LBL-19787 Revised
Preprint

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Submitted to Physical Reports

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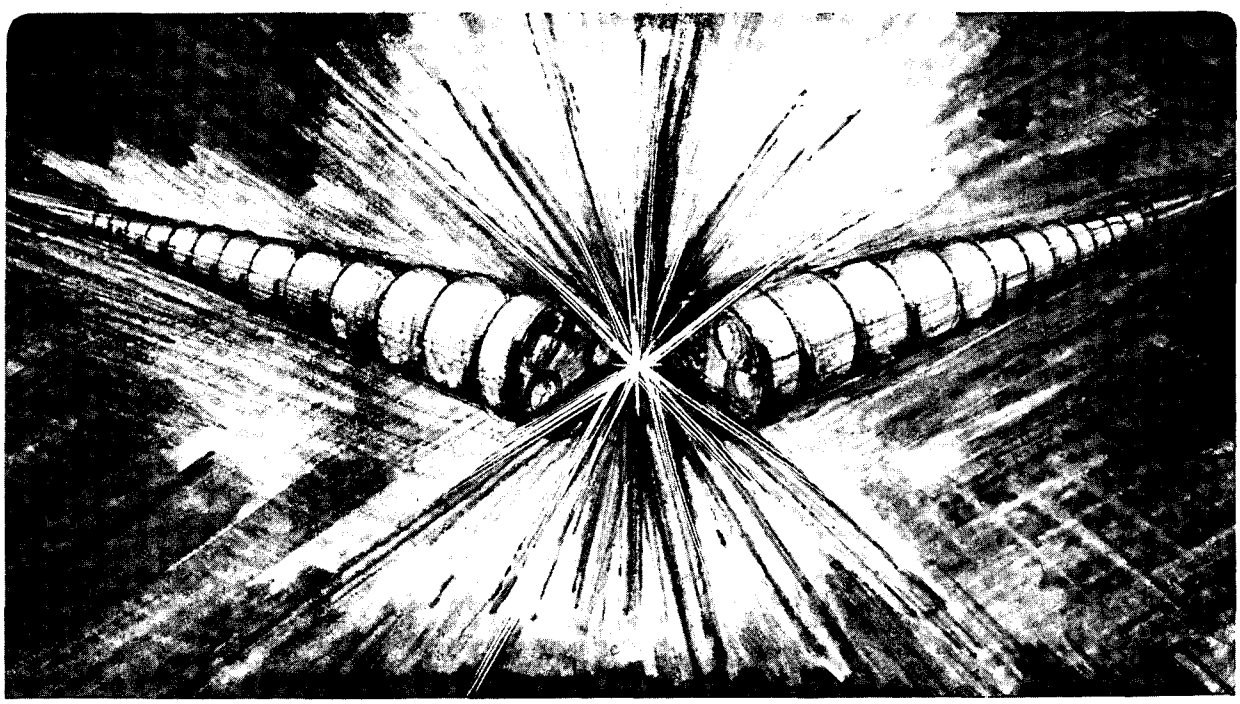
June 1985



Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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LBL-19787 Rev.

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* This work was supported by the Department of Energy under Contract No. DE-AC03-76SF00098, and by the National Science Foundation under grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration.

The Semiclassical Evolution of Wave Packets

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Abstract

The theory of the semiclassical evolution of wave packets is developed as a version of WKB theory in phase space. Special attention is given to the transformation properties of wave packets, their Wigner functions, and their classical analogs under operations in phase space. A complete development of the Heisenberg and metaplectic operators is presented, including their interaction with the Wigner-Weyl formalism and the question of caustics. A metaplectically covariant wave packet propagator is presented and discussed. Finally, a group theoretical discussion of Gaussian wave packets is given.

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Contents

1. Introduction

Wave packet techniques constitute a version of WKB theory in phase space. The appeal of such theories is that they incorporate the known canonical structure of classical mechanics, including Poisson brackets, Poincaré invariants, and the like, into semiclassical mechanics. Phase space is the proper framework for studying classical mechanics, since it provides the arena in which the most general principles of covariance of the equations of motion are expressed, as well as the most general relations between symmetries and invariants. Therefore, on both physical and mathematical grounds, one should not expect the canonical structure of Hamilton's equations to be purely an attribute of classical mechanics, but rather it should have precursors in both quantum mechanics and semiclassical mechanics. For this reason, covariance in phase space can be taken as a guiding principle for semiclassical mechanics, one which can be expected to reveal fundamental relations in their most general form.

Of course, the general outlines of the relation between the canonical structure of classical mechanics and the formalism of quantum mechanics are well known, and go back to Dirac and beyond, even to Hamilton. Nevertheless, a serious and explicit examination of invariance principles in semiclassical mechanics is a rather more recent occurrence, which can be dated from the work of Keller [1958] and Maslov [1972] (see also Maslov and Fedoriuk [1981]). Maslov's theory, which in some ways is a more mathematical version of Keller's, presents semiclassical wave functions and propagators which are, in a sense, invariant under the Fourier transform. The significance of the Fourier transform is that it represents a transformation in phase space of a simple kind, namely an inversion of the roles of q and p.

On the other hand, the majority of WKB work done over the years has dealt almost exclusively with an eikonal representation of wave functions in configuration space. This

approach typically leads to nonphysical infinities at caustics, boundary layer analyses, and connection rules. Nor is this approach merely a version of a phase space theory in disguise; traditional eikonal methods are fundamentally committed to the space in which the wave function is expressed, and are not invariant even under the Fourier transform. This lack of invariance is felt most acutely at caustics, where, say, the **x**-space wave function diverges, but the **p**-space wave function is well behaved.

A fundamental fact about caustics is that they have no invariant meaning in phase space. This is related to the fact that rays in phase space do not focus, because of Liouville's theorem. This is not to say that phase space theories always avoid the practical difficulties of evaluating wave fields in the neighborhood of caustics, such as by the use of special functions or their integral representations. But sometimes they do, as is the case with numerical applications of wave packet techniques.

The above are the main reasons for my interest in this subject, and in my discussion of wave packet propagation I have made a concerted effort to treat q and p on an equal footing, and always to display the transformations properties of the results derived. However, this paper is in no way an attempt to formulate some definitive version of WKB theory on phase space; not only do I not know how to do this, it is not even clear that there is any sense in which some theory should be considered unique. Instead, I have focussed on the specific issue of wave packet propagation, about which much can be said and many definite results derived.

The basic idea underlying the semiclassical propagation of wave packets is very simple. One merely replaces the exact Hamiltonian or other time evolution operator of a wave system by a tractible, usually quadratic, approximation, valid in the neighborhood of the wave packet. It is also an old idea, whose history is hard to trace, and which has certainly been used in many isolated instances for many years. The basic idea is present, for example, in the use of "Gaussian beams" (Keller [1971]; Deschamps [1972]).

But surely no one has done more to advance the theory and practice of wave packet techniques than has the chemist Heller. In a remarkable series of papers (Heller [1975, 1976, 1977a,b, 1985]; Davis and Heller [1979, 1981, 1984]), Heller and coworkers have successfully applied wave packet methods to a number of problems, including classically chaotic systems such as the Henon-Heiles system. Furthermore, recent practical advances in the method by Metiu and coworkers (Heather and Metiu [1985]; Sawada and Metiu [1985]; Sawada, Heather, Jackson and Metiu [1985]) seem to have overcome many of the shortcomings of earlier approaches, and extended their applicability. Although this latter work is too recent to have figured prominently into the thinking underlying this paper, nevertheless it shows that wave packet techniques have every promise of maturing into an important new calculational tool of broad applicability.

This paper, however, is not intended to be a review of Heller's work, and in many respects, expecially those relating to numerical calculations, what I have to say is often simple-minded in comparison to the analyses of Heller. What I have tried to do is to show the structure and transformation properties of wave packets and their time evolution within a phase space framework. As a result, much of the emphasis is group theoretical, and deals with covariance and invariance properties under transformations in phase space.

I have attempted to formulate this presentation in as nontechnical language as possible. I have not used differential geometry at all, and only a minimum of topology, such as is required to discuss the Maslov index. The group theory I have invoked is hardly more than what one encounters in the theory of the ordinary rotation operators in quantum mechanics. Some issues, such as irreducible representations, hardly appear at all, while others, such as the group theoretical properties of caustics, take some attention. Throughout, I have tried to draw parallels between transformations in phase space and the more familiar transformations in configuration space. For example, the Maslov index bears a

strong analogy to the phase shifts which occur in systems with internal degrees of freedom, such as electron spin, and I have emphasized this.

This paper has been substantially influenced by the rather considerable body of mathematical literature which now exists on wave asymptotics. There has been a good deal of activity in this area over the last twenty years, which seems to have been stimulated originally by the work of Maslov. Principal references in this area include Arnold [1967]; Duistermaat [1974]; Guillemin and Sternberg [1977, 1984]; Hormander [1971]; Leray [1981]; Maslov [1972]; Maslov and Fedoriuk [1981]; and Voros [1976, 1977]. I have especially found the work of Voros to be insightful and accessible. Unfortunately, most of this mathematical work is virtually impenetrable to the nonspecialist, and it is difficult for an outsider to master it in detail or even to know what the fundamental ideas are. Furthermore, I know of few instances in which this theory has consciously been applied in a practical way. There is a regrettable communications gap here, which hopefully this paper will help to fill.

Therefore my approach has been to concentrate on concrete calculations and derivations. I have always tried to be explicit in my derivations, and to be complete with phase conventions and practical matrix elements. The theory of the Heisenberg and metaplectic groups which I have invoked is sometimes old, and almost always well understood, at least in the right circles. But I believe that many of my explicit calculations and the physical reasoning which accompanies them are new, although one can never be quite sure about this.

In particular, I am not aware of anything in the published literature quite like my discussion in Sec. 5 of caustics and the metaplectic operators. Nor am I aware of anything like my discussion of the transformation properties of Gaussian wave packets in Sec. 8, although similar things are known to field theorists, who have dealt extensively with cre-

ation and annihilation operators. Furthermore, the ideas underlying the propagator of Eq. (7.27) are current, but I am not aware of any such formula having been written down.

WKB theory and semiclassical mechanics is a truly vast field, in which there are literally thousands of relevant books and research articles. These are spread over many diverse fields, among which there is little communication, such as seismology, electrical engineering, physics, chemistry and mathematics. Therefore it is inevitable that I have neglected to give proper credit for some of the ideas I shall present. It is also inevitable that some of the problems I pose have already been solved. For this I apologize in advance, and merely request that these matters be drawn to my attention by interested readers.

Nevertheless, one can clearly discern in this sea of literature that the evolution of phase space methods in semiclassical theory is the dividing line between the old and the new. It is one of the principal objectives of this paper to provide an accounting of some of the ideas which are involved in any phase space approach to semiclassical mechanics, and to do it in such a way as to be accessible to the largest possible audience. The specific issue of wave packet evolution has been selected as a vehicle for this, partly because it is concrete, and partly because of its demonstrated practical value.

In practical terms, there are two main advantages to the formalism presented in this paper, of which the first is conceptual. The analogies between the classical, phase space picture of dynamics and the quantum mechanical picture, which are represented quantitatively through the medium of symplectic/metaplectic transformations on the Wigner-Weyl formalism, are much stronger than many realize at first. These analogies form a powerful means of conceptualizing problems, formulating the right questions, and understanding the answers. They are also quite astonishing when first encountered.

A second advantage is computational. Most of the calculations involving Gaussian integrals and wave packets to be found in the literature are carried out by brute force

methods, and lead to results in which it is hard to see the fundamental structure. One of the main points of this paper is that the metaplectic operators form the natural transformation group of Gaussians. Because of this, many calculations are reduced to a standard form, in which one need only multiply symplectic matrices to get the desired result.

The applications of WKB theory extend considerably beyond the Schrödinger equation, and this potentially applies to wave packet techniques as well. Therefore I remark that virtually all of the results of this paper are applicable to any wave system, if one merely sets $\hbar = 1$ and replaces $\mathbf{p}$ by $\mathbf{k}$. People who work with classical wave equations tend not to like the Schrödinger equation as an example of WKB theory, becuase it is too restrictive a model. There are three features of the Schrödinger equation which make it special. First, it is a second order differential equation in space, instead of some higher order. In fact, integral equations are common in classical wave systems. Second, the simplest versions of the Schrödinger equation do not involve any q-p ordering issues. And third, the Schrödinger equation has no dissipation, since the Hamiltonian is Hermitian.

Partly in deference to this larger context of wave equations, I have nowhere, except in some inessential examples, made any assumption that the Hamiltonian has the simple form of kinetic plus potential energies, nor have I assumed that it is a quadratic (or any other) polynomial in momentum, or that q-p ordering issues can be neglected. Actually, even for simple Schrödinger Hamiltonians, this would be the right approach to take anyway, since the functional form of kinetic plus potential energies is not invariant under transformations in phase space.

I have, however, assumed that the Hamiltonian is Hermitian. This is definitely a limitation of this paper, although there is no reason why the wave packet methods as developed originally by Heller could not be applied to dissipative systems. However, the transformation properties of such systems involve complex phase space, and it seemed

better to draw the line here with real phase space. Incidentally, there are plenty of reasons to believe that complex phase space would be useful even for conservative systems.

In spite of this attention to a larger class of wave systems, I have written this paper throughout with quantum mechanics in mind. I did this because of the fundamental physical importance of semiclassical mechanics, because it seemed best to work with a specific problem, and because the most sophisticated applications of wave packet techniques seem to be taking place today in quantum mechanics. Besides, the formalism of quantum mechanics, and in particular the Dirac bra-ket notation, is of great value in discussing transformation properties, and it would be pointless not to use it. I do hope, however, that workers in other fields will find this presentation to be useful and illuminating.

This paper is organized as follows. Section 2 presents the fundamental physical picture which is elaborated upon in the rest of the paper. This consists of the Ehrenfest relations and wave packet spreading, seen in classical terms through distribution functions in phase space. In Section 3, the Heisenberg operators are developed and used to formulate a representation of the Ehrenfest relations in phase space. The natural role of the Heisenberg operators in a phase space picture of semiclassical mechanics is discussed, as well as some basic ideas about transformation properties. Sections 4, 5 and 6 define, develop and apply the metaplectic operators, which are responsible for wave packet spreading. There does not seem to be any fully satisfactory presentation of the metaplectic operators in the physics literature, and these sections are partly intended to fill the gap. Section 4 motivates the metaplectic operators, and, by a simple analysis, develops their x-space matrix elements for points not on caustics. Section 5 generalizes these results for points which are on caustics, and presents a rather complete theory of caustics for quadratic Hamiltonians. In Sec. 6 some examples of the practical consequences of the metaplectic operators are developed, including special cases such as the Fourier transform and scaling operations, as well as the transformation properties of the Wigner-Weyl formalism under

metaplectic operations. The latter are essential to the phase space picture of wave packet propagation. In Sec. 7, a semiclassical propagator is developed, using the Heisenberg and metaplectic operators. This is the propagator implicitly used by Heller, and its properties are discussed. Section 8 develops in detail the transformation properties of Gaussian wave packets and Wigner functions under metaplectic operators, and reveals the group theoretical significance of the quantities which appear in Gaussian wave packets. This section is somewhat more technical than the others. Section 8 also contains some results and speculations on simple generalizations of the coherent states. Section 9 contains a discussion of omissions, generalization, and conclusions. Three appendices are provided, which summarize important properties of the symplectic matrices, the Wigner-Weyl formalism, and the standard coherent states.

2. Wave Packets and Classical Nearby Orbits

The time evolution of the center of a wave packet in quantum mechanics is governed, at least approximately, by the Eherenfest relations, which relate this evolution to motion along a classical orbit. In this section it is argued that the evolution of the shape and spreading of the wave packet, in both configuration and momentum space, should also be describable in classical terms, and that in particular it should be related to the classical evolution of a bundle of nearby orbits.

These notions are not new, and can be traced back at least as far as Madelung's [1926] fluid interpretation of quantum mechanics. More recently, Heller [1975] has shown the relationship between wave packet spreading in quantum mechanics and the classical symplectic matrices governing the behavior of nearby orbits. This is the first instance of which I am aware in which this relationship has been explicitly revealed, although Heller employed the quantum mechanical projective representations of the symplectic matrices (the metaplectic operators) only in implicit form. Heller went on to perform a fascinating series of theoretical and computational studies of wave packet evolution. Similar ideas have also been given by Markuvitz [1980], who used the Wigner function as a "quasiparticle" distribution function on phase space. The interesting paper by Bialynicki-Birula [1977] is also to be recommended in this regard. The role of the metaplectic operators in the propagation of light through optical devices has been developed by Bastiaans [1979a,b], Bacry and Cadilhac [1981], Nazarathy and Shamir [1982], Sudarshan, Simon and Mukunda [1983], and others, and discussed rather thoroughly by Guillemin and Sternberg [1984]. Workers in optics seem not to regard the light in an optical device as a "wave packet," although it is treated in the same way as the wave packets in this paper (with time replaced by a spatial coordinate as the independent variable). In this section I provide an independent argument for these ideas, with some examples, and I generalize the context of the discussion.

2.1. Ehrenfest's Theorem and Quadratic Hamiltonians

A proof of Ehrenfest's theorem can be found in any textbook on quantum mechanics, but often the statement of the theorem is vague and imprecise, and usually the thrust of the discussion is somewhat different than what we need here. Therefore I shall begin with Ehrenfest's theorem, and I shall emphasize certain features of it which will be of particular interest to us. I shall do this in the context of a one-dimensional Schrödinger equation with a Hamiltonian of the form

$$H = \frac{\hat{p}^2}{2m} + V(\hat{q}). \tag{2.1}$$

As always in this paper, a hat will be used to distinguish the operators $\hat{q}$, $\hat{p}$ from their counterparts on the classical phase space, q, p, which are numbers. It is also convenient to restrict the use of the symbol x to instances in which we are committed to a configuration space representation, as with the wave function $\psi(x)$, and to reserve the symbol q for cases where we wish to represent something on phase space, or to draw attention to the pairing with p. This distinction cannot always be maintained consistently, nor is it completely logical, since we make no analogous convention for the momentum variable. But we seldom use momentum space wave functions, and, as a practical matter, this convention eliminates considerable confusion. For example, in the x-representation, the operators $\hat{q}$, $\hat{p}$ are represented by $\hat{q}$ = multiplication by x, $\hat{p} = -i\hbar\partial/\partial x$.

A wave function $\psi(x,t)$ which satisfies the Schrödinger equation will endow the expectation values $\langle\hat{q}\rangle$, $\langle\hat{p}\rangle$ with a time dependence, which, by Ehrenfest's theorem, is governed by the equations

$$\begin{aligned} \frac{d}{dt}\langle\hat{q}\rangle &= \frac{\langle\hat{p}\rangle}{m}, \\ \frac{d}{dt}\langle\hat{p}\rangle &= -\left\langle\frac{\partial V}{\partial x}(\hat{q})\right\rangle. \end{aligned} \tag{2.2}$$

These equations are often stated in words by saying that the expectation values $\langle\hat{q}\rangle$, $\langle\hat{p}\rangle$ follow the classical motion. This statement is in general incorrect, as may be seen by noting that Eqs. (2.2) do not in general even form an autonomous system, much less the particular autonomous system offered by Hamilton's equations of classical mechanics. That is, the right hand side of the second of Eqs. (2.2) (the force term) is not in general a function of $\langle\hat{q}\rangle$. The statement in question would be correct if instead of Eqs. (2.2) we had

$$\frac{d}{dt}\langle\hat{q}\rangle = \frac{\langle\hat{p}\rangle}{m},$$
$$\frac{d}{dt}\langle\hat{p}\rangle = -\frac{\partial V}{\partial x}(\langle\hat{q}\rangle). \tag{2.3}$$

These equations, however, are only an approximation, whereas Eqs. (2.2) are exact.

In the special case that the potential is a quadratic function of x, the two sets of equations, (2.2) and (2.3), are, in fact, equivalent, and the expectation values do follow the classical motion, exactly. Indeed, this is the only case they do so, for arbitrary wave packets (and speaking of Hamiltonians of the form (2.1)). For other potentials, Eqs. (2.3) will be approximately correct, if the potential $V(x)$ can be represented to a good accuracy over the extent of the wave packet by expanding it out to quadratic order about the center of the wave packet, $\langle\hat{q}\rangle$. This is not necessarily a semiclassical approximation, because the same approximation occurs entirely within classical mechanics, as shown in Sec. 7.

The case of quadratic potentials is also the most general case in which an initial Gaussian wave packet remains exactly Gaussian in the course of time. Otherwise, the Gaussian property is only maintained approximately, the approximation being the same as just mentioned.

The generalization of these facts to arbitrary Hamiltonians $H(\hat{\mathbf{q}}, \hat{\mathbf{p}})$ in any number of degrees of freedom involves an analogous privileged role for the Hamiltonians which are quadratic functions of $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$ (which are now N-dimensional vectors of operators). Similarly, the generalizations of Eqs. (2.2) will be approximately correct if the classical

Hamiltonian $H(\mathbf{q},\mathbf{p})$ (i.e. an appropriate symbol of the evolution operator $H(\hat{\mathbf{q}},\hat{\mathbf{p}})$) is well approximated in phase space by a quadratic expansion about $\langle\hat{\mathbf{q}}\rangle$, $\langle\hat{\mathbf{p}}\rangle$, over the extent of the wave packet in *both* configuration and momentum space. Expanding in momentum as well as position is usually not an issue in quantum mechanics, where Hamiltonians are at most quadratic in $\hat{\mathbf{p}}$ (including linear terms if a magnetic field is present). But such considerations certainly arise in plasma physics, where Bessel and other functions of $\hat{\mathbf{p}}$ are common. They also arise in optics, where the Hamiltonian involves the square root of polynomials in $\hat{\mathbf{p}}$. (They would also appear in quantum mechanics, if spin were taken into account.)

In any case, consideration of more general time evolution operators does lead to an important consideration, namely that a wave packet should be thought of simultaneously in both its configuration and momentum space forms. One way to deal precisely with such concepts is to use the Wigner function, which is discussed in Appendix B. The Wigner function is a function on the classical phase space $(\mathbf{q},\mathbf{p})$, associated with the wave packet. It is centered on the expectation values $\langle\hat{\mathbf{q}}\rangle$, $\langle\hat{\mathbf{p}}\rangle$, and has widths in the various directions in phase space related to the dispersions, Δq, Δp. The Wigner function of Gaussian wave packets will be discussed more fully in Sec. 8.

It is apparent that in the theory of the semiclassical evolution of wave packets the Hamiltonians which are at most quadratic polynomials in $\hat{\mathbf{q}}$, $\hat{\mathbf{p}}$ play a privileged role, even when they are obtained by expanding more general Hamiltonians about some point $\langle\hat{\mathbf{q}}\rangle$, $\langle\hat{\mathbf{p}}\rangle$ in phase space. A similar privileged role is suggested for the Gaussian wave packets, which as a class are invariant under the time evolution generated by quadratic Hamiltonians.

One may also note that the Gaussian form is invariant under the Fourier transform. This fact is reminiscent of the Maslov theory (Maslov [1972]; Maslov and Fedoriuk [1980]; Blattner and Ralston [1983]; Kravtsov [1968]; Percival [1976]; Weinstein [1979]; Ziolkowski [1980]), in which caustics are circumvented by selective appeal to the Fourier transform. In

a sense, the Maslov theory avoids caustics by being invariant under the Fourier transform, and it is a similar principle of invariance under transformations in phase space which circumvents caustic difficulties in the use of Gaussian wave packets. As is now widely recognized (Arnold [1983]; Berry and Upstill [1980]; Kravtsov and Orlov [1983]), caustics are the results of a kind of projection from objects in phase space (Lagrangian manifolds) down onto configuration space, and they do not have an invariant meaning in phase space. The Fourier transform itself is a part of the theory of quadratic Hamiltonians, as will be shown in Secs. 4-6, and has an interpretation in phase space.

The process of expanding a Hamiltonian out to second order about some point in phase space is important as well in classical mechanics, because it is such an expansion which governs the linearized behavior of classical orbits near some chosen orbit. To develop this idea, it is useful to have a collective notation for coordinates in phase space. Consider a classical system of N degrees of freedom, with phase space coordinates $\mathbf{q}, \mathbf{p}$, which are N-vectors. We will denote the coordinates collectively by $\mathbf{z} = (\mathbf{q}, \mathbf{p})$, which is a $2N$-vector. (This is not to be confused with the complex N-vector $\mathbf{q} + i\mathbf{p}$, which is used in the theory of coherent states. See Appendix C.) When it is necessary to indicate components, we shall let the Latin indices i, j, etc., run over the numbers $1, \ldots, N$, and Greek indices α, β, etc., over the numbers $1, \ldots, 2N$, as in q_i, p_j, z_α.

For some given Hamiltonian $H(\mathbf{q}, \mathbf{p}) = H(\mathbf{z})$, Hamilton's equations can be written in the compact form

$$\frac{d\mathbf{z}}{dt} = \mathbf{J} \cdot \frac{\partial H}{\partial \mathbf{z}}, \tag{2.4}$$

where the $2N \times 2N$ matrix $\mathbf{J}$ is defined by its decomposition into four $N \times N$ matrices,

$$\mathbf{J} = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}. \tag{2.5}$$

The matrix $\mathbf{J}$ is responsible for the Poisson bracket structure of classical mechanics, as is easily seen by noting that

$$\{z_\alpha, z_\beta\} = J_{\alpha\beta}, \tag{2.6}$$

where the curly brackets represent the usual Poisson bracket. More generally, the Poisson bracket of two functions $f(\mathbf{z})$, $g(\mathbf{z})$ is given by

$$\{f,g\} = \frac{\partial f}{\partial z_\alpha} J_{\alpha\beta} \frac{\partial g}{\partial z_\beta}. \tag{2.7}$$

In this paper I sum over repeated indices, except as noted.

A change of coordinates $z'_\alpha = z'_\alpha(z_\beta)$ is a canonical transformation if the Poisson bracket structure is preserved, i.e. if

$$\frac{\partial z'_\alpha}{\partial z_\mu} J_{\mu\nu} \frac{\partial z'_\beta}{\partial z_\nu} = J_{\alpha\beta}. \tag{2.8}$$

In particular, a homogeneous linear transformation $\mathbf{z}' = \mathbf{S} \cdot \mathbf{z}$, for some $2N \times 2N$ matrix $\mathbf{S}$, is a canonical transformation if $\mathbf{S}$ satisfies the matrix equation,

$$\mathbf{S}\mathbf{J}\tilde{\mathbf{S}} = \mathbf{J}, \tag{2.9}$$

where the tilde represents the transpose.

The matrices $\mathbf{S}$ satisfying this equation are the symplectic matrices, which form a group of $N(2N+1)$ dimensions. Important properties of the symplectic matrices are summarized in Appendix A. By Eq. (2.8), even a nonlinear canonical transformation can be characterized in terms of symplectic matrices, by saying that the transformation is canonical if and only if the Jacobian matrix $S_{\alpha\beta} = \partial z'_\alpha / \partial z_\beta$ is symplectic at every point of phase space.

Turning now to the problem of nearby orbits, we let $\mathbf{z}_0$ be some initial conditions, which give rise to an orbit $\mathbf{z}(t)$ under the time evolution generated by $H(\mathbf{z})$ (see Fig. 1). We shall call $\mathbf{z}(t)$ the "reference orbit". We let $\delta\mathbf{z}_0$ be some small displacement in the initial conditions, which gives rise to a nearby orbit in the course of time, described by the displacement $\delta\mathbf{z}(t)$. The displacement $\delta\mathbf{z}(t)$ obeys time-dependent linear equations of motion, obtained by linearizing Eq. (2.4) about the reference orbit,

$$\frac{d}{dt}\delta\mathbf{z} = \mathbf{J} \cdot \mathbf{H}''(t) \cdot \delta\mathbf{z}, \tag{2.10}$$

where the $2N \times 2N$ symmetric matrix $\mathbf{H}''$ is the Hessian matrix of the original Hamiltonian H, evaluated along the reference trajectory,

$$H''_{\alpha\beta} = \frac{\partial^2 H}{\partial z_\alpha \partial z_\beta}\big(\mathbf{z}(t)\big). \tag{2.11}$$

It depends on time, but, once the reference orbit is given, it does not depend on $\mathbf{z}$. Just as $\mathbf{z}$ obeys a Hamiltonian system of equations, so also does $\delta\mathbf{z}$, with the Hamiltonian being given by

$$K(\delta\mathbf{z}, t) = \tfrac{1}{2}\delta\tilde{\mathbf{z}} \cdot \mathbf{H}''(t) \cdot \delta\mathbf{z}, \tag{2.12}$$

which is a homogeneous quadratic polynomial in $\delta\mathbf{q}$, $\delta\mathbf{p}$ (and is explicitly time-dependent).

The general solution to Eq. (2.10) can be written in the form

$$\delta\mathbf{z}(t) = \mathbf{S}(t) \cdot \delta\mathbf{z}_0, \tag{2.13}$$

where $\mathbf{S}(t)$ is a $2N \times 2N$ time-dependent matrix satisfying $\mathbf{S}(0) = \mathbf{I}$. It is also a symplectic matrix, since

$$S_{\alpha\beta}(t) = \frac{\partial z_\alpha(t)}{\partial z_{0\beta}}, \tag{2.14}$$

and since the time evolution of classical Hamiltonian systems generates canonical transformations (i.e. $\mathbf{z}(t)$, considered as a function of $\mathbf{z}_0$, is canonical) (Goldstein [1980]). The matrix $\mathbf{S}(t)$ obeys equations of evolution essentially the same as those of $\delta\mathbf{z}$, namely

$$\frac{d}{dt}\mathbf{S}(t) = \mathbf{J} \cdot \mathbf{H}''(t) \cdot \mathbf{S}(t). \tag{2.15}$$

We note that if the original Hamiltonian happens to be a quadratic function of $\mathbf{q}$,$\mathbf{p}$, then $\mathbf{H}''$ is independent of time, and $\delta\mathbf{z}$ obeys time-independent equations of motion. In that case, $\mathbf{S}(t)$ forms a one-parameter subgroup of the symplectic group.

Clearly there is a strong analogy between the approximation involved in the Ehrenfest relations (2.3) (and in the preservation of the Gaussian form in the course of time), and the linearized behavior of nearby orbits in classical mechanics. This suggests that the

spreading of wave packets can be understood in classical terms, just as the motion of the expectation values $\langle \hat{\mathbf{q}} \rangle$, $\langle \hat{\mathbf{p}} \rangle$ can be so understood.

2.2. A Simple Example

Nevertheless, the spreading of wave packets is often regarded as a purely quantum phenomenon, with no classical analog. Sometimes this spreading is called "quantum diffusion", presumably because of the mathematical similarity between the Schrödinger equation and a diffusion equation under the replacement $t \rightarrow -it$. However, there is not much physical similarity between wave packet spreading and diffusion. For example, an ensemble of classical particles undergoing a simple diffusive process has a dispersion Δx which goes asymptotically in time as $\sqrt{t}$, whereas the dispersion Δx of a free particle wave packet in quantum mechanics is linear in time as $t \rightarrow \infty$. The quantum behavior is more like that of a classical ensemble of particles, not undergoing a diffusive process, but rather evolving independently of each other as free particles, since an initial displacement in velocity δv_0 gives rise to a spatial separation $\delta v_0 \, t$ in the course of time. We shall now develop the example of the free particle more fully, in order to explore this analogy.

We consider first the quantum case. Let $\psi(x,t)$ be the solution to the free particle Schrödinger equation (here in one dimension),

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}, \tag{2.16}$$

with initial conditions

$$\psi_0(x) = \frac{1}{(2\pi L^2)^{1/4}} \exp\left(-\frac{x^2}{4L^2} + \frac{ip_0 x}{\hbar} \right). \tag{2.17}$$

The initial conditions represent a minimum uncertainty wave packet with $\langle \hat{q} \rangle = 0$, $\langle \hat{p} \rangle = p_0$, $\Delta q_0 = L$, $\Delta p_0 = \hbar/2L$. The exact solution is

$$\psi(x,t) = \frac{1}{(2\pi L^2)^{1/4}} \frac{1}{\sqrt{1+\dfrac{i\hbar t}{2mL^2}}} \times \exp\left[-\frac{(x-p_0 t/m)^2}{4L^2\left(1+\dfrac{i\hbar t}{2mL^2}\right)} + \frac{ip_0 x}{\hbar} - \frac{ip_0^2 t}{2m\hbar}\right]. \tag{2.18}$$

If we take the branch cut of the square root to lie just under the negative real axis, then Eq. (2.18) is correct for all t, both positive and negative. We have chosen our wave packet to be minimum uncertainty at $t = 0$, but it is easy to show that an arbitrary Gaussian taken as initial conditions (in one dimension) becomes minimum uncertainty for some value of t (possibly negative).

It follows directly from the solution that the expectation values and dispersions, as functions of time, are given by

$$\langle \hat{q} \rangle = \frac{p_0 t}{m}, \qquad \langle \hat{p} \rangle = p_0, \tag{2.19}$$

$$\Delta q(t) = L\sqrt{1+\frac{\hbar^2 t^2}{4m^2 L^4}}, \qquad \Delta p(t) = \Delta p_0 = \frac{\hbar}{2L}. \tag{2.20}$$

Equations (2.19) verify the Ehrenfest relations, and Eqs. (2.20) show the spreading in x. (For the free particle, there is no spreading in momentum, but more generally, this will occur, too.) The spreading in x appears to vanish as $\hbar \to 0$, thereby seeming to substantiate the notion that the spreading is a purely quantum phenomenon; we shall discuss this issue presently.

Consider now a purely classical analysis of an ensemble of free particles. Let the Liouville density function $f = f(\boldsymbol{z}) = f(q,p)$ be given initially by a Gaussian in phase space, centered at $q = 0$, $p = p_0$:

$$f_0(q,p) = \frac{1}{2\pi LK} \exp\left[-\frac{q^2}{2L^2} - \frac{(p-p_0)^2}{2K^2}\right]. \tag{2.21}$$

The initial dispersions are $\Delta q_0 = L$, $\Delta p_0 = K$. The distribution at any later time is given by

$$f(q,p,t) = f_0(q - \frac{pt}{m}, p) = \frac{1}{2\pi LK} \exp\left[-\frac{(q-pt/m)^2}{2L^2} - \frac{(p-p_0)^2}{2K^2}\right]. \qquad (2.22)$$

A direct calculation of moments gives the average values of q and p and their dispersions,

$$\langle q \rangle = \frac{p_0 t}{m}, \qquad \langle p \rangle = p_0 \qquad (2.23)$$

$$\Delta q(t) = L\sqrt{1 + \frac{K^2 t^2}{m^2 L^2}}, \qquad \Delta p(t) = K. \qquad (2.24)$$

Note in particular the similarity of the formulas for $\Delta q(t)$ in the quantum and classical cases. Again, as in the quantum case, our initial conditions cause Δq to be minimum at $t = 0$, but more generally one can show that an arbitrary Gaussian taken as initial conditions produces a function $\Delta q(t)$ which is minimum for some t.

Figure 2 gives a picture of the time evolution of the free particle ensemble. Suppose we choose the parameters L and K (or the scaling of q and p in the diagram) so that the initial Liouville distribution function has contour lines which are circles in phase space, centered at $q = 0$, $p = p_0$. One of these contour lines is shown in the figure. As time progresses, the center of the distribution function moves to the right along the constant momentum line, $p = p_0$. But the particles above this line have higher velocities than the average, and those below have lower velocities, so the contours of the distribution function gradually shear into ellipses. The result is the spreading characterized by $\Delta q(t)$.

We can now understand better the appearance of $\hbar$ in the quantum formula for the dispersion Δq, Eq. (2.20). It is true that the term $\hbar^2 t^2/4m^2L^4$ approaches zero as $\hbar \to 0$, but only if the other parameters of the problem are held fixed. In Eq. (2.17) we chose an initial wavefunction which was minimum uncertainty, i.e. of quantum dimensions (the quantity $\Delta q \Delta p/\hbar$ is of order unity), and this in effect is responsible for the appearance of $\hbar$ in Eq. (2.20). On the other hand, if we were to choose a classical distribution function, Eq. (2.21), satisfying $LK = \hbar/2$, i.e. one of quantum dimensions, then $\hbar$ would appear in the classical formula, Eq. (2.24), as well. In this case, the classical spreading would

also vanish as $\hbar \to 0$, because the velocity differential in the distribution would go as $\Delta v = \Delta p/m \sim \hbar/mL \to 0$.

There are further subtleties to this analysis, because in a certain sense one has no choice in quantum mechanics except to choose a wave packet of quantum dimensions. For example (speaking in terms of Gaussians), while it is true that $\Delta q \Delta p/\hbar$ at $t = 0$ can be assigned any value not less than $\frac{1}{2}$, even classical (i.e. very large) values, nevertheless in the course of time there will come a moment when the wavepacket is minimum uncertainty and $\Delta q(t)\Delta p(t)/\hbar = \frac{1}{2}$. Obviously there is no analogous requirement for a classical Gaussian ensemble, in which $\hbar$ does not appear, even though $\Delta q \Delta p$ does have some minimum value for some value of t. The resolution of this subtlety involves the distinction between pure and mixed states, about which we will have more to say.

With this analysis in mind, we are encouraged to further push the notion that not only the evolution of expectation values, but also the spreading of wave packets, is comprehensible in classical terms.

3. An Operator Approach to the Ehrenfest Relations

In this section I introduce the Heisenberg operators and use them to describe the evolution of expectation values of wave packets. Issues relating to the spreading will be deferred to later sections.

Heisenberg operators have a long history, going back to Weyl [1927]. They play an important role in the theory of coherent states (Klauder and Sudarshan [1968]), as is discussed in Appendix C. The Wigner-Weyl formalism (see Appendix B) is fundamentally based on these operators, and they provide the most appealing medium through which the canonical structure of classical mechanics can be made to make its appearance in the classical limit.

3.1. Translations in Phase Space

The basic idea of the Heisenberg operators is that they move wave functions around in phase space. Since wave functions are not usually defined on phase space, but rather on configuration space or momentum space (but not both), this notion is as yet imprecise. However, wave functions do have expectation values which can be represented as points on phase space, and Heisenberg operators do move these expectation values around.

To develop this idea, let us extend the notation of the previous section, and write $\hat{\mathbf{z}}$ for the $2N$-vector of operators $(\hat{\mathbf{q}}, \hat{\mathbf{p}})$. These operators do not commute with each other, for we have

$$\left[\hat{z}_\alpha, \hat{z}_\beta\right] = i\hbar J_{\alpha\beta}, \tag{3.1}$$

where $\mathbf{J}$ is the Poisson matrix introduced in Eq. (2.5). For a given state $|\psi\rangle$, the expectation values $\langle\hat{\mathbf{q}}\rangle$, $\langle\hat{\mathbf{p}}\rangle$ may be written collectively as

$$\mathbf{z} = \langle\hat{\mathbf{z}}\rangle = \langle\psi|\hat{\mathbf{z}}|\psi\rangle. \tag{3.2}$$

A Heisenberg operator is parameterized by a point $\mathbf{z}_0$ in phase space, which represents a displacement vector from the origin to $\mathbf{z}_0$. We shall denote this operator by $T(\mathbf{z}_0)$, where T stands for "translation". The operator $T(\mathbf{z}_0)$ has the property that if $|\psi\rangle$ has the expectation value $\mathbf{z}$ given by Eq. (3.2), then $T(\mathbf{z}_0)|\psi\rangle$ has the expectation value $\mathbf{z} + \mathbf{z}_0$. That is,

$$\langle\psi|T(\mathbf{z}_0)^\dagger\,\hat{\mathbf{z}}\,T(\mathbf{z}_0)|\psi\rangle = \mathbf{z} + \mathbf{z}_0. \tag{3.3}$$

This will be satisfied if we have

$$T(\mathbf{z}_0)^\dagger\,\hat{\mathbf{z}}\,T(\mathbf{z}_0) = \hat{\mathbf{z}} + \mathbf{z}_0. \tag{3.4}$$

This equation represents the most fundamental property of the Heisenberg operators. It is, in fact, satisfied by the explicit form of the Heisenberg operators, which we now proceed to construct.

One approach to the Heisenberg operators is to consider first their classical counterparts, which we denote by $T_{cl}(\mathbf{z}_0)$. When acting on points $\mathbf{z}$ in the classical phase space, these classical operators act by simple vector addition, so that

$$T_{cl}(\mathbf{z}_0)\mathbf{z} = \mathbf{z} + \mathbf{z}_0. \tag{3.5}$$

A different version of the classical Heisenberg operators acts on Liouville distribution functions $f(\mathbf{z})$. Here the effect is to move all the particles constituting the distribution function by the same displacement $\mathbf{z}_0$, so that the contour surfaces of $f(\mathbf{z})$ are rigidly displaced forward by $\mathbf{z}_0$. If we write $g = T_{cl}(\mathbf{z}_0)f$ for the new distribution function g, then we have

$$g(\mathbf{z}) = [T_{cl}(\mathbf{z}_0)f](\mathbf{z}) = f(\mathbf{z} - \mathbf{z}_0). \tag{3.6}$$

The minus sign is necessary in Eq. (3.6) to make the classical expectation values come out right, i.e. so that

$$\int \mathbf{z}\, g(\mathbf{z})\, d^{2N}\mathbf{z} = \mathbf{z}_0 + \int \mathbf{z}\, f(\mathbf{z})\, d^{2N}\mathbf{z}. \tag{3.7}$$

This is the correct classical analog of Eq. (3.3), because it shows that classical expectation values are moved forward by $\mathbf{z}_0$.

The classical Heisenberg operators form an Abelian group of $2N$ dimensions, since they represent simple vector addition on phase space. Furthermore, the action of a classical Heisenberg operator constitutes a canonical transformation (if viewed in the passive sense), or a symplectic mapping of phase space onto itself (if viewed in the active sense, which is more common). That is, the transformation

$$\mathbf{z}' = \mathbf{z} + \mathbf{z}_0, \tag{3.8}$$

is canonical, since $\partial z'_\alpha / \partial z_\beta = \delta_{\alpha\beta}$ is a symplectic matrix (the identity matrix is symplectic).

It is convenient to embed this transformation in a family of transformations, by scaling $\mathbf{z}_0$ by a parameter t. That is, we write

$$\mathbf{z}'(t) = \mathbf{z} + t\mathbf{z}_0, \tag{3.9}$$

so that $\mathbf{z}'(0) = \mathbf{z}$ and $\mathbf{z}'(1) = \mathbf{z}'$. This can be viewed as the t-evolution of a classical Hamiltonian, where $\mathbf{z}$ plays the role of an initial condition at $t = 0$, and $\mathbf{z}'$ plays the role of a final condition at $t = 1$. $\mathbf{z}_0$ is a parameter of the Hamiltonian, not the initial condition. This scaling has the effect of embedding the given displacement in a one parameter group of displacements, all along the line in phase space specified by $\mathbf{z}_0$. The Hamiltonian describing this evolution of $\mathbf{z}'$ is parameterized by $\mathbf{z}_0$, so we write $H(\mathbf{z}', \mathbf{z}_0)$ for it. It is easy to find this Hamiltonian; we call on Eq. (2.4) in the form

$$\frac{d}{dt}\mathbf{z}'(t) = \mathbf{J} \cdot \frac{\partial}{\partial \mathbf{z}'} H(\mathbf{z}', \mathbf{z}_0) = \mathbf{z}_0. \tag{3.10}$$

Using the antisymmetric symplectic form $\omega = \mathbf{J}^{-1}$, defined by Eqs. (A.4)-(A.5), we can easily solve for H, and we find

$$H(\mathbf{z}, \mathbf{z}_0) = \tilde{\mathbf{z}} \cdot \omega \cdot \mathbf{z}_0 = \omega(\mathbf{z}, \mathbf{z}_0) = \mathbf{p} \cdot \mathbf{q}_0 - \mathbf{q} \cdot \mathbf{p}_0 \tag{3.11}$$

where we have now dropped the prime. We see that the symplectic form is the classical generator of displacements in phase space.

We now ask for the quantum analog of the classical displacement operator, $T_{cl}(\mathbf{z}_0)$. Since the time evolution operator in quantum mechanics is $e^{-itH/\hbar}$, we postulate the following form for the quantum Heisenberg operator,

$$T(\mathbf{z}_0) = e^{-\frac{i}{\hbar}\omega(\hat{\mathbf{z}},\mathbf{z}_0)} = e^{\frac{i}{\hbar}(\mathbf{p}_0\cdot\hat{\mathbf{q}}-\mathbf{q}_0\cdot\hat{\mathbf{p}})}, \tag{3.12}$$

where we have taken the classical Hamiltonian of Eq. (3.11) and simply replaced $\mathbf{z}$ by the operator vector $\hat{\mathbf{z}}$. (This formula has a classical analog, which relates $T_{cl}(\mathbf{z}_0)$ to the exponential of a certain Liouville operator. The action of this operator on functions f is obtained by forming the Poisson bracket of f with $\omega(\mathbf{z},\mathbf{z}_0)$. The result is precisely Eq. (3.6).)

As before, we can embed the quantum Heisenberg operator in a family parameterized by t, by replacing $\mathbf{z}_0$ by $t\mathbf{z}_0$, and we can consider the t-evolution which results. If $|\psi_0\rangle$ is some initial state, we set $|\psi\rangle = T(t\mathbf{z}_0)|\psi_0\rangle$, and we obtain the following differential equation for $|\psi\rangle$,

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \omega(\hat{\mathbf{z}},\mathbf{z}_0)|\psi\rangle = (\mathbf{q}_0\cdot\hat{\mathbf{p}} - \mathbf{p}_0\cdot\hat{\mathbf{q}})|\psi\rangle, \tag{3.13}$$

which is a version of the Schrödinger equation.

This equation can be solved, and it leads to the matrix elements of $T(\mathbf{z}_0)$. We solve it in the x-representation, i.e. we write $\psi = \psi(\mathbf{x},t)$, so that

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar\mathbf{q}_0\cdot\nabla\psi - (\mathbf{p}_0\cdot\mathbf{x})\psi. \tag{3.14}$$

This equation, being first order in space as well as time, is easily solved by the method of characteristics; if $\psi_0(\mathbf{x})$ is the initial condition, then we find

$$\psi(\mathbf{x},t) = \exp\left[\frac{i}{\hbar}\left(t\mathbf{p}_0\cdot\mathbf{x} - \frac{t^2}{2}\mathbf{p}_0\cdot\mathbf{q}_0\right)\right]\psi_0(\mathbf{x}-t\mathbf{q}_0). \tag{3.15}$$

Setting $t = 1$, we have

$$[T(\mathbf{z}_0)\psi](\mathbf{x}) = e^{\frac{i}{\hbar}(\mathbf{p}_0\cdot\mathbf{x}-\frac{1}{2}\mathbf{p}_0\cdot\mathbf{q}_0)}\psi(\mathbf{x}-\mathbf{q}_0), \tag{3.16}$$

which is an explicit formula for the action of the Heisenberg operator $T(\mathbf{z}_0)$ on wave functions in the x-representation. This may be compared to its classical analog, Eq. (3.6). This result is also easily obtained by applying the Cambell-Baker-Hausdorff formula to Eq. (3.12).

Special cases of this are of interest. If the vector $\mathbf{z}_0$ consists of a displacement purely in configuration space, then we have

$$[T(\mathbf{q}_0, 0)\psi](\mathbf{x}) = \psi(\mathbf{x}-\mathbf{q}_0), \tag{3.17}$$

as one would expect. Similarly, if the displacement is purely in momentum space, then

$$[T(0, \mathbf{p}_0)\psi](\mathbf{x}) = e^{i\mathbf{p}_0\cdot\mathbf{x}/\hbar}\psi(\mathbf{x}), \tag{3.18}$$

which is also to be expected. However, $T(\mathbf{z}_0)$ is more general than either of these cases, and allows simultaneous displacements in both configuration and momentum space. This is necessary, because such simultaneous displacements are actually generated by the semi-classical time evolution of wave packets.

Equation (3.16) gives us immediately the configuration space matrix elements of $T(\mathbf{z}_0)$, which we write in the form

$$\langle\mathbf{x}|T(\mathbf{z}_0)|\mathbf{x}'\rangle = e^{i\mathbf{p}_0\cdot(\mathbf{x}+\mathbf{x}')/2\hbar}\,\delta(\mathbf{x}-\mathbf{x}'-\mathbf{q}_0). \tag{3.19}$$

Further properties follow easily. By Eq. (3.12), the Heisenberg operators are unitary, and in fact

$$T(\mathbf{z}_0)^{-1} = T(-\mathbf{z}_0) = T(\mathbf{z}_0)^\dagger. \tag{3.20}$$

We now consider the commutativity of the Heisenberg operators. The classical Heisenberg operators commute with each other, since they merely represent vector addition:

$$T_{cl}(\mathbf{z}_0)T_{cl}(\mathbf{z}_1) = T_{cl}(\mathbf{z}_1)T_{cl}(\mathbf{z}_0) = T_{cl}(\mathbf{z}_0+\mathbf{z}_1). \tag{3.21}$$

But the quantum Heisenberg operators do not commute, since they are exponentials of linear combinations of the noncommuting operators $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$. Indeed, a simple calculation based on Eq. (3.19) shows that

$$T(\mathbf{z}_0)T(\mathbf{z}_1) = e^{\frac{i}{2\hbar}\omega(\mathbf{z}_0,\mathbf{z}_1)}T(\mathbf{z}_0+\mathbf{z}_1). \tag{3.22}$$

The quantum Heisenberg operators fail to commute, due to the phase factor shown.

Finally, we return to Eq. (3.4), and prove that it is satisfied. One way to do this is to expand out the exponential of Eq. (3.12) and commute the operator $\hat{z}_\alpha$ through the terms. We find, for example,

$$\left[\omega(\hat{\mathbf{z}},\mathbf{z}_0),\hat{z}_\alpha\right] = -i\hbar z_{0\alpha}, \tag{3.23}$$

using Eqs. (3.1) and (A.5). The result is

$$T(\mathbf{z}_0)^\dagger\,\hat{z}_\alpha = (\hat{z}_\alpha + z_{0\alpha})T(\mathbf{z}_0)^\dagger, \tag{3.24}$$

in agreement with Eq. (3.4).

3.2. Discussion

Let us pause to consider Eq. (3.22). Although we have derived this result in the x-representation, the result itself is representation independent. Furthermore, the classical phase space expressions appearing in this result treat q and p on an equal footing. The coupling of q and p is expressed through the symplectic form ω, which is a symplectic invariant (see Eq. (A.6)). The same properties are evident in Eq. (3.12), which is also representation independent. Equations (3.16) and (3.19) do not treat q and p on an equal footing, but that is because they explicitly involve x-space matrix elements, and not because of the Heisenberg operators themselves.

In any practical calculation, one must use some representation, whether it is configuration space or momentum space or some other. But one can think beyond the representation

being used to the objects in the abstract, whether they be vectors in Hilbert space or the operators which act on them. Consider, for example, the vectors in Hilbert space, which are the abstract representatives of the wave functions. In carrying out some calculation, one certainly should expect the result, in the sense of the Hilbert space vector, to be independent of the representation which was used in the calculation. And indeed, this is the normal situation in quantum mechanics.

Yet it is precisely on this account that traditional WKB theory fails. For example, the usual WKB techniques for calculating energy eigenfunctions yield different answers (in the sense of Hilbert space vectors) when carried out in momentum space than they do in configuration space. This is to say that the momentum space WKB wave function is not in general the exact Fourier transform of the configuration space WKB wave function.

Similarly, the usual WKB techniques can be applied in initial value problems to obtain the WKB approximation to the Green's function. This can be done either in configuration space or momentum space, and the result is the respective matrix element of a WKB approximation to the propagator, which in the abstract is an operator on the Hilbert space. Unfortunately, the approximate propagator which results is not the same operator, in general, when the calculation is done in momentum space as it is in configuration space. Again, this is to say that the WKB Green's function in momentum space is not the exact Fourier transform of the WKB Green's function in configuration space.

This situation is usually rationalized by saying that the two wave functions or Green's functions, derived in the two representations, are approximately the Fourier transforms of each other, through the stationary phase approximation. And in fact one can devise a sense in which the two wave functions or Green's functions differ from one another by an amount which is $O(\hbar)$, so that the situation seems to be consistent and satisfactory.

Nevertheless, there is another sense, and an important one physically, in which the two wave functions or Green's functions do not differ by a small amount, but rather have

an infinite difference. This has to do with caustics. Consider, for example, WKB wave functions in one dimension. Carrying out the usual WKB approximation in configuration space yields a wave function $\langle x|\psi_q\rangle$, and carrying it out in momentum space yields another wave function $\langle p|\psi_p\rangle$. The two Hilbert space vectors $|\psi_q\rangle$ and $|\psi_p\rangle$ are not the same vectors, so that the x-space wave function $\langle x|\psi_p\rangle$, which is the exact Fourier transform of the momentum space WKB wave function $\langle p|\psi_p\rangle$, is not the same x-space wave function as $\langle x|\psi_q\rangle$. For most values of x, the difference $\langle x|\psi_p\rangle - \langle x|\psi_q\rangle$ is small, but when x is at a caustic, this difference diverges. Indeed, as is well known (Percival [1977]), when x is near a caustic, the wave function $\langle x|\psi_p\rangle$ is finite and well behaved, and typically displays Airy function behavior, whereas $\langle x|\psi_q\rangle$ diverges.

These considerations suggest that if one could devise a semiclassical approximation which was representation independent, then one would not have difficulties with nonphysical divergences at caustics. At a minimum, this would entail the ability to write down a formula for the semiclassical wave function or propagator which is manifestly representation independent. I shall exhibit such a formula for the semiclassical propagator in Sec. 7; its representation independence is responsible for the fact that wave packet techniques do not have difficulties with caustics. This propagator makes explicit use of the Heisenberg operators, and it is for this reason that I call attention to the manifest representation independence of Eqs. (3.4), (3.12), (3.20), and (3.22).

Actually, representation independence, which guarantees that the results of calculations are independent of the basis employed in Hilbert space, is only one issue in semiclassical mechanics, because it only takes care of the quantum side of the picture. The other side is the classical side, and one might suppose that here we should demand an analogous representation independence, namely invariance with respect to general canonical transformations. Sometimes one does obtain such invariance, as is the case with the phase factor of Eq. (3.27) below when the transport process is carried around a closed loop in phase space.

But in other cases, there is only a more limited form of invariance, namely invariance with respect to linear canonical transformations. For example, the phase of Eq. (3.22) is only invariant under this restricted class of classical canonical transformations.

Furthermore, there are many instances in which classical and quantum objects are coupled together, as in the exponent of Eq. (3.12). Here we require an invariance principle which is coordinated between the classical and quantum objects. Again, in the case of linear canonical transformations, it is possible to develop such a principle, due to the fact that linear canonical transformations have a projective representation in terms of unitary operators on Hilbert space. These are the metaplectic operators, which are discussed in Secs. 4-6. But for more general canonical transformations, such a coordination of classical and quantum invariance principles is not possible.

Such considerations quickly lead into a murky area, where it is difficult to formulate the right questions. However, there are several issues which are clearly related to this question of invariance principles, among them being the matter of "nonlinear canonical transformations of operators," "higher order terms," and the uniqueness of the semiclassical expansion. We shall not pursue these matters any further here, but the interested reader is directed to the discussion of "other quantizations" by Guillemin and Sternberg [1984].

In any case, even with invariance only under linear canonical transformations, we are far ahead of traditional WKB theory, which is invariant only under linear point transformations. It is precisely the lack of an invariance principle in phase space which leads to the caustic difficulties in traditional WKB theory.

3.3. Transport of Wave Functions

The phase factor appearing in Eq. (3.22) has an interesting classical interpretation. It says that if we transport a wave function through phase space, then the result we obtain depends on the path taken. Considering, for example, a simple segmented path such as that shown in Fig. 3, we see that the result of transporting a wave function along the broken path is different from the result along the direct path. This is due to the phase difference $\frac{1}{2}\omega(\mathbf{z}_0, \mathbf{z}_1)$, which, apart from sign, is the first Poincaré invariant associated with the triangle defined by the displacements. (For $N = 1$, it is the area of the triangle in phase space.)

It is also interesting to note that if $\omega(\mathbf{z}_0, \mathbf{z}_1) = 0$, then the transport process is commutative. This fact leads to the notion of a Lagrangian manifold, which is a certain kind of N-dimensional surface in the $2N$-dimensional phase space (Arnold [1978]). The simplest Lagrangian manifold is a Lagrangian plane, which we consider first. A Lagrangian plane can be characterized in at least two equivalent ways. First, a Lagrangian plane has the property that $\omega(\mathbf{z}, \mathbf{z}') = 0$ for any two displacement vectors $\mathbf{z}$, $\mathbf{z}'$ which lie in (or are parallel to) the plane. This means that the transport of wave functions along any two paths which lie in a Lagrangian plane is commutative. Second, a Lagrangian plane is any plane which can be realized as the Q-space resulting from a linear, possibly inhomogeneous, canonical transformation. That is, it is the image of configuration space under some linear canonical transformation. If the transformation is homogeneous, then the Lagrangian plane is the image of configuration space under the action of a symplectic matrix, and it passes through the origin of phase space. Configuration space itself is a Lagrangian plane, as is momentum space, or any plane parallel to these, and many others as well. In particular, transport of wave functions in configuration space is commutative.

More generally, a Lagrangian manifold is the image of configuration space under any (possibly nonlinear) canonical transformation. For example, the invariant tori of integrable

systems are Lagrangian manifolds, because they are the Q-spaces which result from the nonlinear transformation to action-angle variables. The tangent plane to a Lagrangian manifold is a Lagrangian plane, so that infinitesimal displacements lying in a Lagrangian manifold are commutative. These can be integrated, as we do below in Eq. (3.27), to form finite displacements, and the results of these displacements are invariant with respect to continuous deformations of path, as long as the deformations lie in the Lagrangian manifold. However, the transport process is not in general commutative if the two paths reaching the same final endpoint form a closed curve which cannot be smoothly contracted to a point (while remaining on the Lagrangian manifold). This is a topological matter, which arises in the case of the invariant tori, and it leads to quantization conditions. In the special case $N = 1$, any curve (a one-dimensional manifold) in the two-dimensional phase space is a Lagrangian manifold. In particular, curves of constant energy are Lagrangian. For $N > 1$, only special N-dimensional surfaces are Lagrangian, and the surfaces of constant energy are never Lagrangian, since they do not even have the right dimension ($2N-1$ instead of N). Lagrangian manifolds arise naturally in the eikonal representation of wave functions, although they have a significance which goes beyond this, since the eikonal form breaks down at caustics. There is no intrinsic feature of a Lagrangian manifold to signal the presence of a caustic, since the latter is representation-dependent, and the condition $\omega(\mathbf{z}, \mathbf{z}') = 0$ is not.

It is suggestive to imagine that the semiclassical time evolution of a wave packet, which causes the expectation values $\langle\hat{\mathbf{z}}\rangle(t)$ to follow a classical trajectory, is governed by a sequence of near-identity Heisenberg operators. Let us take a classical trajectory $\mathbf{z}(t)$, and segment it into a number if straight sections, as shown in Fig. 4. We consider the product of Heisenberg operators corresponding to these segments,

$$T(\mathbf{z}_n - \mathbf{z}_{n-1}) \ldots T(\mathbf{z}_2 - \mathbf{z}_1) T(\mathbf{z}_1 - \mathbf{z}_0). \tag{3.25}$$

By the product rule (3.22), and by using the antisymmetry of ω, this can be written

$$\exp\left[\frac{i}{2\hbar}\sum_{k=0}^{n-1}\omega(\mathbf{z}_{k+1}-\mathbf{z}_k,\mathbf{z}_k)\right]T(\mathbf{z}_n)T(\mathbf{z}_0)^\dagger. \tag{3.26}$$

In the limit $n\to\infty$, and taking $\mathbf{z}_n=\mathbf{z}(t)$, we obtain a kind of propagator,

$$U(t)=\exp\left[-\frac{i}{2\hbar}\int_0^t\omega(\mathbf{z},\dot{\mathbf{z}})\,dt\right]T\big(\mathbf{z}(t)\big)T(\mathbf{z}_0)^\dagger. \tag{3.27}$$

The integral in this expression is like the Bohr-Sommerfeld phase factor, but it is taken over the symmetrized action $\frac{1}{2}(\mathbf{p}\cdot d\mathbf{q}-\mathbf{q}\cdot d\mathbf{p})$. When transport is performed around a closed curve, the phase factor is unity only if the orbit encloses an area of $2\pi n\hbar$, for some integer n. (The word "area" is correct only for one degree of freedom. More generally, it is the first Poincaré invariant.)

The picture presented by this analysis is incomplete in several respects, and has been given at this point only for its suggestive value. It will be greatly improved upon in Sec. 7. Nevertheless, it is important to show how a semiclassical theory can be founded on constructions which are based on the canonical structure of classical mechanics. After all, this structure should not be expected to abruptly emerge, fully formed, when the classical limit is taken. Instead, this structure should be mirrored somehow in semiclassical mechanics. This illustration and others we shall present show that the Heisenberg operators are a natural medium for expressing the classical canonical structure in quantum and semiclassical mechanics.

3.4. Further Properties of the Heisenberg Operators

I finish this section with some further properties of the Heisenberg operators which will be of use in other places. First we may note that the Heisenberg operators, as defined so far, do not form a group, because of the phase factor in Eq. (3.22). (They are not closed

under multiplication.) However, if we extend their definition to include a phase factor, then we do get a group. We define

$$T(\mathbf{z}_0, \gamma) = e^{i\gamma/\hbar} T(\mathbf{z}_0), \tag{3.28}$$

so that

$$T(\mathbf{z}_0, \gamma_0) T(\mathbf{z}_1, \gamma_1) = T\big(\mathbf{z}_0 + \mathbf{z}_1, \gamma_0 + \gamma_1 + \tfrac{1}{2}\omega(\mathbf{z}_0, \mathbf{z}_1)\big). \tag{3.29}$$

This equation is the group multiplication law for the Heisenberg group, which is $(2N+1)$-dimensional. Unlike its classical counterpart, it is non-Abelian. The name of Heisenberg is attached to this group because its Lie algebra consists essentially of the q-p commutation relations.

Next we derive a pair of orthogonality and completeness formulas which are of great importance for the Wigner-Weyl formalism. The first is

$$\int \frac{d^{2N}\mathbf{z}_0}{(2\pi\hbar)^N} \langle \mathbf{x}|T(\mathbf{z}_0)^\dagger|\mathbf{x}'\rangle \langle \mathbf{y}|T(\mathbf{z}_0)|\mathbf{y}'\rangle = \delta(\mathbf{x}-\mathbf{y}')\delta(\mathbf{y}-\mathbf{x}'). \tag{3.30}$$

This is easily proved by directly using the matrix element of Eq. (3.19). It is a kind of a completeness relation on operator space, and in a formal sense it says that the Heisenberg operators, as given, form an irreducible representation of the Heisenberg group (the abstract group obeying the multiplication law (3.29)).

The second formula is

$$\mathrm{Tr}\big[T(\mathbf{z}_0)^\dagger T(\mathbf{z}_1)\big] = (2\pi\hbar)^N \delta(\mathbf{z}_0 - \mathbf{z}_1), \tag{3.31}$$

where Tr is the trace. This is a kind of orthogonality relation on operator space. It is easy to prove, and often useful.

Finally, I remark that some authors have used an alternative version of the Heisenberg operators, in which Eq. (3.12) is replaced by

$$T(\mathbf{z}_0) = e^{\frac{i}{\hbar}\mathbf{p}_0\cdot\hat{\mathbf{q}}}\, e^{-\frac{i}{\hbar}\mathbf{q}_0\cdot\hat{\mathbf{p}}}. \tag{3.32}$$

For the purposes of semiclassical mechanics, this version is undesirable, because it does not treat q and p on an equal footing. (For example, the factors do not commute. Which one is to be placed first?) For this reason and others, I shall make no use of it.

Although the Heisenberg operators can account for the evolution of the expectation values $\langle \hat{\mathbf{z}} \rangle$ of wave packets, they have no effect on the spreading. For example, when they act on minimum uncertainty Gaussians, they produce other minimum uncertainty Gaussians, with different expectation values $\langle \hat{\mathbf{z}} \rangle$. (These are the coherent states; see Appendix C). On the other hand, we know that wave packet spreading is ubiquitous, as shown by the example of the free particle. To account for spreading, it is necessary to introduce a new class of operators, namely the metaplectic operators.

4. The Metaplectic Operators

Although the Heisenberg operators have been frequently used in physics, the same is not true for the metaplectic operators. This is not due to any intrinsic lack of importance, for, as we shall see, the metaplectic operators go hand in hand with the Heisenberg operators, in the same way that purely spatial rotations combine with purely spatial translations to form the Euclidean group, the group which preserves the Euclidean structure of configuration space. Indeed, the Heisenberg and metaplectic operators include the Euclidean transformations as special cases, and generalize them to the analogous operations on phase space, operations which preserve the symplectic structure of phase space.

Probably the best references on the metaplectic operators which exist in the physics literature are Bargmann [1961], Moshinsky and Quesne [1971], and Kramer, Moshinsky and Seligman [1975]. Bargmann's remarkable and beautiful paper develops the abstract group properties of the metaplectic operators quite thoroughly, and is otherwise notable for his theory of the Hilbert space of analytic functions. It is, however, rather technical, and many of his conventions are contrary to the standards of physics. Also, he dealt only with the coherent state matrix elements of the metaplectic operators, and not their x-space matrix elements. The other references provide valuable additional information, especially Kramer, Moshinsky and Seligman [1975], which presents a theory of complex symplectic transformations. Many of the observations of this paper would probably be placed on a deeper foundation if complex symplectic transformations were incorporated. None of these references, however, deal in a systematic way with the matrix elements of the metaplectic operators near caustics. This is a subject which I will explore in detail in Sec. 5.

There are a number of references in the mathematical literature to the metaplectic operators, among which I may mention Duistermaat and Hörmander [1972]; Guillemin and Sternberg [1977, 1984]; Leray [1975, 1981]; Lion and Vergne [1980]; Shale [1962]; Treve

[1980]; Voros [1976, 1977]; and Weil [1963]; and references contained therein. In most of these there has been little attempt to make the discussion accessible to the nonspecialist, with the exception of the first hundred pages of Guillemin and Sternberg [1984], who have a very interesting discussion of "Fresnel optics." There is no uniformity among these references as to the precise definition of the metaplectic group, although the one I adopt in this paper seems to be the most common. Incidentally, it is from the mathematical literature that the name "metaplectic" is taken.

My presentation is intended to be practical, and I shall emphasize the similarity between the metaplectic operators and the familiar rotation operators of quantum mechanics. I begin by defining and motivating the metaplectic operators in three equivalent ways, before proceeding to an explicit calculation of matrix elements.

4.1. First Approach: Linear Canonical Transformations

Our first approach to the metaplectic operators arises in a natural way when we consider homogeneous linear transformations taking the operator vector $\hat{\mathbf{z}} = (\hat{\mathbf{q}}, \hat{\mathbf{p}})$ into a new operator vector, $\hat{\mathbf{Z}} = (\hat{\mathbf{Q}}, \hat{\mathbf{P}})$. As for the motivation for this question, suffice it for the moment to point out that in the classical nearby orbit problem, the displacement $\delta\mathbf{z}$ evolves according to a time-dependent linear transformation specified by the matrix $\mathbf{S}(t)$, which is symplectic. Let us therefore set

$$\hat{Z}_\alpha = S_{\alpha\beta}\,\hat{z}_\beta, \tag{4.1}$$

for some matrix $\mathbf{S}$. If we demand that the standard commutation relations be satisfied for the new operators $\hat{\mathbf{Z}}$, i.e.

$$\left[\hat{Z}_\alpha, \hat{Z}_\beta\right] = i\hbar J_{\alpha\beta}, \tag{4.2}$$

then we easily see that $\mathbf{S}$ must be symplectic.

In general, the question as to what constitutes a "canonical transformation of operators" is one that is beset with subtleties. However, in the special case of linear transformations, we see that the answer is easy: the classical and quantum cases are identical.

The linear transformation (4.1) specifies a unitary operator $M = M(\mathbf{S})$, parameterized by the symplectic matrix $\mathbf{S}$, such that the relation

$$M(\mathbf{S})^\dagger \, \hat{z}_\alpha \, M(\mathbf{S}) = S_{\alpha\beta} \, \hat{z}_\beta = \hat{Z}_\alpha \tag{4.3}$$

is satisfied. We shall prove this below; for now we merely call attention to the analogous formula obeyed by the Heisenberg operators, Eq. (3.4), as well as the analogous formula in the theory of rotation operators (c.f. Messiah [1961], Eq. XIII.54). This operator $M(\mathbf{S})$ is a metaplectic operator; by Eq. (4.3) it is specified to within an arbitrary phase. The choice of phase can be narrowed by demanding that the operators reproduce the multiplication law of the symplectic matrices. This demand is only partially successful, however; a sign ambiguity remains.

4.2. Second Approach: Quadratic Generators

Our second approach to the metaplectic operators is group theoretical and involves quantum Hamiltonians which are homogeneous quadratic polynomials in $\hat{\mathbf{z}}$. Of course, we are thinking of the quadratic expansion discussed in Sec. 2 (and so successfully exploited by Heller [1975, 1976, 1977a,b]), but in addition there are many Hamiltonians of physical interest of this form. Among these, we mention the harmonic oscillator, a charged particle in a uniform magnetic field, and the components of angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, treated as the generators of rotations. Let us write such a Hamiltonian in the form

$$h = \tfrac{1}{2} \, \hat{z}_\alpha K_{\alpha\beta} \, \hat{z}_\beta, \tag{4.4}$$

for some $2N \times 2N$ symmetric matrix $\mathbf{K}$ (c.f. Eq. (A.13) for the classical analog). We demand that $\mathbf{K}$ be symmetric so that h will be Hermitian; of course, there is no such consideration in the classical case.

The infinitesimal propagator for such a Hamiltonian is an infinitesimal metaplectic operator. Let us put

$$M(\epsilon) = 1 - \frac{i\epsilon}{2\hbar}\, \hat{z}_\alpha K_{\alpha\beta}\, \hat{z}_\beta. \tag{4.5}$$

Then a short calculation shows that

$$M(\epsilon)^\dagger\, \hat{z}_\alpha\, M(\epsilon) = (\delta_{\alpha\beta} + \epsilon J_{\alpha\mu} K_{\mu\beta})\hat{z}_\beta. \tag{4.6}$$

This agrees with Eq. (4.3) if we write $\mathbf{S}(\epsilon) = \mathbf{I} + \epsilon\mathbf{JK}$, which is indeed an infinitesimal symplectic matrix (c.f. Eq. (A.15)). In fact, it is the same symplectic matrix generated by the classical Hamiltonian corresponding to Eq. (4.4). It was this agreement which governed my choice for the positioning of M and $M^\dagger$ in Eq. (4.3).

Next we consider the Lie algebra generated by quadratic Hamiltonians. We write the quantum equivalent of Eq. (A.18),

$$h_i = \tfrac{1}{2}\hat{\mathbf{z}} \cdot \mathbf{K}_i \cdot \hat{\mathbf{z}}, \tag{4.7}$$

for $i = 1, 2, 3$, where $\mathbf{K}_1$ and $\mathbf{K}_2$ are any two given symmetric matrices, and where $\mathbf{K}_3$ is determined by

$$\big[h_1, h_2\big] = i\hbar\, h_3. \tag{4.8}$$

This is meaningful, because the commutator of two quadratic Hamiltonians is another such Hamiltonian. Working out the commutator gives $\mathbf{K}_3 = \mathbf{K}_1\mathbf{J}\mathbf{K}_2 - \mathbf{K}_2\mathbf{J}\mathbf{K}_1$, in agreement with Eq. (A.17).

The fact that quadratic Hamiltonians are closed under the commutator shows that they generate a group; this is the metaplectic group, denoted $Mp(2N)$. And the explicit calculation we have done shows that this group has the same Lie algebra as the classical

symplectic matrices, i.e. the symplectic group $Sp(2N)$. It follows from Lie group theory that in neighborhoods of the identity of the two groups there is a one-to-one correspondence between symplectic matrices and metaplectic operators, which preserves the group multiplication law. For infinitesimal symplectic matrices and metaplectic operators, this association is given explicitly by Eq. (4.6). This is an important concept, because in the classical nearby orbit problem defined by Eq. (2.9), the time evolution of $\delta\mathbf{z}$ proceeds from t to $t+\Delta t$ by multiplication by the infinitesimal symplectic matrix $\mathbf{I}+\Delta t\mathbf{J}\mathbf{H}''(t)$. On the other hand, the semiclassical time evolution of the quantum wave packet proceeds by the action of the uniquely corresponding infinitesimal metaplectic operator,

$$1-\frac{i\Delta t}{2\hbar}\,\hat{\mathbf{z}}\cdot\mathbf{H}''(t)\cdot\hat{\mathbf{z}}. \tag{4.9}$$

However, in spite of this one-to-one correspondence for near-identity operations, the two groups, $Sp(2N)$ and $Mp(2N)$, are not the same group, i.e. the multiplication law for the metaplectic operators cannot, globally speaking, be placed in one-to-one correspondence with that of the symplectic matrices. This is due, in a sense, to the fact that the metaplectic operators carry more information than the symplectic matrices; in fact, one bit more information. This arises in the following way. The classical evolution of nearby orbits produces a symplectic matrix function $\mathbf{S}(t)$, satisfying $\mathbf{S}(0)=\mathbf{I}$. This function can be regarded as a trajectory in the space of symplectic matrices. As discussed in Appendix A, this space has a "hole" in it, and a closed trajectory therefore has a winding number. Now, for most nearby orbit problems, the matrix function $\mathbf{S}(t)$ will not represent a closed curve in the space of symplectic matrices, i.e. it will not satisfy $\mathbf{S}(t)=\mathbf{I}$ for any t except $t=0$. Nevertheless, for the sake of illustration, let us imagine for the moment that $\mathbf{S}(t)$ is closed, since this is the best way to illustrate the double valuedness of the metaplectic operators. This double valuedness is important even when $\mathbf{S}(t)$ is not closed. Corresponding to the symplectic matrix $\mathbf{S}(t)$, there is a metaplectic operator $M(t)$, built up by infinitesimal

compositions in the same way as $\mathbf{S}(t)$. It turns out that if $\mathbf{S}(t)$ is a closed curve with an odd winding number, returning to $\mathbf{S}(T) = \mathbf{I}$ at some time $t = T$, then $M(T)$ is not 1 (the identity), but rather it is -1. On the other hand, if the winding number of $\mathbf{S}(t)$ is even, then $M(T) = +1$.

These facts do not contradict the statement made above, that in neighborhoods of the identity the two groups $Sp(2N)$ and $Mp(2N)$ are isomorphic. This is because, globally speaking, they are not isomorphic; rather, the metaplectic group stands in a 2-to-1 correspondence with the symplectic group. For every symplectic matrix $\mathbf{S}$ (globally speaking), there are two metaplectic operators, $M_1(\mathbf{S})$ and $M_2(\mathbf{S})$. These operators differ by a sign,

$$M_1(\mathbf{S}) = -M_2(\mathbf{S}). \tag{4.10}$$

The relationship between the two groups $Sp(2N)$ and $Mp(2N)$ is very much like that between the complex w- and z-planes for the analytic function $w = z^2$. If the complex number $z = z(t)$, parameterized by t, goes around the origin once, without passing through it, then $w(t)$ goes around twice. (The correct analogy here is to identify $z(t)$ with $M(t)$, and $w(t)$ with $\mathbf{S}(t)$.) In this analogy, the relation between z and w can be expressed through the phase angles, $\theta_z = \arg z$ and $\theta_w = \arg w$, so that $\theta_z = \theta_w/2 + n\pi$, where $n = 0$ or 1. Similarly, a symplectic matrix $\mathbf{S}$ can be associated with an angle $\gamma_S = \arg\det(\mathbf{A} + i\mathbf{B})$, as explained in Appendix A. A metaplectic operator can also be associated with an angle γ_M, which can be understood in terms of the resulting phase when a standard Gaussian wave packet is acted upon by a metaplectic operator. If this metaplectic operator is one of the two shown in Eq. (4.10), then $\gamma_M = \gamma_S/2 + n\pi$, where $n = 0$ or 1. This half-angle relationship is shown explicitly in Eqs. (6.30) and (6.32).

This situation is analogous to the one which obtains in the theory of rotation operators for half-integral angular momenta. In that case, also, there are two rotation operators corresponding to a single classical 3×3 rotation matrix, and these operators differ by a

sign. In the same way that an electron can be rotated by 360° and suffers a phase change of -1, so too, in a sense, can a wave packet be "rotated" in phase space by a continuous operation which classically returns to the identity, but quantum mechanically produces a phase change of -1. However, this property of the metaplectic operators has nothing to do with spin.

Furthermore, just as the double valuedness of electron rotation operators is important even when the classical rotation matrix does not return to the identity, the same is true in the case of metaplectic operators and classical symplectic matrices. For example, in the case of an electron precessing in an inhomogeneous or time-varying magnetic field, the rotation operator describing the precession might never return to the identity, and yet clearly no analysis of the problem could be done without taking the double valuedness into account.

As just indicated, the phase shift produced by the metaplectic operators when the classical symplectic matrix returns to its original value is determined by the winding number of $\mathbf{S}(t)$ in the group $Sp(2N)$. This winding number is one half of the *Maslov index*, which we denote by μ; therefore the phase shift is $e^{i\mu\pi/2}$. The Maslov index for a closed trajectory $\mathbf{S}(t)$ is a topological invariant of the symplectic group, and is invariant under changes of coordinates (in the sense discussed in Appendix A), as well as under continuous deformations of the path $\mathbf{S}(t)$. Later we will relate this version of the Maslov index to the more familiar version, which is expressed in terms of caustics.

4.3. Third Approach: Gaussian Wave Packets

Our third approach to the metaplectic operators is based on Gaussian wave packets. By using Heisenberg operators to move expectation values around in phase space, we know we can transform any Gaussian into one which has $\langle\hat{\mathbf{z}}\rangle = 0$, i.e. one which is situated at

the origin in phase space. We may regard this operation as trivial, so here we consider only Gaussians satisfying $\langle \hat{\mathbf{z}} \rangle = 0$. We also consider only normalized Gaussians. Then the metaplectic operators can be characterized as those operators which map every such Gaussian into another such Gaussian, i.e. the operators which leave the set of all such Gaussians invariant.

It is tolerably apparent that the x-space matrix elements of such an operator must have the form

$$\langle \mathbf{x}|M|\mathbf{x}'\rangle = \text{const.} \times e^{\bar{\mathbf{x}}\mathbf{L}_1\mathbf{x}+\bar{\mathbf{x}}\mathbf{L}_2\mathbf{x}'+\bar{\mathbf{x}}'\mathbf{L}_3\mathbf{x}'}, \tag{4.11}$$

since the quadratic exponent guarantees that a Gaussian will be transformed into another Gaussian. The $N\times N$ matrices $\mathbf{L}_1$ and $\mathbf{L}_3$ are symmetric, and $\mathbf{L}_2$ is arbitrary, for a total count of $N(2N+1)$ parameters. The $\mathbf{L}$ matrices must also be purely imaginary, so that M is unitary (the Gaussians are supposed to remain normalized). In addition to the form (4.11), one must also consider limiting cases of it, which give rise to δ-functions of linear expressions in $\mathbf{x}$ and $\mathbf{x}'$. Obviously, such δ-functions also preserve the Gaussian form. What is perhaps surprising is that the kernels of the form (4.11) are closely related to the symplectic matrices. As a result, it turns out that Gaussian wave packets can be parameterized, in a sense, by symplectic matrices (but not uniquely, as we shall see).

4.4. Configuration Space Matrix Elements of the Metaplectic Operators

We now proceed to calculate the matrix elements of the metaplectic operators, based on our first approach and Eqs. (4.1)–(4.3). This calculation is similar to that employed by Moshinsky and Quesne [1971] and by Bargmann [1961], although Bargmann worked directly in the coherent state basis. It is also related to the analysis of Miller [1974], who considered as well nonlinear operator functions of $\hat{\mathbf{z}}$.

Using the notation of Eq. (A.8), we write the first half of Eq. (4.1) in the form

$$\hat{\mathbf{Q}} = \mathbf{A}\hat{\mathbf{q}} + \mathbf{B}\hat{\mathbf{p}}. \tag{4.12}$$

Because of the commutation relations (4.2), the N components of the operator vector $\hat{\mathbf{Q}}$ are commuting operators, and we can construct their simultaneous eigenstates. We denote these by $|\hat{\mathbf{Q}}(\mathbf{x})\rangle$, to indicate both the operators $\hat{\mathbf{Q}}$ and the eigenvalues $\mathbf{x}$, so that $\hat{\mathbf{Q}}|\hat{\mathbf{Q}}(\mathbf{x})\rangle = \mathbf{x}|\hat{\mathbf{Q}}(\mathbf{x})\rangle$. Similarly, we write $|\hat{\mathbf{q}}(\mathbf{x})\rangle$ for the simultaneous eigenstate of the operators $\hat{\mathbf{q}}$ with eigenvalues $\mathbf{x}$; the simple notation $|\mathbf{x}\rangle$ is ambiguous.

The eigenstates $|\hat{\mathbf{Q}}(\mathbf{x})\rangle$ are determined in the $\hat{\mathbf{q}}$-representation by

$$\langle\hat{\mathbf{q}}(\mathbf{x}')|\hat{\mathbf{Q}}|\hat{\mathbf{Q}}(\mathbf{x})\rangle = \mathbf{x}\langle\hat{\mathbf{q}}(\mathbf{x}')|\hat{\mathbf{Q}}(\mathbf{x})\rangle, \tag{4.13}$$

or

$$\left(\mathbf{A}\mathbf{x}' - i\hbar\mathbf{B}\frac{\partial}{\partial\mathbf{x}'} - \mathbf{x}\right)U(\mathbf{x}',\mathbf{x}) = 0, \tag{4.14}$$

where we abbreviate, $U(\mathbf{x}',\mathbf{x}) = \langle\hat{\mathbf{q}}(\mathbf{x}')|\hat{\mathbf{Q}}(\mathbf{x})\rangle$. For the time being, we assume that the matrix $\mathbf{B}$ is nonsingular, which in effect says that we are away from caustics. We will interpret this condition more fully in Sec. 5; for now we merely note that the symplectic matrices $\mathbf{S}$ such that $\det\mathbf{B} = 0$ form a set of measure zero in the space of all symplectic matrices, and that the possible difficulty $\det\mathbf{B} = 0$ can be removed by introducing an arbitrarily small perturbation into $\mathbf{S}$. Then we have

$$\frac{\partial}{\partial\mathbf{x}'}U(\mathbf{x}',\mathbf{x}) = -\frac{i}{\hbar}\mathbf{B}^{-1}(\mathbf{A}\mathbf{x}' - \mathbf{x})\,U(\mathbf{x}',\mathbf{x}). \tag{4.15}$$

The fact that a solution to this equation exists is guaranteed by the symmetry of the matrix $\mathbf{B}^{-1}\mathbf{A} = \tilde{\mathbf{A}}\tilde{\mathbf{B}}^{-1}$, which follows from the symplectic condition in the form (A.9). It is also equivalent to the fact that the operators $\hat{\mathbf{Q}}$ commute with one another, and therefore possess simultaneous eigenstates. Thus we have

$$U(\mathbf{x}',\mathbf{x}) = f(\mathbf{x})e^{-\frac{i}{2\hbar}(\tilde{\mathbf{x}}'\mathbf{B}^{-1}\mathbf{A}\mathbf{x}' - 2\tilde{\mathbf{x}}'\mathbf{B}^{-1}\mathbf{x})}, \tag{4.16}$$

where $f(\mathbf{x})$ is a normalization/phase factor.

The spectrum of $\hat{\mathbf{Q}}$, like that of $\hat{\mathbf{q}}$, is continuous, so we normalize the states $|\hat{\mathbf{Q}}(\mathbf{x})\rangle$ according to

$$\langle\hat{\mathbf{Q}}(\mathbf{x}')|\hat{\mathbf{Q}}(\mathbf{x})\rangle = \delta(\mathbf{x}-\mathbf{x}'), \tag{4.17}$$

or

$$\int d\mathbf{x}''\, U(\mathbf{x}'',\mathbf{x}')^* U(\mathbf{x}'',\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x}'). \tag{4.18}$$

The integral gives

$$(2\pi\hbar)^N f(\mathbf{x}')^* f(\mathbf{x})\, \delta\big[\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}')\big] = (2\pi\hbar)^N \big|f(\mathbf{x})\big|^2 \big|\det\mathbf{B}\big|\, \delta(\mathbf{x}-\mathbf{x}'), \tag{4.19}$$

so we obtain

$$U(\mathbf{x}',\mathbf{x}) = \frac{e^{i\alpha(\mathbf{x})/\hbar}}{\sqrt{(2\pi\hbar)^N|\det\mathbf{B}|}}\, e^{-\frac{i}{2\hbar}(\mathbf{x}'\mathbf{B}^{-1}\mathbf{A}\mathbf{x}'-2\mathbf{x}'\mathbf{B}^{-1}\mathbf{x})}, \tag{4.20}$$

in which the phase $\alpha(\mathbf{x})$ is still arbitrary.

For any choice of the phase function $\alpha(\mathbf{x})$, the eigenstates $|\hat{\mathbf{Q}}(\mathbf{x})\rangle$ uniquely specify a unitary operator M, defined by

$$M|\hat{\mathbf{Q}}(\mathbf{x})\rangle = |\hat{\mathbf{q}}(\mathbf{x})\rangle. \tag{4.21}$$

That is, M takes an eigenstate of $\hat{\mathbf{Q}}$ with eigenvalues $\mathbf{x}$ into an eigenstate of $\hat{\mathbf{q}}$ with the same eigenvalues. M is uniquely specified because it maps a complete set of states into another complete set. (Here we simply assume that the commuting operators $\hat{\mathbf{Q}}$ form a complete set. This can be verified after the fact.) It is also unitary, because of the normalization condition (4.17). This M causes the first half of Eqs. (4.3) to be satisfied, i.e.

$$M^\dagger\,\hat{\mathbf{q}}\,M = \hat{\mathbf{Q}} = \mathbf{A}\hat{\mathbf{q}} + \mathbf{B}\hat{\mathbf{p}}. \tag{4.22}$$

We would like M to satisfy as well the second half, i.e.

$$M^\dagger\,\hat{\mathbf{p}}\,M = \hat{\mathbf{P}} = \mathbf{C}\hat{\mathbf{q}} + \mathbf{D}\hat{\mathbf{p}}. \tag{4.23}$$

It is not obvious that this can be done, because M is already determined by Eq. (4.21). However, it turns out that by properly choosing the phase $\alpha(\mathbf{x})$, this equation is also satisfied. We show this by taking the matrix element of Eq. (4.23) between the states $\langle\hat{\mathbf{q}}(\mathbf{x}')|$ and $|\hat{\mathbf{Q}}(\mathbf{x})\rangle$, which gives

$$i\hbar\frac{\partial}{\partial\mathbf{x}}U(\mathbf{x}',\mathbf{x}) = \left(\mathbf{C}\mathbf{x}' - i\hbar\mathbf{D}\frac{\partial}{\partial\mathbf{x}'}\right)U(\mathbf{x}',\mathbf{x}), \tag{4.24}$$

or, by substitution of Eq. (4.20),

$$\frac{\partial\alpha(\mathbf{x})}{\partial\mathbf{x}} = (\mathbf{D}\mathbf{B}^{-1}\mathbf{A} - \mathbf{C} - \tilde{\mathbf{B}}^{-1})\mathbf{x}' - \mathbf{D}\mathbf{B}^{-1}\mathbf{x}. \tag{4.25}$$

The term in $\mathbf{x}'$ vanishes according to the symplectic conditions (A.9)–(A.10), which also show that the matrix $\mathbf{D}\mathbf{B}^{-1} = \tilde{\mathbf{B}}^{-1}\tilde{\mathbf{D}}$ is symmetric. Therefore a solution exists, and we have

$$\alpha(\mathbf{x}) = -\tfrac{1}{2}\,\tilde{\mathbf{x}}\mathbf{D}\mathbf{B}^{-1}\mathbf{x} - \hbar\beta, \tag{4.26}$$

where β is a constant.

We see that with this choice of α, i.e. with this choice of phase conventions for the states $|\hat{\mathbf{Q}}(\mathbf{x})\rangle$, we can simultaneously satisfy all $2N$ components of Eq. (4.3), with M defined by Eq. (4.21). We also have phase conventions for the states $|\hat{\mathbf{P}}(\mathbf{k})\rangle$, if we define them by

$$M|\hat{\mathbf{P}}(\mathbf{k})\rangle = |\hat{\mathbf{p}}(\mathbf{k})\rangle. \tag{4.27}$$

(We should not write $|\hat{\mathbf{Z}}(\mathbf{z})\rangle$, because the $2N$ operators $\hat{\mathbf{Z}}$ do not commute and do not possess simultaneous eigenstates.)

We summarize these results by noting that $U(\mathbf{x}',\mathbf{x})^* = \langle\hat{\mathbf{q}}(\mathbf{x})|M|\hat{\mathbf{q}}(\mathbf{x}')\rangle$, or

$$\langle\mathbf{x}|M(\mathbf{S})|\mathbf{x}'\rangle = \frac{e^{i\beta}}{\sqrt{(2\pi\hbar)^N|\det\mathbf{B}|}} \times\exp\left[\frac{i}{2\hbar}\left(\tilde{\mathbf{x}}'\mathbf{B}^{-1}\mathbf{A}\mathbf{x}' - 2\tilde{\mathbf{x}}'\mathbf{B}^{-1}\mathbf{x} + \tilde{\mathbf{x}}\mathbf{D}\mathbf{B}^{-1}\mathbf{x}\right)\right], \tag{4.28}$$

where we have dropped the specification of the operator $\hat{\mathbf{q}}$ in $\langle\mathbf{x}|$, $|\mathbf{x}'\rangle$, this henceforth being understood. The exponent is $i/\hbar$ times the mixed variable generating function

$F_1(\mathbf{x},\mathbf{x}')$ (Goldstein [1980]) which is responsible for the canonical transformation, $\mathbf{z} = \mathbf{S}\mathbf{z}'$, in agreement with Miller [1974].

Next we consider the phase β, which is an essential part of our analysis. This phase is independent of $\mathbf{x}$ and $\mathbf{x}'$, but we will want it to depend on $\mathbf{S}$. As we have seen, in a neighborhood of the identity, the group multiplication law for the metaplectic operators should be the same as that for the symplectic matrices, and we can only bring our result (4.28) into accordance with this if we determine the phase β as a function of $\mathbf{S}$.

Let us therefore consider two symplectic matrices $\mathbf{S}_1$, $\mathbf{S}_2$, and set $\mathbf{S} = \mathbf{S}_1\mathbf{S}_2$. Then we have

$$\mathbf{S} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_1\mathbf{A}_2 + \mathbf{B}_1\mathbf{C}_2 & \mathbf{A}_1\mathbf{B}_2 + \mathbf{B}_1\mathbf{D}_2 \\ \mathbf{C}_1\mathbf{A}_2 + \mathbf{D}_1\mathbf{C}_2 & \mathbf{C}_1\mathbf{B}_2 + \mathbf{D}_1\mathbf{D}_2 \end{pmatrix}. \tag{4.29}$$

Correspondingly, let us compute the matrix element $\langle \mathbf{x}|M(\mathbf{S}_1)M(\mathbf{S}_2)|\mathbf{x}'\rangle$ by inserting a resolution of the identity,

$$\int d\mathbf{y}\, |\mathbf{y}\rangle\langle\mathbf{y}| = 1 \tag{4.30}$$

and integrating over $\mathbf{y}$. We assume that all three matrices, $\mathbf{B}_1$, $\mathbf{B}_2$, $\mathbf{B}$, are nonsingular. Collecting only the terms which depend on $\mathbf{y}$, we have the integral

$$\int d\mathbf{y}\, \exp\left\{ \frac{i}{2\hbar} \left[\tilde{\mathbf{y}}(\mathbf{B}_1^{-1}\mathbf{A}_1 + \mathbf{D}_2\mathbf{B}_2^{-1})\mathbf{y} - 2(\tilde{\mathbf{x}}'\mathbf{B}_2^{-1} + \tilde{\mathbf{x}}\tilde{\mathbf{B}}_1^{-1})\mathbf{y} \right] \right\}. \tag{4.31}$$

The symmetric matrix $\mathbf{B}_1^{-1}\mathbf{A}_1 + \mathbf{D}_2\mathbf{B}_2^{-1}$ can be written $\mathbf{B}_1^{-1}\mathbf{B}\mathbf{B}_2^{-1}$, and when we carry out the integral and collect terms, making liberal use of the identities (A.9)-(A.10), we find that the exponent of the result is precisely the exponent of Eq. (4.28). Furthermore, the leading factors agree in absolute value, so that $M(\mathbf{S}_1\mathbf{S}_2)$ is the same operator as $M(\mathbf{S}_1)M(\mathbf{S}_2)$, to within a phase.

As for the phase itself, we let N_+ and N_- be respectively the numbers of positive and negative eigenvalues of the symmetric matrix $\mathbf{B}_1^{-1}\mathbf{B}\mathbf{B}_2^{-1}$, so that $N_+ + N_- = N$. Then the phase of the result is

$$\beta = \beta_1 + \beta_2 + \frac{N\pi}{4} - \frac{\pi}{2}N_-. \tag{4.32}$$

If this could be written in the form $\beta(\mathbf{S}) = \beta(\mathbf{S}_1) + \beta(\mathbf{S}_2)$, then we would have a unitary representation of the symplectic group. However, we will find in the attempt that this cannot be done, although an appropriate form for $\beta(\mathbf{S})$ does appear. Let us denote the phases of $\det \mathbf{B}_1$, $\det \mathbf{B}_2$, $\det \mathbf{B}$ respectively by $\nu_1\pi$, $\nu_2\pi$, $\nu\pi$, where the ν's take on the values 0 or 1. Then we have

$$N_- \equiv \nu - \nu_1 - \nu_2 \,(\mathrm{mod}\, 2). \tag{4.33}$$

Therefore if we write Eq. (4.32) in the form

$$\left(\beta + \frac{N\pi}{4} + \frac{\nu\pi}{2}\right) = \left(\beta_1 + \frac{N\pi}{4} + \frac{\nu_1\pi}{2}\right) + \left(\beta_2 + \frac{N\pi}{4} + \frac{\nu_2\pi}{2}\right) + \frac{\pi}{2}(\nu - \nu_1 - \nu_2 - N_-), \tag{4.34}$$

we see that the integer in the last term is even. This suggests that we define

$$\beta(\mathbf{S}) = -\frac{N\pi}{4} - \frac{\nu\pi}{2}, \tag{4.35}$$

where $e^{i\nu\pi} = \mathrm{sgn}\det \mathbf{B}$, so that

$$\beta(\mathbf{S}_1\mathbf{S}_2) = \beta(\mathbf{S}_1) + \beta(\mathbf{S}_2) + n\pi, \tag{4.36}$$

where n is an integer.

The result of this analysis is that if we form a one-to-one association between symplectic matrices $\mathbf{S}$ and operators $M(\mathbf{S})$, by using Eq. (4.28) with $\beta(\mathbf{S})$ defined by Eq. (4.35), then the set of operators $M(\mathbf{S})$ that we obtain is not a group. This is so because the set of operators so formed is not closed under multiplication; sometimes (depending on $\mathbf{S}_1$, $\mathbf{S}_2$) when we multiply $M(\mathbf{S}_1)$ with $M(\mathbf{S}_2)$, we obtain, not $M(\mathbf{S}_1\mathbf{S}_2)$, but rather $-M(\mathbf{S}_1\mathbf{S}_2)$, which is not in the set. Therefore in order to obtain a group, we must extend the set of operators to include both $M(\mathbf{S})$ and $-M(\mathbf{S})$ for every symplectic $\mathbf{S}$.

We see that in order to uniquely specify a metaplectic operator, we must not only give the symplectic matrix to which it corresponds, but we must also give the choice of

sign, which we denote by σ. Thus, an unambiguous notation for a metaplectic operator is $M(\mathbf{S},\sigma)$. This operator has x-space matrix elements given by

$$\langle \mathbf{x}|M(\mathbf{S},\sigma)|\mathbf{x}'\rangle = \frac{\sigma}{(2\pi i\hbar)^{N/2}\sqrt{\det \mathbf{B}}} \times \exp\left[\frac{i}{2\hbar}\left(\tilde{\mathbf{x}}'\mathbf{B}^{-1}\mathbf{A}\mathbf{x}' - 2\tilde{\mathbf{x}}'\mathbf{B}^{-1}\mathbf{x} + \tilde{\mathbf{x}}\mathbf{D}\mathbf{B}^{-1}\mathbf{x}\right)\right], \tag{4.37}$$

where $\sigma = \pm 1$. To maintain agreement with our computation of phases above, we will take the branch cut of the square root to lie just under the negative real axis, so that the phase of $\sqrt{\det \mathbf{B}}$ is either 0 or $\pi/2$. Similarly, the phase of $i^{N/2}$ is $N\pi/4$ (we take the square root first, and then raise to the N-th power). Note that with this convention for the phase of the square root, the algebraic rules $\sqrt{xy} = \sqrt{x}\sqrt{y}$ and $\sqrt{1/x} = 1/\sqrt{x}$ are *not* in general true.

Having made this careful analysis of phases, we now partially set it aside, and adopt the following admittedly imprecise but useful notation. We will write $M(\mathbf{S})$, without the sign σ, either when we do not care what the sign is, or when a formula as written is true for one or more of the possible choices of signs, or when the sign cancels. For example, we now display a pair of fundamental results,

$$M(\mathbf{S}_1)M(\mathbf{S}_2) = \pm M(\mathbf{S}_1\mathbf{S}_2), \tag{4.38}$$

and

$$M(\mathbf{S})^{-1} = M(\mathbf{S})^\dagger = \pm M(\mathbf{S}^{-1}). \tag{4.39}$$

This notation tends to be useful, because for many purposes it is more important to recognize the 2-to-1 association than it is to work with some explicit representation of it, such as the conventions developed here for σ. (Later we will see other conventions, as well.)

An important case in which the sign cancels is when the combination $M(\mathbf{S})^\dagger$, $M(\mathbf{S})$ occur together. One example of this has already been given, in Eq. (4.3), and it will occur

again, in other conjugation formulas. These are examples of the fact that the product $Mp(2N)^{\dagger} \times Mp(2N)$ transforms, not according to the metaplectic group, but according to the classical symplectic matrices (as can be seen in Eq. (4.3)). The analogous fact in the theory of rotation operators is that, even for half-integral angular momenta, vector operators transform under conjugations according to the classical 3×3 rotation matrices, and do not have any double valuedness. For example, the electron spin operator $\mathbf{S} = (\hbar/2)\sigma$ transforms as an ordinary 3-vector. Analogously, the operator vector $\hat{\mathbf{z}}$ transforms as an ordinary $2N$-vector in phase space.

We shall not display the mixed **x**- and **p**-space, or full **p**-space, matrix elements of $M(\mathbf{S}, \sigma)$, since these are easily obtained by replacing **S** by **JS** or $\mathbf{SJ}^{-1}$ or $\mathbf{JSJ}^{-1}$, as we shall show in Sec. 6. Furthermore, even if such results were displayed, they would be incomplete, since **x** and **p** are vectors, so that the Fourier transform can be carried out on any subset of the components of **x** or **p**. All these possible matrix elements are easily obtained from Eq. (4.37) by multiplying symplectic matrices.

5. Metaplectic Operators and Caustics

As is evident from Eq. (4.37), the matrix element $\langle \mathbf{x}|M(\mathbf{S})|\mathbf{x}'\rangle$ diverges when $\det \mathbf{B} \to 0$. In this section I will show that this divergence is a kind of caustic, and I will develop limiting forms for the metaplectic matrix elements as the caustic is approached.

5.1. Caustics and Divergences

The word "caustic" often raises alarm bells. When a caustic is approached, one has the expectation that some approximation is breaking down, and is leading to nonphysical infinities. Furthermore, various singularities and discontinuities are expected, such as a discontinuity of the phase. Let us therefore address these issues in connection with the metaplectic matrix elements.

First, I emphasize that the derivation of Eq. (4.37) involved no approximation. It began with Eq. (4.3) and led directly to the metaplectic matrix elements of Eq. (4.37). Therefore the divergence as $\det \mathbf{B} \to 0$ is not the result of some approximation breaking down, but rather it is correct and real. Next, we may note that the divergence in question is not in a wave function, but rather in the matrix elements of an operator. In fact, as I shall show, when $\det \mathbf{B} \to 0$, the matrix element $\langle \mathbf{x}|M(\mathbf{S})|\mathbf{x}'\rangle$ assumes the form of δ-functions of linear combinations of $\mathbf{x}$ and $\mathbf{x}'$. These δ-functions represent perfectly well behaved operators, as can be seen in the special case $\mathbf{S} = \mathbf{I}$, where $M(\mathbf{S}) = \pm 1$ and $\langle \mathbf{x}|M(\mathbf{S})|\mathbf{x}'\rangle = \pm\delta(\mathbf{x} - \mathbf{x}')$. In other words, it is the $\mathbf{x}$-space matrix element which is diverging, not the operator itself in any intrinsic sense. In fact, the metaplectic operators are quite well behaved; they are not only bounded for all values of $\mathbf{S}$, they are, by construction, unitary.

Next we consider the question of discontinuities. This is a real question, because if we compute a matrix function $\mathbf{S}(t)$ in a classical nearby orbit problem, and similarly the corresponding metaplectic operator $M(t) = M\big(\mathbf{S}(t)\big)$, we would like to know if $M(t)$ will

suffer a discontinuity when we cross a caustic, i.e. when $\det \mathbf{B}(t) \to 0$. The answer is that the operator $M(t)$ itself is perfectly continuous as the caustic is crossed, although its **x**-space matrix elements will diverge as the caustic is approached, and the sign σ of Eq. (4.37) may undergo a discontinuity on crossing the caustic. Indeed, in this section we shall determine the rules for the sign changes in σ, based on the requirement that $M(t)$ be continuous.

To say that $M(t)$ is continuous as we cross a caustic means that the operator difference $M(t+\Delta t) - M(t)$ is small when Δt is small, even when the two times straddle a caustic. However, since the difference of the **x**-space matrix elements is not small in this situation, we should say what is meant by a small operator difference. There are actually several different ways to define continuity of operators (Reed and Simon [1980]), but the fact is that for all reasonable definitions of continuity, the familily of metaplectic operators $M(t)$ which we have in mind is continuous for all t. In a practical sense, it comes down to this. If $|\psi_0\rangle$ is some fixed state, and properly a member of Hilbert space, so that $\langle\psi_0|\psi_0\rangle$ is finite, then $M(t+\Delta t)|\psi_0\rangle - M(t)|\psi_0\rangle$ is small (in the sense of the usual norm on Hilbert space) when Δt is small. (This is strong continuity.) This means in particular that if $|\psi_0\rangle$ represents a wave packet which is being propagated in time by an operation represented by $|\psi(t)\rangle = M(t)|\psi_0\rangle$, then $|\psi(t)\rangle$ undergoes no discontinuity or divergence of any kind when the caustic is crossed. This is part of the reason why wave packet techniques do not suffer from caustic difficulties.

On the other hand, if $|\psi_0\rangle$ is a "state" like $|\mathbf{x}\rangle$, which is not normalizable, then there may be divergences, as indeed we see there are from Eq. (4.37). In other words, the caustic divergences of Eq. (4.37) are the fault of the **x**-representation, and not of the metaplectic operators themselves. That is also why the matrix **B** seems to play a privileged role; in another representation, such as the momentum representation, another submatrix of **S** would take the place of **B** in determining divergences. None of these submatrices has any

privileged role in phase space. On the other hand, if we were to use matrix elements of $M(\mathbf{S})$ taken between proper Hilbert space vectors, such as harmonic oscillator eigenstates, then there would be no divergences at all. In particular, the coherent state matrix elements of the metaplectic operators are always finite and continuous.

Therefore several questions of strategy arise here. First, if the **x**-space matrix elements have divergences, then why do we not use, say, momentum space matrix elements? The answer to this is that the states $|\mathbf{p}\rangle$ are not normalizable either, and thus the momentum space matrix elements also have divergences. It is true, however, that the divergences of the momentum space matrix elements $\langle \mathbf{p}|M(\mathbf{S})|\mathbf{p}'\rangle$ usually occur at different locations within the space of symplectic matrices, although the overall structure of the divergences is the same as in the case of the configuration space matrix elements. In fact, one can show that when the **x**-space matrix element diverges, there always exists some combination of **x**- and **p**-components with respect to which the matrix element of $M(\mathbf{S})$ is finite and well behaved. This fact is one of the essential ingredients in the Maslov theory, and it allows one to make a practical analysis of the divergences of the **x**-space matrix elements by a selective appeal to the Fourier transform. We do not take this approach in this section, but rather we stay with the **x**-space matrix elements. But we do set up the practical machinery which would be required for the Fourier transform approach; this is most of the work anyway, and the interested reader can easily fill in the missing details. In any case, since the overall structure of the caustic singularities is the same in any representation obtained from the **x**-representation by a partial or a complete Fourier transform, we are in effect solving all cases at once by dealing only with the **x**-representation. (In fact, the caustic structure is the same in any representation obtained from the **x**-representation by *any* fixed, passive metaplectic transformation. The structure, although not the actual locations, of the caustic singularities is an invariant of the symplectic group.)

Second, if wave packet techniques do not lead to caustic difficulties, and if divergences can be avoided by using, say, coherent state matrix elements, then why do we not switch to these matrix elements here, and simply forget about the **x**-representation? The answer is that we could do this, and in a sense the contents of this section are not, strictly speaking, necessary for the subject of wave packet propagation. (The reader who is only interested in wave packet propagation could skip this section without much loss of continuity.) Nevertheless, the coherent state basis is less familiar and in some respects less convenient to use than the **x**-basis. Furthermore, the divergence of the metaplectic matrix elements at caustics is an important part of the theory of caustics, and sheds considerable light on the general phenomenon. It is also an interesting subject in its own right, and contributes to an understanding of why nonphysical divergences at caustics do not occur in wave packet techniques, or, for that matter, in any semiclassical approach based on invariance principles in phase space. In addition, one of our aims in this paper is to present a reasonably complete accounting of the properties of the metaplectic operators, and the caustic singularities are certainly a part of it. In later sections we shall make some use of the **x**-space matrix elements of $M(\mathbf{S})$ when $\det \mathbf{B} = 0$.

Besides, caustics are physically real, if not in the sense of infinities in the wave field in configuration space, at least in the sense of the enhancement of wave intensity at certain locations and the evanescent penetration into classically forbidden regions. This is true in spite of the fact that caustics have no invariant meaning in phase space. The general theory of caustics involves catastrophe theory, as reviewed by Berry and Upstill [1980] and Kravtsov and Orlov [1983], and an interesting question would be to relate wave packet methods to this general theory. We will not do this here, but rather leave it as a problem for the future.

The caustics we encounter in this section are of a rather special kind, because of our focus on quadratic Hamiltonians. We will find no Airy functions, nor any of their

generalizations. Catastrophe theory in the usual sense does not enter, because quadratic Hamiltonians produce linear maps on phase space, which always take Lagrangian planes into other such planes. These can and do have singular projections onto configuration space, but the singularities are not stable with respect to small perturbations, even linear ones.

Our discussion of caustics begins with a classical analysis, and then proceeds to a discussion of the metaplectic matrix elements when $\det \mathbf{B} \to 0$.

5.2. A Classical Picture of Caustics for Quadratic Hamiltonians

To deal with the case $\det \mathbf{B} = 0$, it is well to begin with a classical analysis. For the time being, let us assume that we are dealing with a classical Hamiltonian which is a quadratic function of $\mathbf{z}$, and which may be time-dependent. Ultimately, of course, we are interested in the linearized behavior around some reference orbit, in which a quadratic Hamiltonian is only an approximation. But for the sake of simplicity, we shall momentarily assume that our quadratic Hamiltonian is globally valid in phase space. When we have completed this analysis, we will say a few words about how the results can be interpreted in the nearby orbit problem.

Let us suppose that some initial conditions $\mathbf{z}_i$ at $t = 0$ give rise to an orbit $\mathbf{z}(t)$, reaching final point $\mathbf{z}_f$ at time t_f. Then we know that the final condition is related to the initial condition by some symplectic matrix $\mathbf{S}$, which depends only on t_f. That is, we have $\mathbf{z}_f = \mathbf{S}(t_f)\mathbf{z}_i$.

The correct analogy between this situation and the matrix element (4.37) is to identify $\mathbf{x}'$ with the configuration space part of $\mathbf{z}_i$, and $\mathbf{x}$ with the configuration space part of $\mathbf{z}_f$. Furthermore, we identify $\mathbf{S}(t_f)$ with the symplectic matrix $\mathbf{S}$ appearing in Eq. (4.37). That is, we take $\mathbf{x}' = \mathbf{q}_i$ and $\mathbf{x} = \mathbf{q}_f$, so that we are interested in classical orbits which start at

$\mathbf{x}'$ at $t = 0$ and reach $\mathbf{x}$ at $t = t_f$. The reason for considering such orbits in connection with Eq. (4.37) comes from an interpretation of the matrix element as a Green's function, since a Green's function indicates the final wave field at position $\mathbf{x}$ and time t_f due to an initial δ-function disturbance at position $\mathbf{x}'$ at time $t = 0$.

Consequently, we are interested in orbits for which the initial and final positions are given. Of course, if the initial position and momentum were given, then we would have a unique orbit, but since instead we have initial and final positions, it is not clear that any such orbit exists, or, if it does, whether it is unique. Let us therefore consider the first half of the transformation equations $\mathbf{z} = \mathbf{S}\mathbf{z}'$ (where $\mathbf{z}' = \mathbf{z}_i$, $\mathbf{z} = \mathbf{z}_f$) in the form

$$\mathbf{B}\mathbf{p}' = \mathbf{x} - \mathbf{A}\mathbf{x}'. \tag{5.1}$$

If knowledge of $\mathbf{x}$ and $\mathbf{x}'$ implies a unique determination of the initial momentum $\mathbf{p}'$, then we have a unique orbit. Therefore we ask, under what conditions, for fixed $\mathbf{S}$ and chosen $\mathbf{x}$, $\mathbf{x}'$, does there exist an initial momentum $\mathbf{p}'$ which will satisfy this relation? Clearly, if $\det \mathbf{B} \neq 0$, then $\mathbf{p}'$ exists and is unique, and is given by

$$\mathbf{p}' = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{A}\mathbf{x}'). \tag{5.2}$$

On the other hand, if $\det \mathbf{B} = 0$, then in general there will not exist a solution, and the chosen final point $\mathbf{x}$ simply cannot be reached by an orbit beginning at $\mathbf{x}'$. This will be the case if the right hand side of Eq. (5.1) is not orthogonal to the left null eigenvectors of $\mathbf{B}$, i.e. the vectors $\mathbf{u}$ such that $\tilde{\mathbf{u}} \cdot \mathbf{B} = 0$. Mathematically, these left null eigenvectors are covectors in the dual space to $\mathbf{x}$-space, and they span the kernel of $\tilde{\mathbf{B}}$; they can be interpreted as momentum vectors in $\mathbf{p}$-space, because the expression $\tilde{\mathbf{u}} \cdot \mathbf{x}$ occurs in the orthogonality condition. The general situation is illustrated in Fig. 5. Let us suppose that there are n linearly independent left null eigenvectors $\mathbf{u}$ of $\mathbf{B}$, which we denote by $\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(n)}$, which we arrange as column vectors in an $N \times n$ matrix $\mathbf{U}_n$. The number n is the corank of $\mathbf{B}$, i.e. the dimensionality of the kernel or nullity of $\mathbf{B}$, and we shall call it

the *order* of the caustic. We denote the rank of $\mathbf{B}$ by r, so that $n+r=N$. The symplectic condition places no restriction on the rank of $\mathbf{B}$, so that n can take on any value between 0 and N. $\mathbf{B}$ can even vanish, as happens in the case $\mathbf{S}=\mathbf{I}$. In any case, we conclude that a solution $\mathbf{p}'$ to Eq. (5.1) exists only if

$$\tilde{\mathbf{U}}_n(\mathbf{x}-\mathbf{A}\mathbf{x}')=0. \tag{5.3}$$

On the other hand, if $\mathbf{x}$ and $\mathbf{x}'$ are chosen so that Eq. (5.3) is satisfied, then a solution for $\mathbf{p}'$ does exist, but it is not unique. In this case the general solution of Eq. (5.1) is given by

$$\mathbf{p}'=\mathbf{p}'_0+\sum_{i=1}^{n}c_i\mathbf{v}^{(i)}, \tag{5.4}$$

where $\mathbf{p}'_0$ is a particular solution to Eq. (5.1), and where we have represented an arbitrary linear combination of the *right* null eigenvectors of $\mathbf{B}$, i.e. the vectors $\mathbf{v}$ such that $\mathbf{B}\cdot\mathbf{v}=0$. (Later we will provide an explicit formula for $\mathbf{p}'$, including the particular solution $\mathbf{p}'_0$.) The linearly independent set $\mathbf{v}^{(1)},\ldots,\mathbf{v}^{(n)}$ span the kernel of $\mathbf{B}$, and can also be arranged column-wise into an $N\times n$ matrix $\mathbf{V}_n$. The vectors $\mathbf{v}^{(i)}$ represent physically momentum vectors in $\mathbf{p}'$-space. The set of all $\mathbf{p}'$ vectors which map onto the same final $\mathbf{x}$ point (i.e. by following an orbit with initial conditions $\mathbf{x}'$, $\mathbf{p}'$) is represented by an n-dimensional plane in $\mathbf{p}'$-space. If $\mathbf{p}'=0$ is a possible solution to Eq. (5.1), then this plane passes through the origin of $\mathbf{p}'$-space, i.e. it is the kernel of $\mathbf{B}$; otherwise it is an n-dimensional plane parallel to the kernel of $\mathbf{B}$.

Let us imagine that at $t=0$ an infinite number of particles are emitted from $\mathbf{x}'$, with all possible initial momenta $\mathbf{p}'$, and distributed, say, uniformly in $\mathbf{p}'$. This would correspond to an initial condition of a wave equation, $\psi_i(\mathbf{x}_i)=\delta(\mathbf{x}_i-\mathbf{x}')$, since the Fourier transform of the δ-function has uniform density in momentum. Classically, it corresponds to the initial N-dimensional Lagrangian plane in the phase space $\mathbf{z}'$ specified by $\mathbf{x}_i=\mathbf{x}'$, $\mathbf{p}_i=\mathbf{p}'=$ anything.

The spatial density of particles is infinite at $\mathbf{x}'$ at $t = 0$. But at final point $\mathbf{x}$ at the later time t_f, the spatial density will be finite if $\det \mathbf{B} \neq 0$, since only one initial momentum $\mathbf{p}'$ gives an orbit arriving at $\mathbf{x}$. However, if $\det \mathbf{B} = 0$, then there are two cases. If $\mathbf{x}$ and $\mathbf{x}'$ are such that Eq. (5.3) is not satisfied, then there are no orbits arriving at $\mathbf{x}$, and the density at $\mathbf{x}$ is zero. But if $\mathbf{x}$ and $\mathbf{x}'$ do satisfy Eq. (5.3), then there is an n-dimensional infinity of initial momenta which map onto $\mathbf{x}$, and the density of particles is infinite at $\mathbf{x}$.

We see that if $\det \mathbf{B} = 0$, then the distribution of particles in $\mathbf{x}$-space (considering now $\mathbf{x}$ variable and $\mathbf{x}'$ fixed) is concentrated with infinite density on a surface specified by Eq. (5.3). This is the caustic surface, and it is an r-dimensional plane. Equation (5.3) shows that the left null eigenvectors $\mathbf{u}^{(i)}$ are all orthogonal to the caustic surface, and determine its orientation. If $\mathbf{x}'$ is such that $\tilde{\mathbf{U}}_n \mathbf{A} \cdot \mathbf{x}' = 0$, then this plane passes through the origin of $\mathbf{x}$-space, and is the image of $\mathbf{B}$; otherwise it is parallel to the image of $\mathbf{B}$.

For an arbitrary matrix taken out of context, there is no particular relation between the left and right null eigenvectors. But the symplectic condition provides additional structure, and gives us such a relation for the matrix $\mathbf{B}$. Let us consider a left null eigenvector $\mathbf{u}$, which we multiply by the matrix $\tilde{\mathbf{A}}$. Then by Eq. (A.9) we have $\mathbf{B}\tilde{\mathbf{A}}\mathbf{u} = \mathbf{A}\tilde{\mathbf{B}}\mathbf{u} = 0$, and we see that $\tilde{\mathbf{A}}\mathbf{u}$ is a right null eigenvector of $\mathbf{B}$. If we let $\tilde{\mathbf{A}}$ act on the entire linearly independent set $\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(n)}$ of left null eigenvectors, we obtain a set of n right null eigenvectors, and we would like to know if these are linearly independent. We cannot assume that $\det \mathbf{A} \neq 0$, because $\mathbf{A}$ may be singular, even when $\mathbf{B}$ is also singular. But the symplectic condition imposes constraints on the simultaneous singularity of the two matrices $\mathbf{A}$ and $\mathbf{B}$, because $\det \mathbf{S} = 1$. This means in particular that if some linear combination of rows of $\mathbf{B}$ should vanish, then the same linear combination of rows of $\mathbf{A}$ cannot vanish, because if it did, there would be a vanishing linear combination of rows of $\mathbf{S}$. Therefore the collection of vectors $\{\tilde{\mathbf{u}}^{(i)} \cdot \mathbf{A}, i = 1, \ldots, n\}$ are linearly independent, and

they provide us (taking the transpose) with a basis for the kernel of $\mathbf{B}$. In other words, with no loss of generality, we can take

$$\mathbf{V}_n = \tilde{\mathbf{A}}\mathbf{U}_n, \tag{5.5}$$

which we shall henceforth do.

Clearly it is desirable, in dealing with the caustic surface, to introduce coordinates in which the surface is oriented in a simple way. We do this as follows. In addition to the vectors $\mathbf{u}^{(i)}$, $i = 1, \ldots, n$, we choose r more such vectors $u^{(i)}$, $i = n+1, \ldots, N$, so that the whole collection of N vectors is linearly independent. Since the first n $\mathbf{u}^{(i)}$ are orthogonal to the caustic surface, the remaining r $\mathbf{u}^{(i)}$ define coordinates on the caustic surface. We arrange these new r vectors column-wise into an $N \times r$ matrix $\mathbf{U}_r$, which can be appended to the right of $\mathbf{U}_n$ to form an invertible $N \times N$ matrix $\mathbf{U}$. There are, of course, many ways to choose these r vectors, and no choice has any privileged role. The same is true for the choice of the particular linearly independent combination of left null eigenvectors of $\mathbf{B}$, which form the columns of $\mathbf{U}_n$. We do not demand orthogonality for any of these vectors, because orthogonality has no invariant meaning under symplectic transformations. To demand orthogonality would only cloud the fundamental issues.

Next, we define new coordinates $\mathbf{y}$ in $\mathbf{x}$-space by

$$\mathbf{y} = \tilde{\mathbf{U}}\mathbf{x}. \tag{5.6}$$

Sometimes we decompose $\mathbf{y}$ into its first n and remaining r components, $\mathbf{y}_n$ and $\mathbf{y}_r$, which are respectively n- and r-dimensional vectors, so that $\mathbf{y}_n = \tilde{\mathbf{U}}_n\mathbf{x}$, $\mathbf{y}_r = \tilde{\mathbf{U}}_r\mathbf{x}$. Then in terms of the new coordinates, the caustic surface is specified by an equation involving only $\mathbf{y}_n$,

$$\mathbf{y}_n = \tilde{\mathbf{U}}_n\mathbf{A}\mathbf{x}' = \tilde{\mathbf{V}}_n\mathbf{x}', \tag{5.7}$$

which is constant if $\mathbf{x}'$ is fixed. The remaining components of $\mathbf{y}$, $\mathbf{y}_r$, represent coordinates on the caustic surface.

Similarly, we perform a change of coordinates in $\mathbf{x}'$-space to simplify expression for the kernel of $\mathbf{B}$. (This is really a change of basis in $\mathbf{p}'$-space, which induces a dual basis in $\mathbf{x}'$-space.) As with $\mathbf{U}$, we fill out the $N\times n$ matrix $\mathbf{V}_n$ with r more columns, denoted collectively by $\mathbf{V}_r$, which is an $N\times r$ matrix, to form altogether an invertible $N\times N$ matrix $\mathbf{V}$. (We cannot take $\mathbf{V}_r = \tilde{\mathbf{A}}\mathbf{U}_r$, because when $\det\mathbf{A} = 0$, the resulting $\mathbf{V}$ would be singular. We cannot assume any relation between $\mathbf{U}_r$ and $\mathbf{V}_r$.) We then set

$$\mathbf{y}' = \tilde{\mathbf{V}}\mathbf{x}', \tag{5.8}$$

and similarly write $\mathbf{y}'_n = \tilde{\mathbf{V}}_n\mathbf{x}'$, $\mathbf{y}'_r = \tilde{\mathbf{V}}_r\mathbf{x}'$. The r-dimensional plane in $\mathbf{x}'$-space which is perpendicular to the kernel of $\mathbf{B}$ is now specified by $\mathbf{y}'_n = 0$, $\mathbf{y}'_r =$ anything, and we see that the vector $\mathbf{y}'_r$ serves as a coordinate vector on this plane. The equation for the caustic surface now takes on the simple form,

$$\mathbf{y}_n = \mathbf{y}'_n. \tag{5.9}$$

These changes of coordinates induce dual changes of coordinates in $\mathbf{p}$- and $\mathbf{p}'$-space. We define

$$\begin{aligned}\mathbf{k} &= \mathbf{U}^{-1}\mathbf{p},\\ \mathbf{k}' &= \mathbf{V}^{-1}\mathbf{p}',\end{aligned} \tag{5.10}$$

which cause the transformations $(\mathbf{x},\mathbf{p}) \to (\mathbf{y},\mathbf{k})$ and $(\mathbf{x}',\mathbf{p}') \to (\mathbf{y}',\mathbf{k}')$ to be canonical (they are both point transformations). In effect, we have replaced our symplectic matrix $\mathbf{S}$ by $\mathbf{S}_0\mathbf{S}\mathbf{S}_1^{-1}$, where

$$\mathbf{S}_0 = \begin{pmatrix}\tilde{\mathbf{U}} & 0\\ 0 & \mathbf{U}^{-1}\end{pmatrix}, \qquad \mathbf{S}_1 = \begin{pmatrix}\tilde{\mathbf{V}} & 0\\ 0 & \mathbf{V}^{-1}\end{pmatrix}. \tag{5.11}$$

This causes the replacements $\mathbf{A} \mapsto \tilde{\mathbf{U}}\mathbf{A}\tilde{\mathbf{V}}^{-1}$, $\mathbf{B} \mapsto \tilde{\mathbf{U}}\mathbf{B}\mathbf{V}$, $\mathbf{C} \mapsto \mathbf{U}^{-1}\mathbf{C}\tilde{\mathbf{V}}^{-1}$, $\mathbf{D} \mapsto \mathbf{U}^{-1}\mathbf{D}\mathbf{V}$, which we denote respectively by $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$. The change of coordinates makes it natural to partition each of these into their $n\times n$, $n\times r$, $r\times n$, and $r\times r$ submatrices, denoted $\mathbf{a}_{nn}$, $\mathbf{a}_{nr}$,

$\mathbf{a}_{rn}$, $\mathbf{a}_{rr}$, etc. By using the relations $\tilde{\mathbf{U}}_n\mathbf{B} = 0$, $\mathbf{B}\mathbf{V}_n = 0$, and the symplectic conditions (A.9), we find a simplification in many of the submatrices, which are summarized by

$$\mathbf{a} = \begin{pmatrix} \mathbf{I}_{nn} & 0 \\ \mathbf{a}_{rn} & \mathbf{a}_{rr} \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{b}_{rr} \end{pmatrix},$$

$$\mathbf{c} = \begin{pmatrix} \mathbf{c}_{nn} & \mathbf{c}_{nr} \\ \mathbf{c}_{rn} & \mathbf{c}_{rr} \end{pmatrix}, \qquad \mathbf{d} = \begin{pmatrix} \mathbf{I}_{nn} & \mathbf{d}_{nr} \\ 0 & \mathbf{d}_{rr} \end{pmatrix}. \tag{5.12}$$

We note in particular that the $r \times r$ matrix $\mathbf{b}_{rr}$ has rank r and is, therefore, invertible.

We can now give a complete and explicit solution to the inversion problem (5.1). Writing this out in the new coordinates, we have

$$\begin{aligned} 0 &= \mathbf{y}_n - \mathbf{y}'_n, \\ \mathbf{b}_{rr}\mathbf{k}'_r &= \mathbf{y}_r - \mathbf{a}_{rn}\mathbf{y}'_n - \mathbf{a}_{rr}\mathbf{y}'_r. \end{aligned} \tag{5.13}$$

A solution for $\mathbf{k}'$ exists only when $\mathbf{y}_n = \mathbf{y}'_n$, whereupon the solution takes the form

$$\begin{aligned} \mathbf{k}'_n &= \text{anything}, \\ \mathbf{k}'_r &= \mathbf{b}_{rr}^{-1}\left(\mathbf{y}_r - \mathbf{a}_{rn}\mathbf{y}'_n - \mathbf{a}_{rr}\mathbf{y}'_r\right). \end{aligned} \tag{5.14}$$

This classical solution will prove to be of value in analyzing the matrix element (4.37).

5.3. Phase Space Picture of Caustics

It is enlightening to view this classical picture of caustics which we have developed from the standpoint of phase space. Figure 6 shows the general situation in the case $N = 1$; unfortunately, it is not easy to represent phase space in a diagram when $N > 1$, so some imagination must be used in the general case.

The initial condition at time $t = 0$ is $q_i = x'$, as shown in the figure. The ensemble of initial particles, all satisfying $q_i = x'$ and uniformly distributed in the initial momentum p', is represented by the vertical line L_0. In higher dimensions, L_0 is an N-dimensional

plane, because it is a copy of momentum space. It is also a Lagrangian plane, as explained in Sec. 3.

As time progresses, the points constituting L_0 follow their respective orbits, and produce the new Lagrangian plane L_1 at some time t_1. L_1 is still a plane, because the Hamiltonian, by hypothesis, is quadratic, and generates linear equations of motion. It is also Lagrangian, because Lagrangian manifolds evolve into other Lagrangian manifolds under Hamilton's equations. This new Lagrangian plane L_1 (a line in the diagram) has a nonsingular projection onto configuration space, and the final particle density at any point x at time t_1 is finite (such as $x = x_1$ in the figure). This corresponds to the case $\det \mathbf{B} \neq 0$.

Later, however, at time t_2, we suppose that the Lagrangian plane has turned over and become vertical, as shown by the line L_2 in the diagram. Now if we choose a final point such as $x = x_2$, we see that the final density of particles is zero, since no orbits arrive at x_2 at time t_2. But if we choose $x = x_3$ as a final point, then the density of particles is infinite, and we have a caustic. This corresponds to the case $\det \mathbf{B} = 0$, and we see that the caustic "surface" in the diagram is just the one point $x = x_3$ (which is zero-dimensional).

Let us now consider the more general case of a nonquadratic Hamiltonian, which has a quantum propagator $U(t) = e^{-itH/\hbar}$ and Green's function $\langle \mathbf{x}|U(t)|\mathbf{x}'\rangle$. Again, as shown in Fig. 7, the appropriate classical picture is one in which initial particles are spread uniformly in momentum over the initial Lagrangian plane L_0. Now, however, in the course of time the Lagrangian surface distorts and does not remain a plane (although it is still Lagrangian), and it turns into the curved surface L_1 at time t_1.

Let us consider first the final point $x = x_1$ at time t_1 in the figure. We will speak in one-dimensional terms for a moment. We see that there are two orbits which reach $x = x_1$ from x' in the given time, one with initial conditions $\mathbf{z}_1' = (x', p_1')$ and final conditions $\mathbf{z}_1 = (x_1, p_1)$, and the other below the q-axis (not labelled). The particle density at x_1

is a sum of two terms, coming from these two orbits and orbits nearby them. However, both contributions are finite, because the tangent line to L_1 at the point $\mathbf{z}_1$ has a finite slope (and similarly for the second orbit below). This finite slope is similar to that of the Lagrangian line L_1 in Fig. 6. The tangent line to L_1 at $\mathbf{z}_1$ in Fig. 7 is evidently the image of a small piece of the initial Lagrangian line L_0 at $\mathbf{z}'_1$, under the linearized classical evolution which results from treating $\mathbf{z}_1(t)$ as a reference orbit. This linearized evolution is described by the symplectic matrix $\mathbf{S}_1(t)$, as discussed in Sec. 2.

The tangent line to L_1 at $\mathbf{z}_1$ generalizes in higher dimensions to a piece of a Lagrangian plane which is tangent to the (generally curved) Lagrangian manifold. And the finite slope of the tangent line at $\mathbf{z}_1$ in Fig. 7 generalizes to the nonsingularity of the projection of this tangent plane onto configuration space. As in our discussion above, this nonsingularity condition is equivalent to $\det \mathbf{B}_1(t_1) \neq 0$, where $\mathbf{B}_1(t)$ is the submatrix of $\mathbf{S}_1(t)$. Therefore, there is no caustic at x_1 at time t_1.

Next we consider the point $x = x_2$ at time t_1. Now there are no orbits arriving at x_2 in the given time, and the density of classical particles is zero.

Finally we consider the point $x = x_3$ at time t_1. In this case the tangent to the Lagrangian surface at $\mathbf{z}_3$ has infinite slope, so the density of classical particles at x_3 is infinite, and we have a caustic. In higher dimensions, this caustic would be indicated by the vanishing of $\det \mathbf{B}_3(t_1)$, where $\mathbf{B}_3(t)$ is the submatrix of $\mathbf{S}_3(t)$, obtained by treating $\mathbf{z}_3(t)$ as a reference orbit.

Although in Fig. 7 the caustic "surface" is just one point, in higher dimensions it is a real surface, generally curved, in configuration space. Figure 8 is an attempt to illustrate this for the case $N = 2$. Every point on this surface is characterized by the fact that it the projection of a Lagrangian manifold onto configuration space is singular there. This Lagrangian manifold is the image under the classical evolution of the initial

Lagrangian manifold, which is the momentum plane situated at $\mathbf{x}'$ at $t = 0$. Furthermore, a classical orbit $\mathbf{z}(t)$ starting from the initial Lagrangian manifold and arriving at the final one contributes to a caustic there if the submatrix $\mathbf{B}(t)$ of the symplectic matrix $\mathbf{S}(t)$, obtained by linearizing about $\mathbf{z}(t)$, is singular at the final time. The local orientation of the caustic surface in configuration space is determined by the left null eigenvectors $\mathbf{u}$ of $\mathbf{B}(t)$, as in our analysis above of quadratic Hamiltonians. (Usually there is only one left null eigenvector when $\det \mathbf{B} = 0$, and the caustic surface is $(N-1)$-dimensional.)

Note that the caustic at x_3 in Fig. 7 is not due to a turning point, since the orbit $\mathbf{z}_3(t)$ continues without turning around. Turning points are associated with caustics only in normal mode (i.e. energy eigenfunction) problems, not in initial value problems such as we are considering here.

However, the caustic can be associated with a focussing of rays in configuration space. We can see this by noting that an orbit which is nearby $\mathbf{z}_3(t)$ in Fig. 7, differing from it by a first order displacement $\delta p'$ in initial momentum, arrives at the final point with only a second order displacement in position. This is to say that the quantity $(\partial x/\partial p')_{x'}$ vanishes; in higher dimensions, the analog is the vanishing of the determinant of the matrix $(\partial x_i/\partial p'_j)_{\mathbf{x}'}$, which is none other than the matrix $\mathbf{B}$. In higher dimensions, the first order displacements $\delta \mathbf{p}'$ in initial momentum must lie in the kernel of $\mathbf{B}$ in order to get only second order displacements in the final position.

We see that for any given orbit $\mathbf{z}(t)$, the caustics which it encounters during its time evolution are determined by the vanishing of $\det \mathbf{B}(t)$, which can occur successively at different times. Any of these caustics can be of any order, and, as we shall see, there is a directionality to their crossing, so that they can be counted in either a positive or a negative sense (at least for first order caustics; see below for details). The total count of caustics along a segment of an orbit, including multiplicities and directionality of crossing,

is the Maslov index of the orbit segment. This version of the Maslov index differs somewhat from the one discussed in Sec. 4, as I shall explain presently.

We can also see that the caustics are not so much a property of the orbit $\mathbf{z}(t)$ itself as they are of the symplectic matrix $\mathbf{S}(t)$ describing the linearized motion about the orbit. In fact, even this statement is misleading, for the following reasons. Suppose that instead of the Green's function $\langle \mathbf{x}|U(t)|\mathbf{x}'\rangle$, we were to look at the mixed matrix element of the propagator, $\langle \mathbf{x}|U(t)|\mathbf{p}'\rangle$. The classical picture for this case is indicated in Fig. 9. Since the initial wave disturbance is now a δ-function in momentum space, the initial Lagrangian manifold is not a copy of momentum space, but rather a copy of configuration space with constant momentum p'. As this Lagrangian manifold evolves in time to a later Lagrangian manifold L_1, caustics may indeed develop, as shown by the points x_1 and x_2 and the orbit $\mathbf{z}(t)$. But now the caustics are indicated by the vanishing of the determinant of $(\partial x_i/\partial x'_j)_{\mathbf{p}'}$, which is the $\mathbf{A}$ submatrix of $\mathbf{S}(t)$. Finally, suppose we were interested in the full momentum space Green's function, $\langle \mathbf{p}|U(t)|\mathbf{p}'\rangle$. In this case we still have the same initial Lagrangian manifold L_0 shown in Fig. 9, but the caustics at the later time are now determined by the projection of L_1 onto momentum space, not configuration space. This gives the one caustic $p = p_1$ shown in the figure, corresponding to the singularity of the $\mathbf{C}$ submatrix.

As a result, there is no meaning to the number of caustics encountered by an orbit $\mathbf{z}(t)$ when it is taken out of context. Even when we consider the matrix function $\mathbf{S}(t)$, obtained by linearizing about $\mathbf{z}(t)$, there is still, in general, no meaning to the number of caustics in some time interval. To specify the number of caustics, one must indicate not only $\mathbf{S}(t)$, but also the initial Lagrangian plane (or small piece of one) which is to be transported by $\mathbf{z}(t)$ and rotated by $\mathbf{S}(t)$, as well as the space onto which it is to be projected. This latter space is usually configuration space or momentum space, both of which themselves are Lagrangian planes, but more generally it can be any Lagrangian plane.

Therefore the symplectic matrix function $\mathbf{S}(t)$, taken out of context, does not specify any caustics or Maslov index. It is only when $\mathbf{S}(t)$ is associated with some initial Lagrangian plane to be rotated, and some final Lagrangian plane to be projected upon, that caustics have any meaning. It is for this reason that caustics cannot be considered to have any invariant meaning in phase space. Similarly, the metaplectic operators $M(\mathbf{S})$ are, in any intrinsic sense, oblivious of caustic issues, at least until we place them in some context, such as by looking at the matrix element $\langle \mathbf{x}|M(\mathbf{S})|\mathbf{x}'\rangle$. The metaplectic operators themselves are, in a sense, true phase space objects, and ideally suited for the expression of a theory of semiclassical mechanics on phase space.

However, if one is interested in caustics, then the most satisfactory objects to look at are the Lagrangian planes. The orientation of these planes can be specified by symplectic matrices, but with some redundancy, because more than one symplectic matrix can rotate a Lagrangian plane into some fixed final position (e.g. one can always rotate coordinates on the plane itself, without changing the orientation). Therefore the most satisfactory treatment of caustics does not deal with the space of symplectic matrices, but rather with the space of Lagrangian planes (Arnold [1967]). We do not take this approach in this paper, mainly in order to avoid any unnecessary proliferation of abstract spaces, and we shall stay with the symplectic matrices as the descriptors of caustics.

Finally, I should point out that in wave packet propagation, one is not so much interested in Green's functions *per se* as in some matrix element such as $\langle \mathbf{x}|M(\mathbf{S})|\psi_0\rangle$, where $|\psi_0\rangle$ represents some initial wave packet (say a Gaussian). The initial wave packet does not generally correspond to any initial Lagrangian manifold, so its time evolution does not involve caustic issues.

I turn now to the metaplectic operators and their matrix elements when $\det \mathbf{B} \to 0$.

5.4. Metaplectic Matrix Elements Near Caustics

Equation (4.37) was derived on the assumption that $\det \mathbf{B} \neq 0$, and we now seek the corresponding expression when $\det \mathbf{B} = 0$. We could simply return to the differential equations (4.14) and (4.24) and reanalyze them, but this would not give us the phase of the result. Instead, we shall represent our $\mathbf{S}$ with $\det \mathbf{B} = 0$ as the product of two symplectic matrices $\mathbf{S}_1\mathbf{S}_2$, where $\det \mathbf{B}_1$ and $\det \mathbf{B}_2$ are nonzero. However, if we were to do this with fixed $\mathbf{S}_1$ and $\mathbf{S}_2$, then we would miss a fact of fundamental importance, namely that the metaplectic operators themselves (as in contrast to their matrix elements) are continuous as a caustic is approached and crossed.

We shall examine this situation by embedding the symplectic matrix $\mathbf{S}$ with $\det \mathbf{B} = 0$ in a family $\mathbf{S}(\epsilon)$, which satisfies $\det \mathbf{B}(\epsilon) \neq 0$ for $\epsilon \neq 0$, where ϵ is confined to a finite (but possibly small) neighborhood of zero. Clearly this is the appropriate thing to do when $\mathbf{S}(t)$ results from the classical nearby orbit problem, since typically we will have $\det \mathbf{B}(t) = 0$ only at an isolated point of time $t = t_c$ (where c stands for "caustic").

In this analysis we require a different sense to the term "caustic surface" than was used in the preceding discussion of the classical picture of caustics. There the caustic surface was seen as a surface (in fact, an n-dimensional plane) in $\mathbf{x}$-space. Here, since we are considering the time evolution of $\mathbf{S}(t)$ in the space of symplectic matrices, we shall speak of the caustic surface somewhat differently. It is convenient to do this in terms of the space of the $\mathbf{B}$ matrices, because the caustics are determined by the vanishing of $\det \mathbf{B}$. We could look at things in the larger space of symplectic matrices, but that is not necessary, since only the $\mathbf{B}$ matrix is needed to determine caustics. A trajectory $\mathbf{S}(t)$ in the space of symplectic matrices gives rise to another trajectory $\mathbf{B}(t)$ in $\mathbf{B}$-matrix space, and a caustic occurs when $\det \mathbf{B}(t) = 0$. Therefore we shall now speak of the caustic surface as the surface in $\mathbf{B}$-matrix space where $\det \mathbf{B} = 0$. If there is any possibility of confusion

between this terminology and the caustic surface in **x**-space, we shall indicate explicitly which is meant.

The space of **B** matrices is a simple vector space with N^2 dimensions. Every possible **B** matrix is allowed as a submatrix of a symplectic matrix, so every possible point of this space is accessible by some orbit $\mathbf{B}(t)$. One can easily see this by considering the matrix

$$\mathbf{S} = \begin{pmatrix} \mathbf{I} & \mathbf{B} \\ 0 & \mathbf{I} \end{pmatrix}, \tag{5.15}$$

which is symplectic for every possible **B**.

As we pointed out in Sec. 4, for any given **S** with $\det \mathbf{B} = 0$, it is always possible to introduce a small perturbation (even maintaining the symplectic condition) such that the perturbed **S** has $\det \mathbf{B} \neq 0$. We shall explicitly construct such a perturbation below. This fact has a simple geometrical interpretation in terms of **B**-matrix space. Since the condition $\det \mathbf{B} = 0$ amounts to one constraint on N^2 variables, the caustic surface in **B**-matrix space is a surface of lower dimensionality than that of the whole space, so there is plenty of "room" to move away from it.

It turns out that if we restrict consideration to points on the caustic surface where the corank of **B** is 1, i.e. the points representing first order caustics, then these points form a smooth surface of dimensionality $N^2 - 1$, i.e. one less than the dimensionality of the whole space. Therefore a matrix function $\mathbf{B}(t)$ undergoing a first order caustic at $t = t_c$ can be pictured as shown in Fig. 10. We assume that $\mathbf{B}(t)$ punctures the surface transversally, and does not, for example, touch it tangentially and then pull away again.

In this case we see that the existence of the caustic is stable under small perturbations to the trajectory $\mathbf{B}(t)$. Although an individual matrix **B** can be pulled away from the caustic surface by means of a small perturbation, nevertheless a whole trajectory $\mathbf{B}(t)$ will still have a first order caustic when it is perturbed. The only thing that will happen is that the time t_c at which the caustic occurs will shift by a small amount, as will also the

null eigenvector of $\mathbf{B}$ which determines the orientation of the caustic surface in $\mathbf{x}$-space. Furthermore, we see that in the case of a first order caustic, there are two sides to the caustic surface. These correspond to the positive and negative senses of traversal which are used in determining the Maslov index.

As for second order caustics, the set of points where $\operatorname{corank}\mathbf{B} = 2$ is also a smooth surface, but it has dimensionality $N^2 - 4$, three less than the first order caustic surface. The second order caustic surface obviously must be connected to the first order caustic surface, because by introducing a small perturbation into $\mathbf{B}$ when $\operatorname{rank}\mathbf{B} = N - 2$, we can get rid of one of the linear dependencies of its rows or columns. However, the two surfaces connect in such a way that their combination is not a smooth manifold (Golubitsky and Guillemin [1973]).

The situation is a little hard to see geometrically, because even in the simplest case of $N = 2$, we are dealing with a 4-dimensional space of $\mathbf{B}$ matrices. Nevertheless, the diagram of Fig. 11, representing surfaces in 3-dimensional space, gives the right idea. The first order caustic surface looks like a cone (which extends out to infinity in both directions), omitting the apex. The apex itself is the second order caustic surface, represented with zero dimensions due to the inadequacy of the diagram, but actually having dimensionality $N^2 - 4$.

Now we can get an idea of what happens when $\mathbf{B}(t)$ passes through a second order caustic, although the cone diagram is only an approximation to the real situation in higher dimensional space, and is in some ways misleading. There are two possibilities, as shown in Figs. 12 and 13. Figure 12 shows how a small perturbation introduced into the trajectory $\mathbf{B}(t)$ may cause the caustic to be bypassed altogether. In other words, unlike first order caustics, second order caustics sometimes disappear completely under a small perturbation. On the other hand, Fig. 13 shows that sometimes a small perturbation will cause a second order caustic to bifurcate into two first order caustics, both occurring at times near t_c. We

can also see that a second order caustic can be approached from more than two inequivalent directions.

The general situation for an n-th order caustic is similar, but more complicated. As we shall see, the possible classes of directions from which an n-th order caustic can be approached depends on the number of positive and negative eigenvalues of a certain $n \times n$ matrix $\mathbf{G}$, defined below in Eq. (5.33). In all cases, however, a small perturbation can be introduced to cause an n-th order caustic to break up into a cluster of some number of first order caustics (possibly none at all). For this reason, the Maslov index is often reckoned in terms of first order caustics only (although this is not really necessary).

Let us now return to some symplectic matrix of interest $\mathbf{S}$ satisfying $\det \mathbf{B} = 0$. We shall embed this in a family $\mathbf{S}(\epsilon)$ defined by

$$\mathbf{S}(\epsilon) = \mathbf{T}(\epsilon)\mathbf{S}, \tag{5.16}$$

where $\mathbf{T}(\epsilon)$ is symplectic and satisfies $\mathbf{T}(0) = \mathbf{I}$, where $\mathbf{S} = \mathbf{S}(0)$, and where we require $\det \mathbf{B}(\epsilon) \neq 0$ when $\epsilon \neq 0$. We can find such a $\mathbf{T}(\epsilon)$ in the following way. Writing $\mathbf{z} = \mathbf{S}\mathbf{z}'$, we note that if $\mathbf{z}'$ is purely in the momentum direction, and if its momentum components are purely in the subspace defined by the kernel of $\mathbf{B}$, then $\mathbf{z}$ is also purely in the momentum direction. That is, if we choose $\mathbf{z}'$ to be of the form $(0, \mathbf{v}^{(i)})$, for $1 \leq i \leq n$, then

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \begin{pmatrix} 0 \\ \mathbf{v}^{(i)} \end{pmatrix} = \begin{pmatrix} 0 \\ \mathbf{u}^{(i)} \end{pmatrix}, \tag{5.17}$$

where we have used Eq. (A.9) to show that $\mathbf{D}\mathbf{v}^{(i)} = \mathbf{D}\tilde{\mathbf{A}}\mathbf{u}^{(i)} = \mathbf{u}^{(i)}$. The geometrical significance of this is that the original Lagrangian plane, specified by $\mathbf{x}' = 0$, $\mathbf{p}' =$ anything, has been rotated under $\mathbf{S}$ into a final configuration in which it is partially perpendicular to $\mathbf{x}$-space (in an n-dimensional subspace, spanned by the vectors $\mathbf{u}^{(i)}$, $i = 1, \ldots, n$, which are linearly independent). Our task in choosing $\mathbf{T}(\epsilon)$ will be to rotate the n phase space vectors on the right hand side of Eq. (5.17) so that they have a nonsingular projection onto $\mathbf{x}$-space.

These considerations lead to the following choice for $\mathbf{T}(\epsilon)$,

$$\mathbf{T}(\epsilon) = \begin{pmatrix} \mathbf{I} & \epsilon\tilde{\mathbf{U}}^{-1}\mathbf{U}^{-1} \\ 0 & \mathbf{I} \end{pmatrix}, \tag{5.18}$$

which is symplectic for all values of ϵ, and which gives

$$\mathbf{S}(\epsilon) = \begin{pmatrix} \mathbf{A} + \epsilon\tilde{\mathbf{U}}^{-1}\mathbf{U}^{-1}\mathbf{C} & \mathbf{B} + \epsilon\tilde{\mathbf{U}}^{-1}\mathbf{U}^{-1}\mathbf{D} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}. \tag{5.19}$$

This particular parameterization constitutes only one of the possible directions of approach to the caustic. We note that $\mathbf{B}(\epsilon)$ is now nonsingular in some neighborhood of $\epsilon = 0$, since

$$\mathbf{B}(\epsilon) = \tilde{\mathbf{U}}^{-1}(\mathbf{b} + \epsilon\mathbf{d})\mathbf{V}^{-1}, \tag{5.20}$$

and since

$$\mathbf{b} + \epsilon\mathbf{d} = \begin{pmatrix} \epsilon\mathbf{I}_{nn} & \epsilon\mathbf{d}_{nr} \\ 0 & \mathbf{b}_{rr} + \epsilon\mathbf{d}_{rr} \end{pmatrix}. \tag{5.21}$$

Indeed, we have

$$\det \mathbf{B}(\epsilon) = \epsilon^n \left[\beta + O(\epsilon)\right], \tag{5.22}$$

where

$$\beta = \det \mathbf{b}_{rr} \det(\mathbf{UV})^{-1}. \tag{5.23}$$

The quantity β depends on the particular linear combinations which were used in selecting the left null eigenvectors of $\mathbf{B}$, i.e. the choice of basis for the kernel of $\tilde{\mathbf{B}}$. But its sign is independent of this choice, and depends only on the original symplectic matrix $\mathbf{S}$. Nor does β depend on how the remaining r columns of the matrices $\mathbf{U}$ and $\mathbf{V}$ were chosen. If $n = N$, so that $\mathbf{b}_{rr}$ is vacuous, we shall interpret $\det \mathbf{b}_{rr}$ as $+1$.

Since we now have $\det \mathbf{B}(\epsilon) \neq 0$ for $\epsilon \neq 0$, we can make use of our previous result, Eq. (4.37). It is convenient to call on our transformations (5.6) and (5.8) to the variables $\mathbf{y}$, $\mathbf{y}'$. We also note that

$$(\mathbf{b} + \epsilon\mathbf{d})^{-1} = \begin{pmatrix} \frac{1}{\epsilon}\mathbf{I}_{nn} & -\mathbf{d}_{nr}\mathbf{b}_{rr}^{-1} \\ 0 & \mathbf{b}_{rr}^{-1} \end{pmatrix} + O(\epsilon). \tag{5.24}$$

Keeping only terms which will not vanish as $\epsilon \to 0$, we have

$$\langle \mathbf{x}|M\big(\mathbf{S}(\epsilon),\sigma\big)|\mathbf{x}'\rangle = \frac{\sigma}{(2\pi i\hbar)^{N/2}\sqrt{\epsilon^n\beta}} \times \exp\Big[\frac{i}{2\epsilon\hbar}(\mathbf{y}_n-\mathbf{y}'_n)^2 + \frac{i}{2\hbar}Q(\mathbf{y},\mathbf{y}')\Big], \tag{5.25}$$

where

$$Q(\mathbf{y},\mathbf{y}') = \tilde{\mathbf{y}}'\mathbf{Q}_1\mathbf{y}' - 2\tilde{\mathbf{y}}'\mathbf{Q}_2\mathbf{y} + \tilde{\mathbf{y}}\mathbf{Q}_3\mathbf{y}, \tag{5.26}$$

and where

$$\mathbf{Q}_1 = \begin{pmatrix} \mathbf{c}_{nn} - \mathbf{d}_{nr}\mathbf{b}_{rr}^{-1}\mathbf{a}_{rn} & \tilde{\mathbf{a}}_{rn}\tilde{\mathbf{b}}_{rr}^{-1} \\ \mathbf{b}_{rr}^{-1}\mathbf{a}_{rn} & \mathbf{b}_{rr}^{-1}\mathbf{a}_{rr} \end{pmatrix},$$

$$\mathbf{Q}_2 = \begin{pmatrix} 0 & -\mathbf{d}_{nr}\mathbf{b}_{rr}^{-1} \\ 0 & \mathbf{b}_{rr}^{-1} \end{pmatrix},$$

$$\mathbf{Q}_3 = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{d}_{rr}\mathbf{b}_{rr}^{-1} \end{pmatrix}. \tag{5.27}$$

The matrices $\mathbf{Q}_1$ and $\mathbf{Q}_3$ are symmetric.

Now letting $\epsilon \to 0$, we have the following result for the metaplectic matrix element when $\det \mathbf{B} = 0$:

$$\langle \mathbf{x}|M(\mathbf{S},\sigma)|\mathbf{x}'\rangle = \frac{\sigma\sigma_1}{(2\pi i\hbar)^{r/2}\sqrt{\beta}}\,\delta^n(\mathbf{y}_n-\mathbf{y}'_n)\,\exp\Big[\frac{i}{2\hbar}Q(\mathbf{y},\mathbf{y}')\Big]. \tag{5.28}$$

The quantity σ_1 is either $+1$ or -1, depending on n and the signs of ϵ and β. We shall not give explicit rules for this sign, because our derivation is based on a particular path of approach to the caustic, and because we shall give the more general formula below (for an arbitrary approach). Nevertheless, this result illustrates the fact that when $\det \mathbf{B} = 0$, as when $\det \mathbf{B} \neq 0$, there is a 2-to-1 sign ambiguity in relating a symplectic matrix to a corresponding metaplectic operator. One can also show the overall consistency of this result, i.e. that the group multiplication law $M(\mathbf{S}_1)M(\mathbf{S}_2) = \pm M(\mathbf{S}_1\mathbf{S}_2)$ is valid even when any or all of the matrices $\mathbf{B}_1$, $\mathbf{B}_2$, $\mathbf{B}$ are singular. The matrix element of Eq. (5.28)

is independent of any of the choices that were involved in setting up the matrices $\mathbf{U}$ and $\mathbf{V}$ (i.e. the choice of basis in $\ker \mathbf{B}$, or coordinates on the caustic surface, etc.).

We see from this result that the matrix element of the metaplectic operator, considered as a function of $\mathbf{x}$ and $\mathbf{x}'$, becomes a δ-function concentrated on the caustic surface in $\mathbf{x}$-space when $\det \mathbf{B} = 0$. There is also a phase, which is a function of position along the caustic surface in $\mathbf{x}$-space. Although the matrix element diverges, it does so only as a δ-function, which represents a perfectly well-behaved operator $M(\mathbf{S})$. (Of course, the operator is still unitary, as it must be.)

Special cases of this result are of interest. If $\mathbf{B} = 0$, then the symplectic condition requires that $\mathbf{A}$ be nonsingular and that $\mathbf{D} = \tilde{\mathbf{A}}^{-1}$. In this case we can take $\mathbf{U} = \mathbf{I}$, so that $\mathbf{V} = \tilde{\mathbf{A}}$. Then we have

$$\langle \mathbf{x}|M(\mathbf{S})|\mathbf{x}'\rangle = \frac{\pm 1}{\sqrt{\det \mathbf{A}^{-1}}}\, \delta(\mathbf{x} - \mathbf{A}\mathbf{x}')\, \exp\Big[\frac{i}{2\hbar}\tilde{\mathbf{x}}' \cdot \mathbf{C} \cdot \mathbf{x}'\Big]. \tag{5.29}$$

If further $\mathbf{C} = 0$, then the phase vanishes, and we have the matrix elements for a linear point transformation (and a representation of the group $GL(N, \mathbb{R})$). Finally, if in addition $\mathbf{A} = \mathbf{I}$, so that $\mathbf{S}$ is overall the identity, we have

$$\langle \mathbf{x}|M(\mathbf{I})|\mathbf{x}'\rangle = \pm\delta(\mathbf{x} - \mathbf{x}'), \tag{5.30}$$

i.e. $M(\mathbf{I}) = \pm 1$.

There are important conclusions to be drawn from these results. Our whole derivation has been based on continuity arguments, which are relevant because we want the time dependent operator $M(t) = M\big(\mathbf{S}(t), \sigma(t)\big)$ to be a continuous function of time when $\mathbf{S}(t)$ is determined by the classical analysis of nearby orbits. As long as $\mathbf{S}(t)$ does not cross a caustic surface, then the expression (4.37) is valid, and continuity of $M(t)$ is guaranteed by the continuity of the matrix element. This in turn implies that $\sigma(t)$ must be constant. Next, when we approach a caustic surface, continuity of $M(t)$ demands that the matrix

element assume the form (5.28) with σ_1 uniquely determined. But when we cross to the other side, and enter a region where Eq. (4.37) is valid again, we must change the sign of σ if the value of σ_1 was dependent on the direction in which Eq. (5.28) was evaluated. This is so because only by so doing can we guarantee that the product $\sigma\sigma_1$ is independent of the direction in which the caustic surface is approached. In other words, the quantity $\sigma(t)$ may discontinuously change sign when a caustic surface is crossed by $\mathbf{S}(t)$, in order that $M(t)$ be continuous.

Our conclusions so far are incomplete, because we have shown how to determine σ_1 on the caustic surface, and hence the possible sign flip of σ when crossing it, only for the particular path $\mathbf{S}(\epsilon)$ given by Eqs. (5.16) and (5.19). The actual path $\mathbf{S}(t)$ generated by a classical orbit will usually be a different one. Let us therefore replace $\mathbf{T}(\epsilon)$ with the infinitesimal symplectic matrix generated by the classical Hamiltonian at $t = t_c$, i.e. let us set

$$\mathbf{W}(\tau) = \mathbf{I} + \tau\mathbf{J}\mathbf{K} + O(\tau^2), \tag{5.31}$$

where $\tau = t - t_c$ and $\mathbf{K} = \mathbf{H}''(t_c)$, in accordance with Eqs. (2.10) and (A.15). Then we write

$$\mathbf{S}(\tau) = \mathbf{W}(\tau)\mathbf{S}, \tag{5.32}$$

where $\mathbf{S} = \mathbf{S}(0)$ is on the caustic surface.

As before, we would like to have $\det \mathbf{B}(\tau) \neq 0$ for some finite neighborhood around $\tau = 0$. However, in general this will not be so; it is perfectly possible for $\mathbf{B}(t)$ to run along the caustic surface, or for the rank of $\mathbf{B}(t)$ to drop in steps. In any case, it is straightforward to show that if the following $n \times n$ symmetric matrix is nonsingular,

$$\mathbf{G} = \tilde{\mathbf{U}}_n \mathbf{K}_{\mathbf{pp}} \mathbf{U}_n, \tag{5.33}$$

where $\mathbf{K}_{\mathbf{pp}}$ is the $N \times N$ lower right submatrix of $\mathbf{K}$, then $\det \mathbf{B}(\tau) \neq 0$ for $\tau \neq 0$ in some finite interval about $\tau = 0$. But if $\mathbf{G}$ is singular, then the curve $\mathbf{B}(t)$ is tangent to the

caustic surface at $t = t_c$, and may even lie in it. It is also interesting that the condition $\det \mathbf{G} \neq 0$ is the same one required in order to have $\mathbf{B}(\tau)^{-1} = O(1/\tau)$ (instead of $O(1/\tau^2)$ or something stronger).

In the name of simplicity, therefore, we shall assume here that $\det \mathbf{G} \neq 0$. We note, however, that in quantum mechanics the matrix $\mathbf{K_{pp}}$ is the inverse mass tensor, and is always positive definite. Therefore in quantum mechanics, $\mathbf{B}(t)$ always crosses the caustic surface transversally.

The rest of the analysis proceeds exactly as before, by introducing the coordinates $\mathbf{y}$, $\mathbf{y}'$ and the matrices $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$. The calculation, however, is somewhat tedious, so I shall merely quote the results. In the first place, except for σ_1, Eq. (5.28) emerges as the metaplectic matrix element, showing that to within a sign the form given is independent of the path used to reach the caustic surface. The quantity σ_1 itself is given by the following rules, which depend on the numbers of positive and negative eigenvalues of $\mathbf{G}$, denoted respectively by n_+ and n_-. If $\tau \to 0$ from negative values (the same direction the time will take), then, writing $\sigma_1 = (-1)^\nu$, we have $\nu = n_+/2$ if n_+ is even. If n_+ is odd and $\beta > 0$, then $\nu = (n_+ + 1)/2$. If n_+ is odd and $\beta < 0$, then $\nu = (n_+ - 1)/2$. If $\tau \to 0$ from positive values, then the rules are the same as those just given, with n_+ replaced by n_-. These rules uniquely determine whether or not σ must change sign when $\mathbf{S}(t)$ crosses the caustic, in order to ensure continuity of $M(t)$.

We shall now define the Maslov index in terms of caustics. Suppose we have a symplectic matrix function $\mathbf{S}(t)$ and a corresponding metaplectic operator $M(t) = M\big(\mathbf{S}(t), \sigma(t)\big)$. The sign $\sigma(t)$ is determined by demanding that $M(t)$ be continuous in t. At some time t such that $\mathbf{S}(t)$ does not lie on a caustic, the $\mathbf{x}$-space matrix element of $M(t)$ is given by Eq. (4.37). The constant phase $e^{-iN\pi/4}$ is independent of time, so we ignore it, and we look at the phase of $\sigma/\sqrt{\det \mathbf{B}}$. If $\det \mathbf{B} > 0$, this quantity has the phase ± 1, and if

$\det \mathbf{B} < 0$, it has the phase $\pm i$. Therefore in all cases, we can write

$$\arg \frac{\sigma}{\sqrt{\det \mathbf{B}}} = \mu \frac{\pi}{2}, \tag{5.34}$$

where μ is defined modulo 4. The integer μ is the Maslov index. Since both σ and $\operatorname{sgn} \det \mathbf{B}$ are constant away from caustics, the Maslov index is a constant function of t until a caustic is crossed. If it is a first order caustic, then the sign of $\det \mathbf{B}$ will change, as may also σ. In any case, the Maslov index will either increment or decrement by 1 on crossing the first order caustic. If it is a higher order caustic, it can be broken up into first order caustics by a small perturbation, or it can be treated directly by the rules given above for σ. The results are the same in either case.

In Sec. 4 another version of the Maslov index was given, namely twice the winding number of $\mathbf{S}(t)$ when $\mathbf{S}(t)$ is a closed curve in the space of symplectic matrices. If $\mathbf{S}(t)$ is closed, the corresponding $M(t)$, determined by continuity, need not be a closed curve in the space of metaplectic operators. But the increment of the Maslov index along $M(t)$, for one period of $\mathbf{S}(t)$, obtained by counting caustics, is the same as twice the winding number of $\mathbf{S}(t)$. In other words, for closed curves $\mathbf{S}(t)$, the two versions of the Maslov index are the same.

It is not hard to see that this is true, on the basis of the mixed $\mathbf{x}$-space and coherent state matrix elements we shall develop in the next section. But it is rather remarkable, because when $\mathbf{S}(t)$ is not closed, the Maslov index has no invariant meaning, since it depends on the choice of initial and final Lagrangian planes. For closed $\mathbf{S}(t)$, however, this dependency cancels, and the count of caustics is the same for any choice of Lagrangian planes.

One cannot help but have mixed feelings about this analysis of caustics. On the one hand, caustics are physically important and interesting in their own right, and they lead to some pretty mathematics. On the other hand, their noninvariance in phase space

keeps reasserting itself, and the mathematics involved is the kind in which it is easier to prove theorems than it is to apply one's conclusions in a practical way. Altogether, it seems that the use of the **x**-representation in developing the intrinsic properties of the metaplectic operators is an awkward and inelegant approach, although it can be and has been done with full mathematical rigor. In the next section we shall examine some alternative representations of the metaplectic operators, which are not only more practical and theoretically cleaner, but which are also of direct relevance to wave packet propagation.

6. Applications of the Metaplectic Operators

We are now prepared to explore the consequences of the metaplectic operators, whose most important properties are summarized by Eqs. (4.3), (4.21), (4.27), (4.37), (4.38), and (5.28). I shall begin by discussing the active and passive points of view in the use of the metaplectic operators, and by presenting some examples. One of these shows that a change from the **x**-basis to the **p**-basis, i.e. the Fourier transform, is a passive metaplectic transformation corresponding to the symplectic matrix $\mathbf{S} = \mathbf{J}$. The second example shows how scaling transformations can be represented as passive metaplectic transformations, and dispenses with the scale factors which are often introduced into practical calculations involving coherent states. Following this, we discuss the interaction between Heisenberg and metaplectic operators, and we display a number of formulas showing how various symbols transform under Heisenberg and metaplectic conjugations. Finally, we discuss the coherent state matrix elements of the metaplectic operators, and some of their suggestive properties.

6.1. Active Versus Passive

The metaplectic operators, like the symplectic matrices, can be used in either an active or passive manner, and both are useful (see Appendix A for the case of symplectic matrices). Mostly we have been taking the active point of view with the metaplectic operators, as is appropriate when thinking of wave packet evolution, but we implicitly sneaked in a passive operation with our introduction of the symplectic matrices $\mathbf{S}_0$ and $\mathbf{S}_1$ in Eq. (5.11). In either point of view, the algebra is the same; however, the operations themselves are conceptually quite distinct, and it is worthwhile to keep them straight.

In the active point of view, we take a state $|\psi_1\rangle$ (say with wave function $\psi_1(\mathbf{x})$) and map it into a new state $|\psi_2\rangle = M(\mathbf{S})|\psi_1\rangle$ under the action of a metaplectic operator. The

wave function of the new state, $\psi_2(\mathbf{x})$, is computed using the matrix elements of Eq. (4.37) or (5.28),

$$\psi_2(\mathbf{x}) = \int d\mathbf{x}' \, \langle \hat{\mathbf{q}}(\mathbf{x}) | M(\mathbf{S}) | \hat{\mathbf{q}}(\mathbf{x}') \rangle \, \psi_1(\mathbf{x}'), \tag{6.1}$$

where we have temporarily restored our notation which displays both the operators and their eigenvalues. In the active point of view, the symplectic matrix $\mathbf{S}$ has components with physical dimensions such that the physical dimensions of the components of $\mathbf{z}$ are preserved, component-wise, under the transformation $\mathbf{Z} = \mathbf{S}\mathbf{z}$, in accordance with the classical idea that $\mathbf{z}$ and $\mathbf{Z}$ represent distinct points of phase space in the same coordinate system. For example, if $\mathbf{q}$ and $\mathbf{p}$ represent ordinary physical position and momentum, then the submatrix $\mathbf{A}$ of $\mathbf{S}$ is dimensionless, while $\mathbf{B}$ has dimensions of length/momentum, etc. When $\mathbf{S}$ arises from linearizing in a classical nearby orbit problem, these physical dimensions emerge automatically from Hamilton's equations, and $\hbar$ does not appear in the components of $\mathbf{S}$. Similarly, when we use Eq. (4.3) in the active point of view to define new operators $\hat{\mathbf{Z}} = \mathbf{S}\hat{\mathbf{z}} = M(\mathbf{S})^\dagger \, \hat{\mathbf{z}} \, M(\mathbf{S})$, the physical dimensions of the components of $\hat{\mathbf{Z}}$ are the same, component-wise, as those of $\hat{\mathbf{z}}$. Finally, we note that the original and transformed wave functions $\psi_1(\mathbf{x})$, $\psi_2(\mathbf{x})$ in Eq. (6.1) have the same physical dimensions (length$^{-N/2}$ if $\mathbf{x}$ is ordinary physical position), and that they represent distinct physical states, both being expressed in the same basis.

But sometimes it is convenient to introduce symplectic matrices which do not preserve physical dimensions. Consider, for example, the transformation which results from taking $\mathbf{S} = \mathbf{J}$. Classically, we have

$$\begin{pmatrix} \mathbf{Q} \\ \mathbf{P} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{p} \\ -\mathbf{q} \end{pmatrix}. \tag{6.2}$$

This transformation inverts the roles of $\mathbf{q}$ and $\mathbf{p}$, so that if $\mathbf{q}$ and $\mathbf{p}$ are ordinary position and momentum, then $\mathbf{Q}$ no longer has the same physical dimensions as $\mathbf{q}$. Similarly, the operators $\hat{\mathbf{Q}}$, $\hat{\mathbf{P}}$ defined by Eq. (4.3) now have opposite physical dimensions from $\hat{\mathbf{q}}$, $\hat{\mathbf{p}}$.

Another example is a scaling operation, used to change dimensions or to introduce dimensionless variables. Suppose $\mathbf{q}$, $\mathbf{p}$ represent ordinary position and momentum, and that some problem has a characteristic scale length a in $\mathbf{x}$-space. For example, in the harmonic oscillator, we would take $a = \sqrt{\hbar/m\omega}$. Then the following symplectic transformation could be used to introduce a new dimensionless variable $\mathbf{Q}$:

$$\begin{pmatrix} \mathbf{Q} \\ \mathbf{P} \end{pmatrix} = \begin{pmatrix} \frac{1}{a}\mathbf{I} & 0 \\ 0 & a\mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}. \tag{6.3}$$

The new variable $\mathbf{P}$ is not dimensionless, but rather has the dimensions of $\hbar$. If we wish $\mathbf{Q}$ and $\mathbf{P}$ to appear with the same dimensions (namely $\hbar^{1/2}$), we could take

$$\begin{pmatrix} \mathbf{Q} \\ \mathbf{P} \end{pmatrix} = \begin{pmatrix} (\sqrt{\hbar}/a)\mathbf{I} & 0 \\ 0 & (a/\sqrt{\hbar})\mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}. \tag{6.4}$$

If a is given by its harmonic oscillator value of $\sqrt{\hbar/m\omega}$, then this symplectic matrix is independent of $\hbar$, whereas that of Eq. (6.3) is not (holding m and ω fixed).

These are examples of passive transformations, which classically represent a change of coordinates on phase space. The vectors $\mathbf{z}$ and $\mathbf{Z}$ on the two sides of Eqs. (6.2)–(6.4) represent the same point of phase space, expressed in two different coordinate systems. A similar interpretation occurs in the quantum picture. We still use Eq. (4.3) as it stands to define new operators $\hat{\mathbf{Z}}$, but these no longer have the same physical dimensions, componentwise, as the old operators $\hat{\mathbf{z}}$.

Let us examine these passive transformations quantum mechanically. We take some state $|\psi\rangle$, which has wavefunction $\psi(\mathbf{x}) = \langle\hat{\mathbf{q}}(\mathbf{x})|\psi\rangle$, and ask for the wave wave function of the same state with respect to a new basis specified by the operators $\hat{\mathbf{Q}}$. We denote this new wave function by $\phi(\mathbf{Q}) = \langle\hat{\mathbf{Q}}(\mathbf{Q})|\psi\rangle$. Then, applying Eq. (4.21), we have

$$\phi(\mathbf{Q}) = \int d\mathbf{x}' \, \langle\hat{\mathbf{q}}(\mathbf{Q})|M(\mathbf{S})|\hat{\mathbf{q}}(\mathbf{x}')\rangle\psi(\mathbf{x}'). \tag{6.5}$$

This has the same form as Eq. (6.1), but a different interpretation. Now $\phi(\mathbf{Q})$ and $\psi(\mathbf{x}')$ represent the same state, but with respect to a different basis. The wavefunctions $\phi(\mathbf{Q})$ and $\psi(\mathbf{x}')$ may also have different physical dimensions.

These issues are really quite elementary, but they are capable of causing a great deal of confusion. Therefore we will illustrate them with some examples. Consider first the inversion of $\mathbf{q}$ and $\mathbf{p}$ specified by Eq. (6.2). Since we now have $\hat{\mathbf{Q}} = \hat{\mathbf{p}}$, the change of basis indicated by Eq. (6.5) must correspond to a transformation to the momentum space wave function. To bring this out, we replace the symbol $\mathbf{Q}$ in Eq. (6.5) by $\mathbf{p}$, since $\hat{\mathbf{Q}}$, and therefore its eigenvalues $\mathbf{Q}$, now have physical dimensions of momentum, and since the symbol $\mathbf{Q}$ is a dummy in this equation anyway. We also use Eq. (4.37) with $\mathbf{A} = \mathbf{D} = 0$, $\mathbf{B} = \mathbf{I}$, and we take $\sigma = +1$. Then Eq. (6.5) becomes

$$\phi(\mathbf{p}) = \int \frac{d\mathbf{x}'}{(2\pi i\hbar)^{N/2}}\, e^{-i\mathbf{p}\cdot\mathbf{x}'/\hbar}\psi(\mathbf{x}'), \tag{6.6}$$

which, apart from the overall phase, is the usual momentum space wave function.

We see that the Fourier transform itself is a metaplectic operator, and that the group of metaplectic operators constitutes a generalization of the Fourier transform. This observation allows us to easily write down the mixed $\mathbf{x}$- and $\mathbf{p}$-space, and full $\mathbf{p}$-space, matrix elements of the metaplectic operators. For example, the matrix element $\langle \mathbf{x}|M(\mathbf{S})|\mathbf{p}'\rangle$ is given by replacing $\mathbf{S}$ in Eq. (4.37) or (5.28) by $\mathbf{S}\mathbf{J}^{-1}$, and replacing $\mathbf{x}'$ by $\mathbf{p}'$. Similarly, we obtain $\langle \mathbf{p}|M(\mathbf{S})|\mathbf{x}'\rangle$ by making the replacements $\mathbf{S} \rightarrow \mathbf{J}\mathbf{S}$, $\mathbf{x} \rightarrow \mathbf{p}$; and $\langle \mathbf{p}|M(\mathbf{S})|\mathbf{p}'\rangle$ by the replacements $\mathbf{S} \rightarrow \mathbf{J}\mathbf{S}\mathbf{J}^{-1}$, $\mathbf{x} \rightarrow \mathbf{p}$, and $\mathbf{x}' \rightarrow \mathbf{p}'$.

The Fourier transform also sometimes appears in the active sense, such as in the time evolution of the harmonic oscillator during a quarter period (in the appropriately scaled variables). In the active sense, the transformation of Eq. (6.2) appears as a 90° active rotation of objects in phase space in a clockwise (negative) direction. The metaplectic operators, in their greater generality, allow for arbitrary angles of rotation, along with

scaling and other transformations which constitute the linear canonical transformations. These are important, because the actual time evolution of wave packets consists of such transformations. Rotations in the usual sense, i.e. orthogonal transformations, do not have any invariant meaning in phase space, because canonical transformations do not respect any Euclidean metric. Nevertheless, considerations of the transformations which are both orthogonal and symplectic does lead to important conclusions, as indicated in Appendix A.

As another example of a passive transformation, let us consider the scaling operation (6.4) which introduces the variables $\mathbf{Q}$, $\mathbf{P}$ with symmetrized physical dimensions. We write the matrix element of Eq. (5.29) in the following form, where we have taken $\mathbf{A} = (\sqrt{\hbar}/a)\mathbf{I}$, $\mathbf{C} = 0$:

$$\langle \hat{\mathbf{q}}(\mathbf{Q})|M(\mathbf{S})|\hat{\mathbf{q}}(\mathbf{x}')\rangle = \left(\frac{\hbar}{a^2}\right)^{N/4} \delta\left(\mathbf{Q} - (\sqrt{\hbar}/a)\mathbf{x}'\right). \tag{6.7}$$

We apply this to the wave function

$$\psi(\mathbf{x}) = \frac{1}{(\pi a^2)^{N/4}} e^{-\tilde{\mathbf{x}}\cdot\mathbf{x}/2a^2}, \tag{6.8}$$

which, if $a = \sqrt{\hbar/m\omega}$, is the ground state of the isotropic harmonic oscillator. (Even if the physical system of interest has nothing to do with harmonic oscillators, it might be reasonable to consider the state given by Eq. (6.8) anyway, such as when using coherent states. In that case, a is merely some spatial scale of interest.) Then we find

$$\phi(\mathbf{Q}) = \frac{1}{(\pi\hbar)^{N/4}} e^{-\tilde{\mathbf{Q}}\cdot\mathbf{Q}/2\hbar} \tag{6.9}$$

Had we used the transformation of Eq. (6.3) instead of (6.4), our result would be in completely dimensionless form. However, we shall generally prefer the transformation (6.4), which treats $\mathbf{Q}$ and $\mathbf{P}$ symmetrically, and which leaves $\hbar$ explicitly in the result (6.9). This will be used later for ordering purposes. We also note that the wave function $\chi(\mathbf{P})$ of the same state appearing in Eqs. (6.8) and (6.9), expressed in the $\hat{\mathbf{P}}$-basis, is

$$\chi(\mathbf{P}) = \frac{1}{(\pi\hbar)^{N/4}} e^{-\tilde{\mathbf{P}}\cdot\mathbf{P}/2\hbar}, \tag{6.10}$$

which shows the effects of the symmetrized dimensions.

If our physical system has different scale lengths in different directions, then for the purposes of setting up coherent states, it might be advisable to replace the scalar a^2 in Eq. (6.8) with a diagonal matrix, containing different quantities a_i^2, $i = 1, \ldots, N$, in its diagonal slots. It is clear that the same analysis used above, with appropriate modifications to the symplectic matrix of Eq. (6.4), will go through with minor modifications, and will yield the same symmetrized wave functions appearing in Eqs. (6.9)–(6.10). The significance of this fact is that for the purposes of developing coherent states, it suffices to consider only wave functions of the form (6.9)–(6.10). All others, with correct physical scaling, can be obtained from these by a fixed, passive metaplectic transformation.

Indeed, there may not be any reason to restrict oneself to diagonal matrices, or even point transformations, in Eq. (6.4). There has often been a concern, in using coherent states for physical systems which are not harmonic oscillators, of how best to choose the fundamental wave packet from which all the other coherent states are derived (the fiducial state; see Appendix C). Our considerations here do not answer this question, but they do show what the freedom of choice is: We can choose any wave packet which is derived from Eq. (6.9) as the result of a passive metaplectic transformation. As we shall see, this means any Gaussian wave packet, minimum uncertainty or not.

Let us now return to the active transformation $|\psi_2\rangle = M(\mathbf{S})|\psi_1\rangle$, the $\mathbf{x}$-representation of which is given in Eq. (6.1). If we wish to express this in the $\mathbf{Q}$-representation, defined by Eq. (6.4) or some appropriate generalization of it, then we can simply combine matrix elements in the obvious way. For example, if we write $\phi_1(\mathbf{Q})$, $\phi_2(\mathbf{Q})$ for the wave functions of $|\psi_1\rangle$, $|\psi_2\rangle$ in the $\hat{\mathbf{Q}}$-basis, then we have

$$\begin{aligned}\psi_1(\mathbf{x}') = \langle \hat{\mathbf{q}}(\mathbf{x}')|\psi_1\rangle &= \int d\mathbf{Q}' \, \langle \hat{\mathbf{q}}(\mathbf{x}')|\hat{\mathbf{Q}}(\mathbf{Q}')\rangle\langle \hat{\mathbf{Q}}(\mathbf{Q}')|\psi_1\rangle \\ &= \int d\mathbf{Q}' \, \langle \hat{\mathbf{q}}(\mathbf{x}')|M(\mathbf{S}_0)^\dagger|\hat{\mathbf{q}}(\mathbf{Q}')\rangle\phi_1(\mathbf{Q}'), \qquad (6.11)\end{aligned}$$

where we have used Eq. (4.21) and where $\mathbf{S}_0$ is the symplectic matrix of Eq. (6.4) (or its appropriate generalization). By similarly transforming $\psi_2(\mathbf{x})$ into $\phi_2(\mathbf{Q})$, Eq. (6.1) becomes

$$\phi_2(\mathbf{Q}) = \int d\mathbf{Q}' \, \langle \hat{\mathbf{q}}(\mathbf{Q}) | M(\mathbf{S}_0 \mathbf{S} \mathbf{S}_0^{-1}) | \hat{\mathbf{q}}(\mathbf{Q}') \rangle \, \phi_1(\mathbf{Q}'). \tag{6.12}$$

The sign choice for $M(\mathbf{S}_0)$ cancels, and the result has algebraically the same form as Eq. (6.1), with $\mathbf{S}$ replaced by the conjugation $\mathbf{R} = \mathbf{S}_0 \mathbf{S} \mathbf{S}_0^{-1}$. This new symplectic matrix $\mathbf{R}$ is dimensionless, if the original $\mathbf{S}$ appearing in Eq. (6.1) preserved physical dimensions (as it should, if it represents an active transformation, and as it must, if $\mathbf{S}$ is derived from a classical nearby orbit problem).

Furthermore, if $\mathbf{S}$ is derived from a classical nearby orbit problem, as discussed in Sec. 2, then there is no need to compute $\mathbf{S}(t)$ in the original $\mathbf{q}$, $\mathbf{p}$ variables and then conjugate with $\mathbf{S}_0$. Instead, we can do the classical problem in the $(\mathbf{Q}, \mathbf{P})$ coordinates, and directly obtain $\mathbf{R}(t)$. Indeed, conjugating Eq. (2.15) with $\mathbf{S}_0$ gives

$$\frac{d}{dt}\mathbf{R}(t) = \mathbf{J}\mathbf{K}''(t)\mathbf{R}(t), \tag{6.13}$$

where

$$\mathbf{K}''(t) = \tilde{\mathbf{S}}_0^{-1} \mathbf{H}''(t) \mathbf{S}_0^{-1}. \tag{6.14}$$

The matrix $\mathbf{K}''$ is symmetric, like $\mathbf{H}''$, and is the Hessian matrix of a transformed classical Hamiltonian $\mathbf{K}$, defined by

$$K(\mathbf{Z}) = H(\mathbf{z}) = H(\mathbf{S}_0^{-1}\mathbf{Z}). \tag{6.15}$$

K is the result of performing the classical canonical transformation $\mathbf{Z} = \mathbf{S}_0 \mathbf{z}$ on $H(\mathbf{z})$, and it therefore correctly describes the time evolution of the coordinates $\mathbf{Z} = (\mathbf{Q}, \mathbf{P})$, with symmetrized physical dimensions, along any orbit $\mathbf{Z}(t)$, as well as the small displacements $\delta\mathbf{Z}(t)$ about such an orbit. In addition, if $H(\mathbf{z})$ is the ordinary Weyl symbol (see Appendix

B) of the quantum Hamiltonian $H(\hat{\mathbf{z}})$, then $K(\mathbf{Z})$ will be the ordinary Weyl symbol of the quantum Hamiltonian

$$K(\hat{\mathbf{Z}}) = H(\mathbf{S}_0^{-1}\hat{\mathbf{Z}}) = M(\mathbf{S}_0)H(\hat{\mathbf{Z}})M(\mathbf{S}_0)^\dagger = H(\hat{\mathbf{z}}). \tag{6.16}$$

This follows by the use of Eq. (4.3), and some properties of the Weyl symbol under metaplectic conjugation, which we shall discuss presently. These operations are examples of "metaplectic covariance," to which we shall return.

The upshot of this analysis is that, with no loss of generality, and maintaining full ability to restore variables with physical dimensions and scale lengths, we can work entirely with the variables $(\mathbf{Q}, \mathbf{P})$ with symmetrized dimensions, both classically and quantum mechanically. Furthermore, if we are using coherent states, we can use the simple form given in Eq. (6.9) for the fiducial state, again with no loss of generality.

Therefore in the sequel we make the following notational changes. We simply forget about our original $\mathbf{z}$'s and the transformations to $\mathbf{Z}$'s, etc., and replace $\mathbf{Z}$ by $\mathbf{z}$, $\mathbf{R}$ by $\mathbf{S}$, K by H, etc. That is, we return to our original notation, except that now it is understood that $\mathbf{q}$ and $\mathbf{p}$ have the same dimensions of $\hbar^{1/2}$. Our symplectic matrices $\mathbf{S}(t)$ arising in the nearby orbit problem are now dimensionless, and any issue of physical scale lengths does not enter into our considerations.

6.2. The Semidirect Product

There is an interesting interplay between the Heisenberg and metaplectic operators, which also involves the Wigner-Weyl formalism and coherent states. We begin with an important conjugation formula, which follows from Eq. (4.3). If we let $\mathbf{z}_0$ be a displacement vector in phase space, then we have

$$M(\mathbf{S})^\dagger \omega(\mathbf{z}_0, \hat{\mathbf{z}}) M(\mathbf{S}) = \omega(\mathbf{z}_0, \mathbf{S}\hat{\mathbf{z}}) = \omega(\mathbf{S}^{-1}\mathbf{z}_0, \hat{\mathbf{z}}), \tag{6.17}$$

by use of Eq. (A.6). Combining this with Eq. (3.12), we obtain the important result,

$$M(\mathbf{S})^\dagger\, T(\mathbf{z}_0)\, M(\mathbf{S}) = T(\mathbf{S}^{-1}\mathbf{z}_0). \tag{6.18}$$

Equation (6.18) is often of use in the analysis of coherent states. Suppose, for example, we are interested in the action of a metaplectic operator on the coherent state $|\mathbf{z}\rangle$. we have

$$M(\mathbf{S})|\mathbf{z}\rangle = M(\mathbf{S})T(\mathbf{z})|0\rangle = T(\mathbf{S}\mathbf{z})M(\mathbf{S})|0\rangle. \tag{6.19}$$

The result can be obtained by letting $M(\mathbf{S})$ act first on the fiducial state, and then translating by a Heisenberg operator (both of which are easier than evaluating $M(\mathbf{S})|\mathbf{z}\rangle$ directly).

Equation (6.18) also allows us to combine the Heisenberg and metaplectic groups into a single group, which encompasses all linear canonical transformations, both homogeneous and inhomogeneous. Returning to the notation of Eqs. (3.28)–(3.29), we define the operator $M(\mathbf{z}, \gamma, \mathbf{S})$ by

$$M(\mathbf{z}, \gamma, \mathbf{S}) = T(\mathbf{z}, \gamma)M(\mathbf{S}). \tag{6.20}$$

This operator is a member of the inhomogeneous metaplectic group, which we shall denote by $IMp(2N)$. It is the semidirect product of the Heisenberg and metaplectic groups, and its group multiplication law is

$$M(\mathbf{z}_0, \gamma_0, \mathbf{S}_0)M(\mathbf{z}_1, \gamma_1, \mathbf{S}_1) = \pm M\big(\mathbf{z}_0 + \mathbf{S}_0\mathbf{z}_1, \gamma_0 + \gamma_1 + \tfrac{1}{2}\omega(\mathbf{z}_0, \mathbf{S}_0\mathbf{z}_1), \mathbf{S}_0\mathbf{S}_1\big). \tag{6.21}$$

In this paper we shall mostly keep the Heisenberg and metaplectic operators separate, because it is algebraically simpler to do so. In Sec. 7 we shall develop a wave packet propagator which is an operator in $IMp(2N)$.

There is a sense in which the phase space of classical mechanics emerges from quantum mechanics as the space of the Heisenberg operators $T(\mathbf{z})$. If these are augmented by the phase factor $e^{i\gamma/\hbar}$, as in Eq. (3.28), then we have a candidate for a "semiclassical phase space," which is the group manifold for the Heisenberg group, and which has the

topology $\mathbb{R}^{2N} \times S^1$. ($S^1$ is the circle.) The simultaneous time evolution of $\mathbf{z}(t)$ and $\gamma(t)$, such as indicated by Eqs. (3.25)–(3.27), then appears as a single trajectory in this space, and the Bohr-Sommerfeld quantization rules (without any factors of $\frac{1}{2}$) take on an interesting geometrical interpretation (namely, energy eigenstates correspond to periodic orbits). More generally, one can take the semiclassical phase space to the be group manifold of $IMp(2N)$, in which a single trajectory represents the simultaneous time evolution of $\mathbf{z}(t)$, $\gamma(t)$, and $M(t)$. (As it turns out, this evolution itself is a Hamiltonian system.) The EBK quantization rules (Keller [1958], Percival [1977]) are closly related to the geometry and topology of this space (Voros [1976, 1977]). There is some interesting mathematics here, but since it is not always clear how this impacts the practical problems of wave packet evolution, we shall pursue it no further.

6.3. Interaction of Heisenberg and Metaplectic Operators and Symbols

The Heisenberg and metaplectic operators also interact with the Wigner-Weyl formalism. Let A be some operator with Weyl symbols $\tilde{a}(\mathbf{z})$, $a(\mathbf{z})$ (see Appendix B), and let $B = T(\mathbf{z}_0)\, A\, T(\mathbf{z}_0)^\dagger$, with symbols $\tilde{b}(\mathbf{z})$, $b(\mathbf{z})$. Then it follows immediately from Eqs. (B.2)–(B.3) that

$$\begin{aligned} \tilde{b}(\mathbf{z}) &= e^{\frac{i}{\hbar}\omega(\mathbf{z}_0,\mathbf{z})}\tilde{a}(\mathbf{z}), \\ b(\mathbf{z}) &= a(\mathbf{z}-\mathbf{z}_0). \end{aligned} \tag{6.22}$$

Under conjugation by $T(\mathbf{z}_0)$, the ordinary Weyl symbol is translated in phase space by $\mathbf{z}_0$, exactly like a classical function on phase space under the action of the classical translation operator, $T_{cl}(\mathbf{z}_0)$, as given by Eq. (3.6). We can state this succinctly by writing

$$\mathrm{Sym}\left(T(\mathbf{z}_0) A\, T(\mathbf{z}_0)^\dagger\right) = T_{cl}(\mathbf{z}_0)\,\mathrm{Sym}\, A, \tag{6.23}$$

where $\mathrm{Sym}\, A$ refers to the ordinary Weyl symbol of the operator A. In particular, if A is the projection operator $|\psi\rangle\langle\psi|$, so that $a(\mathbf{z})$ is the Wigner function $W(\mathbf{z})$ of the state $|\psi\rangle$,

then the Wigner function corresponding to the transformed state $T(\mathbf{z}_0)|\psi\rangle$ is $W(\mathbf{z}-\mathbf{z}_0)$. The Wigner function has been rigidly translated in phase space.

Before developing analogous formulas for the metaplectic operators, it is useful to have a notation for their classical analogs (which are multiplications by symplectic matrices). Following the notation of Eqs. (3.5)–(3.6), we define the classical operator $M_{cl}(\mathbf{S})$ by

$$M_{cl}(\mathbf{S})\mathbf{z} = \mathbf{S}\mathbf{z}, \tag{6.24}$$

when acting on points, and by

$$\left(M_{cl}(\mathbf{S})f\right)(\mathbf{z}) = f(\mathbf{S}^{-1}\mathbf{z}), \tag{6.25}$$

when acting on functions on the classical phase space.

Now let $B = M(\mathbf{S})A\,M(\mathbf{S})^\dagger$, and consider the Weyl symbols of the operators A and B. By using Eq. (6.18) and (B.2)–(B.3), we have

$$\begin{aligned} \tilde{b}(\mathbf{z}) &= \tilde{a}(\mathbf{S}^{-1}\mathbf{z}), \\ b(\mathbf{z}) &= a(\mathbf{S}^{-1}\mathbf{z}). \end{aligned} \tag{6.26}$$

We state this rule for the ordinary Weyl symbol in the form,

$$\mathrm{Sym}\left(M(\mathbf{S})A\,M(\mathbf{S})^\dagger\right) = M_{cl}(\mathbf{S})\,\mathrm{Sym}\,A. \tag{6.27}$$

The choice of sign for $M(\mathbf{S})$ cancels. Again, if $W(\mathbf{z})$ is the Wigner function of the state $|\psi\rangle$, then the Wigner function of $M(\mathbf{S})|\psi\rangle$ is $W(\mathbf{S}^{-1}\mathbf{z})$. In all these cases, the ordinary Weyl symbol or Wigner function has transformed exactly as one would expect under the active, classical canonical transformation specified by the symplectic matrix $\mathbf{S}$, i.e. under the mapping $\mathbf{Z} = \mathbf{S}\mathbf{z}$. The inverse of $\mathbf{S}$ appears in these formulas for the same reason that $\mathbf{z}-\mathbf{z}_0$ appears in Eqs. (3.6) and (6.20): the value of the old function at the old point is equal to the value of the new function at the new point.

Incidentally, we see that Eqs. (6.15) and (6.16) also have the same mathematical form as our results here, and essentially for the same mathematical reasons. But Eqs. (6.15)

and (6.16) represented a passive transformation, so their interpretation is different. There we did not have old points and new points; rather, there was only one point, expressed in the two coordinate systems $\mathbf{z}$ and $\mathbf{Z} = \mathbf{S}_0\mathbf{z}$. The matrix $\mathbf{S}_0^{-1}$ appears in Eq. (6.15) because we were eliminating the old variables $\mathbf{z}$ in $H(\mathbf{z})$ in favor of the new, in order to get $K(\mathbf{Z})$.

Equations (6.22)–(6.27) form the basis of "metaplectic covariance." The idea behind this concept is that, just as the results of classical mechanics should not depend on the canonical coordinate system used, so also should the results of semiclassical mechanics not depend on the canonical operator vector $\hat{\mathbf{z}}$ which is used in the semiclassical calculations. Insofar as one restricts oneself to linear canonical transformations, these goals are easily achieved, and they are based on the transformation rules just derived. Suppose, for example, we have a semiclassical problem involving some Hamiltonian and possibly other operators, which produces a semiclassical wave function $\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle$. In the process of carrying out the semiclassical calculation, we use the coordinate system $(\mathbf{z} = \mathbf{q}, \mathbf{p})$ on the classical phase space. If the semiclassical theory is metaplectically covariant, then our results will be the same if, on the quantum side, we act on the state $|\psi\rangle$ with some fixed Heisenberg or metaplectic operator, and conjugate all operators such as the Hamiltonian by the same operator; and, on the classical side, we perform the canonical change of coordinates corresponding to the fixed Heisenberg or metaplectic operator. In particular, metaplectic covariance implies covariance under the Fourier transform. As discussed in Sec. 3, traditional WKB theory has no such principle of covariance, and this fact is closely associated with the existence of nonphysical caustic singularities.

The coherent state wave functions and symbols also have simple transformation properties under the Heisenberg operators. If $|\psi\rangle$ is some state with coherent state wave function $\psi_{cs}(\mathbf{z})$ (see Appendix C), then the state $T(\mathbf{z}_0)|\psi\rangle$ has coherent state wave function

$$\langle \mathbf{z}|T(\mathbf{z}_0)|\psi\rangle = e^{\frac{i}{2\hbar}\omega(\mathbf{z}_0,\mathbf{z})}\psi_{cs}(\mathbf{z} - \mathbf{z}_0). \tag{6.28}$$

The coherent state wave function is rigidly translated, and multiplied by a phase factor (which depends on position in phase space). Likewise, if A is an operator with coherent state symbol $a_{cs}(\mathbf{z})$, then the coherent state symbol of $T(\mathbf{z}_0)AT(\mathbf{z}_0)^\dagger$ is

$$\langle \mathbf{z}|T(\mathbf{z}_0)AT(\mathbf{z}_0)^\dagger|\mathbf{z}\rangle = a_{cs}(\mathbf{z}-\mathbf{z}_0). \tag{6.29}$$

That is, the coherent state symbol transforms exactly as the ordinary Weyl symbol under conjugation by Heisenberg operators. The transformation of coherent state symbols under metaplectic conjugation is more complicated, and will be dealt with later.

6.4. Coherent State Matrix Elements

When a Gaussian wave packet evolves according to the semiclassical approximation discussed in Sec. 2, its spreading and certain of its other features are governed by the action of a metaplectic operator. Therefore we now examine this action.

We begin with the standard fiducial coherent state given by Eq. (C.4), denoted $|0\rangle$. We do not at first consider the other coherent states, because they are obtained from this one by the action of Heisenberg operators, an essentially trivial operation. Nor do we consider more general Gaussians, for, as we shall see, they are contained in our result. Therefore we consider the state $M(\mathbf{S})|0\rangle$. We compute this in the $\mathbf{x}$-representation, using Eq. (4.37) when $\det \mathbf{B} \neq 0$. The calculation is straightforward, and yields

$$\langle \mathbf{x}|M(\mathbf{S})|0\rangle = \frac{1}{(\pi\hbar)^{N/4}} \frac{\sigma}{\sqrt{\det(\mathbf{A}+i\mathbf{B})}} \exp\left[-\frac{1}{2\hbar}\tilde{\mathbf{x}}(\mathbf{D}-i\mathbf{C})(\mathbf{A}+i\mathbf{B})^{-1}\mathbf{x}\right]. \tag{6.30}$$

It is convenient in this expression (and in Eq. (6.32)) to take the branch cut of the square root to lie just under the positive real axis.

This is a result of some significance. First we note that the matrix $(\mathbf{D}-i\mathbf{C})(\mathbf{A}+i\mathbf{B})^{-1}$ is symmetric (and complex), as follows from the identities of Eq. (A.9)–(A.10). It also has

a real part which is positive definite, since

$$(\mathbf{D}-i\mathbf{C})(\mathbf{A}+i\mathbf{B})^{-1} = (\mathbf{D}-i\mathbf{C})(\tilde{\mathbf{A}}-i\tilde{\mathbf{B}})\left[(\mathbf{A}+i\mathbf{B})(\tilde{\mathbf{A}}-i\tilde{\mathbf{B}})\right]^{-1}$$
$$= \left[\mathbf{I}-i(\mathbf{D}\tilde{\mathbf{B}}+\mathbf{C}\tilde{\mathbf{A}})\right](\mathbf{A}\tilde{\mathbf{A}}+\mathbf{B}\tilde{\mathbf{B}})^{-1}. \qquad (6.31)$$

The final expression in this equation depends only on the components of the matrix $\mathbf{S}\tilde{\mathbf{S}}$, for reasons explained in Sec. 8. Next we note that the complex matrix $\mathbf{A}+i\mathbf{B}$ is never singular, for if it were, there would exist some vanishing linear combination of its rows. Splitting this linear combination into its real and imaginary parts, we see that there would be a simultaneous vanishing linear combination of the rows of $\mathbf{A}$ and $\mathbf{B}$, which would imply that $\mathbf{S}$ was singular. Since $\det\mathbf{S}=+1$, this is impossible. Therefore, although Eq. (6.30) was derived from Eq. (4.37) on the assumption that $\det\mathbf{B}\neq 0$, it is easy to extend it by continuity to the case $\det\mathbf{B}=0$, since the expression is continuous in all components of the symplectic matrix $\mathbf{S}$, including $\mathbf{B}$. Therefore Eq. (6.30) is valid as it stands, even for $\det\mathbf{B}=0$.

The quantity σ appearing in Eq. (6.30) has the values ± 1, but it is not the same σ appearing in Eq. (4.37). The relation between the two is complicated, but the overall situation regarding the 2-to-1 association between metaplectic operators and symplectic matrices is much more clear here than it was in Eq. (4.37). In particular, we note that there is absolutely no problem when $\det\mathbf{B}\to 0$, because this matrix element is nonsingular for all symplectic matrices $\mathbf{S}$. If we have a function $\mathbf{S}=\mathbf{S}(t)$ derived by linearizing about a classical orbit, and we wish to guarantee the continuity of $M(\mathbf{S}(t))$ as a function of time, then, as shown by the complicated rules for sign flips of σ on crosssing caustics, the matrix element of Eq. (4.37) is quite awkward to use. Here, however, we need only change the sign of σ when the square root in Eq. (6.30) crosses over onto the second Riemann sheet. This is simple, and can easily be implemented numerically.

Equation (6.30) does not uniquely specify the metaplectic operator it came from, because we have a fixed ket on the right in the matrix element, instead of an arbitrary

member of complete basis. To remedy this situation, we compute the mixed $\mathbf{x}$-space and coherent state matrix element, according to Eq. (6.19). The analysis is straightforward, and the result can be put into the form

$$\begin{aligned}\langle \mathbf{x}|M(\mathbf{S})|\mathbf{z}\rangle = \frac{1}{(\pi\hbar)^{N/4}}\frac{\sigma}{\sqrt{\det(\mathbf{A}+i\mathbf{B})}}\exp\Big(-\frac{1}{2\hbar}|\varsigma|^2\Big) \\ \times\exp\Big\{\frac{1}{\hbar}\Big[-\tfrac{1}{2}\tilde{\mathbf{x}}(\mathbf{D}-i\mathbf{C})(\mathbf{A}+i\mathbf{B})^{-1}\mathbf{x} \\ +\sqrt{2}\,\tilde{\varsigma}(\mathbf{A}+i\mathbf{B})^{-1}\mathbf{x}-\tfrac{1}{2}\tilde{\varsigma}(\mathbf{A}+i\mathbf{B})^{-1}(\mathbf{A}-i\mathbf{B})\varsigma\Big]\Big\},\end{aligned} \tag{6.32}$$

where we use the notation of Appendix C to distinguish the complex N-vector ς from the real $2N$-vector $\mathbf{z}$. The matrix $(\mathbf{A}+i\mathbf{B})^{-1}(\mathbf{A}-i\mathbf{B})$ is complex symmetric.

Unlike Eq. (6.30), the matrix element of Eq. (6.32) does contain full information about the metaplectic operator, because of the completeness of the coherent states $|\mathbf{z}\rangle$. It also provides a unique specification of the symplectic matrix $\mathbf{S}$ on the right hand side, as may be seen by noting that the complex symplectic matrix $\mathbf{S}' = \mathbf{S}\mathbf{W}^{-1}$, where $\mathbf{W}$ is given by Eq. (A.31), has components,

$$\mathbf{S}' = \frac{1}{\sqrt{2}}\begin{pmatrix}\mathbf{A}-i\mathbf{B} & -i(\mathbf{A}+i\mathbf{B}) \\ -i(\mathbf{D}+i\mathbf{C}) & \mathbf{D}-i\mathbf{C}\end{pmatrix}. \tag{6.33}$$

The components of $\mathbf{S}$ can therefore be reconstructed from a knowledge of the matrices appearing in the exponent of Eq. (6.32).

Furthermore, Eq. (6.32) shows quite simply and rigorously the double covering of the symplectic group by the metaplectic group, which is expressed via the double Riemann surface required for the complex square root. The double covering is manifested through the overall phase of the Gaussian wave packet appearing in Eq. (6.32). This is related to the phase γ_S, defined by

$$\gamma_S = \arg\det(\mathbf{A}+i\mathbf{B}), \tag{6.34}$$

which is discussed in Appendix A. If we denote the overall phase of Eq. (6.32) by $e^{-i\gamma_M}$, then we have

$$\gamma_M = \tfrac{1}{2}\gamma_S + n\pi, \tag{6.35}$$

where $n = 0$ if $\sigma = +1$, and $n = 1$ if $\sigma = -1$. The phase γ_M evolves continuously in time, unlike the Maslov index (which has discontinuities at caustics), and in a sense it is a continuous version of the Maslov index.

In this interpretation, the discontinuities in phase which are usually associated with caustics are smoothed out, and take place continuously along a whole orbit. However, one should not make too much of this idea, since neither the Maslov index nor the phase γ_M are invariants in phase space. (Specifically, the angle γ_S is not preserved under symplectic conjugation.) It is only when the matrix function $\mathbf{S}(t)$ is periodic that there is any invariant meaning to the elapsed γ_S or Maslov index; in that case, γ_S is an integral multiple of 2π, γ_M is an integral multiple of π, and the Maslov index is even.

It is also curious to note that had we blindly substituted the components of the complex $\mathbf{S}'$ directly into Eq. (4.37), not worrying about the fact that $\mathbf{S}'$ is complex, we would have arrived at Eq. (6.32) in all of its details, except for the factor $\exp(-|\varsigma|^2/2\hbar)$. Similarly, had we blindly substituted the components of the complex $\mathbf{W}^{-1}$ of Eq. (A.31) into Eq. (4.37), again, except for the factor $\exp(-|\varsigma|^2/2\hbar)$, we would have arrived at the coherent state matrix element $\langle \mathbf{x}|\mathbf{z}\rangle$ of Eq. (C.9). These observations suggest an important role for the theory of the complex symplectic group (Kramer, Moshinsky, and Seligman [1975]; Weissman [1982]). Perhaps there is a sense in which the use of coherent states to avoid caustic difficulties is analogous to the analytic continuation methods so common in ordinary WKB theory (Berry and Mount [1972]; Fröman and Fröman [1965]). It would especially be of interest to know what invariant significance there is to the phenomenon of Stokes' lines (which, being tied to caustics, are certainly not invariant in the usual formulation of WKB theory). Some interesting analysis of complex manifolds, using the formalism of Stokes' lines, has been carried out by Berk and Pfirsch [1980], and is in need of deeper understanding.

The mixed x-space/coherent state matrix element of Eq. (6.32) is most useful in the kind of wave packet analysis performed by Heller, but it is also useful to have the full coherent state matrix elements. These are obtained in a straightforward manner from Eqs. (6.32) and (C.9). The result is

$$\langle \mathbf{z}|M(\mathbf{S})|\mathbf{z}'\rangle = \frac{\sigma}{\sqrt{\det \mathbf{\Lambda}}} \exp\left[-\tfrac{1}{2\hbar}\left(|\varsigma|^2 + |\varsigma'|^2\right)\right] \times \exp\left[\frac{1}{\hbar}\left(\tfrac{1}{2}\tilde{\varsigma}^*\mathbf{\Gamma}^*\mathbf{\Lambda}^{-1}\varsigma^* + \tilde{\varsigma}'\mathbf{\Lambda}^{-1}\varsigma^* - \tfrac{1}{2}\tilde{\varsigma}'\mathbf{\Lambda}^{-1}\mathbf{\Gamma}\varsigma'\right)\right], \qquad (6.36)$$

where the complex $N\times N$ matrices $\mathbf{\Lambda}$, $\mathbf{\Gamma}$ are given by Eq. (A.40). The matrix $\mathbf{\Lambda}$ is always nonsingular. This result was first derived by Bargmann [1961], who worked directly in the coherent state representation. It also arises in semiclassical operations on the coherent state path integral (Klauder [1978]). The quantity σ appearing here is not the same σ as in Eq. (4.37) or (6.32).

Because of the completeness of the coherent states, one can in principle use purely coherent state matrix elements to carry out any calculation. Such calculations involve integrals over the Liouville-Gibbs measure on the classical phase space, $d^{2N}\mathbf{z}/(2\pi\hbar)^N$, and Bargmann [1961] has given rules, involving analytic continuation, for carrying out such integrals.

Finally, we note an interesting fact concerning the ordinary eigenstates $|\mathbf{x}\rangle$ and $|\mathbf{p}\rangle$ of position and momentum, namely that these can be seen as limiting cases of coherent states, under the action of metaplectic operators. Since the states $|\mathbf{x}\rangle$, $|\mathbf{p}\rangle$ are not normalized, whereas the coherent states are, one must change the norm in the limiting process. We introduce the following symplectic matrix,

$$\mathbf{S}(\alpha) = \begin{pmatrix} \alpha\mathbf{I} & 0 \\ 0 & \frac{1}{\alpha}\mathbf{I} \end{pmatrix}, \qquad (6.37)$$

which is a simple scaling operation. Then we have

$$\lim_{\alpha \to 0} \quad \frac{1}{(4\alpha^2\pi\hbar)^{N/4}} T(\mathbf{x},0)\, M\big(\mathbf{S}(\alpha)\big)|0\rangle = |\mathbf{x}\rangle,$$

$$\lim_{\alpha \to 0} \quad \frac{1}{(4\alpha^2\pi\hbar)^{N/4}} T(0,\mathbf{p})\, M\big(\mathbf{S}(\alpha)\big)^{\dagger} |0\rangle = |\mathbf{p}\rangle, \tag{6.38}$$

where $|0\rangle$ is the standard fiducial coherent state of Eq. (C.4), and where we have taken $\sigma = +1$. One can use these limiting forms to retrieve Eq. (4.37) from Eq. (6.32) or (6.36).

We turn now to the use of Heisenberg and metaplectic operators in wave packet propagation.

7. A Semiclassical Wave Packet Propagator

We are now prepared to assemble our results and to develop a semiclassical propagator for wave packets. We begin by developing a classical nearby orbit propagator for localized Liouville distribution functions. We then extend this analysis to the quantum case, and explore the strong analogies between the quantum and classical picture. The quantum wave packet propagator is then used to create a semiclassical propagator for arbitrary initial wave functions. This propagator has a number of problematic aspects, which we discuss and relate to some fundamental questions of semiclassical mechanics.

7.1. A Classical Propagator in the Nearby Orbit Approximation

Let us return to the discussion of Sec. 2 and make a classical analysis of the time evolution of a distribution function $f(\mathbf{z},t)$ in the nearby orbit approximation. Let us suppose, as illustrated in Fig. 14, that at $t = 0$ the initial distribution function $f_0(\mathbf{z})$ has expectation values $\langle \mathbf{z} \rangle = \mathbf{z}_0$. These act as initial conditions for an orbit $\mathbf{z}_r(t)$, which we shall take as a reference orbit. We expect that if $f_0(\mathbf{z})$ is localized about $\mathbf{z}_0$, then the time evolution of $\langle \mathbf{z} \rangle(t)$ will follow the reference orbit, and be the same as $\mathbf{z}_r(t)$.

To relate this idea to the nearby orbit approximation, we begin with the exact Liouville equation for the evolution of $f(\mathbf{z},t)$,

$$\frac{\partial f}{\partial t} + \{f,H\} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{z}} \cdot \mathbf{J} \cdot \frac{\partial H}{\partial \mathbf{z}} = 0. \tag{7.1}$$

$H = H(\mathbf{z})$ is the classical Hamiltonian, about which we make no assumptions (e.g. it does not necessarily have the form of kinetic plus potential energies). We compute the time derivative of the expectation values $\langle \mathbf{z} \rangle(t)$, as is standard in classical kinetic theory, to obtain

$$\frac{d}{dt}\langle \mathbf{z} \rangle = -\int \mathbf{z} \left(\frac{\partial f}{\partial \mathbf{z}} \cdot \mathbf{J} \cdot \frac{\partial H}{\partial \mathbf{z}} \right) d^{2N}\mathbf{z}. \tag{7.2}$$

Integration by parts and the use of the antisymmetry of $\mathbf{J}$ then gives us the classical version of Ehrenfest's theorem,

$$\frac{d}{dt}\langle \mathbf{z} \rangle = \mathbf{J} \cdot \left\langle \frac{\partial H}{\partial \mathbf{z}} \right\rangle . \tag{7.3}$$

Just as in Eqs. (2.2), this result is exact, but it does not imply that $\langle \mathbf{z} \rangle(t)$ follows the reference orbit. Nor is it a version of Hamilton's equations, because the average of $\partial H/\partial \mathbf{z}$ on the right hand side, while it is a function of t, in general is not a function of $\langle \mathbf{z} \rangle(t)$.

If, however, $f_0(\mathbf{z})$ is localized about $\mathbf{z}_0$, then we can expect $f(\mathbf{z},t)$ to be localized about $\langle \mathbf{z} \rangle(t)$, at least for limited time intervals, and we can expand $H(\mathbf{z})$ about $\langle \mathbf{z} \rangle(t)$. Carrying this out to second order, we have

$$\begin{aligned} H(\mathbf{z}) \approx H(\langle \mathbf{z} \rangle) + (\mathbf{z} - \langle \mathbf{z} \rangle) \cdot \frac{\partial H}{\partial \mathbf{z}}(\langle \mathbf{z} \rangle) \\ + \tfrac{1}{2}(\mathbf{z} - \langle \mathbf{z} \rangle) \cdot \frac{\partial^2 H}{\partial \mathbf{z} \partial \mathbf{z}} \cdot (\mathbf{z} - \langle \mathbf{z} \rangle). \end{aligned} \tag{7.4}$$

The final term involves the same matrix $\mathbf{H}''$ introduced in Eq. (2.11). Using this approximation in Eq. (7.3), the term in $\mathbf{H}''$ cancels, and we have

$$\frac{d}{dt}\langle \mathbf{z} \rangle = \mathbf{J} \cdot \frac{\partial H}{\partial \mathbf{z}}(\langle \mathbf{z} \rangle), \tag{7.5}$$

which is the classical analog of Eq. (2.3). This equation has the solution $\langle \mathbf{z} \rangle(t) = \mathbf{z}_r(t)$, and we see that classical expectation values do follow the reference orbit in the nearby orbit approximation.

However, the reference orbit gives only partial information about the time evolution of $f(\mathbf{z},t)$. More complete information results when we introduce the symplectic matrix defined by Eq. (2.15). Referring to Fig. 14, we can see pictorially what effect the evolution of nearby orbits has on the evolution of $f(\mathbf{z},t)$. Not only does the expectation value $\langle \mathbf{z} \rangle(t)$ move along the reference orbit $\mathbf{z}_r(t)$, but also the shape and spreading of $f(\mathbf{z},t)$ about $\mathbf{z}_r(t)$ changes in time. This can be conceived of as a symplectic "rotation" in phase space; we put the word in quotes because a symplectic matrix includes scaling and stretching

operations, as well as rotations. Sample contour lines of f are shown in the figure to illustrate this effect.

It is convenient to describe the net effect of the time evolution of f in the nearby orbit approximation as a three-step process. In the first step, we move $f_0(\mathbf{z})$ rigidly from $\mathbf{z}_0$ to the origin. This can be done with the classical displacement operator, $T_{cl}(\mathbf{z}_0)^{-1}$. In the second step, we rotate f into its final orientation by means of the symplectic matrix $\mathbf{S}(t)$, which is the solution to Eq. (2.15). This can be accomplished with the operator $M_{cl}\left(\mathbf{S}(t)\right)$, defined by Eqs. (6.24)–(6.25). In the final step, we rigidly translate the rotated f into its final position at $\mathbf{z}_r(t)$, using the translation operator $T_{cl}\left(\mathbf{z}_r(t)\right)$.

Combining these operations, we have a classical propagator $U_{cl}(t,\mathbf{z})$, based on the nearby orbit approximation, which has the form

$$U_{cl}(t,\mathbf{z}_0) = T_{cl}\big(\mathbf{z}_r(t)\big) M_{cl}\big(\mathbf{S}(t)\big) T_{cl}(\mathbf{z}_0)^{-1}. \tag{7.6}$$

The approximate time evolution of f is then given by

$$f(\mathbf{z},t) = \left[U_{cl}(t,\mathbf{z}_0) f_0\right](\mathbf{z}), \tag{7.7}$$

or, by explicitly writing out the action of $U_{cl}(t,\mathbf{z}_0)$,

$$f(\mathbf{z},t) = f_0\Big(\mathbf{S}(t)^{-1}\big(\mathbf{z}-\mathbf{z}_r(t)\big)+\mathbf{z}_0\Big). \tag{7.8}$$

Note that we have made no assumptions about $f_0(\mathbf{z})$, other than that it be localized. In particular, it need not be Gaussian. Note also tht we are not expanding $f(\mathbf{z},t)$ about $\langle\mathbf{z}\rangle$; we have only expanded the Hamiltonian. The evolution (7.8) is nonlinear in f, because $\mathbf{z}_0$ depends on f_0.

A less pictorial derivation of Eq. (7.8) can also be given. Let us assume that $f(\mathbf{z},t)$ has the form shown in Eq. (7.8), but without making any assumptions about $\mathbf{z}_r(t)$ or $\mathbf{S}(t)$. In particular, we do not assume that $\mathbf{z}_r(t)$ is an allowable orbit, or that $\mathbf{z}_r(t) = \langle\mathbf{z}\rangle(t)$, or that $\mathbf{S}(t)$ is symplectic. In general, of course, a solution of this form does not exist, and

cannot be made to satisfy the Liouville equation. However, if we expand $H(\mathbf{z})$ to second order about $\mathbf{z}_r(t)$, as in Eq. (7.4), and substitute into the Liouville equation, then we find that $\mathbf{z}_r(t)$ and $\mathbf{S}(t)$ are uniquely determined.

Indeed, Eq. (7.8) gives

$$\frac{\partial f}{\partial t} = \frac{\partial f_0}{\partial \mathbf{z}} \cdot \left[\dot{\mathbf{S}}^{-1}(\mathbf{z} - \mathbf{z}_r) - \mathbf{S}^{-1}\dot{\mathbf{z}}_r\right],$$

$$\frac{\partial f}{\partial \mathbf{z}} = \frac{\partial f_0}{\partial \mathbf{z}} \cdot \mathbf{S}^{-1}, \tag{7.9}$$

where $\partial f_0/\partial \mathbf{z}$ is evaluated at the argument shown in Eq. (7.8). Substituting this into the Liouville equation and using the second order expansion of $H(\mathbf{z})$ about $\mathbf{z}_r$, we find

$$\frac{\partial f_0}{\partial \mathbf{z}} \cdot \left[\dot{\mathbf{S}}^{-1}(\mathbf{z} - \mathbf{z}_r) - \mathbf{S}^{-1}\dot{\mathbf{z}}_r + \mathbf{S}^{-1}\mathbf{J}\mathbf{H}' + \mathbf{S}^{-1}\mathbf{J}\mathbf{H}''(\mathbf{z} - \mathbf{z}_r)\right] = 0, \tag{7.10}$$

where $\mathbf{H}'$ is the vector $(\partial H/\partial \mathbf{z})(\mathbf{z}_r)$, and $\mathbf{H}''$ is the matrix of Eq. (2.11), evaluated at $\mathbf{z}_r$. Collecting terms in powers of $\mathbf{z} - \mathbf{z}_r$, and using $\mathbf{S}\dot{\mathbf{S}}^{-1} + \dot{\mathbf{S}}\mathbf{S}^{-1} = 0$, we find

$$\dot{\mathbf{z}}_r = \mathbf{J}\mathbf{H}'$$

$$\dot{\mathbf{S}} = \mathbf{J}\mathbf{H}''\mathbf{S}, \tag{7.11}$$

in agreement with the results of Sec. 2 on nearby orbits.

It is also of interest to compute the second moments of f under the time evolution specified by Eq. (7.8). We define a $2N \times 2N$ correlation matrix,

$$C_{\alpha\beta} = \big\langle \big(z_\alpha - \langle z_\alpha \rangle\big)\big(z_\beta - \langle z_\beta \rangle\big) \big\rangle = \langle z_\alpha z_\beta \rangle - \langle z_\alpha \rangle \langle z_\beta \rangle. \tag{7.12}$$

Then a direct calculation of moments based on Eq. (7.8) gives

$$\mathbf{C}(t) = \mathbf{S}(t)\mathbf{C}(0)\tilde{\mathbf{S}}(t). \tag{7.13}$$

Thus, not only the first moments of f, but also the second, can be expressed simply in terms of the parameters of the nearby orbit problem.

7.2. The Quantum Propagator in the Nearby Orbit Approximation

We shall now perform a similar analysis in the quantum case. Let us suppose we have an initial state $|\psi_0\rangle$ which represents a wave packet of finite norm. It need not be Gaussian. This wave packet has expectation values $\langle\hat{\mathbf{z}}\rangle$ at $t = 0$ which we denote by $\mathbf{z}_0$.

On the analogy of the classical propagator of Eq. (7.6), we shall look for solutions $|\psi\rangle = |\psi(t)\rangle$ to the Schrödinger equation in the form

$$|\psi\rangle = e^{i\gamma(t)/\hbar} T\left(\mathbf{z}(t)\right) M\left(\mathbf{S}(t)\right) T(\mathbf{z}_0)^\dagger |\psi_0\rangle, \tag{7.14}$$

where $\mathbf{z}(t)$, $\mathbf{S}(t)$, and $\gamma(t)$ are functions of time yet to be determined. This approach is essentially the same as Heller's [1975], although Heller built the time evolution into the parameters of a Gaussian wave packet, and we have placed it into the operators. This approach has the advantage the $|\psi_0\rangle$ need not be Gaussian. In order to satisfy the initial conditions, we must have $\gamma = 0$, $\mathbf{z} = \mathbf{z}_0$, and $\mathbf{S} = \mathbf{I}$ at $t = 0$. Furthermore, the sign of $M(\mathbf{S})$ is chosen at $t = 0$ so that $M(\mathbf{I}) = +1$; continuity will then determine the sign of $M\left(\mathbf{S}(t)\right)$ at all later times.

In order to substitute Eq. (7.14) into the Schrödinger equation, we need formulas for the time derivatives of $T\left(\mathbf{z}(t)\right)$ and $M\left(\mathbf{S}(t)\right)$. For the Heisenberg operator, we use Eq. (3.22) to write

$$T(\mathbf{z} + \dot{\mathbf{z}}\Delta t) = \exp\Big[-\frac{i\Delta t}{2\hbar}\omega(\dot{\mathbf{z}}, \mathbf{z})\Big] T(\dot{\mathbf{z}}\Delta t) T(\mathbf{z}). \tag{7.15}$$

Using Eq. (3.12) for the term $T(\dot{\mathbf{z}}\Delta t)$ and expanding the exponentials to first order in Δt, we have

$$T(\mathbf{z} + \dot{\mathbf{z}}\Delta t) = \left\{1 - \frac{i\Delta t}{\hbar}\left[\omega(\hat{\mathbf{z}}, \dot{\mathbf{z}}) - \tfrac{1}{2}\omega(\mathbf{z}, \dot{\mathbf{z}})\right]\right\} T(\mathbf{z}). \tag{7.16}$$

From this we can compute the time derivative of $T(\mathbf{z})$, which we write in the form

$$\frac{d}{dt}T(\mathbf{z}) = -\frac{i}{\hbar}\left[\omega(\hat{\mathbf{z}} - \mathbf{z}, \dot{\mathbf{z}}) + \tfrac{1}{2}\omega(\mathbf{z}, \dot{\mathbf{z}})\right] T(\mathbf{z}). \tag{7.17}$$

We treat the metaplectic operators similarly. First we write

$$M\left(\mathbf{S}(t+\Delta t)\right) = M(\mathbf{S}+\Delta t\dot{\mathbf{S}}) = M\left((\mathbf{I}+\Delta t\dot{\mathbf{S}}\mathbf{S}^{-1})\mathbf{S}\right)$$
$$= M(\mathbf{I}+\Delta t\dot{\mathbf{S}}\mathbf{S}^{-1})M(\mathbf{S}), \tag{7.18}$$

where we use Eq. (4.38). The + sign is taken in the decomposition of the product because the first factor is near identity, and we demand continuity. The near identity symplectic matrix in the first factor must have the form $\mathbf{I}+\Delta t\mathbf{J}\mathbf{K}$, where $\mathbf{K}$ is symmetric, as in Eq. (A.15). Therefore $\mathbf{K} = -\mathbf{J}\dot{\mathbf{S}}\mathbf{S}^{-1}$, and we can use Eq. (4.5) to write

$$M\big(\mathbf{S}(t+\Delta t)\big) = \left(1+\frac{i\Delta t}{2\hbar}\,\hat{\mathbf{z}}\cdot\mathbf{J}\dot{\mathbf{S}}\mathbf{S}^{-1}\cdot\hat{\mathbf{z}}\right)M\big(\mathbf{S}(t)\big). \tag{7.19}$$

This finally shows that

$$\frac{d}{dt}M(\mathbf{S}) = \frac{i}{2\hbar}\left(\hat{\mathbf{z}}\cdot\mathbf{J}\dot{\mathbf{S}}\mathbf{S}^{-1}\cdot\hat{\mathbf{z}}\right)M(\mathbf{S}). \tag{7.20}$$

We now compute the time derivative of $|\psi\rangle$. The term in $(d/dt)M(\mathbf{S})$ is multiplied on the left by $T(\mathbf{z})$, so we commute this through the leading factor of Eq. (7.20), using Eq. (4.3). This replaces $\hat{\mathbf{z}}$ by $\hat{\mathbf{z}}-\mathbf{z}$, so that altogether our result can be written in the form

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \left[-\dot{\gamma}+\omega(\hat{\mathbf{z}}-\mathbf{z},\dot{\mathbf{z}})+\tfrac{1}{2}\omega(\mathbf{z},\dot{\mathbf{z}})-\tfrac{1}{2}\,(\hat{\mathbf{z}}-\mathbf{z})\cdot\mathbf{J}\dot{\mathbf{S}}\mathbf{S}^{-1}\cdot(\hat{\mathbf{z}}-\mathbf{z})\right]|\psi\rangle, \tag{7.21}$$

where $\mathbf{z}$ means the $\mathbf{z}(t)$ appearing in Eq. (7.14). The leading factor, not surprisingly, is a quadratic polynomial in $\hat{\mathbf{z}}-\mathbf{z}$; it represents an element of the Lie algebra of $IMp(2N)$.

As in the classical case, a time dependent state of the form (7.4) is not in general a solution to the Schrödinger equation, unless we approximate the Hamiltonian in terms of nearby orbits. However, the Schrödinger Hamiltonian is a function of the operators $\hat{\mathbf{z}}$, not the classical phase space coordinates $\mathbf{z}$, so we need to develop a sense for what this approximation means. Of course, this is no problem for the simple Hamiltonians of quantum mechanics, in which the kinetic energy is already quadratic in momentum, and there are no ordering issues. In that case, we merely expand the potential $V(\mathbf{x})$ about $\mathbf{q}$,

where $\mathbf{q}$ is the configuration space part of $\mathbf{z}$. More generally, however, there are ordering issues to be dealt with.

Therefore we call on the Wigner-Weyl formalism, and proceed somewhat heuristically. We denote the ordinary Weyl symbol of $H(\hat{\mathbf{z}})$ by $H(\mathbf{z})$, and we let the Wigner function of $|\psi\rangle$ be $W(\mathbf{z})$. By Eq. (B.20), the Wigner function is centered in phase space on the point $\langle\psi|\hat{\mathbf{z}}|\psi\rangle$. We shall assume that it is well localized about this point, and that it takes on substantial values only within roughly one unit cell of phase space, with volume $(2\pi\hbar)^N$. If we use the phase space coordinates $(\mathbf{q}, \mathbf{p})$ with symmetrized dimensions, as discussed in Sec. 6, then the Wigner function will have, according to our assumptions, a scale length in phase space which is $O(\hbar^{1/2})$ in any direction. We do not assume that the Wigner function is smooth, nor do we expand it about its mean value.

Actually, it is known (Balazs and Jennings [1984], Berry [1977], Heller [1976]) that in general the Wigner function is highly oscillatory in phase space, and may be quite extended. The degree to which this is true, of course, depends on the state $|\psi\rangle$, and it is not clear what restrictions $|\psi\rangle$ must satisfy in order to produce the kind of localized Wigner function we have in mind here. In the case of Gaussians, however, the Wigner function is easily calculated, and, for reasonable Gaussians at least, it has the kind of localization in phase space we are describing. For more general wave functions, perhaps it is easiest to sidestep the question and simply to define a "wave packet" as a state whose Wigner function is localized. Although certain rigorous statements can be made about the approximation scheme we are developing here (Hepp [1974], Hagedorn [1980]), we shall be satisfied with a partly intuitive picture.

In any case, if $|\psi(t)\rangle$ has the form postulated in Eq. (7.14), then the Wigner function $W(\mathbf{z}, t)$ is centered on the point $\mathbf{z}(t)$. We show this by directly computing $\langle\psi|\hat{\mathbf{z}}|\psi\rangle$, using Eqs. (3.4) and (4.3):

$$\begin{aligned}\langle\psi|\hat{\mathbf{z}}|\psi\rangle &= \langle\psi_0|T(\mathbf{z}_0)M(\mathbf{S})^\dagger T\big(\mathbf{z}(t)\big)^\dagger \hat{\mathbf{z}}\, T\big(\mathbf{z}(t)\big) M(\mathbf{S})T(\mathbf{z}_0)^\dagger|\psi_0\rangle \\ &= \langle\psi_0|T(\mathbf{z}_0)M(\mathbf{S})^\dagger \left[\hat{\mathbf{z}} + \mathbf{z}(t)\right] M(\mathbf{S})T(\mathbf{z}_0)^\dagger|\psi_0\rangle \\ &= \langle\psi_0|T(\mathbf{z}_0) \left[\mathbf{S}\hat{\mathbf{z}} + \mathbf{z}(t)\right] T(\mathbf{z}_0)^\dagger|\psi_0\rangle \\ &= \langle\psi_0| \left[\mathbf{S}(\hat{\mathbf{z}} - \mathbf{z}_0) + \mathbf{z}(t)\right] |\psi_0\rangle = \mathbf{z}(t), \end{aligned} \tag{7.22}$$

where we have used $\langle\psi_0|\hat{\mathbf{z}}|\psi_0\rangle = \mathbf{z}_0$ in the last step.

Therefore we shall assume that the time evolution of the Wigner function can be approximated by expanding the Weyl symbol $H(\mathbf{z})$ of the Hamiltonian about $\mathbf{z}(t)$, which we take out to quadratic order as in Eq. (7.4). This produces a quadratic polynomial in $\hat{\mathbf{z}} - \mathbf{z}(t)$, which can be interpreted as the symbol of an approximate quantum Hamiltonian. Inverting the Weyl symbol relations is easy for quadratic polynomials in $\mathbf{z}$, and we obtain the approximation

$$H(\hat{\mathbf{z}};t) \approx H\big(\mathbf{z}(t)\big) + \big(\hat{\mathbf{z}} - \mathbf{z}(t)\big) \cdot \mathbf{H}'\big(\mathbf{z}(t)\big) + \tfrac{1}{2}\big(\hat{\mathbf{z}} - \mathbf{z}(t)\big) \cdot \mathbf{H}''\big(\mathbf{z}(t)\big) \cdot \big(\hat{\mathbf{z}} - \mathbf{z}(t)\big). \tag{7.23}$$

The scalar H, the vector $\mathbf{H}' = \partial H/\partial \mathbf{z}$, and the matrix $\mathbf{H}''$ represent the ordinary Weyl symbol of the exact quantum Hamiltonian, and are functions of time through $\mathbf{z}(t)$.

This expression is not necessarily an expansion in $\hbar$. This is most easily seen in the $\mathbf{q}$, $\mathbf{p}$ variables with symmetrized dimensions introduced in Sec. 6. The expansion of the Weyl symbol should be valid out to a distance in phase space of order $\hbar^{1/2}$ about $\mathbf{z}(t)$, on the basis of our assumptions about the Wigner function. However, $H(\mathbf{z})$ is a function of the dimensionless variables $\mathbf{q}/\sqrt{\hbar}$, $\mathbf{p}/\sqrt{\hbar}$, so all terms in Eq. (7.23) are of the same order in $\hbar$. The expansion (7.23) really represents an assumption about the smoothness of the Hamiltonian, which can be tested in individual cases. One also has considerable latitude in the choice of the initial state $|\psi_0\rangle$, which can be used to optimize the validity of the expansion. In some cases, Eq. (7.23) can be seen as an expansion in the inverse quantum number.

In any case, we can now combine Eqs. (7.21) and (7.23) in the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle. \tag{7.24}$$

Collecting terms on each side by powers of $\hat{\mathbf{z}} - \mathbf{z}$, we obtain the equations

$$\begin{aligned}
\dot{\gamma} &= \tfrac{1}{2}\omega(\mathbf{z}, \dot{\mathbf{z}}) - H\big(\mathbf{z}(t)\big), \\
\dot{\mathbf{z}} &= \mathbf{J}\mathbf{H}'\big(\mathbf{z}(t)\big), \\
\dot{\mathbf{S}} &= \mathbf{J}\mathbf{H}''\big(\mathbf{z}(t)\big)\mathbf{S}.
\end{aligned} \tag{7.25}$$

The last two of these are the equations for the classical orbit and the symplectic matrix describing nearby orbits; and the first is a phase, due essentially to the noncommutativity of the Heisenberg operators. It is like the Bohr-Sommerfeld phase, but symmetrized in q and p, since

$$\gamma(t) = \tfrac{1}{2}\int_0^t dt\,(\mathbf{p}\cdot\dot{\mathbf{q}} - \mathbf{q}\cdot\dot{\mathbf{p}}) - Ht. \tag{7.26}$$

Here we have assumed that the original Hamiltonian is time-independent, so that $H(\mathbf{z})$ is constant along the orbit $\mathbf{z}(t)$, and can be taken out of the time integral. However, if H does have an explicit (but slow) dependence on time, then Eqs. (7.25) are still valid, and we need only keep $H(\mathbf{z}, t)$ inside the time integral in Eq. (7.26).

Collecting our results, we can now write down a semiclassical wave packet propagator, which is the quantum analog of Eq. (7.6):

$$U(t, \mathbf{z}_0) = e^{i\gamma(t)/\hbar}\,T\big(\mathbf{z}(t)\big)M\big(\mathbf{S}(t)\big)T(\mathbf{z}_0)^\dagger. \tag{7.27}$$

Apart from the phase γ and the double valuedness of the metaplectic operators, this carries exactly the same information as the classical propagator, and it shows that wave packets can be propagated on the basis of (nearly) purely classical calculations. This, of course, is the practical goal of any semiclassical theory.

Although this propagator preserves the norm of the state it acts upon, it is not unitary in the usual sense, because it is not even a linear operator. It is nonlinear for the same reason as its classical counterpart, i.e. the parameter $\mathbf{z}_0$ depends on the initial state.

When this propagator is used to advance wave packets in time, the expectation values $\langle \mathbf{z} \rangle(t)$ follow the trajectory $\mathbf{z}(t)$, as shown by Eq. (7.22). Furthermore, by Eq. (7.25), $\mathbf{z}(t)$ is seen to be a classical orbit. However, just as in the classical case, the reference orbit alone gives somewhat limited information about the wave packet. Let us therefore compute the second moments of the wave packet about the central orbit.

As in the classical case, we define a $2N \times 2N$ correlation matrix $\mathbf{C}$,

$$C_{\alpha\beta} = \left\langle \frac{\hat{z}_\alpha \hat{z}_\beta + \hat{z}_\beta \hat{z}_\alpha}{2} \right\rangle - \langle \hat{z}_\alpha \rangle \langle \hat{z}_\beta \rangle. \tag{7.28}$$

Because the components of $\hat{\mathbf{z}}$ do not commute with each other, we have symmetrized the first term to obtain a real quantity. Inverting the Weyl symbol relations for a quadratic polynomial in $\mathbf{z}$ automatically produces this symmetrization, because real symbols correspond to Hermitian operators. We note that $C_{\alpha\beta}$ contains all the quantities Δq_i^2, Δp_i^2 which would be of interest in investigating questions of minimum uncertainty, as well as all the cross terms.

A direct calculation of $C_{\alpha\beta}$, carried out exactly as in Eq. (7.22), shows that the quantum correlation matrix obeys exactly the same rules as in the classical case, i.e. Eq. (7.13) is still valid. This is the generalization of the spreading of the free particle wave packet, as discussed in Sec. 2.

We can go beyond the calculation of moments and give a precise description of the evolution of the Wigner function of $|\psi\rangle$ under the propagator (7.27). We let the Wigner function of $|\psi_0\rangle$ be $W_0(\mathbf{z})$. Then, using Eqs. (6.22) and (6.26), we find that the Wigner function of $U(t, \mathbf{z}_0)|\psi_0\rangle$ is

$$W(\mathbf{z}, t) = W_0\Big(\mathbf{S}(t)^{-1}(\mathbf{z} - \mathbf{z}(t)) + \mathbf{z}_0\Big). \tag{7.29}$$

This is exactly the same behavior displayed in the classical Liouville function, Eq. (7.8).

A principal benefit of this analysis is a conceptual one, since wave packet spreading, in both configuration and momentum space, can now be seen in purely classical terms. This picture also clearly shows the limitations of Eq. (7.27) as a wave packet propagator. For example, it is known classically that distributions of particles which are initially localized in phase space do not remain localized in the course of time. In most cases, the spreading is at least linear in time, and for chaotic systems, it is exponential in time, as determined by the Liapunov exponents (Lichtenberg and Lieberman [1983]).

For certain systems, however, the classical spreading of a distribution of particles is periodic in time. These are systems whose Hamiltonians are action variables, which have the properties that not only are the orbits they generate periodic, but also the period is constant from one orbit to the next. Thus, after one period, a classical distribution function reassembles itself exactly, and if any spreading does occur, it is followed by contraction. This is not to say that the corresponding quantum evoltion will be exactly periodic, but at least within the quadratic nearby orbit approximation it will be so. If furthermore the action variable which is being treated as a Hamiltonian happens to be a quadratic function of q's and p's, then the propagator (7.27) will be exact, and the spreading of the quantum wave packet will be periodic and hence bounded. More generally, the propagator will be valid only for limited periods of time, which can be determined quantitatively by an analysis of the separation of classical orbits.

Nevertheless, there are many problems for which the time limitation is not an impediment. Some of these are discussed by Heller [1975, 1976]; others include the transmission of light through optical devices, as discussed by Guillemin and Sternberg [1984], and the use of "Gaussian beams" (Keller [1971], Deschamps [1972], Červený and Pšenčík [1979], Červený, Popov and Pšenčík [1982]). Another interesting example concerns the motion of charged particles in inhomogeneous magnetic fields. If the inhomogeneities are weak, then

the motion is approximated by the uniform field solution. The latter, however, is represented by a quadratic Hamiltonian, whose propagator is a metaplectic operator. Taking account of the inhomogeneities as a perturbation will surely result in a wave packet propagator of the form (7.27), although to my knowledge the details of this have never been worked out. This problem is important in recent $g-2$ experiments (Ford [1978]), and in other areas.

Another limitation of the propagator (7.27) is its failure to deal with tunneling. If the reference orbit $\mathbf{z}(t)$ is inside a separatrix, then it will stay there forever, and no tunneling will occur. However, the classical analog we have developed shows clearly what the problem is, and what must be done to fix it. Although tunneling is usually considered a purely quantum effect, there is a simple classical analog. Suppose, for example, that the initial Liouville distribution function is Gaussian in phase space, and that the reference orbit is inside a separatrix. In the exact classical solution, particles in the tail of the distribution will be outside the separatrix, and will classically "tunnel." However, this effect is lost when the approximate classical propagator (7.6) is used. Clearly, in order to correctly describe tunneling, one must propagate more than one wave packet. (This, however, is a naive picture. The basic fact is that neither Eq. (7.27) nor its classical analog is valid for long periods of time in the neighborhood of an unstable fixed point.)

It is possible that the limitation on time intervals allowed in Eq. (7.27) can be turned into an advantage, by providing one with a means for studying the statistical properties of quantum chaos. Presumably quantum chaos differs from classical chaos in that not only do the phase space positions of the particles or wave packets mix, but also the linear superposition of the wave packets gives rise to a mixing of their phases. It is likely that a simple analysis along these lines would lead to interesting results. For chaotic systems, it is known that initially smooth Lagrangian manifolds become tangled up in the course of time (Berry, Balazs, Tabor and Voros [1979]), and this is certainly related to the time limitations

imposed on the propagator (7.27). Some interesting studies relating wave packet evolution and quantum chaos have been carried out by Heller [1985].

The wave packet $|\psi_0\rangle$ appearing in Eq. (7.14) need not be Gaussian, and it seems that sometimes it is useful to consider more general wave packets. For example, the light entering an optical system can be treated as a single wave packet, whose reference orbit is the optical axis (Guillemin and Sternberg [1984]).

If, however, $|\psi_0\rangle$ is a Gaussian, then we have the advantage of being able to carry out the action of the metaplectic operator in closed form. Suppose, for example, that $|\psi_0\rangle$ is the standard coherent state centered at $\mathbf{z}_0$ at $t = 0$. That is, let $|\psi_0\rangle = T(\mathbf{z}_0)|0\rangle$, where $|0\rangle$ is the standard fiducial state of Eq. (C.4). When we apply the propagator (7.27) to this initial state, the Heisenberg operator $T(\mathbf{z}_0)$ cancels, and we have

$$|\psi(t)\rangle = e^{i\gamma(t)/\hbar}\, T\big(\mathbf{z}(t)\big) M\big(\mathbf{S}(t)\big)|0\rangle. \tag{7.30}$$

The $\mathbf{x}$-space representation of this is easily worked out, by using Eqs. (6.30) and (3.16), and we find

$$\begin{aligned}\langle \mathbf{x}|\psi(t)\rangle = {} & \frac{1}{(\pi\hbar)^{N/4}} \frac{1}{\sqrt{\det(\mathbf{A}+i\mathbf{B})}} \\ & \times \exp\left\{ \frac{1}{\hbar}\left[i\gamma + i\tilde{\mathbf{p}}\cdot\mathbf{x} - \frac{i}{2}\tilde{\mathbf{p}}\cdot\mathbf{q} \right.\right. \\ & \left.\left. - \frac{1}{2}(\tilde{\mathbf{x}}-\tilde{\mathbf{q}})\cdot(\mathbf{D}-i\mathbf{C})(\mathbf{A}+i\mathbf{B})^{-1}\cdot(\mathbf{x}-\mathbf{q}) \right] \right\}. \end{aligned} \tag{7.31}$$

If one does not want to use the standard fiducial coherent state $|0\rangle$, then it can be replaced by $M(\mathbf{S}_0)|0\rangle$, where $\mathbf{S}_0$ is some fixed symplectic matrix. This form encompasses all possible Gaussian wave packets as initial conditions, as shown in Sec. 8. Then Eq. (7.30) is still valid, with $\mathbf{S}(t)$ replaced by the product $\mathbf{S}(t)\mathbf{S}_0$. In other words, one only needs to multiply symplectic matrices.

7.3. A Semiclassical Propagator for Arbitrary Initial Conditions

Of course, wave packets do not constitute the most general initial conditions that one might be interested in. However, an arbitrary initial condition $|\psi_0\rangle$ can be represented as a linear combination of wave packets, and these can be propagated individually. From an analytical standpoint, it is most convenient to use the coherent states for this purpose (Klauder and Sudarshan [1968]). Let us therefore decompose $|\psi_0\rangle$ into coherent states, by using the coherent state wave function, as in Appendix C. For the initial state, we can write a modified form of Eq. (C.12),

$$|\psi_0\rangle = \int \frac{d^{2N}\mathbf{z}_0}{(2\pi\hbar)^N}\, T(\mathbf{z}_0)|0\rangle\langle\mathbf{z}_0|\psi_0\rangle. \tag{7.32}$$

Applying the propagator (7.27) to each wave packet individually then gives us a semiclassical propagator, applicable to any initial wave function,

$$U(t) = \int \frac{d^{2N}\mathbf{z}_0}{(2\pi\hbar)^N}\, e^{i\gamma(t)/\hbar}\, T\big(\mathbf{z}(t)\big) M\big(\mathbf{S}(t)\big)|0\rangle\langle\mathbf{z}_0|. \tag{7.33}$$

Of course, this propagator is subject to the same limitations on time interval as was Eq. (7.27). This propagator is not directly useful in numerical work, because it requires an infinite number of orbits. But it does have analytical promise, which mostly seems to be as yet unrealized.

Nevertheless, certain aspects of this propagator are problematical. For example, it does not form a group, i.e. $U(t_2 + t_1) \neq U(t_2)U(t_1)$. There is a certain amount of arbitrariness to the manner in which an initial wave function is decomposed into wavepackets. We have chosen the standard coherent states for convenience, but many other choices could be made. For any reasonable choice for this decomposition, some error will be introduced as the wave packets are propagated, due to the approximations inherent in Eq. (7.27). This error hopefully will be small, but it will differ from one choice of initial wave packets to another. However, when we apply, say $U(t_1)$ to an initial wave function, the final state

is not represented as a linear combination of the same class of wave packets as the initial state, due to wave packet spreading. Therefore if we follow $U(t_1)$ by $U(t_2)$, the effect at time t_1 is to stop, add up all the final wave packets created by $U(t_1)$, which by now have spread, and express the sum again in terms of the given initial set. In a sense, therefore, $U(t)$ creates a privileged role for the time $t = 0$. In fact, since wave packet spreading generally degrades the accuracy of Eq. (7.27), we can see that the product $U(t_2)U(t_1)$ will be more accurate than $U(t_2+t_1)$. Therefore this failure of $U(t)$ to form a group is another manifestation of the time limitation imposed on the wave packet propagator (7.27), and one can see that for short times, the group composition law is approximately obeyed, the approximation being of the same order as that inherent in Eq. (7.27). It is an interesting question as to whether any semiclassical propagator can form a group. Of course, one does not ask this question out of love for group theory, but rather because any privileged role for the time $t = 0$ is unphysical. In any case, it is not clear that this question has ever been addressed.

A slight consolation in this is the fact that the classical analog of Eq. (7.32) would suffer from the same problem. If an initial distribution function $f_0(\mathbf{z})$ were decomposed into small packets at $t = 0$, and each of these packets were propagated forward by Eq. (7.6), then the classical packets would also spread, and again a privileged role would be created for the time $t = 0$. The only exception would be if the classical packets were so small that they became δ-functions, in which case the classical propagator would be exact. Of course, we have no such option in the quantum case.

A worse problem for Eq. (7.32) is that $U(t)$ is not unitary. A unitary operator preserves scalar products, and our propagator (7.33) does not do this. The overcompleteness of the coherent states is an inessential obstacle in seeing this, so let us simply consider two initial coherent states, $|\mathbf{z}_0\rangle$ and $|\mathbf{z}'_0\rangle$, both of which are to be propagated by Eq. (7.27). Then at a later time we have

$$\langle \mathbf{z}_0|U(t,\mathbf{z}_0)^\dagger U(t,\mathbf{z}_0')|\mathbf{z}_0'\rangle = e^{i[\gamma'(t)-\gamma(t)]/\hbar}\,\langle 0|M(\mathbf{S})^\dagger T(\mathbf{z})^\dagger T(\mathbf{z}')M(\mathbf{S}')|0\rangle. \tag{7.34}$$

In general, this is not equal to $\langle \mathbf{z}_0|\mathbf{z}_0'\rangle$, although it is possible to see that for limited times it is approximately equal to it.

Suppose first of all that $\mathbf{z}_0$ and $\mathbf{z}_0'$ are close together, and that $\mathbf{z}(t)$, $\mathbf{z}'(t)$ remain close together over the time interval of interest, so that $\delta\mathbf{z}_0 = \mathbf{z}_0' - \mathbf{z}_0$ and $\delta\mathbf{z}(t) = \mathbf{z}'(t) - \mathbf{z}(t)$ are small. Then we can assume that $\mathbf{S} \approx \mathbf{S}'$, so that $\delta\mathbf{z}(t) = \mathbf{S}\delta\mathbf{z}_0$. Using this and Eq. (6.18), we can write the matrix element on the right in the form

$$e^{-\frac{i}{2\hbar}\omega(\mathbf{z},\delta\mathbf{z})}\,\langle 0|T(\delta\mathbf{z}_0)|0\rangle. \tag{7.35}$$

On the other hand, if we carry out $\gamma'(t) - \gamma(t)$ to first order in $\delta\mathbf{z}$, and make use of the fact that

$$\int_0^t dt\,\omega(\dot{\mathbf{z}},\delta\mathbf{z}) = -\int_0^t dt\,\delta\mathbf{z}\cdot\frac{\partial H}{\partial \mathbf{z}} = -\delta E\,t, \tag{7.36}$$

where δE is the difference in energy between the two orbits, then we find

$$\gamma'(t) - \gamma(t) \approx \tfrac{1}{2}\omega(\mathbf{z},\delta\mathbf{z}) - \tfrac{1}{2}\omega(\mathbf{z}_0,\delta\mathbf{z}_0). \tag{7.37}$$

As a result, the right hand side of Eq. (7.34) becomes

$$e^{-\frac{i}{2\hbar}\omega(\mathbf{z}_0,\delta\mathbf{z}_0)}\,\langle 0|T(\delta\mathbf{z}_0)|0\rangle = \langle 0|T(\mathbf{z}_0)^\dagger T(\mathbf{z}_0')|0\rangle = \langle \mathbf{z}_0|\mathbf{z}_0'\rangle, \tag{7.38}$$

and the scalar product is preserved.

On the other hand, if $\mathbf{z}_0$ and $\mathbf{z}_0'$ are widely separated, then both the initial and final matrix elements are exponentially small in their respective separations (see Eq. (C.18)), so scalar products are again approximately conserved. Altogether, we conclude that $U(t)$ will be approximately unitary, as long as the nearby orbit approximation remains valid.

Perhaps these difficulties have to do with the impossibility of mapping groups of unitary operators onto classical groups of canonical transformations in a natural way. The exceptions to this rule include the Heisenberg and metaplectic groups, for which the

classical and quantum Lie algebras are identical, and in this sense it is not surprising that for quadratic Hamiltonians all the difficulties with Eq. (7.33) fall away, and $U(t)$ becomes the exact propagator. In effect, the Heisenberg and metaplectic operators are used in Eq. (7.33) to represent nonlinear canonical transformations locally in phase space, but the small pieces do not exactly "fit" together.

In this sense it is interesting that Eq. (7.33) represents a semiclassical version of a "nonlinear canonical transformation of operators," where the canonical transformation in question is that generated by the classical time evolution. In general, there is no unique way of making a correspondence between a classical canonical transformation and a quantum unitary operator. This is evidently true even in a semiclassical sense, due to the arbitrariness involved in the representation of the initial wave function as a linear combination of wave packets. Nevertheless, Eq. (7.33) is one candidate for such a correspondence.

Another candidate has been proposed by Miller [1974], and exploited by him with great success. Miller's semiclassical version of a canonical transformation of operators is based on the traditional eikonal approach to WKB theory, rather than wave packets, so its immediate relation to the propagators considered here is not immediately clear. It would be an interesting problem to explore this connection.

The next section is motivated by one of the issues raise here, namely the privileged role played by the standard coherent states in our formalism. Although it is widely recognized that there is no particular reason to use the standard fiducial state of Eq. (C.4), nevertheless the arbitrariness of this choice is especially driven home by the troubles it causes here, such as the failure of $U(t)$ to form a group. Therefore in the next section we shall examine Gaussian wave packets from a larger perspective than that of coherent states and the Heisenberg operators which are used to create them. Although our results will not solve any of the difficulties raised in this section, they do form an important analysis of Gaussian

wave packets in general, which should be of value in any application of Gaussians in practical problems.

8. Gaussian Wave Packets

As I pointed out in Sec. 4, the metaplectic operators constitute the natural transformation group of the Gaussian wave packets. In this section I shall explore these transformation properties in detail. I begin by considering the Wigner functions of Gaussians, which give us an interesting interpretation of Gaussian wave packets in phase space, and show that there is no invariant meaning to the concept of minimum uncertainty. I also show that these Wigner functions are invariant under $U(N)$ transformations, and I discuss some questions relating to pure and mixed states. Next I examine the transformation properties of the Gaussian wave packets themselves, and show that they are invariant under $SU(N)$ transformations. Finally, I raise some questions about the nonuniqueness of the standard coherent states, and make a few observations.

8.1. The Wigner Function of Gaussians

Let us begin by assembling some facts about Gaussians, derived in a straightforward manner in the **x**-representation. We shall consider only Gaussians which satisfy $\langle \hat{\mathbf{z}} \rangle = 0$, since any Gaussian which does not satisfy this condition is easily transformed into one which does, by the trivial operation of applying a Heisenberg operator. We shall also consider only normalized Gaussians. The most general Gaussian of this kind has the form

$$\psi(\mathbf{x}) = \left(\frac{\det \mathbf{a}}{(\pi\hbar)^N}\right)^{\frac{1}{4}} \exp\left[-i\gamma - \frac{1}{2\hbar}\,\tilde{\mathbf{x}}\cdot(\mathbf{a}+i\mathbf{b})\cdot\mathbf{x}\right], \tag{8.1}$$

where γ is a phase and the $N\times N$ matrices **a**, **b** are real and symmetric. The matrix **a** is also positive definite, so that ψ is normalizable.

The topology of the space of positive definite symmetric matrices is the same as that of the symmetric matrices, since one space is converted into the other by the invertible operations of taking the exponential or logarithm. Therefore, since both **a** and

$\mathbf{b}$ have $N(N+1)/2$ independent parameters, the space of Gaussians has the topology $\mathbb{R}^{N(N+1)} \times S^1$, where the circle S^1 represents the phase γ.

It is straightforward to calculate the Wigner function $W(\mathbf{z})$ of the Gaussian (8.1), by using Eq. (B.6). The result can be written

$$W(\mathbf{z}) = 2^N \exp\Big(-\frac{1}{\hbar}\tilde{\mathbf{z}} \cdot \mathbf{G} \cdot \mathbf{z}\Big), \tag{8.2}$$

where the $2N \times 2N$ matrix $\mathbf{G}$ is given by

$$\mathbf{G} = \begin{pmatrix} \mathbf{a} + \mathbf{b}\mathbf{a}^{-1}\mathbf{b} & \mathbf{b}\mathbf{a}^{-1} \\ \mathbf{a}^{-1}\mathbf{b} & \mathbf{a}^{-1} \end{pmatrix}. \tag{8.3}$$

Although in general the Wigner function of a state may take on negative values, we see that for Gaussians it is strictly positive. The matrix $\mathbf{G}$ is real and symmetric, and, not surprisingly, positive definite. This follows by noting that

$$\tilde{\mathbf{z}} \cdot \mathbf{G} \cdot \mathbf{z} = \tilde{\mathbf{q}} \cdot \mathbf{a} \cdot \mathbf{q} + (\tilde{\mathbf{q}}\mathbf{b} + \tilde{\mathbf{p}}) \cdot \mathbf{a}^{-1} \cdot (\mathbf{b}\mathbf{q} + \mathbf{p}) \geq 0, \tag{8.4}$$

with equality only if $\mathbf{q} = \mathbf{p} = 0$.

What is perhaps more surprising is that $\mathbf{S}$ is also symplectic (Bastiaans [1979b]). This is easily proved by directly showing that $\mathbf{GJG} = \mathbf{J}$. This means that $\mathbf{G}$ is a member of the $\mathbf{T}$-space of positive definite symmetric symplectic matrices discussed in Appendix A, and that it can be uniquely represented as the exponential of $\mathbf{JK}_s$ for some symmetric $\mathbf{K}_s$ in the s-subspace of the Lie algebra of $Sp(2N)$. This is the first sign of the intimate connection between Gaussians and the polar decomposition of the symplectic matrices.

Furthermore, it is easy to show that every positive definite symmetric symplectic matrix can be realized through the Wigner function of some Gaussian. To see this, we note that if $|\psi\rangle$ in Eq. (8.1) is taken to be the standard fiducial state $|0\rangle$ of Eq. (C.4), then $\mathbf{a} = \mathbf{I}$ and $\mathbf{b} = 0$, so that $\mathbf{G} = \mathbf{I}$, and the Wigner function of the standard fiducial state is

$$W_0(\mathbf{z}) = 2^N e^{-\mathbf{z} \cdot \mathbf{z}/\hbar}. \tag{8.5}$$

Next, we use Eq. (6.26) to show that the Wigner function of the state $M(\mathbf{S})|0\rangle$ is $W_0(\mathbf{S}^{-1}\mathbf{z})$, so that the $\mathbf{G}$ matrix corresponding to the Gaussian $M(\mathbf{S})|0\rangle$ is given by

$$\mathbf{G} = \tilde{\mathbf{S}}^{-1}\mathbf{S}^{-1}. \tag{8.6}$$

Thus, if we are given some positive definite symmetric symplectic matrix $\mathbf{G}$, we can always put it into this form by taking $\mathbf{S}^{-1} = \sqrt{\mathbf{G}}$, which is the unique positive definite square root of $\mathbf{G}$. This is also symplectic, as shown either by the polar decomposition, or by noting that if $\mathbf{G} = \exp(\mathbf{J}\mathbf{K}_s)$, then we can take $\mathbf{S} = \exp(-\frac{1}{2}\mathbf{J}\mathbf{K}_s)$. Therefore the space of the Wigner functions of Gaussians is identical to the space of the positive definite symmetric symplectic matrices, which has the topology $\mathbb{R}^{N(N+1)}$. Incidentally, we see that whereas every Gaussian wave function has a Gaussian Wigner function, the converse is not true; many Gaussian distribution functions are not the Wigner functions of Gaussian wave packets.

Next we compute the correlation matrix $\mathbf{C}$, defined by Eq. (7.28), for Gaussians. Although it is straightforward to do this directly in the $\mathbf{x}$-representation, it is easier to do it through the Wigner function. First we note that the Weyl symbol of the operator $(\hat{z}_\alpha\hat{z}_\beta + \hat{z}_\beta\hat{z}_\alpha)/2$ is simply $z_\alpha z_\beta$. Equation (B.19) then shows us that

$$C_{\alpha\beta} = 2^N \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N}\, z_\alpha z_\beta\, e^{-\mathbf{z}\cdot\mathbf{G}\cdot\mathbf{z}/\hbar}. \tag{8.7}$$

Using the fact that $\mathbf{G}$ can be written in the form (8.6), and also that $\det\mathbf{S} = 1$, we make the substitution $\mathbf{z} = \mathbf{S}\mathbf{z}'$ to obtain

$$C_{\alpha\beta} = S_{\alpha\mu}S_{\beta\nu}\int \frac{d^{2N}\mathbf{z}'}{(\pi\hbar)^N}\, z'_\mu z'_\nu\, e^{-\mathbf{z}'\cdot\mathbf{z}'/\hbar} = \frac{\hbar}{2}S_{\alpha\mu}S_{\beta\mu}, \tag{8.8}$$

or, by noting that $\mathbf{G}^{-1} = \mathbf{S}\tilde{\mathbf{S}}$,

$$\mathbf{C} = \frac{\hbar}{2}\mathbf{G}^{-1}. \tag{8.9}$$

Therefore, by using Eq. (A.11), we have

$$\mathbf{C} = \frac{\hbar}{2}\begin{pmatrix} \mathbf{a}^{-1} & -\mathbf{a}^{-1}\mathbf{b} \\ -\mathbf{b}\mathbf{a}^{-1} & \mathbf{a} + \mathbf{b}\mathbf{a}^{-1}\mathbf{b} \end{pmatrix}. \tag{8.10}$$

A similar calculation has been presented by Bastiaans [1979b].

This matrix contains in its diagonal elements all the variances Δq_i^2, Δp_i^2. If we define a minimum uncertainty wave packet as one which satisfies $\Delta q_i \Delta p_i = \hbar/2$, for $i = 1, \ldots, N$, then the usual analysis of the minimum uncertainty condition shows that $\mathbf{a}$ is diagonal and $\mathbf{b} = 0$. Therefore minimum uncertainty wave packets are characterized by $\mathbf{G}$ and $\mathbf{C}$ matrices which are diagonal.

These results can be seen pictorially in phase space. By Eq. (8.2), the contour surfaces of the Wigner function in phase space are the same as those of the positive definite quadratic form $\tilde{\mathbf{z}} \cdot \mathbf{G} \cdot \mathbf{z}$, which are ellipsoids. We pick out one of these for convenience, the ellipsoid $\tilde{\mathbf{z}} \cdot \mathbf{G} \cdot \mathbf{z} = 2\pi\hbar$, and call it the "Wigner ellipsoid." It is indicated schematically in Fig. 15. The volume enclosed by the Wigner ellipsoid is of the order of a unit cell in phase space, i.e. $(2\pi\hbar)^N$, and it indicates the principal region of concentration of the Wigner function.

The principal axes of the Wigner ellipsoid indicate the directions in phase space along which the rate of decrease of the Wigner function is stationary with respect to small variations in direction. The rate of decrease itself is measured with respect to the distance $s^2 = \tilde{\mathbf{z}} \cdot \mathbf{z}$. Since this distance is not invariant under symplectic transformations, neither are the principal axes, but they are interesting to consider nonetheless.

We denote the eigenvectors of $\mathbf{G}$ by $\mathbf{e}_\alpha$, where α is not a component index, but rather distinguishes the eigenvectors, and we let the corresponding eigenvalues be λ_α, so that

$$\mathbf{G}\mathbf{e}_\alpha = \lambda_\alpha \mathbf{e}_\alpha \tag{8.11}$$

(no sum on α). Since $\mathbf{G}$ is symmetric and positive definite, the eigenvectors $\mathbf{e}_\alpha$ are real and can be chosen to form an orthogonal set, and the eigenvalues are real and positive. As shown in Appendix A, if λ is an eigenvalue of $\mathbf{G}$, then so is $1/\lambda$, and in fact the eigenvalues can be arranged in $(\lambda, 1/\lambda)$ pairs. One can show that these pairs can be made

to correspond to the q-p axes of a canonical coordinate system. This is easiest when the eigenvalues are distinct, but it can be proven in any case. If we normalize the eigenvectors so that their tips lie on the Wigner ellipsoid, i.e. so that $\mathbf{e}_\alpha \cdot \mathbf{e}_\alpha = 2\pi\hbar/\lambda_\alpha$, then the total volume spanned by the eigenvectors is $(2\pi\hbar)^N$.

If the Gaussian from which $\mathbf{G}$ was derived is minimum uncertainty, then the principal axes of the Wigner ellipsoid can be chosen to be parallel to the q-p coordinate axes, and conversely. If the Gaussian is not minimum uncertainty, then the products $\Delta q_i \Delta p_i$ are greater than $\hbar/2$ because of the angles of the projections of the Wigner ellipsoid onto the coordinate axes. In a sense, therefore, Gaussians which are not minimum uncertainty appear so only because they are viewed from the wrong symplectic frame; in the right frame, every Gaussian is minimum uncertainty. This fact is also suggested by the rules of statistical mechanics, which assign quantum states a phase space volume of $(2\pi\hbar)^N$, whether or not they are minimum uncertainty in the usual sense. This is another reason not to assign any privileged role to the standard coherent states.

However, one must be careful in the use of the Wigner ellipsoid, because its principal axes are not symplectic invariants. That is, suppose a Gaussian $|\psi\rangle$ has a Wigner function specified by the matrix $\mathbf{G}$, with eigenvectors $\mathbf{e}_\alpha$. Then if we replace $|\psi\rangle$ by $M(\mathbf{S})|\psi\rangle$, $\mathbf{G}$ is replaced by $\tilde{\mathbf{S}}^{-1}\mathbf{G}\mathbf{S}^{-1}$, but the new eigenvectors are *not* given by $\mathbf{S}\mathbf{e}_\alpha$. This is clear because the eigenvectors always form an orthogonal set, and symplectic matrices do not respect orthogonality relations. In general, the relation between the old and new eigenvectors is not simple.

In particular, this means that we cannot align the Wigner ellipsoid along some Lagrangian manifold, and expect the alignment to persist in the course of time. The orientation of the tangent plane to the Lagrangian manifold is correctly described by the symplectic matrix which represents the linearized flow along some orbit, but the eigenvectors of the Wigner ellipsoid are not.

Furthermore, there is no simple relation between the eigenvectors of the Wigner ellipsoid and those of the symplectic matrix describing the linearized flow. The eigenvectors of the latter need not even be real, nor do they necessarily form a complete set. They are useful, however, in describing the exponential instability of chaotic systems; presumably in the course of time for such a system, the Wigner ellipsoid gets stretched out along the unstable manifold (Arnold and Avez [1968]). These questions have apparently not been investigated deeply.

Because the Wigner function is bilinear in the state $|\psi\rangle$, it transforms according to the group $Sp(2N)$, not $Mp(2N)$, as shown explicitly by Eq. (6.26). Furthermore, the Wigner function of any Gaussian can be derived from that of the standard Gaussian, as we showed in Eqs. (8.5) and (8.6). Therefore Wigner functions of Gaussians can be parameterized by symplectic matrices. However, this parameterization is not unique; more than one symplectic matrix will yield the same final Wigner function, or, to say the same thing, there is a family of symplectic matrices which will leave the Wigner function invariant.

The family in question depends on the Wigner function under consideration; it consists of the symplectic matrices $\mathbf{S}$ such that $\tilde{\mathbf{S}}^{-1}\mathbf{G}_0\mathbf{S}^{-1} = \mathbf{G}_0$, where the positive definite symmetric symplectic matrix $\mathbf{G}_0$ represents the chosen Wigner function. This family forms a group, which is a subgroup of $Sp(2N)$, and it is the isotropy or stationary subgroup of the chosen Wigner function. It is easiest to see what this subgroup is when we let the Wigner function be the standard one of Eq. (8.5), since in that case we have $\mathbf{G}_0 = \mathbf{I}$. Then the invariance condition becomes $\tilde{\mathbf{S}}^{-1}\mathbf{S}^{-1} = \mathbf{I}$, which shows that $\mathbf{S}$ must be orthogonal. Therefore the isotropy subgroup of the standard Wigner function is the intersection $Sp(2N) \cap O(2N)$, which, as shown in Appendix A, is isomorphic to the group $U(N)$. For any other Wigner function, specified by $\mathbf{G}_0$, the isotropy subgroup is the conjugate subgroup of $U(N)$ under the action of $\sqrt{\mathbf{G}_0}$. Therefore the Wigner functions are parameterized uniquely by the coset spaces with respect to $U(N)$, or,

$$\text{Space of Wigner functions of Gaussians} \sim \frac{Sp(2N)}{U(N)}. \tag{8.12}$$

This space is not a group, because $U(N)$ is not an invariant subgroup of $Sp(2N)$. This again is related to the fact that there is no privileged role for the standard fiducial state, insofar as canonical transformations in phase space are concerned.

Because the matrix **G** does not contain the full information which is in the symplectic matrix **S** describing the evolution of nearby orbits, there is considerable redundancy in the matrix **S** when it is used to advance the Wigner function of Gaussian wave packets according to Eq. (7.29). In fact, we see that out of $N(2N+1)$ independent parameters which are necessary to specify **S**, only $N(N+1)$ of them, or approximately half, are actually used in the time evolution. At first sight this seems to suggest an opportunity for making the numerical integration of Eq. (2.15) more efficient, by keeping only the subset of variables which are actually needed. However, this is probably not practical, since Eq. (2.15) is linear, and the $2N$ columns of **S** decouple from one another, and evolve independently. It is probably not worth it to replace Eq. (2.15) by a coupled, nonlinear system, even if the total number of variables is reduced.

Nevertheless, there is theoretical interest in the redundancy indicated by Eq. (8.12), because it says that the time evolution of a Gaussian wave packet requires less information than would be required for the analogous classical problem of nearby orbits. Evidently, this is related to the fact that the matrix **G** must be symplectic. It might be reasonable to consider classical distributions which are Gaussian in phase space, as we did in Sec. 2, but there would be no reason in classical mechanics to demand that the quadratic form in the exponent be symplectic. However, since Wigner functions are capable of representing both pure and mixed states, one might suspect that the privileged role for symplectic quadratic forms has to do with this distinction.

Let us therefore consider a distribution function of the form

$$f(\mathbf{z}) = 2^N \sqrt{\det \mathbf{F}}\, \exp\Big(-\frac{1}{\hbar}\tilde{\mathbf{z}} \cdot \mathbf{F} \cdot \mathbf{z}\Big), \tag{8.13}$$

where we make no assumptions about $\mathbf{F}$ except that it be positive definite and symmetric. There is no guarantee that this distribution function can be realized as a Wigner function at all, either for a pure or a mixed state. Because f is real, it does correspond to some Hermitian operator ρ, but ρ must be positive semidefinite and satisfy $\mathrm{Tr}\,\rho = 1$ if it is to be interpreted as a density operator. It is easy to show that $\mathrm{Tr}\,\rho = 1$, because of the normalization we imposed on $f(\mathbf{z})$. But it is more difficult to see whether ρ is positive semidefinite.

Therefore we shall pose a more refined question, which is easier to answer. We shall ask what conditions must be imposed on $\mathbf{F}$ so that $f(\mathbf{z})$ will represent the Wigner function of a pure state. In this case, we need not directly prove positive semidefiniteness, because the density operator for a pure state is a projection operator, and satisfies $\rho^2 = \rho$.

It seems easiest to examine this condition through the alternative Weyl symbol of Eq. (B.2). Using Eq. (B.4), we find

$$\tilde{f}(\mathbf{z}) = \exp\Big(\frac{1}{4\hbar}\tilde{\mathbf{z}} \cdot \mathbf{J}\mathbf{F}^{-1}\mathbf{J} \cdot \mathbf{z}\Big). \tag{8.14}$$

Next, we use the Weyl product rule in the form (B.8) to compute the alternative Weyl symbol of ρ^2, which we denote by $\tilde{f}^2(\mathbf{z})$. We find

$$\tilde{f}^2(\mathbf{z}) = \sqrt{\det \mathbf{F}}\, \exp\Big[\frac{1}{8\hbar}\tilde{\mathbf{z}} \cdot (\mathbf{J}\mathbf{F}^{-1}\mathbf{J} - \mathbf{F}) \cdot \mathbf{z}\Big]. \tag{8.15}$$

Therefore $\tilde{f}^2(\mathbf{z}) = \tilde{f}(\mathbf{z})$, i.e. $\rho^2 = \rho$, if and only if $\mathbf{F}\mathbf{J}\mathbf{F} = \mathbf{J}$, which shows that $\mathbf{F}$ is symplectic. Therefore the distribution function (8.13) represents a pure state if and only if $\mathbf{F}$ is symplectic. In particular, the distribution function of Eq. (2.21) represents a pure state if and only if $LK = \hbar/2$.

Equation (8.13) can also represent mixed states. One example is the Wigner function of a harmonic oscillator in thermal equilibrium with a heat bath. However, not every

distribution function of the form (8.13) represents a Wigner function. One example is the case $\mathbf{F} = c\mathbf{I}$, where $c > 1$ is a constant. I do not know in general what condition $\mathbf{F}$ must satisfy in order that the operator corresponding to $f(\mathbf{z})$ should be positive semidefinite.

While we are on the subject of redundant information, I shall point out some interesting facts about Eq. (2.15), the evolution equation for $\mathbf{S}$. This is a matrix equation, nominally in $4N^2$ variables, although there are only $N(2N+1)$ independent components in $\mathbf{S}$. The redundancy is due to the Poincaré invariants, which are constants of the motion of Eq. (2.15). Since there are $N(2N-1)$ independent Poincaré invariants, and since $N(2N-1) + N(2N+1) = 4N^2$, the total parameter count comes out right. What is more interesting is that Eq. (2.15) is a Hamiltonian system in its own right, whose phase space is the $4N^2$-dimensional space of all $2N \times 2N$ matrices. The Poincaré invariants are generators of a symmetry group in this space, which turns out to be $O(2N)$. Therefore out of the remaining $N(2N+1)$ independent parameters in $\mathbf{S}$, some can be evaluated by quadratures. This system is a prime candidate for the theory of "reduction" (Abraham and Marsden [1978]), and I shall report on it in more detail in the future.

8.2. Transformation Properties of Gaussians Under $Mp(2N)$

We turn now from Wigner functions to Gaussian wave packets themselves, and consider their transformation properties under the metaplectic operators. First we ask whether any Gaussian wave packet can be realized from any other through the action of a metaplectic operator. If so, then any Gaussian can be realized in the course of time in semiclassical wave packet evolution. To answer this question, it is sufficient to ask whether any Gaussian $|\psi\rangle$ can be reached from the standard Gaussian $|0\rangle$, i.e. whether we can write

$$|\psi\rangle = M(\mathbf{S}, \sigma)|0\rangle \tag{8.16}$$

for some metaplectic operator $M(\mathbf{S},\sigma)$. We shall take $|\psi\rangle$ to be given in the form (8.1), and we shall search for $M(\mathbf{S},\sigma)$, where σ is defined by Eq. (6.30) or (6.32).

Certainly, if Eq. (8.16) is to be satisfied, then the Wigner functions of the two sides must be equal. But we have just shown that there always exist symplectic matrices which cause the Wigner functions to be equal; they all have the form

$$\mathbf{S} = \frac{1}{\sqrt{\mathbf{G}}}\mathbf{R}, \tag{8.17}$$

where $\mathbf{G}$ is the positive definite symmetric symplectic matrix appearing in the Wigner function of $|\psi\rangle$, as shown explicitly by Eq. (8.3), and $\mathbf{R}$ is an element of the $U(N)$ subgroup of $Sp(2N)$, as shown by Eq. (A.23).

However, there is an alternative form of Eq. (8.17) which is more useful and equally valid. Instead of factoring $\mathbf{G}$ by its square root, we write $\mathbf{G} = \tilde{\mathbf{S}}_0^{-1}\mathbf{S}_0^{-1}$, where

$$\mathbf{S}_0 = \begin{pmatrix} \mathbf{c}^{-1} & 0 \\ -\mathbf{b}\mathbf{c}^{-1} & \mathbf{c} \end{pmatrix}, \tag{8.18}$$

in which $\mathbf{c} = \sqrt{\mathbf{a}}$, i.e. the positive definite square root of $\mathbf{a}$. One can easily show that $\mathbf{S}_0$ is symplectic. Therefore every $\mathbf{S}$ which makes the Wigner functions of the two sides of Eq. (8.16) agree has the form $\mathbf{S} = \mathbf{S}_0\mathbf{R}$, or

$$\mathbf{S} = \begin{pmatrix} \mathbf{c}^{-1}\mathbf{X} & \mathbf{c}^{-1}\mathbf{Y} \\ -\mathbf{b}\mathbf{c}^{-1}\mathbf{X} - \mathbf{c}\mathbf{Y} & -\mathbf{b}\mathbf{c}^{-1}\mathbf{Y} + \mathbf{c}\mathbf{X} \end{pmatrix}, \tag{8.19}$$

where $\mathbf{U} = \mathbf{X} + i\mathbf{Y}$ is unitary.

On the other hand, equality of Wigner functions does not imply equality of wave functions, because the overall phase is lost on going to the Wigner function. Therefore we must make the phases of the two sides of Eq. (8.16) agree in order to solve for $M(\mathbf{S},\sigma)$. As it turns out, this will place further restrictions of $\mathbf{S}$ and uniquely determine σ. (Incidentally, a more obvious approach to the transformation of Gaussians would be to transform annihilation operators, since every Gaussian has an annihilation operator, and these transform

under metaplectic conjugation according to Eq. (4.3). But this approach would give us no information about the phases.)

Therefore we use Eqs. (8.1) and (6.30) to equate phases, and we have

$$\gamma = n\pi + \tfrac{1}{2} \arg\det(\mathbf{A} + i\mathbf{B}), \tag{8.20}$$

where $n = 0$ if $\sigma = +1$, and $n = 1$ if $\sigma = -1$. The matrices $\mathbf{A}$ and $\mathbf{B}$ must be restricted to the form shown in Eq. (8.19) to make the Wigner functions agree, so we have

$$\arg\det(\mathbf{A} + i\mathbf{B}) = \arg\det(\mathbf{X} + i\mathbf{Y}) = \arg\det\mathbf{U}, \tag{8.21}$$

since $\mathbf{c}$ is positive definite. On the other hand, as indicated in Appendix A, every unitary $\mathbf{U}$ can be uniquely written in the form $\mathbf{U} = \mathbf{U}_s\mathbf{U}_0 = \mathbf{U}_0\mathbf{U}_s$, where $\mathbf{U}_s$ is a member of $SU(N)$ and $\mathbf{U}_0 = e^{i\alpha/N}\mathbf{I}$, where $0 \le \alpha < 2\pi$. Thus, we have $\det\mathbf{U} = \det\mathbf{U}_0 = e^{i\alpha}$, and the angle α and the integer n are uniquely determined by the following rules: If $0 \le \gamma < \pi$, then $n = 0$ and $\alpha = 2\gamma$; if $\pi \le \gamma < 2\pi$, then $n = 1$ and $\alpha = 2(\gamma - \pi)$.

Altogether, we see that there always exists a metaplectic operator $M(\mathbf{S}, \sigma)$ which will satisfy Eq. (8.16), and that it is not unique. The sign σ is uniquely determined, but $\mathbf{S}$ is not, since it must have the form $\mathbf{S} = \mathbf{S}_0\mathbf{R}_0\mathbf{R}_s$, where $\mathbf{S}_0$ is given by Eq. (8.18), where $\mathbf{R}_0$ is given by Eq. (A.30) with $\beta = \alpha/N$, and where $\mathbf{R}_s$ has the form (A.23), where $\mathbf{X} + i\mathbf{Y}$ is an arbitrary member of $SU(N)$.

As in the case of the Wigner functions, there is a family of metaplectic operators which will leave any given Gaussian invariant, and this family forms a group. This group is a subgroup of $Mp(2N)$, and it is the isotropy subgroup of the given Gaussian. Again, it is easiest to see what this subgroup is when the given Gaussian is the fiducial state $|0\rangle$ itself; in that case, $\mathbf{S}_0 = \mathbf{I}$ and $\alpha = 0$, so $\mathbf{R}_0 = \mathbf{I}$ also. Therefore all metaplectic operators which leave the fiducial state invariant have the form $M(\mathbf{R}_s, +1)$, where $\mathbf{R}_s$ is a member of the symplectic representation of $SU(N)$. These operators, naturally, form a representation of

$SU(N)$ within the metaplectic group, and therefore the isotropy subgroup of the standard fuducial Gaussian is simply $SU(N)$. More generally, the isotropy subgroup of an arbitrary Gaussian is the conjugate subgroup of $SU(N)$ under the action of $\mathbf{S}_0\mathbf{R}_0$. This shows that the Gaussian wave packets parameterize the coset spaces of $Mp(2N)$ with respect to $SU(N)$, or,

$$\text{Space of Gaussian wave packets} \sim \frac{Mp(2N)}{SU(N)}. \tag{8.22}$$

Again, as in the case of Wigner functions, the propagation of Gaussian wave packets requires less than the full information contained in the metaplectic operators, namely $N^2 + N + 1$ parameters instead of $N(2N + 1)$.

In the special case $N = 1$, the group $SU(1)$ is zero-dimensional and essentially vacuous. Furthermore, the matrices $\mathbf{a}$ and $\mathbf{b}$ reduce to scalars a, b, with $a > 0$. Therefore for $N = 1$, the solution $M(\mathbf{S}, \sigma)$ of Eq. (8.16) is unique, and the quantities a, b, γ uniquely parameterize the metaplectic operator, and form a coordinate system on the group manifold of $Mp(2)$.

8.3. Possible Generalizations of the Coherent States

The following comments are some observations and speculations on possible generalizations of the coherent states, which are motivated by the manifest nonuniqueness of the standard coherent states. We have seen this nonuniqueness in several ways, all of which ultimately come down to the fact that the standard coherent states have no invariant meaning in phase space, i.e. that they are not invariant under the action of metaplectic operators. This means, among other things, that the selection of the standard fiducial state depends on the coordinate system used in phase space; it is not invariant even under scaling operations. Furthermore, standard coherent states do not remain standard in the course of time, when they are advanced by the wave packet propagator of Sec. 7. This

fact brings about a privileged role for the time $t = 0$, which has no physical significance. Finally, the coherent states give rise to a metric on phase space, as shown in Eq. (C.10); this has no classical significance, and it is hard to understand why it should appear in a semiclassical theory.

From a purely mathematical standpoint, it would seem logical to generalize the completeness relation (C.2), which is essentially a Haar integral over the Heisenberg group, into some analogous integral over the inhomogeneous metaplectic group, $IMp(2N)$. However, it is not clear to me how this would work out, although it would presumably involve the irreducible representations of $IMp(2N)$. Nor is it clear what physical meaning the result would have, since it would include Gaussian wave packets with very long and thin Wigner ellipsoids.

Therefore I shall take a more limited approach here, and simply consider the generalization of the coherent states which results when the standard fiducial state $|0\rangle$ is replaced by $M(\mathbf{S}_0)|0\rangle$, for some fixed symplectic matrix $\mathbf{S}_0$. Many authors who have written about coherent states, apparently sensing their nonuniqueness, have introduced scale factors into the definition of the fiducial state, and left these scale factors as free parameters of the analysis. These scale factors represent simple point transformations, so what we are proposing here is a generalization of this approach, in that we are considering arbitrary linear canonical transformations, and allowing the entire symplectic matrix $\mathbf{S}_0$ to be a free parameter. Since, as we have shown, any Gaussian wave packet can be realized from the standard one by the action of some metaplectic operator, our use of $M(\mathbf{S}_0)|0\rangle$ as a fiducial state is equivalent to taking an arbitrary Gaussian for this state. Furthermore, apart from phase factors, we can expect $\mathbf{S}_0$ to appear in our results only through the combination $\mathbf{G}_0 = \tilde{\mathbf{S}}_0^{-1}\mathbf{S}_0^{-1}$.

However, at the same time, this approach is quite naive, since it does not solve any of the nonuniqueness issues mentioned above. Nor is it the best approach to take in

practical problems, where one often wants to represent a given wave function as a linear combination of Gaussians which are related to $|0\rangle$ by different matrices $\mathbf{S}_0$. (This question has been addressed in an interesting paper by Davis and Heller [1979]). Therefore I offer the following results mainly for their suggestive value, in the hopes that they will help clarify the larger picture.

Let us write $|0, \mathbf{S}_0\rangle = M(\mathbf{S}_0)|0\rangle$ for our nonstandard fiducial state, and let us define a complete set of coherent states by

$$|\mathbf{z}, \mathbf{S}_0\rangle = T(\mathbf{z})|0, \mathbf{S}_0\rangle = T(\mathbf{z})M(\mathbf{S}_0)|0\rangle. \tag{8.23}$$

These are complete in the same way as the standard coherent states, as explained in Appendix C.

We could now go through all the formulas we have for the standard coherent states, and generalize them to our nonstandard version, which would explicitly display the dependence on $\mathbf{S}_0$. In all cases, the calculations merely involve multiplications of symplectic matrices, due to the rules developed in Sec. 6. To take a complicated example, consider Bargmann's matrix element (6.36). If we generalize this, we have

$$\langle \mathbf{z}, \mathbf{S}_0|M(\mathbf{S})|\mathbf{z}', \mathbf{S}_0\rangle = \langle \mathbf{S}_0^{-1}\mathbf{z}|M(\mathbf{S}_0^{-1}\mathbf{S}\mathbf{S}_0)|\mathbf{S}_0^{-1}\mathbf{z}'\rangle, \tag{8.24}$$

by using Eq. (6.18), so that the generalized version can be expressed in terms of the standard version. It is not particularly illuminating to write this out explicitly, although one can show that it depends on $\mathbf{S}_0$ only through the combination $\mathbf{G}_0 = \tilde{\mathbf{S}}_0^{-1}\mathbf{S}_0^{-1}$.

To take another example, let us consider the generalized coherent state symbol of an operator, defined by

$$a_{cs}(\mathbf{z}, \mathbf{S}_0) = \langle \mathbf{z}, \mathbf{S}_0|A|\mathbf{z}, \mathbf{S}_0\rangle, \tag{8.25}$$

as in Eq. (C.15). In order to relate this to the standard coherent state symbol, we can first relate it to the ordinary Weyl symbol $a(\mathbf{z})$. We proceed exactly as in Eqs. (C.20)-(C.22).

Thus, we have

$$a_{cs}(\mathbf{z},\mathbf{S}_0) = \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N}\ \langle 0|M(\mathbf{S}_0)^\dagger T(\mathbf{z})^\dagger T(\mathbf{z}')T(\mathbf{z})M(\mathbf{S}_0)|0\rangle\ \tilde{a}(\mathbf{z}')$$

$$= \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N}\ \exp\Big[-\frac{i}{\hbar}\omega(\mathbf{z},\mathbf{z}') - \frac{1}{4\hbar}(\tilde{\mathbf{z}}'\cdot\mathbf{G}_0\cdot\mathbf{z}')\Big]\ \tilde{a}(\mathbf{z}')$$

$$= \int \frac{d^{2N}\mathbf{z}'}{(\pi\hbar)^N}\ \exp\Big(-\frac{1}{\hbar}\,\tilde{\mathbf{z}}'\cdot\mathbf{G}_0\cdot\mathbf{z}'\Big)\ a(\mathbf{z}+\mathbf{z}')$$

$$= \exp\Big[\frac{\hbar}{4}\Big(\frac{\partial}{\partial\mathbf{z}}\cdot\mathbf{G}_0^{-1}\cdot\frac{\partial}{\partial\mathbf{z}}\Big)\Big]\ a(\mathbf{z}), \tag{8.26}$$

where $\mathbf{G}_0^{-1} = \mathbf{S}_0\tilde{\mathbf{S}}_0$. This result can be combined with Eq. (C.22) to obtain a formula connecting $a_{cs}(\mathbf{z},\mathbf{S}_0)$ with the standard version, $a_{cs}(\mathbf{z})$.

What is interesting about this calculation is that it proceeds exactly as in the standard case, except that the standard coherent state metric, expressed through $2|\varsigma|^2 = \tilde{\mathbf{z}}\cdot\mathbf{z}$, is replaced by $\tilde{\mathbf{z}}\cdot\mathbf{G}_0\cdot\mathbf{z}$. In effect, the use of alternative coherent states has introduced an alternative metric. Although these alternative metrics have no more classical significance than the standard one, perhaps there is consolation in the fact that not just any metric is allowed, but rather only symplectic ones.

It is hoped that some of these observations will prove useful in gaining a deeper understanding of the semiclassical role of coherent states.

9. Conclusions

I shall conclude this paper by discussing some outstanding omissions and possible generalizations.

The first of these concerns the relationship between wave packet propagation and the more traditional approaches to WKB theory, including the Hamilton-Jacobi equation, the Maslov method, and EBK quantization. The general outlines of this relationship are clear; the Fourier transform in time of the propagator yields both the energy levels and the projection operators onto the subspaces spanned by the energy eigenstates. If the energy levels are nondegenerate, then these projection operators specify the energy eigenfunctions, to within an overall phase. In multidimensional integrable systems, the classical action variables are the symbols or approximate symbols of the complete set of commuting observables which occur in quantum mechanics. The symmetry operations generated by these observables can be treated semiclassically in the same way as the time propagator itself, and will lead to orbits in phase space which encircle the invariant torus. The metaplectic operators describing nearby orbits are an essential part of this picture, because they provide the Maslov index in the EBK quantization conditions.

There exist published accounts of the relationship between wave packet propagation and Hamilton-Jacobi theory, but I do not believe they are correct, because they fail to take into account the time dependence of the symplectic matrix $\mathbf{S}(t)$ which is responsible for wave packet spreading. This cannot be neglected, because it is this time dependence which provides the Maslov index in the quantization condition. On the other hand, the fact that $\mathbf{S}(t)$ is not usually periodic denies one of any simple picture of phase reinforcement in the time evolution of a single wave packet.

Instead, the way to extract the quantization conditions and the semiclassical energy eigenfunctions from a wave packet analysis, at least for integrable systems, is to propagate

the wave packet in the angle variables, by using the conjugate action variables as Hamiltonians. Unlike the time evolution, the angle evolution produces a symplectic matrix $\mathbf{S}(\theta)$ which is always periodic in θ, and which, therefore, corresponds to a definite Maslov index over a single period. These symplectic matrices are periodic because the action variables generate periodic orbits in phase space whose periods are independent of initial conditions. This means in particular that nearby orbits have the same period as the reference orbit. For example, one finds that the z-component of orbital angular momentum, L_z, gives a Maslov index of 0, whereas the magnitude of orbital angular momentum L gives a Maslov index of 2. (The observable L^2 is not an action, and does not possess a Maslov index.)

Since the action variables commute with the Hamiltonian, they and the Hamiltonian possess simultaneous eigenstates. Therefore propagating in the angle variables works as well as propagating in time for finding energy eigenstates. Indeed, the angle propagator works better, due to the periodicity of $\mathbf{S}(\theta)$. When the semiclassical propagator corresponding to one of the action variables is Fourier transformed in the conjugate angle, one obtains both the eigenvalues of the actions and the projection operators onto the subspaces spanned by the action eigenstates. This is just as with the energy, except that the integral in the Fourier transform need be taken only over a finite interval (one period). The action eigenvalues which emerge are the EBK values, $I_n = (n + \mu/4)\hbar$, where μ is the Maslov index corresponding to the action I. The projection operators select the subspaces corresponding to a single (necessarily one-dimensional) irreducible representation of the symmetry corresponding to the given action. A nondegenerate energy eigenstate results when the product of all these projection operators, one for each degree of freedom, is applied to a single initial wave packet.

Although the energy levels which emerge from this analysis are the same as in the EBK theory, the energy eigenfunctions are different. They are, of course, free from caustics, and they bear a close relation to the continuous representation eigenstates I have discussed

previously (Littlejohn [1985]). They are also closely related to the eigenstates which Heller has produced in some of his numerical work, and it is easy to see that they represent a kind of an average over the classical invariant torus.

More generally, other invariant manifolds besides the invariant tori of integrable systems should be of interest. For example, there is considerable evidence to suggest the importance of periodic orbits in the quantization of nonintegrable systems (Gutzwiller [1971, 1973, 1977], Miller [1975], and Tabor [1983]). The calculations of McDonald [1979] and McDonald and Kaufman [1985] on the stadium problem show that certain high mode eigenstates of this nonintegrable system seem to be dominated by a single periodic orbit. Heller [1985] has also examined the stadium problem, and recognized a role for the periodic orbits in the "scarring" of wave functions. There must be a way of attaching a Maslov index to such periodic orbits and explaining their important role in quantization, but I do not know what it is.

A second neglected issue is that of spin, or more generally, multicomponent wave equations. These are, of course, very important in practice, whereas this paper has dealt exclusively with a scalar wave equation. Equations which are higher order than first in time also fall into this category, since they can be represented as first order equations on multicomponent wave fields. Multicomponent wave equations have been neglected here because the emphasis of this paper is on transformation and invariance properties, and it is not clear what invariance properties one should expect for multicomponent objects in a phase space picture. It does seem clear, however, on the basis of traditional WKB theory and other considerations, that multicomponet wave equations will lead to $U(n)$ gauge fields on some kind of phase space, for some integer n. Some interesting results along this line have been obtained by Berry [1984, 1985], Simon [1983], Wilczek and Zee [1984], and Wilkinson [1984], but how these results couple with transformations on phase

space is not completely clear. Another interesting issue in multicomponent wave equations is mode conversion, which is a kind of tunneling.

Another interesting question is that of higher order corrections in the wave packet propagator. The classical side of this question has been well developed by Dragt and coworkers (Dragt [1982], Dragt and Forest [1983]), using a Lie-algebraic theory of nonlinear polynomial symplectic maps. The quantum side seems less well developed, although one proposal for dealing with higher order corrections has been made by Heller [1975], and there generally seems to be interest in this question. The development of a more accurate propagator for a single wave packet would be of use in optics, but perhaps less so in quantum mechanics, where there remain issues to be dealt with even at lowest order. For example, going to higher order will not eliminate the difficulties in the neighborhood of a separatrix, where the topology of the classical orbits changes and wave packets split.

Finally, let me raise the interesting question of symmetries and invariants, which, as mentioned in the introduction, is a primary motivation for using a phase space picture in the first place. It seems that the irreducible representations of a symmetry group in quantum mechanics are analogous to the coadjoint orbits (Abraham and Marsden [1978]) as they are used in classical mechanics (Weinstein [1979]), at least for Lie groups. Nevertheless, probably no one has taken a serious look at this to see how it could be of benefit in semiclassical calculations. It would not be hard to do this, but it would require a closer examination of symmetry groups and the practical matters of wave packet techniques than has been taken in this paper.

Acknowledgements

I am grateful for several useful conversations with Alex Dragt, Eric Heller, Allan Kaufman, Walter Kohn, Horia Metiu, Steve Omohundro, Bob Schrieffer, Philippe Similon, Alan Weinstein, and Eyvind Wichmann, from each of whom I received valuable information. I would especially like to thank Alan Weinstein for pointing out to me several references which I would otherwise not have known about, and also Yukkei Hui and Mary Silber for careful reading of the manuscript and the detection of several errors. I am also grateful to the Institute for Theoretical Physics of the University of California at Santa Barbara, which provided the support which made this work possible, and to the organizers of the workshop, "Stochasticity, Turbulence, and Long-Time Behavior in Plasmas," for inviting me to participate in this program and for their encouragement of this work.

This work was supported by the Department of Energy under contract No. DE-AC0376SF00098, and by the National Science Foundation under grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration.

Appendix A. Symplectic Matrices

In this appendix I outline some of the principal properties of the symplectic matrices, while attempting to keep the technical language to a minimum. A readable account of some of the matters covered here (and some others as well) has been given by Dragt [1982], and the use of symplectic matrices in optics has been discussed by Guillemin and Sternberg [1984]. More mathematical treatments may be found in Arnold [1978], Bargmann [1961], Guillemin and Sternberg [1977], Leray [1981], Weil [1963], and references therein.

Symplectic matrices are defined by Eqs. (2.5) and (2.9). A symplectic matrix $\mathbf{S}$ specifies a homogeneous linear canonical transformation, $\mathbf{z}' = \mathbf{S}\mathbf{z}$, or a linearized version of a nonlinear canonical transformation. Sometimes these represent a change of coordinates (the passive point of view), so that $\mathbf{z}$ and $\mathbf{z}'$ are the coordinates of the same point in two different coordinate systems; and sometimes they represent a linear mapping of phase space onto itself (the active point of view), so that $\mathbf{z}$ and $\mathbf{z}'$ are coordinates of distinct points in the same coordinate system. The latter case arises, for example, as the result of the time evolution of Hamiltonians which are quadratic in $\mathbf{z}$.

Since the matrix $\mathbf{J}$ of Eq. (2.5) is antisymmetric and orthogonal, we have $\mathbf{J}^{-1} = -\mathbf{J} = \tilde{\mathbf{J}}$. We also have $\det \mathbf{J} = 1$. Therefore by Eq. (2.9) it follows that $(\det \mathbf{S})^2 = 1$, so $\mathbf{S}^{-1}$ exists. It is then easy to prove that if $\mathbf{S}$, $\mathbf{S}_1$, $\mathbf{S}_2$ are symplectic, then so are $\tilde{\mathbf{S}}$, $\mathbf{S}^{-1}$, and $\mathbf{S}_1\mathbf{S}_2$. The $2N \times 2N$ identity matrix $\mathbf{I}$, as well as $\mathbf{J}$ itself, are also symplectic. Therefore the symplectic matrices form a group, denoted by $Sp(2N)$. Since $\mathbf{S}^{-1} = -\mathbf{J}\tilde{\mathbf{S}}\mathbf{J}$, it is easy to invert symplectic matrices (see Eq. (A.11) below).

An important fact is $\det \mathbf{S} = +1$ (never -1). It is easy to prove this using exterior algebra (Arnold [1978]); otherwise the proof involves manipulations of permutations (Hamermesh [1962]).

Let the secular equation of a symplectic matrix $\mathbf{S}$ be denoted by

$$\det(\mathbf{S} - \lambda\mathbf{I}) = \lambda^{2N} + a_1\lambda^{2N-1} + \ldots + a_{2N} = 0. \qquad (A.1)$$

All eigenvalues λ are nonzero, since $\det \mathbf{S} \neq 0$. Then one can show that

$$\lambda^{2N} \det(\mathbf{S} - \frac{1}{\lambda}\mathbf{I}) = \det(\mathbf{S} - \lambda\mathbf{I}). \qquad (A.2)$$

Therefore the secular equation has the symmetry $a_0 = a_{2N}$, $a_1 = a_{2N-1}$, etc., where $a_0 = 1$. This means that if λ is an eigenvalue with some multiplicity, then $1/\lambda$ is also an eigenvalue with the same multiplicity. Therefore all eigenvalues $\lambda \neq 1$ can be arranged in $(\lambda, 1/\lambda)$ pairs. Since the total number of eigenvalues is $2N$, the multiplicity of $\lambda = 1$ is even, and all eigenvalues, including $\lambda = 1$, can be arranged in $(\lambda, 1/\lambda)$ pairs.

It is often of interest to see when some feature of a problem is invariant under canonical transformations. We consider a linear canonical change of coordinates, $\mathbf{y} = \mathbf{S}_0 \cdot \mathbf{z}$ for fixed symplectic $\mathbf{S}_0$. Then a mapping $\mathbf{z}' = \mathbf{S} \cdot \mathbf{z}$ becomes, in the new coordinates, $\mathbf{y}' = \mathbf{S}_0\mathbf{S}\mathbf{S}_0^{-1} \cdot \mathbf{y}$. Therefore the conjugation relation, $\mathbf{S} \mapsto \mathbf{S}_0\mathbf{S}\mathbf{S}_0^{-1}$, represents a canonical change of coordinates. In this context, $\mathbf{S}$ represents an active transformation, and $\mathbf{S}_0$ a passive one.

The action differential $\mathbf{p} \cdot d\mathbf{q}$, is familiar in classical and semiclassical mechanics, but it is not invariant under canonical transformations, even linear ones. This fact is related to the appearance of caustics in traditional WKB theory. (It is, however, invariant under point transformations in configuration space). This form of the action differential tends to occur in calculations which are committed to a configuration space representation, as traditional WKB theory often is. In momentum space, the differential $-\mathbf{q} \cdot d\mathbf{p}$ occurs, and this is not invariant either. In this work a more useful quantity is the symmetrized action differential, $\frac{1}{2}(\mathbf{p} \cdot d\mathbf{q} - \mathbf{q} \cdot d\mathbf{p})$. To formalize this, we introduce the symplectic form ω, defined as follows. For any two vectors in phase space $\mathbf{z}_1 = (\mathbf{q}_1, \mathbf{p}_1)$, $\mathbf{z}_2 = (\mathbf{q}_2, \mathbf{p}_2)$, we

define

$$\omega(\mathbf{z}_1, \mathbf{z}_2) = \mathbf{p}_1 \cdot \mathbf{q}_2 - \mathbf{p}_2 \cdot \mathbf{q}_1. \tag{A.3}$$

We will sometimes write this as $\tilde{\mathbf{z}}_1 \cdot \omega \cdot \mathbf{z}_2$, where now ω represents the matrix

$$\omega = \begin{pmatrix} 0 & -\mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix}. \tag{A.4}$$

This matrix differs only by a sign from the matrix $\mathbf{J}$ of Eq. (2.5), and the use of two different symbols for the two matrices is, strictly speaking, not necessary, at least for the purposes of this paper. We do so anyway because ω and $\mathbf{J}$ have rather different meanings in an abstract sense ($\mathbf{J}$ is contravariant and ω is covariant), and because they tend to be used in rather different ways. The matrix ω corresponds to the Lagrange brackets of classical mechanics, just as $\mathbf{J}$ corresponds to the Poisson brackets (c.f. Eq. (2.6)). An important relation is $\omega = \mathbf{J}^{-1}$, or

$$\omega_{\alpha\beta} J_{\beta\mu} = \delta_{\alpha\mu}. \tag{A.5}$$

The matrix ω, like $\mathbf{J}$, is itself symplectic.

The symplectic form ω is invariant under linear canonical transformations, i.e.

$$\omega(\mathbf{S}\mathbf{z}_1, \mathbf{S}\mathbf{z}_2) = \omega(\mathbf{z}_1, \mathbf{z}_2), \tag{A.6}$$

for all vectors $\mathbf{z}_1$, $\mathbf{z}_2$ and all symplectic matrices $\mathbf{S}$. In particular, the symmetrized action differential,

$$\tfrac{1}{2}\omega(\mathbf{z}, \dot{\mathbf{z}}) = \tfrac{1}{2}(\mathbf{p} \cdot \dot{\mathbf{q}} - \mathbf{q} \cdot \dot{\mathbf{p}}) \tag{A.7}$$

is a symplectic invariant.

It is convenient to partition a $2N \times 2N$ symplectic matrix $\mathbf{S}$ into four $N \times N$ matrices,

$$\mathbf{S} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}. \tag{A.8}$$

The definition (2.8) is equivalent to either of the two sets of equations,

$$\mathbf{A}\tilde{\mathbf{D}} - \mathbf{B}\tilde{\mathbf{C}} = \mathbf{I},$$

$$\mathbf{A}\tilde{\mathbf{B}} = \mathbf{B}\tilde{\mathbf{A}},$$

$$\mathbf{C}\tilde{\mathbf{D}} = \mathbf{D}\tilde{\mathbf{C}}, \qquad (A.9)$$

or

$$\tilde{\mathbf{A}}\mathbf{D} - \tilde{\mathbf{C}}\mathbf{B} = \mathbf{I},$$

$$\tilde{\mathbf{A}}\mathbf{C} = \tilde{\mathbf{C}}\mathbf{A},$$

$$\tilde{\mathbf{B}}\mathbf{D} = \tilde{\mathbf{D}}\mathbf{B}, \qquad (A.10)$$

which imply one another. (One does not have to assume that $\mathbf{B}$ is nonsingular.) The matrices $\mathbf{A}\tilde{\mathbf{B}}$, $\mathbf{C}\tilde{\mathbf{D}}$, $\tilde{\mathbf{A}}\mathbf{C}$, $\tilde{\mathbf{B}}\mathbf{D}$ are symmetric. $\mathbf{S}^{-1}$ is given by

$$\mathbf{S}^{-1} = \begin{pmatrix} \tilde{\mathbf{D}} & -\tilde{\mathbf{B}} \\ -\tilde{\mathbf{C}} & \tilde{\mathbf{A}} \end{pmatrix}, \qquad (A.11)$$

which is often useful. Although $\det \mathbf{S} = 1$, any one of the submatrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ may be singular (indeed, they may vanish). In fact, any one of the submatrices can take on any value, although once this value is assigned, the remaining submatrices are constrained by the symplectic condition.

For $N = 1$, the only constraint imposed on a 2×2 matrix by the symplectic condition is that its determinant be +1, i.e. that it represent an area preserving map. (In higher dimensions there are further constraints.) We write a 2×2 symplectic matrix in the form

$$\mathbf{S} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad (A.12)$$

where $ad - bc = 1$. In the four-dimensional space specified by a, b, c, d, the constraint $ad - bc = 1$ produces a three-dimensional surface which is a kind of a hyperboloid of revolution. This can be seen by writing $a = x_1 + x_2$, $b = x_3 + x_4$, $c = x_3 - x_4$, $d = x_1 - x_2$, so that $x_1^2 - x_2^2 - x_3^2 + x_4^2 = 1$. This surface is a bit hard to picture, but the most important

facts are that it is connected, and that it has a "hole" in it. This surface is topologically equivalent to the solid interior of a torus, not including the surface, or of a slab with opposite faces identified (a periodic slab).

When a 2×2 symplectic matrix is parameterized by some parameter t, $\mathbf{S} = \mathbf{S}(t)$, we can picture a curve in the surface $ad - bc = 1$. If the curve is closed, it has a winding number, indicating how many times $\mathbf{S}(t)$ went around the "hole". This winding number is closely related to the Maslov index. There are several versions of the Maslov index; the one appearing in this context is especially interesting, because it is a symplectic invariant. This version of the Maslov index is twice the winding number of $\mathbf{S}(t)$.

Matrix functions $S(t)$ occurring in wave packet propagation are not usually periodic, and so do not give rise to closed curves in the space of symplectic matrices (the group manifold). Therefore, they do not have a winding number, nor a Maslov index in the sense defined here. Periodic matrix functions occur more commonly in Hamilton-Jacobi theory. In any case, the topological features revealed by considering closed curves are important for wave packet propagation.

The situation is not very much different in higher dimensions. The matrices constituting $Sp(2N)$ form an $N(2N+1)$-dimensional surface in the $4N^2$-dimensional space of all $2N \times 2N$ matrices. As in the case $N = 1$, this surface is connected and has one "hole" in it, and hence closed curves $\mathbf{S}(t)$ have a unique winding number (which is one half of the Maslov index). A more detailed and precise discussion of the topology of $Sp(2N)$ is given below.

Symplectic matrices arise classically in the solution of Hamilton's equations for Hamiltonians which are quadratic functions of $\mathbf{z}$. Let $h(\mathbf{z})$ be such a Hamiltonian, specified by a $2N \times 2N$ symmetric matrix $\mathbf{K}$:

$$h(\mathbf{z}) = \tfrac{1}{2}\tilde{\mathbf{z}} \cdot \mathbf{K} \cdot \mathbf{z}. \qquad (A.13)$$

Here we assume that $\mathbf{K}$ is time-independent. Then the solution to Hamilton's equations, Eq. (2.4), is given by $\mathbf{z}(t) = \mathbf{S}(t) \cdot \mathbf{z}_0$, where

$$\mathbf{S}(t) = \exp(t\mathbf{JK}). \tag{A.14}$$

This family of matrices $\mathbf{S}(t)$ forms a one-parameter subgroup of $Sp(2N)$, since $\mathbf{S}(t_1)\mathbf{S}(t_2) = \mathbf{S}(t_1 + t_2)$. Depending on the matrix $\mathbf{K}$, this family may be bounded or unbounded.

Not every symplectic matrix can be written in the form (A.14), but every symplectic matrix can be written as a product of such forms, for different $\mathbf{K}$'s. This follows from the fact that $Sp(2N)$ is connected. See Eq. (A.22).

An infinitesimal symplectic matrix has the form

$$\mathbf{S}(\epsilon) = \mathbf{I} + \epsilon\mathbf{JK}, \tag{A.15}$$

where $\mathbf{K}$ is symmetric. This follows directly by substituting Eq. (A.15) into the definition (2.9). Thus, there is a one-to-one correspondence between $2N \times 2N$ symmetric matrices and infinitesimal symplectic matrices. Since there are $N(2N+1)$ linearly independent symmetric matrices $\mathbf{K}$, this number is the dimensionality of $Sp(2N)$.

The Lie algebra of $Sp(2N)$ is obtained by taking the matrix commutator of infinitesimal symplectic matrices. If $\mathbf{K}_1$ and $\mathbf{K}_2$ are symmetric, then

$$[\mathbf{JK}_1, \mathbf{JK}_2] = \mathbf{JK}_3, \tag{A.16}$$

where

$$\mathbf{K}_3 = \mathbf{K}_1\mathbf{JK}_2 - \mathbf{K}_2\mathbf{JK}_1, \tag{A.17}$$

so that $\mathbf{K}_3$ is also symmetric.

The same Lie algebra occurs in classical quadratic Hamiltonians. We write

$$h_i(\mathbf{z}) = \tfrac{1}{2}\tilde{\mathbf{z}} \cdot \mathbf{K}_i \cdot \mathbf{z}, \tag{A.18}$$

for $i = 1, 2, 3$. If $\mathbf{K}_1$ and $\mathbf{K}_2$ are given symmetric matrices which define h_1 and h_2, and we define $\mathbf{K}_3$ by the Poisson bracket relation,

$$\{h_1, h_2\} = h_3, \tag{A.19}$$

then we find that $\mathbf{K}_3$ is given by Eq. (A.16). Equation (A.19) is meaningful, because the Poisson bracket of two quadratic Hamiltonians is another such Hamiltonian.

Although $\mathbf{K}$ is symmetric and $\mathbf{J}$ is antisymmetric, the product $\mathbf{JK}$ does not in general possess any symmetry. However, we can divide the space of all symmetric matrices $\mathbf{K}$ (a vector space of $N(2N+1)$ dimensions) into two subspaces, which we call the a-subspace and the s-subspace. If the product $\mathbf{JK}$ is antisymmetric, then $\mathbf{K}$ belongs to the a-subspace, and if the product is symmetric, then $\mathbf{K}$ belongs to the s-subspace. An arbitrary $\mathbf{K}$ does not belong to either subspace, but it can be represented uniquely as a sum of matrices which do. That is, the decomposition $\mathbf{K} = \mathbf{K}_a + \mathbf{K}_s$ is unique. The a-subspace is N^2-dimensional, and the s-subspace is $N(N+1)$-dimensional.

The a-subspace is closed under the commutator (A.16), and generates a subgroup of $Sp(2N)$. The matrices of this subgroup are exponentials of antisymmetric matrices, and are, therefore, orthogonal $2N \times 2N$ matrices. They are also symplectic, so they constitute the intersection of the two groups, $Sp(2N) \cap O(2N)$. This subgroup is isomorphic to $U(N)$ (see below).

The s-subspace is not closed under the commutator (A.16), and it does not generate a subgroup. Nevertheless, the exponential of all matrices of the form $\mathbf{JK}_s$ is an important subset of $Sp(2N)$. Since these are exponentials of symmetric matrices, they are all positive definite symmetric. Conversely, a positive definite, symmetric and symplectic matrix $\mathbf{T}$ has a unique symmetric logarithm (as can be seen by diagonalizing it), and therefore corresponds to a unique $\mathbf{K}$ in the s-subspace. Therefore the topology of the positive definite symmetric symplectic matrices is the same as that of the s-subspace, namely

$\mathbb{R}^{N(N+1)}$. These matrices arise in the Wigner functions of Gaussian wave packets (see Sec. 8).

A general theorem (the polar decomposition) states that *any* invertible matrix $\mathbf{S}$ can be *uniquely* written as the product of a positive definite symmetric matrix $\mathbf{T}$ and an orthogonal matrix $\mathbf{R}$:

$$\mathbf{S} = \mathbf{TR} \tag{A.20}$$

This follows by considering the matrix $\mathbf{S}\tilde{\mathbf{S}}$, which is positive definite and symmetric, and has, therefore, a unique positive definite square root, which we define to be $\mathbf{T}$. One then easily shows that $\mathbf{R} = \mathbf{T}^{-1}\mathbf{S}$ is orthogonal.

However, if $\mathbf{S}$ is symplectic, then so are $\mathbf{T}$ and $\mathbf{R}$. This follows by noting that

$$(\mathbf{JTJ}^{-1})(\mathbf{JRJ}^{-1}) = \mathbf{JSJ}^{-1} = \tilde{\mathbf{S}}^{-1} = \mathbf{T}^{-1}\mathbf{R}. \tag{A.21}$$

On both sides we have a product of a positive definite matrix and an orthogonal matrix. Since the polar decomposition is unique, we have $\mathbf{JTJ}^{-1} = \mathbf{T}^{-1}$ and $\mathbf{JRJ}^{-1} = \mathbf{R}$, which shows that both $\mathbf{T}$ and $\mathbf{R}$ are symplectic.

Every $\mathbf{T}$ matrix can be uniquely represented as the exponential of $\mathbf{JK}_s$ for some symmetric $\mathbf{K}_s$ in the s-subspace, and every $\mathbf{R}$ matrix can be represented as the exponential of $\mathbf{JK}_a$ for some symmetric $\mathbf{K}_a$ in the a-subspace (but not uniquely, because some matrices in the a-subspace generate one-parameter subgroups which are periodic). Therefore any symplectic matrix $\mathbf{S}$ can be written in the form

$$\mathbf{S} = \exp(\mathbf{JK}_s)\exp(\mathbf{JK}_a). \tag{A.22}$$

A matrix $\mathbf{R}$ which is both orthogonal and symplectic must satisty both $\mathbf{RJ}\tilde{\mathbf{R}} = \mathbf{J}$ and $\mathbf{R}\tilde{\mathbf{R}} = \tilde{\mathbf{R}}\mathbf{R} = \mathbf{I}$. From these relations we can show that the form (A.8) must satisfy $\mathbf{D} = \mathbf{A}$ and $\mathbf{B} = -\mathbf{C}$. Therefore we write $\mathbf{R}$ in the form

$$\mathbf{R} = \begin{pmatrix} \mathbf{X} & \mathbf{Y} \\ -\mathbf{Y} & \mathbf{X} \end{pmatrix}, \tag{A.23}$$

where $\mathbf{X}$ and $\mathbf{Y}$ satisfy

$$\mathbf{X}\tilde{\mathbf{X}} + \mathbf{Y}\tilde{\mathbf{Y}} = \mathbf{I},$$

$$\mathbf{X}\tilde{\mathbf{Y}} - \mathbf{Y}\tilde{\mathbf{X}} = 0. \qquad (A.24)$$

Therefore the $N\times N$ complex matrix $\mathbf{U} = \mathbf{X} + i\mathbf{Y}$ satisfies $\mathbf{U}\mathbf{U}^\dagger = \mathbf{I}$, and is unitary. Conversely, every $N\times N$ unitary matrix $\mathbf{U} = \mathbf{X} + i\mathbf{Y}$, when converted into a $2N\times 2N$ real matrix via Eq. (A.23), produces an orthogonal symplectic matrix. Furthermore, the group multiplication law is reproduced, i.e. $\mathbf{R}(\mathbf{U}_1)\mathbf{R}(\mathbf{U}_2) = \mathbf{R}(\mathbf{U}_1\mathbf{U}_2)$. Therefore the $\mathbf{R}$ matrices form a $2N$-dimensional real representation of the group $U(N)$, i.e.

$$Sp(2N) \cap O(2N) \sim U(N). \qquad (A.25)$$

(This representation is reducible; see Eq. (A.41).)

Since the polar decomposition is unique, and since the space of $\mathbf{T}$ matrices has the topology of $\mathbb{R}^{N(N+1)}$, $Sp(2N)$ has the topology of the product,

$$Sp(2N) \sim \mathbb{R}^{N(N+1)} \times U(N). \qquad (A.26)$$

In the special case $N = 1$, the group $U(1)$ merely consists of the complex phase factors $e^{i\alpha}$, and has the topology of a circle, denoted S^1. Therefore

$$Sp(2) \sim \mathbb{R}^2 \times S^1, \qquad (A.27)$$

which shows the appearance of the periodic slab mentioned earlier.

For $N > 1$ we call on the fact that for any unitary $\mathbf{U}$, $\det \mathbf{U} = e^{i\alpha}$ is a phase factor. Therefore $\mathbf{U}$ can be uniquely written as

$$\mathbf{U} = e^{i\alpha/N}\mathbf{U}_0, \qquad (A.28)$$

where $\det \mathbf{U}_0 = 1$, and $0 \le \alpha < 2\pi$. The matrix $\mathbf{U}_0$ is an element of the group $SU(N)$, which is simply connected. Therefore, topologically speaking, we have

$$Sp(2N) \sim \mathbb{R}^{N(N+1)} \times SU(N) \times S^1. \qquad (A.29)$$

The group $Sp(2N)$ is the product of a simply connected space with a circle. The circle provides the "hole" mentioned earlier, and the corresponding winding number and Maslov index.

Because $SU(N)$ is a subgroup of $U(N)$, it is also represented as a subgroup of $Sp(2N)$. The symplectic matrices comprising the representation of $SU(N)$ are $\mathbf{R}$ matrices of the form (A.23), with $\det(\mathbf{X}+i\mathbf{Y}) = 1$. Similarly, unitary matrices which represent multiplication by a phase factor, $\mathbf{U} = e^{i\beta}\mathbf{I}$, are represented within $Sp(2N)$ by $\mathbf{R}$ matrices of the form

$$\mathbf{R}(\beta) = \begin{pmatrix} \cos\beta\mathbf{I} & \sin\beta\mathbf{I} \\ -\sin\beta\mathbf{I} & \cos\beta\mathbf{I} \end{pmatrix}. \tag{A.30}$$

In principle, one can use the following algorithm for determining the winding number of a closed curve $\mathbf{S}(t)$ in the space of symplectic matrices. For each t, we apply the polar decomposition, to get $\mathbf{S}(t) = \mathbf{T}(t)\mathbf{R}(t)$. We discard the positive definite symmetric part $\mathbf{T}(t)$, and write $\mathbf{R}(t)$ in the form (A.23), so that $\mathbf{X}(t) + i\mathbf{Y}(t) = \mathbf{U}(t)$ is unitary. We then factor $\mathbf{U}(t)$ according to Eq. (A.28), to obtain the angle $\alpha(t)$. That is, we set

$$\alpha(t) = \arg\det(\mathbf{X}+i\mathbf{Y}). \tag{A.31}$$

The winding number is then determined directly from $\alpha(t)$.

In practice, however, the polar decomposition is awkward to use, and the following alternative algorithm works just as well. Instead of using the angle $\alpha(t)$, we use the angle $\gamma(t)$, defined directly in terms of $\mathbf{S}(t)$ by

$$\gamma(t) = \arg\det(\mathbf{A}+i\mathbf{B}). \tag{A.32}$$

The angle $\gamma(t)$ gives the same winding number as $\alpha(t)$ for the following reason. We decompose $\mathbf{S}(t)$ into a product of three matrices,

$$\mathbf{S}(t) = \begin{pmatrix} \mathbf{T}_1 & \mathbf{T}_2 \\ \tilde{\mathbf{T}}_2 & \mathbf{T}_3 \end{pmatrix} \begin{pmatrix} \cos\alpha/N\,\mathbf{I} & \sin\alpha/N\,\mathbf{I} \\ -\sin\alpha/N\,\mathbf{I} & \cos\alpha/N\,\mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{X}_0 & \mathbf{Y}_0 \\ -\mathbf{Y}_0 & \mathbf{X}_0 \end{pmatrix}, \tag{A.33}$$

where $\mathbf{T}_1$ and $\mathbf{T}_3$ are symmetric and positive definite and where $\det(\mathbf{X}_0 + i\mathbf{Y}_0) = +1$. Multiplying this out, we have

$$\mathbf{A} + i\mathbf{B} = e^{i\alpha/N}(\mathbf{T}_1 + i\mathbf{T}_2)(\mathbf{X}_0 + i\mathbf{Y}_0), \tag{A.34}$$

or

$$\det(\mathbf{A} + i\mathbf{B}) = e^{i\alpha} \det \mathbf{T}_1 \det(\mathbf{I} + i\mathbf{T}_1^{-1}\mathbf{T}_2). \tag{A.35}$$

By the symplectic condition (A.9) applied to $\mathbf{T}$, the matrix $\mathbf{T}_1^{-1}\mathbf{T}_2$ is symmetric, so the eigenvalues of $\mathbf{I} + i\mathbf{T}_1^{-1}\mathbf{T}_2$ are complex numbers of the form $1 + i\lambda$, with λ real. When $\mathbf{S}(t)$ goes through one period, these eigenvalues execute closed paths which are strictly to the right of the imaginary axis, and which do not, therefore, encircle the origin. Thus, the winding number determined by $\alpha(t)$ is the same as that determined by $\gamma(t)$.

Especially in work on coherent states, it is sometimes useful to consider complex symplectic matrices. These are defined in the same way as real ones, and satisfy the relations (A.9-A.11). A complex symplectic matrix of some importance is

$$\mathbf{W} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{I} & i\mathbf{I} \\ i\mathbf{I} & \mathbf{I} \end{pmatrix}, \tag{A.36}$$

which is also symmetric and unitary. This matrix is responsible for the complex classical canonical transformation which takes $(\mathbf{q}, \mathbf{p})$ into creation/annihilation variables,

$$\begin{aligned} \varsigma &= \frac{1}{\sqrt{2}}(\mathbf{q} + i\mathbf{p}), \\ i\varsigma^* &= \frac{1}{\sqrt{2}}(i\mathbf{q} + \mathbf{p}). \end{aligned} \tag{A.37}$$

A useful complex representation of $Sp(2N)$ is obtained by conjugating the real one with $\mathbf{W}$. We write

$$\mathbf{S}_c = \mathbf{W}\mathbf{S}\mathbf{W}^{-1}, \tag{A.38}$$

where the subscript c denotes the complex representation. Since $\mathbf{W}$ is complex symplectic, so is $\mathbf{S}_c$. $\mathbf{S}_c$ partitions as follows:

$$\mathbf{S}_c = \begin{pmatrix} \mathbf{\Lambda}^* & -i\mathbf{\Gamma}^* \\ i\mathbf{\Gamma} & \mathbf{\Lambda} \end{pmatrix}, \tag{A.39}$$

where the $N \times N$ complex matrices $\mathbf{\Lambda}, \mathbf{\Gamma}$ are given by

$$\mathbf{\Lambda} = \tfrac{1}{2}[(\mathbf{A} + \mathbf{D}) + i(\mathbf{B} - \mathbf{C})],$$

$$\mathbf{\Gamma} = \tfrac{1}{2}[(\mathbf{A} - \mathbf{D}) - i(\mathbf{B} + \mathbf{C})]. \qquad (A.40)$$

My notation is based on that of Bargmann [1961].

The $\mathbf{R}$ matrices become especially simple in the complex representation. We have

$$\mathbf{R}_c = \begin{pmatrix} \mathbf{U}^* & 0 \\ 0 & \mathbf{U} \end{pmatrix}, \qquad (A.41)$$

where $\mathbf{U} = \mathbf{X} + i\mathbf{Y}$ is unitary.

Although the polar decomposition is useful for many purposes, it is not invariant under symplectic transformations. That is, the matrix $\mathbf{S}_0\mathbf{R}\mathbf{S}_0^{-1}$ is not in general orthogonal, even if $\mathbf{R}$ is. However, the set of matrices $\mathbf{S}_0\mathbf{R}\mathbf{S}_0^{-1}$, for all orthogonal symplectic $\mathbf{R}$, does form a representation of $U(N)$ which is just as good as the "standard" one we have been using, in the sense that the same topological conclusions can be drawn (the topology does not change under a change of coordinates).

In fact, there is not very much about the symplectic matrices which is invariant under a conjugation. Neither the $\mathbf{R}$ subgroup, nor the $\mathbf{T}$ subspace, nor the phase angle α, nor the decomposition of the Lie algebra into a- and s-type subspaces is invariant. However, the winding number of a closed curve $\mathbf{S}(t)$ is an invariant, as also is the secular equation (A.1).

Neither $U(N)$ nor $SU(N)$ is an invariant subgroup of the symplectic group $Sp(2N)$, and the coset spaces $Sp(2N)/U(N)$ and $Sp(2N)/SU(N)$ are not groups. The Lie subalgebra consisting of the a-type matrices $\mathbf{K}_a$ is not invariant under the adjoint representation of $Sp(2N)$.

Other subgroups of $Sp(2N)$ are of physical interest. A linear point transformation is represented by a symplectic matrix in which $\mathbf{B} = \mathbf{C} = 0$, which means that $\mathbf{A}$ is nonsingular

and $\mathbf{D} = \tilde{\mathbf{A}}^{-1}$. Such a symplectic matrix represents the transformation $\mathbf{q}' = \mathbf{A} \cdot \mathbf{q}$, $\mathbf{p}' = \tilde{\mathbf{A}}^{-1} \cdot \mathbf{p}$. In the special case that $\mathbf{A}$ is orthogonal, we have a classical rotation operator,

$$\mathbf{S} = \begin{pmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{A} \end{pmatrix}, \tag{A.42}$$

where $\mathbf{A}\tilde{\mathbf{A}} = \mathbf{I}$. The symplectic matrices of this form constitute a representation of the group $O(N)$, which is a subgroup of the group $U(N)$ discussed above (i.e. Eq. (A.42) has the form of Eq. (A.23), with $\mathbf{X} = \mathbf{A}$, $\mathbf{Y} = 0$). If $N = 3$, then a one-parameter subgroup of this group represents rotations about some fixed axis in physical space, and it forms a closed curve in $Sp(2N)$ of period 2π with respect to the angle of rotation. The winding number of this curve in $Sp(2N)$ is zero, which is responsible for the fact that the components of orbital angular momentum are quantized in integral multiples of $\hbar$. In this case the semiclassical quantization is exact, because the components of orbital angular momentum are quadratic functions of q, p. More generally, as is easily seen on the basis of Eq. (A.32), the angle γ corresponding to any point transformation is zero. The only way to get a nontrivial Maslov index is to engage both position and momentum simultaneously in an operation on phase space.

Appendix B. The Wigner-Weyl Formalism

This appendix summarizes and develops a symplectic notation for the Wigner-Weyl formalism, in order to show its intimate relation to the Heisenberg and metaplectic operators. Recent reviews or other articles of interest on the Wigner-Weyl formalism include Berezin and Šubin [1972], Balazs and Jennings [1984], Carruthers and Zachariasen [1983], Hillery, O'Connell, Scully and Wigner [1984], McDonald [1983], and Mizrahi [1984]. More mathematical treatments of symbol theory and applications are given by Dubinskii [1982], Grossman, Loupias and Stein [1968], Hörmander [1971], Treve [1980], Voros [1976, 1977], and Weinstein [1975]. Part of the mathematical interest in symbols is in proving theorems about partial differential equations, in which rigorous statements concerning domains of definition are important. In this appendix, we mostly ignore such issues.

Unfortunately, most of the accessible references on the Wigner-Weyl formalism fail to emphasize its representation independence, nor do they make its fundamental symplectic invariance manifest. The purpose of this appendix is primarily to draw attention to such features, as well as to provide a summary of useful formulas.

We begin with symbols. In general, a symbol is some way of representing an operator on Hilbert space in terms of functions defined on some space with a classical interpretation. In all important cases, this space has dimensionality $2N$, and the representation is linear. For example, the x-space matrix element of an operator A, $\langle \mathbf{x}|A|\mathbf{x}'\rangle$, can be interpreted as a symbol on the space $(\mathbf{x},\mathbf{x}')$. The two point dielectric function $\epsilon(\mathbf{x},\mathbf{x}')$ used in plasma physics falls into this category. One can also use the mixed x- and p-space, or full p-space, matrix elements. Clearly, these symbols uniquely specify the operator in question.

If an operator A is a simple function of the operators $(\hat{\mathbf{q}},\hat{\mathbf{p}}) = \hat{\mathbf{z}}$ (see Eq. (3.1)), then one can obtain a symbol for A simply by replacing $(\hat{\mathbf{q}},\hat{\mathbf{p}})$ by their classical counterparts $(\mathbf{q},\mathbf{p}) = \mathbf{z}$, without regard to ordering, and dropping all terms of order $\hbar$ or higher (which

could be present in the original expression for A, or which could be introduced by changing the ordering of the $\hat{q}$'s and $\hat{p}$'s). We will call this the *principal symbol*, which can be interpreted as a function $a = a(\mathbf{q}, \mathbf{p})$ on the classical phase space. This symbol does not uniquely specify the operator it was derived from, because of the neglect of ordering issues. In most cases of interest in quantum mechanics, the principal symbol of the quantum Hamiltonian is the classical Hamiltonian. However, the principal symbol is not always defined. For example, the propagator $U(t) = e^{-itH/\hbar}$ does not have a power series expansion in $\hbar$, and therefore the principal symbol does not exist. The same is generally true for projection operators $|\psi\rangle\langle\psi|$. In cases in which other symbols, such as the Wigner-Weyl symbol or the coherent state symbol, have power series expansions in $\hbar$, the leading term (i.e. the $O(\hbar^0)$ term) is identical with the principal symbol. This is to say that these other symbols differ from one another only by higher order terms in $\hbar$, assuming that they have an expansion in $\hbar$ at all, and that these differences amount to different ordering conventions.

By adopting some ordering convention and keeping all terms in $\hbar$, one can obtain symbols which do uniquely represent the corresponding operator. Suppose, for example, we commute all $\hat{p}$'s to the right and all $\hat{q}$'s to the left in the expression for some operator A, and then replace the $\hat{q}$'s and $\hat{p}$'s by their classical counterparts. Then we obtain the "q-before-p symbol" (called the ordinary symbol by McDonald [1983]). This symbol is extensively used in the mathematical literature, and is especially suggestive for differential operators in x-space. It also tends to appear in WKB theory based on the Hamilton-Jacobi equation. However, it has some unpleasant properties, such as the asymmetry it introduces between q and p, and the fact that Hermitian operators do not in general have real symbols. Similarly, one can define the p-before-q symbol, which has similar drawbacks.

The Feynman path integral leads to symbols. However, if the time evolution operator (the Hamiltonian) involves any nontrivial ordering issues, then the definition of the symbol

gets mixed up with the procedure used to discretize the paths, as discussed by Feynman and Hibbs [1965], Schulman [1981], and Langouche, Roekaerts, and Tirapegui [1982]. If the q-before-p ordering is adopted, then the path discretization is easier, but then we return to the unpleasant features of the q-before-p symbol. We shall not deal with these issues, nor shall we make any use in this paper of the q-before-p symbol.

The coherent state symbol emerges from the coherent state path integral (Klauder [1978], Schulman [1981]). It is discussed in Appendix C.

The most satisfactory symbol is the Weyl symbol. It comes in two versions, which we denote by $\tilde{a}(\mathbf{z})$ and $a(\mathbf{z})$ for some operator A. These are sometimes called the covariant and contravariant versions. The symbol $\tilde{a}(\mathbf{z})$, which we shall call the *alternative Weyl symbol*, is defined implicitly by

$$A = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N}\, \tilde{a}(\mathbf{z})T(\mathbf{z}). \tag{B.1}$$

In other words, $\tilde{a}(\mathbf{z})$ is the expansion coefficient in a representation of A in terms of a linear combination of Heisenberg operators. The fact that such a representation exists and is unique (modulo domain questions, which we ignore) is due to the irreducibility of the Heisenberg operators. Explicitly, if such an $\tilde{a}(\mathbf{z})$ exists, then by Eq. (3.31) it must be given by

$$\tilde{a}(\mathbf{z}) = \mathrm{Tr}\big[T(\mathbf{z})^\dagger A\big]. \tag{B.2}$$

Conversely, if we take this $\tilde{a}(\mathbf{z})$ and substitute it into the integral of Eq. (B.1), then use of Eq. (3.30) shows that the result is just A.

The second version of the Weyl symbol, $a(\mathbf{z})$, which we shall call the *ordinary Weyl symbol*, is the Fourier transform in phase space of the one just given, where the phase of the exponent in the Fourier transform is given in terms of the symplectic form ω (see Eqs. (A.3)-(A.4)). This symbol is the one usually considered as the Weyl symbol proper,

and it is defined by

$$a(\mathbf{z}) = \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N}\, \tilde{a}(\mathbf{z}')\, e^{\frac{i}{\hbar}\omega(\mathbf{z}',\mathbf{z})}. \qquad (B.3)$$

Inverting this gives

$$\tilde{a}(\mathbf{z}) = \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N}\, a(\mathbf{z}')\, e^{\frac{i}{\hbar}\omega(\mathbf{z}',\mathbf{z})}. \qquad (B.4)$$

The signs in the exponents of these expressions are correct. Both symbols $\tilde{a}(\mathbf{z})$ and $a(\mathbf{z})$ uniquely specify the corresponding operator, and are defined even when the principal symbol is not.

Since the association between operators and Weyl symbols is invertible, one can in principle use the Weyl symbol to perform exact quantum mechanical calculations on a classical-looking phase space, with no approximation. In addition, if one is interested in semiclassical approximations, then certain properties of the Weyl symbol make it especially attractive for this purpose as well, such as the ease with which the canonical structure of classical mechanics makes its appearance in the Wigner-Weyl formalism. As a result, several authors have explored the use of the Weyl symbol in semiclassical mechanics (Berry [1977], Bialynicki-Birula [1977], Carruthers and Zachariasen [1983], Heller [1976, 1977b], Smith [1978], and Springborg [1984]). The full promise of this approach has probably not yet been realized.

If the operator A is Hermitian and has Weyl symbols $\tilde{a}(\mathbf{z})$, $a(\mathbf{z})$, then the symbols of the operator $A^\dagger$ are respectively $\tilde{a}(-\mathbf{z})^*$ and $a(\mathbf{z})^*$. In particular, the ordinary Weyl symbol of a Hermitian operator is real. In most cases in quantum mechanics, the ordinary Weyl symbol of the quantum Hamiltonian is the classical Hamiltonian, and agrees with the principal symbol. In plasma physics, the Weyl symbol of the dielectric operator is the local dispersion relation $\epsilon(\mathbf{x}, \mathbf{k})$, and has been used in WKB analyses by Berk and Pfirsch [1980] and others.

The relationship between the Weyl symbols and the x-space matrix elements is given by

$$\tilde{a}(\mathbf{z}) = \int d^N\mathbf{x}\, e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}\, \langle \mathbf{x} + \tfrac{1}{2}\mathbf{q}|A|\mathbf{x} - \tfrac{1}{2}\mathbf{q}\rangle, \tag{B.5}$$

and

$$a(\mathbf{z}) = \int d^N\mathbf{s}\, e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}\, \langle \mathbf{q} + \tfrac{1}{2}\mathbf{s}|A|\mathbf{q} - \tfrac{1}{2}\mathbf{s}\rangle, \tag{B.6}$$

where $\mathbf{z} = (\mathbf{q}, \mathbf{p})$. This follows easily from the formulas above and Eq. (3.19). Equation (B.6) shows that the ordinary Weyl symbol is the Fourier transform of the x-space kernel of the operator A, taken over the difference variable $\mathbf{s} = \mathbf{x} - \mathbf{x}'$, while holding the sum variable $\mathbf{q} = (\mathbf{x} + \mathbf{x}')/2$ fixed. One often has reason to interpret the difference variable as "rapidly varying," whereas the sum variable is "slowly varying." Thus, the Weyl symbol has the nature of a local Fourier transform (de Bruijn [1973]), and leads to such things as local dispersion relations.

Special cases of the Weyl symbols are of interest. If the operator $A = 1$, then $\tilde{a}(\mathbf{z}) = (2\pi\hbar)^N\, \delta(\mathbf{z})$ and $a(\mathbf{z}) = 1$. If $A = \hat{z}_\alpha$, $\alpha = 1, \ldots 2N$, then

$$\tilde{a}(\mathbf{z}) = (2\pi\hbar)^N i\hbar J_{\alpha\beta} \frac{\partial\delta(\mathbf{z})}{\partial z_\beta}, \tag{B.7}$$

and $a(\mathbf{z}) = z_\alpha$. More generally, if A is a polynomial in $\hat{\mathbf{z}}$, then $\tilde{a}(\mathbf{z})$ consists of δ-functions and their derivatives at $\mathbf{z} = 0$, and $a(\mathbf{z})$ is a polynomial in $\mathbf{z}$. $\tilde{a}(\mathbf{z})$ can be nonzero away from $\mathbf{z} = 0$, but only if A is not a polynomial in $\hat{\mathbf{z}}$.

Consider three operators A, B, C such that $C = AB$, and let their Weyl symbols be $\tilde{a}$, $\tilde{b}$, $\tilde{c}$, a, b, c. Then

$$\tilde{c}(\mathbf{z}) = \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N}\, e^{\frac{i}{2\hbar}\omega(\mathbf{z}',\mathbf{z})}\, \tilde{a}(\mathbf{z}')\tilde{b}(\mathbf{z} - \mathbf{z}'). \tag{B.8}$$

The corresponding formula for $c(\mathbf{z})$ cannot be reduced to a single integral:

$$c(\mathbf{z}) = \int \frac{d^{2N}\mathbf{z}'\, d^{2N}\mathbf{z}''}{(4\pi\hbar)^{2N}}\, e^{\frac{i}{2\hbar}\omega(\mathbf{z}',\mathbf{z}'')}\, a(\mathbf{z} + \tfrac{1}{2}\mathbf{z}')b(\mathbf{z} - \tfrac{1}{2}\mathbf{z}''). \tag{B.9}$$

However, by expansion in Taylor series and repeated integration by parts, the equation for $c(\mathbf{z})$ can be formally written as a power series in $\hbar$:

$$c(\mathbf{z}) = a(\mathbf{z}) \exp\left(\frac{i\hbar}{2}\overleftrightarrow{\mathrm{L}}\right) b(\mathbf{z}), \tag{B.10}$$

where $\overleftrightarrow{\mathrm{L}}$ is the "Janus operator,"

$$\overleftrightarrow{\mathrm{L}} = \frac{\overleftarrow{\partial}}{\partial z_\alpha} J_{\alpha\beta} \frac{\overrightarrow{\partial}}{\partial z_\beta}, \tag{B.11}$$

in which the two partial derivatives act in opposite directions (the left one on $a(\mathbf{z})$, the right one on $b(\mathbf{z})$). The first few terms of Eq. (B.10) are

$$c(\mathbf{z}) = a(\mathbf{z})b(\mathbf{z}) + \frac{i\hbar}{2}\{a, b\} + O(\hbar^2), \tag{B.12}$$

where the curly bracket is the Poisson bracket. Since the operators A and B in general do not commute, whereas multiplication of functions on phase space does commute, the symbol of the product of two operators cannot simply be the ordinary product of the symbols. However, Eq. (B.12) shows that the leading term is the ordinary product, and that there are corrections of higher order in $\hbar$. It is interesting that the first correction involves the classical Poisson bracket.

Equation (B.10) is called the Groenewold [1946] formula, or, as we shall call it, the *Weyl product rule.* It must be used with caution, especially if the symbols $a(\mathbf{z})$ or $b(\mathbf{z})$ are not simple power series in $\hbar$. In particular, if they are the symbols of propagators or projection operators (i.e. Wigner functions), then they are likely to have an essential singularity in $\hbar$ at $\hbar = 0$, invalidating the ordering indicated in Eq. (B.12) and jeopardizing the convergence of the series. Nevertheless, the series (B.12) shows the emergence of the classical Poisson bracket in the symbol formalism, and provides powerful persuasion that an approach to semiclassical mechanics based on the Heisenberg operators is the correct approach. The operation of Eq. (B.10) has been denoted $c = a * b$ by Bayen et al. [1978], and used by them to develop a path integral (see also Sharan [1979]). A similar path integral has been discussed by Berezin and Šubin [1972] and Berezin [1980].

If instead of $C = AB$, we take $C = AB - BA = [A, B]$, then we obtain

$$c(\mathbf{z}) = a(\mathbf{z}) \exp\left(\frac{i\hbar}{2}\overleftrightarrow{\mathrm{L}}\right) b(\mathbf{z}) - b(\mathbf{z}) \exp\left(\frac{i\hbar}{2}\overleftrightarrow{\mathrm{L}}\right) a(\mathbf{z}). \qquad (B.13)$$

Expanding this out to the first few terms gives

$$c(\mathbf{z}) = i\hbar\{a, b\} + O(\hbar^3), \qquad (B.14)$$

which shows the relationship between the quantum mechanical commutator and the classical Poisson bracket.

Equation (B.13) provides the definition of the Moyal [1949] bracket, which we distinguish from the Poisson bracket by the subscript M:

$$c(\mathbf{z}) = i\hbar\{a, b\}_M. \qquad (B.15)$$

Like the Poisson bracket, the Moyal bracket is antisymmetric and satisfies the Jacobi identity, but it is not a derivation (i.e. a bilinear operation involving first order differential operators). It is in a sense a nonlocal operation on phase space, as can be seen by putting it into an integral form like Eq. (B.9). The approximation of the Moyal bracket by the classical Poisson bracket (i.e. keeping only the first term in Eq. (B.14)) is related to the approximation involved in wave packet propagation, as discussed in Sec. 2.

The trace of an operator is given in terms of its Weyl symbols by

$$\mathrm{Tr}\, A = \tilde{a}(0) = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N}\, a(\mathbf{z}). \qquad (B.16)$$

The Hermitian scalar product of two operators is given in terms of their Weyl symbols by

$$\mathrm{Tr}(A^\dagger B) = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N}\, \tilde{a}(\mathbf{z})^* \tilde{b}(\mathbf{z}) = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N}\, a(\mathbf{z})^* b(\mathbf{z}). \qquad (B.17)$$

The final equality is a version of Parcival's theorem.

Given a state $|\psi\rangle$, one can associate with it a function on the classical phase space which has most of the properties one would expect for a classical Liouville probability density function. This is the Wigner function $W(\mathbf{z})$, and it is the ordinary Weyl symbol

of the projection operator $|\psi\rangle\langle\psi|$. Since this operator is Hermitian, the Wigner function is real. Assuming that $|\psi\rangle$ is normalized, Eq. (B.16) immediately gives

$$\int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N} W(\mathbf{z}) = 1. \tag{B.18}$$

If A is any operator, then Eq. (B.17) gives

$$\langle\psi|A|\psi\rangle = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N} W(\mathbf{z}) a(\mathbf{z}). \tag{B.19}$$

In particular, setting $A = \hat{\mathbf{z}}$, we have

$$\langle\hat{\mathbf{z}}\rangle = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N} W(\mathbf{z})\, \mathbf{z}. \tag{B.20}$$

If $|\chi\rangle$ is some state with Wigner function $\mathrm{V}(\mathbf{z})$, then

$$|\langle\chi|\psi\rangle|^2 = \mathrm{Tr}(|\chi\rangle\langle\chi|\psi\rangle\langle\psi|) = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N} V(\mathbf{z}) W(\mathbf{z}). \tag{B.21}$$

In particular, if $|\chi\rangle = |\mathbf{x}\rangle$, we have $V(\mathbf{z}) = V(\mathbf{q},\mathbf{p}) = \delta(\mathbf{x}-\mathbf{q})$, as one can easily show by use of Eq. (3.19). Therefore Eq. (B.21) becomes

$$|\psi(\mathbf{x})|^2 = \int \frac{d^N\mathbf{p}}{(2\pi\hbar)^N} W(\mathbf{x},\mathbf{p}), \tag{B.22}$$

which shows that the integral of the Wigner function over momentum is the probability density in configuration space. Similarly, if $|\chi\rangle = |\mathbf{p}\rangle$, we find

$$|\phi(\mathbf{p})|^2 = \int \frac{d^N\mathbf{q}}{(2\pi\hbar)^N} W(\mathbf{q},\mathbf{p}), \tag{B.23}$$

where $\phi(\mathbf{p})$ is the momentum space wave function, so that the integral of the Wigner function over position is the probability density in momentum space.

In all of the properties (B.18)-(B.23), the Wigner function behaves exactly like a classical Liouville probability density function $f(\mathbf{z})$ on phase space (apart from the factor $(2\pi\hbar)^N$). However, unlike the Liouville function, the Wigner function may take on negative values.

The Wigner function $W(\mathbf{z})$ associated with a state $|\psi\rangle$ is a nonlinear function of the state, and does not obey linear superposition. The overall phase of $|\psi\rangle$ is lost on going to

the Wigner function; apart from this, $|\psi\rangle$ can be reconstructed from $W(\mathbf{z})$ (assuming that $W(\mathbf{z})$ represents a pure state).

In statistical mechanics, the Wigner function is taken to be the Weyl symbol of the density operator ρ. This includes the previous usage of the Wigner function as a special case, i.e. when $\rho = |\psi\rangle\langle\psi|$. It is in this context that the Wigner function was first used by Wigner [1932]. This generalization produces obvious modifications to Eqs. (B.19)-(B.23), e.g. the left hand side of Eq. (B.19) becomes $\mathrm{Tr}(\rho A)$.

Given a real function $f(\mathbf{z})$ on the phase space, one would like to know if it represents a Wigner function, i.e. the symbol of some density operator ρ. One can in principle invert the Weyl symbol relations to find the Hermitian operator corresponding to $f(\mathbf{z})$. If the result is a density operator, it must be positive semidefinite and satisfy $\mathrm{Tr}\,\rho = 1$. However, the positive semidefiniteness condition seems difficult to interpret in the Wigner-Weyl formalism, so that it is not easy to tell if a given $f\mathbf{z})$ represents a Wigner function (Voros [1976, 1977]).

Appendix C. Coherent States

Coherent states can be traced back to Schrödinger [1926], but they have attracted special interest in recent years, since the work of Glauber [1963]. They are reviewed by de Groot and Suttorp [1972], Klauder and Skagerstan [1985], Klauder and Sudarshan [1968], and Schulman [1981]. Generalizations have been proposed or developed by Klauder [1979, 1982], Nieto and Simmons [1979], Perelemov [1977], and Yaffe [1982]. The purpose of this appendix is to summarize some important facts about coherent states, while at the same time relating them to the symplectic formalism of this paper and emphasizing their features which are representation independent.

We take any normalized state $|0\rangle$ and act on it with the Heisenberg operators $T(\mathbf{z})$ (given by Eqs. (3.12) and (3.19)) in order to define the new states,

$$|\mathbf{z}\rangle = T(\mathbf{z})|0\rangle. \tag{C.1}$$

The vector $\mathbf{z}$ is the real $2N$-dimensional coordinate vector on the classical phase space. The $2N$-dimensional family of states $|\mathbf{z}\rangle$ provides a resolution of the identity,

$$\int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N} \, |\mathbf{z}\rangle\langle\mathbf{z}| = 1, \tag{C.2}$$

as follows immediately from Eq. (3.30). This fact is a result of the irreducibility of the Heisenberg operators, and has nothing to do with the state $|0\rangle$, apart from the fact that it is normalized. In particular, it has nothing to do with Gaussians. Because of this, Klauder [1978] has called $|0\rangle$ the "fiducial" state.

If the state $|0\rangle$ satisfies $\langle 0|\hat{\mathbf{z}}|0\rangle = 0$, then by Eq. (3.4) we have

$$\langle\mathbf{z}|\hat{\mathbf{z}}|\mathbf{z}\rangle = \mathbf{z}. \tag{C.3}$$

The states $|\mathbf{z}\rangle$ can then be seen as wave packets, centered at location $\mathbf{z}$ in phase space (their Wigner functions will be so centered). If in addition the fiducial state $|0\rangle$ is taken

to be the state with the **x**-space wave function,

$$\langle \mathbf{x}|0\rangle = \frac{1}{(\pi\hbar)^{N/4}} e^{-\tilde{\mathbf{x}}\cdot\mathbf{x}/2\hbar}, \tag{C.4}$$

then the states $|\mathbf{z}\rangle$ form what we shall call the *standard coherent states.* See Sec. 6 for a discussion of the units chosen for **x** in this equation. This appendix deals only with standard coherent states.

Equation (C.4) represents the ground state of the isotropic harmonic oscillator, which is an eigenstate of the annihilation operator with eigenvalue 0. Therefore we introduce the operators $\hat{\varsigma}$, $\hat{\varsigma}^\dagger$,

$$\begin{pmatrix} \hat{\varsigma} \\ i\hat{\varsigma}^\dagger \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{I} & i\mathbf{I} \\ i\mathbf{I} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{q}} \\ \hat{\mathbf{p}} \end{pmatrix}, \tag{C.5}$$

which are creation/annihilation operators. The matrix shown is the complex symplectic matrix **W** of Eq. (A.36). The operators $\hat{\varsigma}$, $i\hat{\varsigma}^\dagger$ therefore play the role of $\hat{\mathbf{Q}}$, $\hat{\mathbf{P}}$ in Eq. (4.1), and the commutation relations (4.2) are satisfied. However, they are not Hermitian. The classical counterpart of Eq. (C.5) is given in Appendix A, and produces the classical complex canonical variables ς, $i\varsigma^*$. Either one of these (a complex N-vector) contains the same information as the $2N$-dimensional real vector **z** (assuming **q** and **p** are real).

By Eq. (3.4) we have

$$T(\mathbf{z}_0)^\dagger\, \hat{\varsigma}\, T(\mathbf{z}_0) = \hat{\varsigma} + \varsigma_0, \tag{C.6}$$

and therefore

$$\hat{\varsigma}|\mathbf{z}_0\rangle = \varsigma_0|\mathbf{z}_0\rangle. \tag{C.7}$$

The standard coherent states $|\mathbf{z}_0\rangle$ are eigenstates of the annihilation operator with eigenvalue ς_0.

In this sense, the coherent states $|\mathbf{z}\rangle$ are like the states $|\hat{\mathbf{Q}}(\mathbf{Q})\rangle$ discussed in Sec. 4, and the transformation connecting the **q**-basis and the coherent state basis is a special kind of metaplectic transformation, related to the complex symplectic matrix **W** of Eq. (C.5)

and (A.36). No doubt a fully satisfactory theory of coherent states would involve the complex generalization of the symplectic group (and the nonunitary generalization of the metaplectic group). Probably the theory of Kramer, Moshinsky, and Seligman [1975] could be applied here, and would result in a deeper understanding of the coherent states, but to my knowledge this has not specifically been done. In any case, the present analogy is imperfect, because a Hermitian $\hat{\mathbf{Q}}$ has both eigenkets and eigenbras, both outside Hilbert space, whereas the non-Hermitian $\hat{\varsigma}$ has good eigenkets within Hilbert space, but no eigenbras. ($\hat{\varsigma}^\dagger$ has eigenbras, but not eigenkets.) See also Weissman [1982], who treats complex canonical transformations.

The q-basis wave functions for the coherent states are given by

$$\begin{aligned}\langle \mathbf{x}|\mathbf{z}\rangle &= \langle \mathbf{x}|T(\mathbf{z})|0\rangle \\ &= \frac{1}{(\pi\hbar)^{N/4}} \exp\left\{\frac{1}{\hbar}\left[-\tfrac{1}{2}(\tilde{\mathbf{x}}-\tilde{\mathbf{q}})\cdot(\mathbf{x}-\mathbf{q}) + i\tilde{\mathbf{p}}\cdot\mathbf{x} - \frac{i}{2}\tilde{\mathbf{p}}\cdot\mathbf{q}\right]\right\}. \qquad (C.8)\end{aligned}$$

This follows from Eq. (3.19). In terms of the complex vector ς, this can also be written

$$\langle \mathbf{x}|\mathbf{z}\rangle = \frac{1}{(\pi\hbar)^{N/4}} \exp\left\{\frac{1}{\hbar}\left[-\tfrac{1}{2}|\varsigma|^2 - \tfrac{1}{2}\tilde{\mathbf{x}}\cdot\mathbf{x} - \tfrac{1}{2}\tilde{\varsigma}\cdot\varsigma + \sqrt{2}\,\tilde{\mathbf{x}}\cdot\varsigma\right]\right\}, \qquad (C.9)$$

where

$$|\varsigma|^2 = \tilde{\varsigma}^*\cdot\varsigma = \tfrac{1}{2}\tilde{\mathbf{z}}\cdot\mathbf{z} = \tfrac{1}{2}(\tilde{\mathbf{q}}\cdot\mathbf{q} + \tilde{\mathbf{p}}\cdot\mathbf{p}). \qquad (C.10)$$

This equation represents a kind of Euclidean metric on the classical phase space, which arises from the choice made in Eq. (C.4) for the fiducial state. This metric makes its appearance in semiclassical calculations based on coherent states, and all representation independent quantities which arise in such calculations can be expressed in terms of this metric and the symplectic form ω. Of course, only the latter has a purely classical significance.

Equation (C.2) provides a means of defining wave functions on phase space. We denote such a function by $\psi_{cs}(\mathbf{z})$, which is given in terms of $\psi(\mathbf{x})$ by

$$\psi_{cs}(\mathbf{z}) = \langle \mathbf{z}|\psi\rangle = \int d\mathbf{x}\, \langle \mathbf{z}|\mathbf{x}\rangle\langle \mathbf{x}|\,\psi\rangle = \int d\mathbf{x}\, \langle \mathbf{z}|\mathbf{x}\rangle\psi(\mathbf{x}). \qquad (C.11)$$

The inverse of this is

$$\psi(\mathbf{x}) = \int \frac{d^{2N}\mathbf{z}}{(2\pi\hbar)^N} \langle \mathbf{x}|\mathbf{z}\rangle \, \psi_{cs}(\mathbf{z}). \qquad (C.12)$$

Unlike the Wigner function, the coherent state wave function $\psi_{cs}(\mathbf{z})$ is a linear functional of $\psi(\mathbf{x})$, and obeys linear superposition. However, it lacks the compelling uniqueness of the Wigner function, since its definition is dependent on the choice of the fiducial state, and because of the over-completeness of the coherent states. It is interesting to note that the coherent state wave function is a form of the Weyl symbol, since

$$\psi_{cs}(\mathbf{z}) = \mathrm{Tr}\left[T(\mathbf{z})^\dagger |\psi\rangle\langle 0|\right]. \qquad (C.13)$$

One can also define coherent state matrix elements for an operator A. These are given by

$$A_{cs}(\mathbf{z}, \mathbf{z}') = \langle \mathbf{z}|A|\mathbf{z}'\rangle. \qquad (C.14)$$

The operator A, and hence its full coherent state matrix elements, are uniquely determined by the diagonal values alone (Klauder [1978], Mizrahi [1984]),

$$a_{cs}(\mathbf{z}) = A_{cs}(\mathbf{z}, \mathbf{z}) = \langle \mathbf{z}|A|\mathbf{z}\rangle. \qquad (C.15)$$

We call $a_{cs}(\mathbf{z})$ the *coherent state symbol* of A. It arises in the coherent state path integral (modulo some issues of path discretization), and in other places as well.

The coherent state wave function $\psi_{cs}(\mathbf{z})$ has the property that the quantity

$$e^{|\varsigma|^2/2\hbar}\psi_{cs}(\mathbf{z}) \qquad (C.16)$$

is an entire analytic function of ς^* (i.e. of its N complex components). Similarly, the quantity

$$e^{(|\varsigma|^2+|\varsigma'|^2)/2\hbar}A_{cs}(\mathbf{z}, \mathbf{z}') \qquad (C.17)$$

is an entire analytic function of both ς^* and ς'. Much has been made of these facts by Bargmann [1961], who has developed a theory of the Hilbert space of analytic functions. A readable introduction to this subject has been given by Schulman [1981].

The coherent states are complete but not orthogonal, since

$$\langle \mathbf{z}|\mathbf{z}'\rangle = \exp\left[\frac{1}{\hbar}\left(-\tfrac{1}{2}|\varsigma|^2 - \tfrac{1}{2}|\varsigma'|^2 + \tilde{\varsigma}^* \cdot \varsigma'\right)\right]$$

$$= \exp\left\{\frac{1}{\hbar}\left[-\tfrac{1}{2}|\varsigma - \varsigma'|^2 - \tfrac{i}{2}\omega(\mathbf{z},\mathbf{z}')\right]\right\}, \qquad (C.18)$$

where

$$\omega(\mathbf{z},\mathbf{z}') = i(\tilde{\varsigma}^* \cdot \varsigma' - \tilde{\varsigma} \cdot \varsigma'^*). \qquad (C.19)$$

The overlap of the coherent states falls off exponentially as $\mathbf{z}$ and $\mathbf{z}'$ separate from each other in phase space, as measured by the distance specified by the coherent state metric, Eq. (C.10). The phase is the symplectic form. Perhaps the coherent state metric should be interpreted as a symmetric, complex extension of the antisymmetric, real symplectic form. As shown in Sec. 8, the coherent state metric has a symplectic interpretation.

The nonorthogonality of the coherent states is a reflection of the fact that they are grossly overcomplete. This leads to their "reproducing kernel," as discussed by Klauder [1978]. The overcompleteness can be greatly reduced by restricting consideration to those coherent states situated on lattice sites in phase space, defined by the unit **q-p** cell of volume $(2\pi\hbar)^N$. One can also use any lattice obtained from this one by the action of a symplectic matrix (a symplectic lattice). This is obviously a kind of a semiclassical result, but I do not know what its significance is. See Bacry, Grossman and Zak [1975], Lion and Vergne [1980], Perelemov [1971, 1977], Schulman [1981], and von Neumann [1955].

A relationship between the coherent state symbol $a_{cs}(\mathbf{z})$ and the Weyl symbols $\tilde{a}(\mathbf{z})$, $a(\mathbf{z})$ for some operator A can be derived as follows. We write

$$a_{cs}(\mathbf{z}) = \langle 0|T(\mathbf{z})^\dagger A\, T(\mathbf{z})|0\rangle$$

$$= \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N}\, \langle 0|T(\mathbf{z})^\dagger T(\mathbf{z}')T(\mathbf{z})|0\rangle\, \tilde{a}(\mathbf{z}')$$

$$= \int \frac{d^{2N}\mathbf{z}'}{(2\pi\hbar)^N} \exp\left[-\frac{i}{\hbar}\omega(\mathbf{z},\mathbf{z}') - \frac{1}{2\hbar}|\varsigma'|^2\right] \tilde{a}(\mathbf{z}'), \qquad (C.20)$$

where we have used Eqs. (3.22) and (C.18). Next, application of Eq. (B.4) gives

$$a_{cs}(\mathbf{z}) = \int \frac{d^{2N}\mathbf{z}'}{(\pi\hbar)^N} e^{-\frac{2}{\hbar}|\varsigma'|^2} a(\mathbf{z}+\mathbf{z}'). \qquad (C.21)$$

The ordinary Weyl symbol in the integrand can be expanded in powers of $\overline{\mathbf{z}'}$, yielding integrals which are moments of Gaussians. These can all be done, giving finally

$$a_{cs}(\mathbf{z}) = \exp\left[\frac{\hbar}{4}\left(\frac{\partial^2}{\partial \mathbf{q}^2} + \frac{\partial^2}{\partial \mathbf{p}^2}\right)\right] a(\mathbf{z}). \qquad (C.22)$$

This result is subject to the same warnings surrounding the Weyl product rule, Eq. (B.10). But it shows explicitly that for operators whose symbols are powers series in $\hbar$, the leading term of both the coherent state symbol and ordinary Weyl symbol is the same (and is identical with the principal symbol). The phase space Laplacian appearing in Eq. (C.22) involves the inverse or contravariant version of the coherent state metric. It will be generalized in Sec. 8.

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Figure Captions

1. Nearby orbits in classical mechanics. The solid curve is the reference orbit, and the dotted curve is the orbit nearby.

2. The classical time evolution of a Gaussian ensemble of free particles. The velocity differential causes the circle to shear into an ellipse.

3. The Heisenberg operators do not commute, due to the overall phase. The phase is the first Poincaré invariant associated with the triangle.

4. Heisenberg operators can be used to move a wave function along a curve in phase space.

5. The left null eigenvectors **u** of **B** lie in **p**-space. They are orthogonal to the caustic surface, which lies in **x**-space and is parallel to the image of **B**. The right null eigenvectors **v** of **B** lie in **p**′-space; they span the kernel of **B**. The diagram illustrates the case $n = 1$, $r = 2$, $N = 3$.

6. Lagrangian planes and caustics for a quadratic Hamiltonian in one dimension. The initial condition is x'. The final point x_3 is a caustic of the Lagrangian plane L_2.

7. Caustics and Lagrangian manifolds for nonlinear Hamiltonians. The final point $\mathbf{x}_3$ lies on a caustic associated with Lagrangian manifold L_1.

8. Caustics in a multidimensional problem. The Lagrangian manifold L has a singular projection onto configuration space at the point **x**. The caustic surface is a curve in configuration space, whose tangent is determined by the null eigenvectors of **B**. **B** is the submatrix of the symplectic matrix governing orbits nearby the reference orbit $\mathbf{z}(t)$.

9. Classical picture corresponding to the mixed **x**- and **p**-space Green's function.

10. The matrix function $\mathbf{B}(t)$ passes through a first order caustic. There are two sides to the caustic surface.

11. The set of points in $\mathbf{B}$ matrix space where $\det \mathbf{B} = 0$ do not form a smooth surface where the rank of $\mathbf{B}$ drops.

12. Sometimes a second order caustic is avoided altogether by introducing a small perturbation into $\mathbf{B}(t)$.

13. Sometimes a second order caustic bifurcates into two first order caustics under a small perturbation.

14. The evolution of localized Liouville distribution functions in the nearby orbit approximation.

15. The Wigner ellipsoid in phase space. Some Gaussians appear to be more than minimum uncertainty because they are viewed from the wrong symplectic frame.

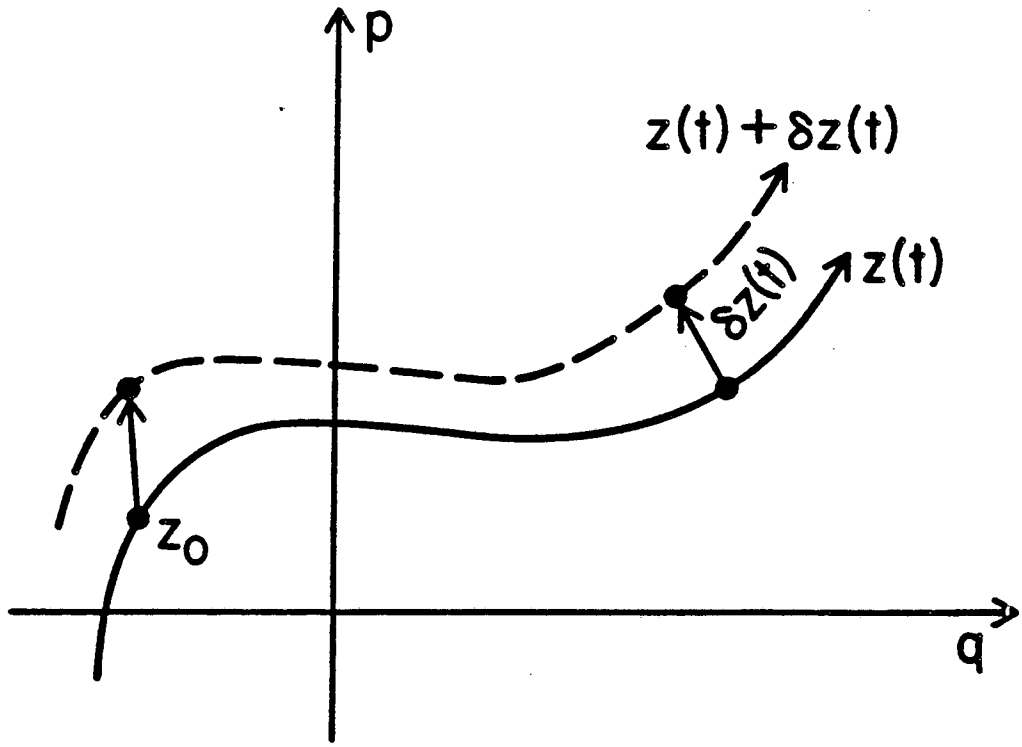

Fig. 1

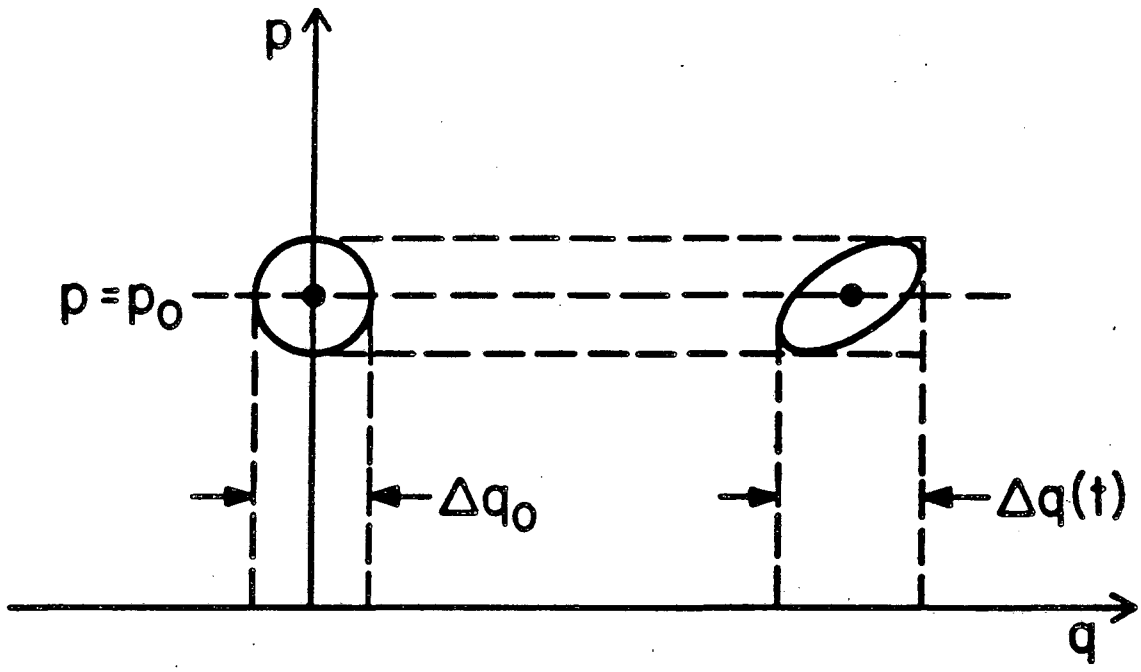

Fig. 2

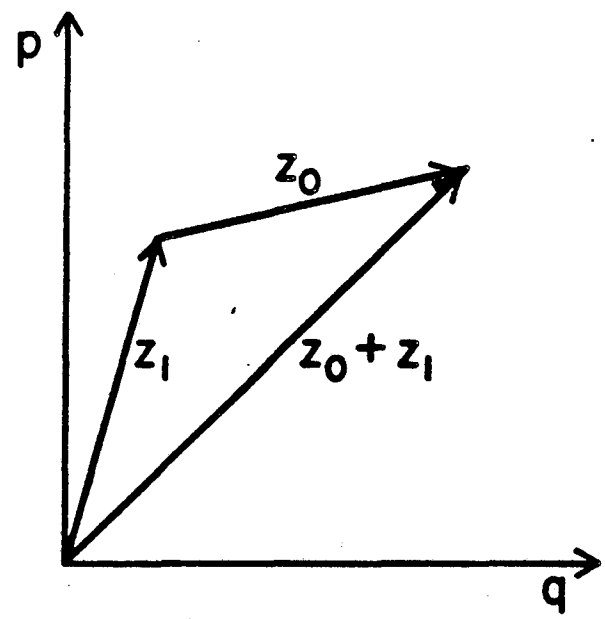

Fig. 3

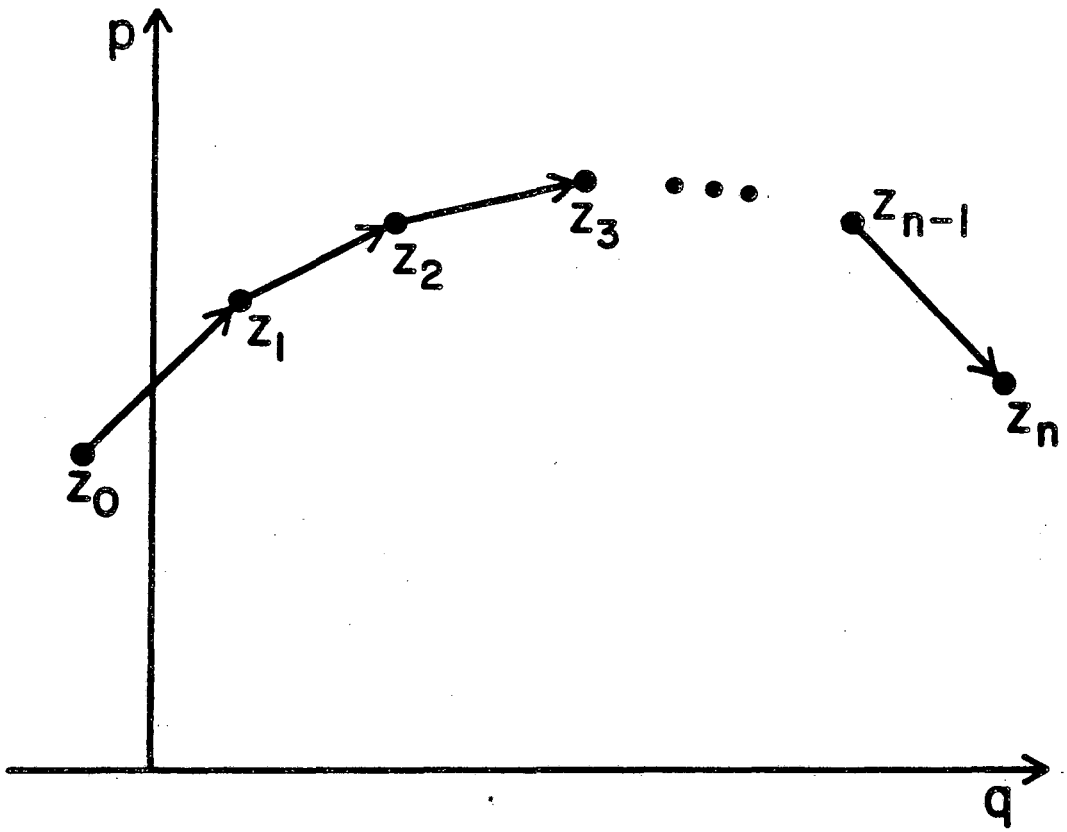

Fig. 4

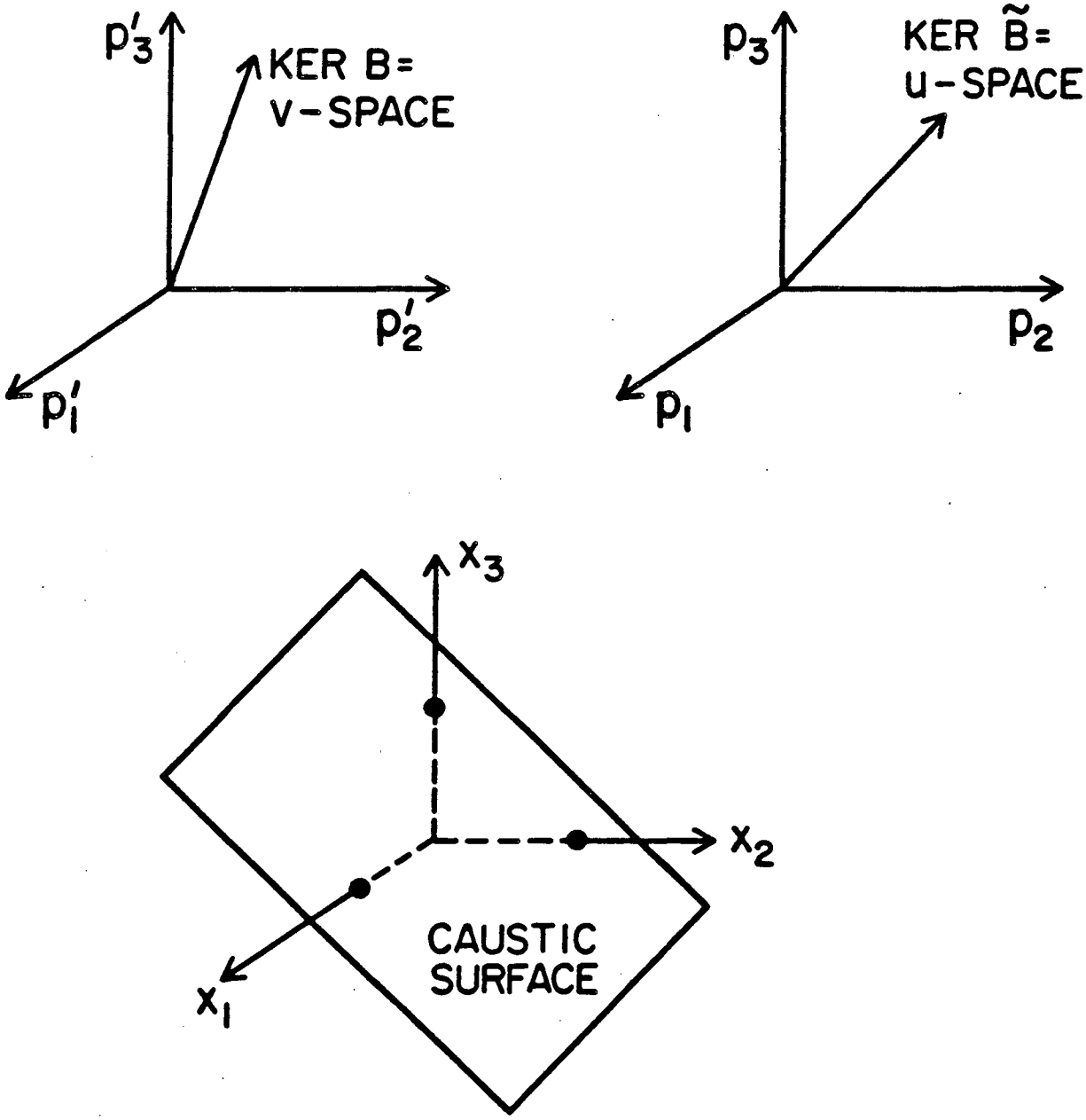
p'_3
KER B=
V-SPACE
p'_2
p'_1
p_3
KER $\tilde{B}$=
u-SPACE
p_2
p_1
x_3
x_2
x_1
CAUSTIC
SURFACE

Fig. 5

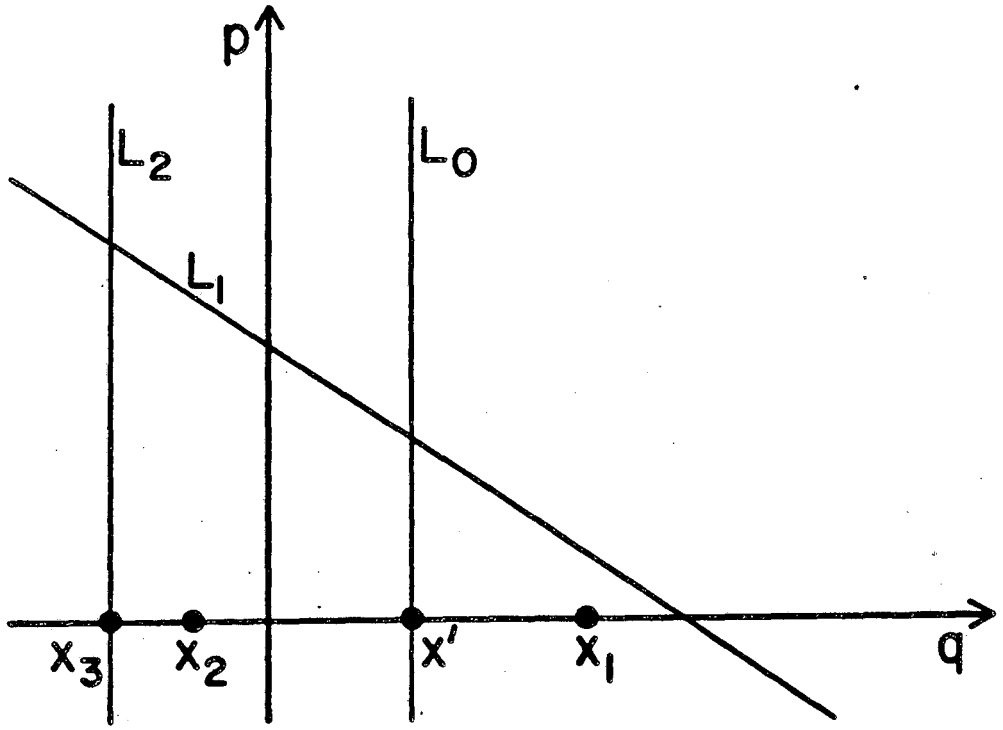

Fig. 6

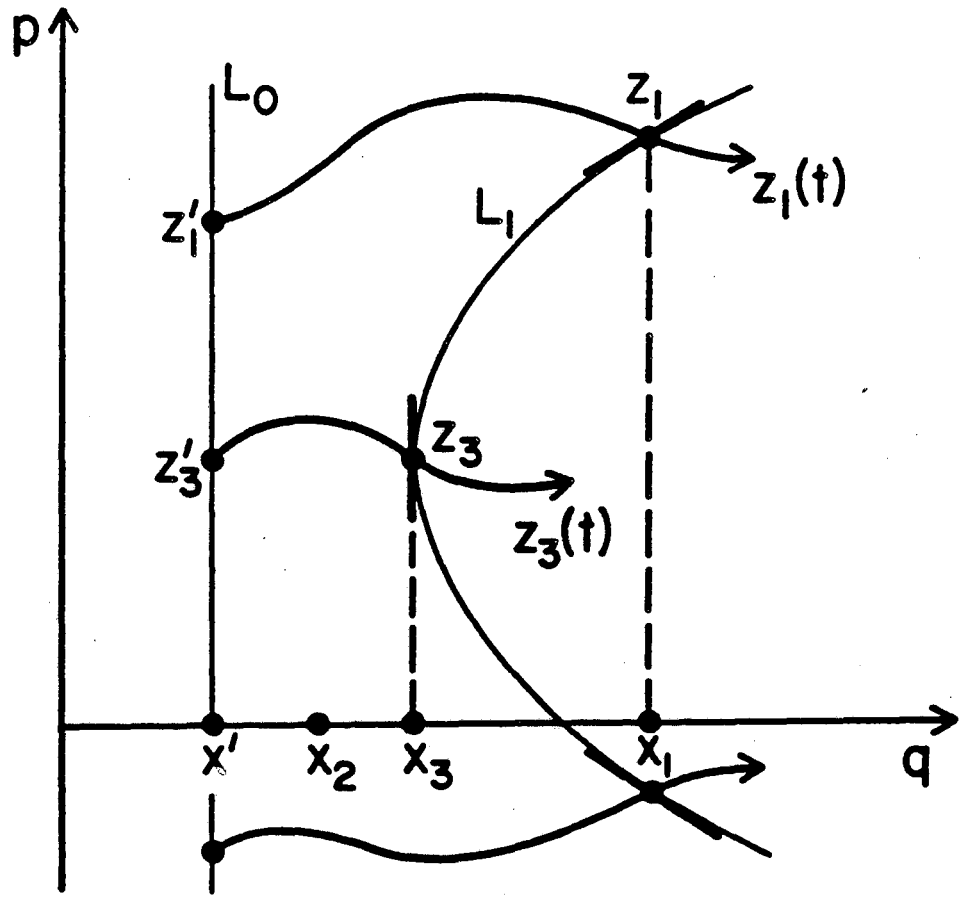

Fig. 7

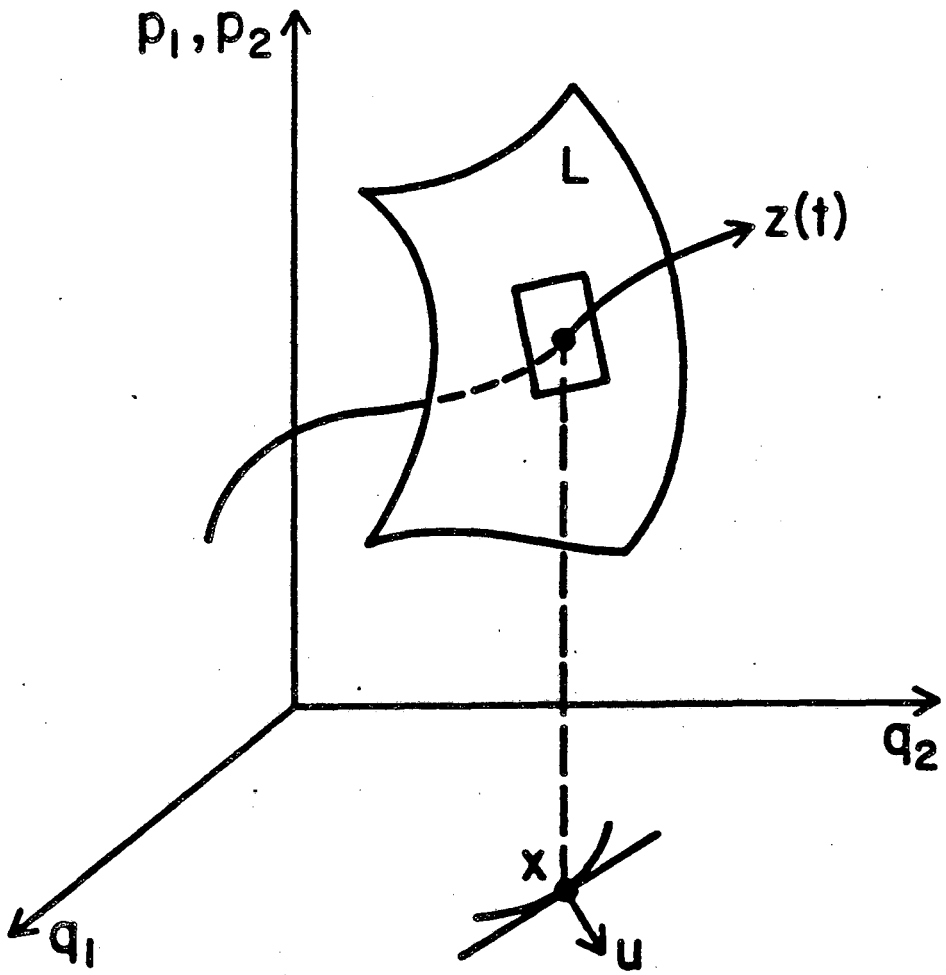

Fig. 8

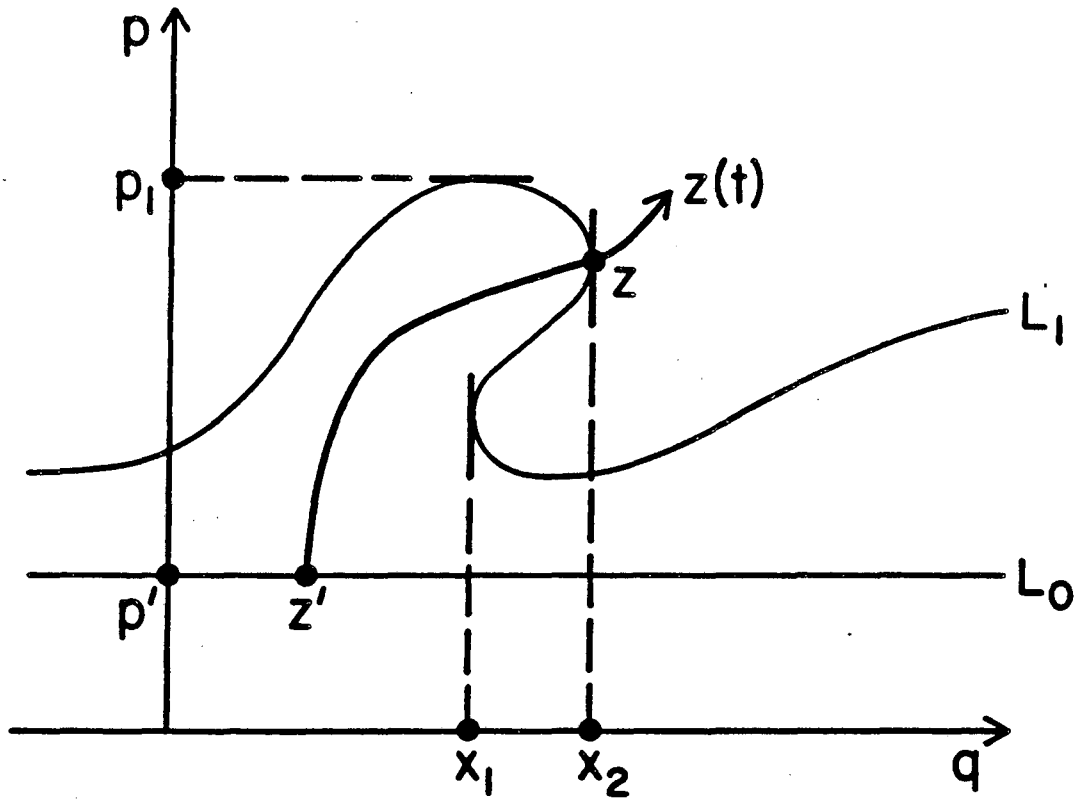

Fig. 9

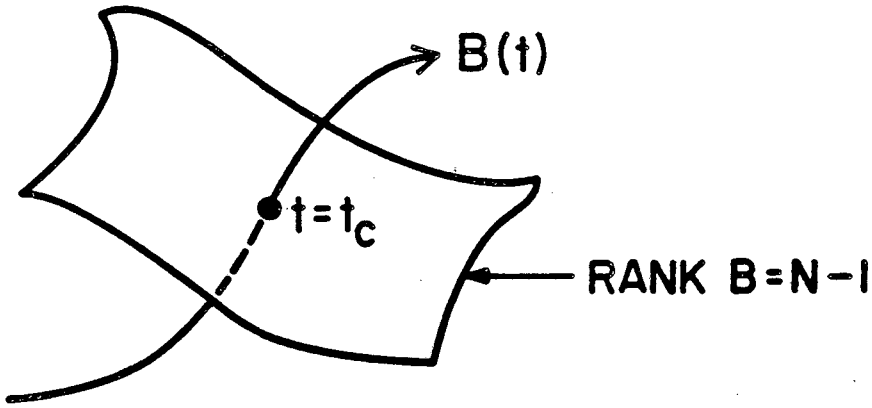

Fig. 10

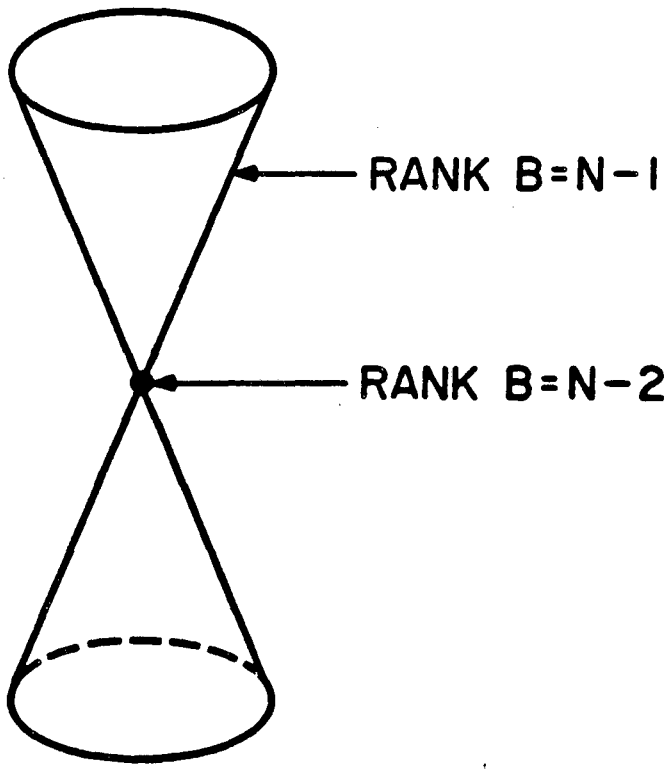

Fig. 11

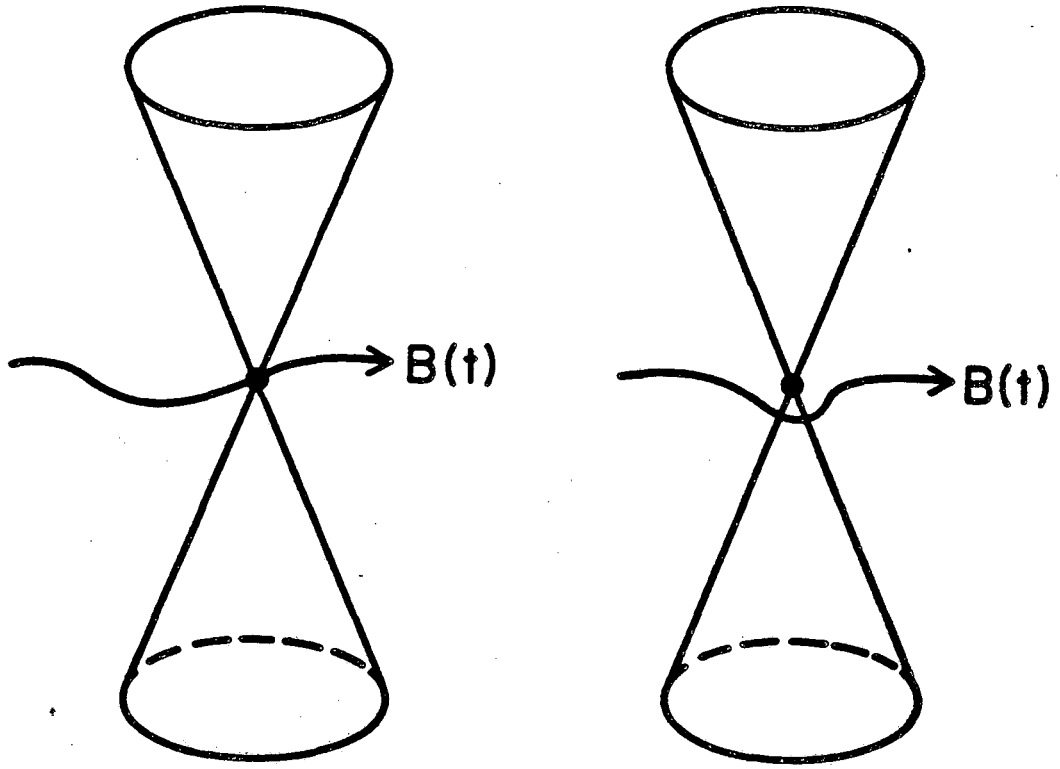

Fig. 12

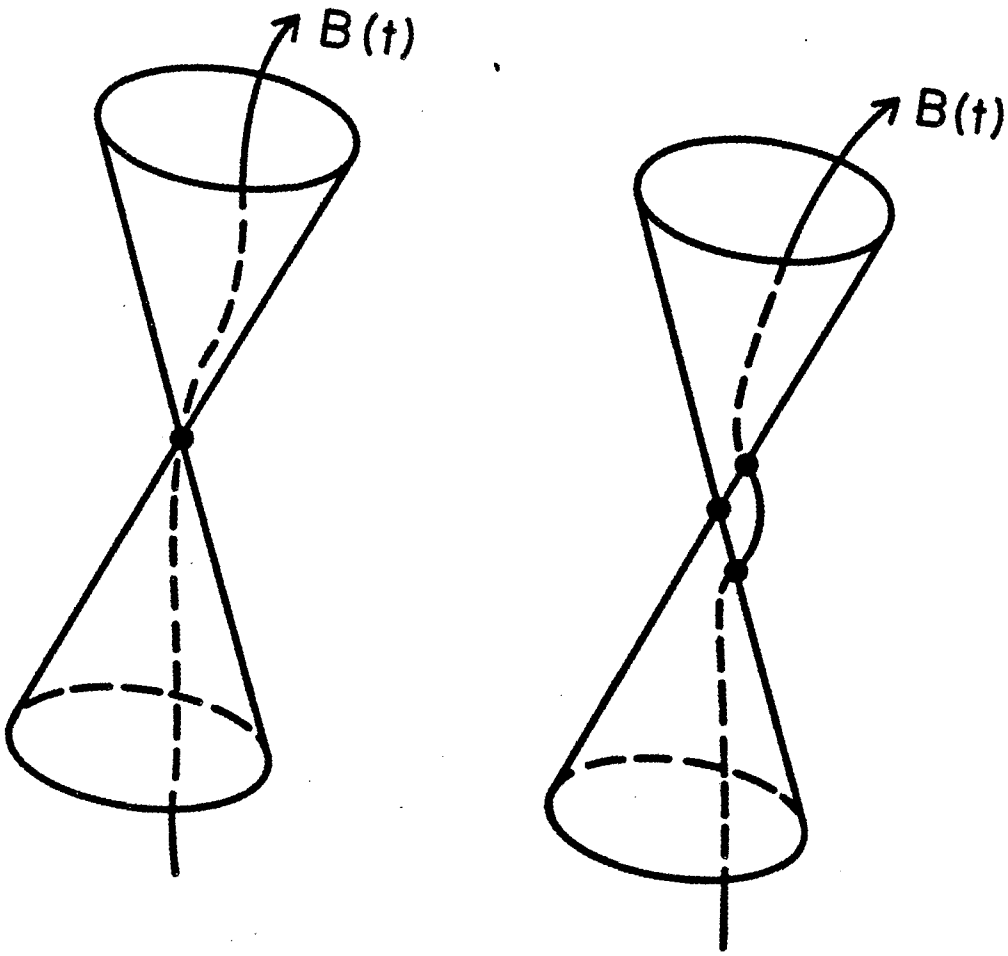

Fig. 13

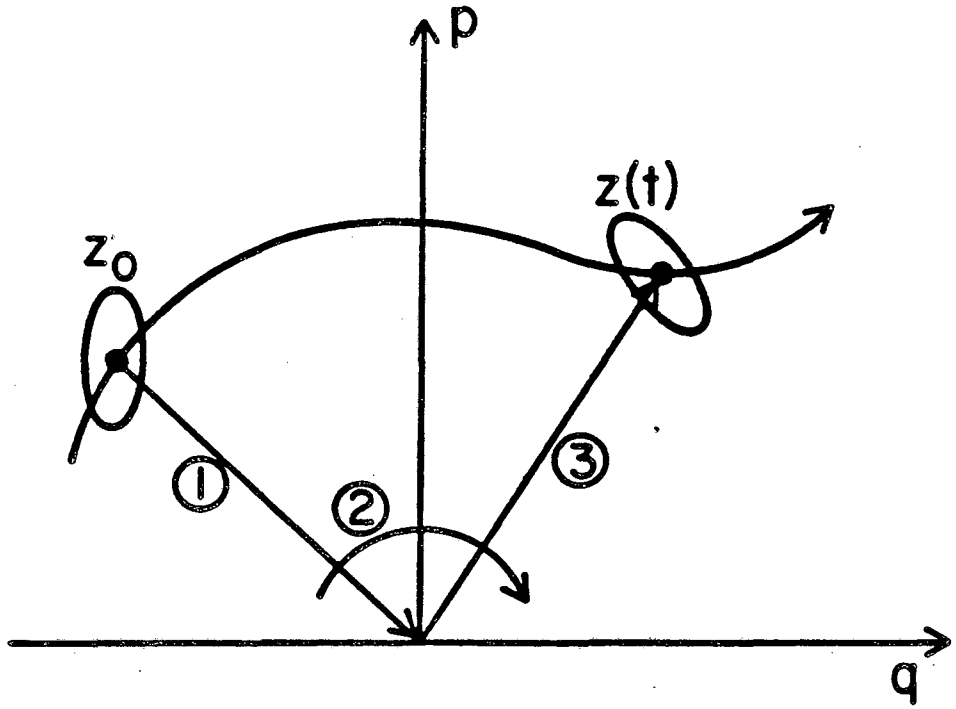

Fig. 14

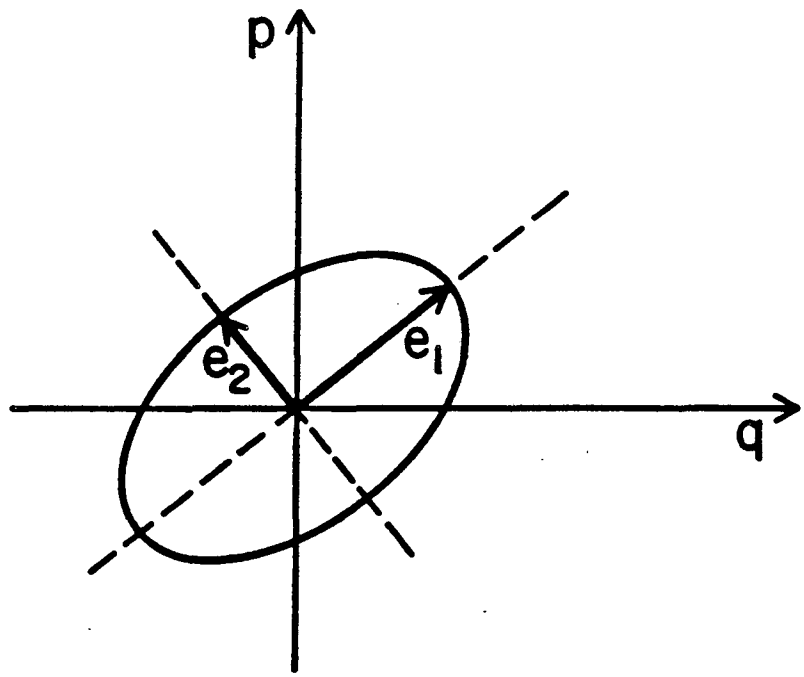

Fig. 15

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