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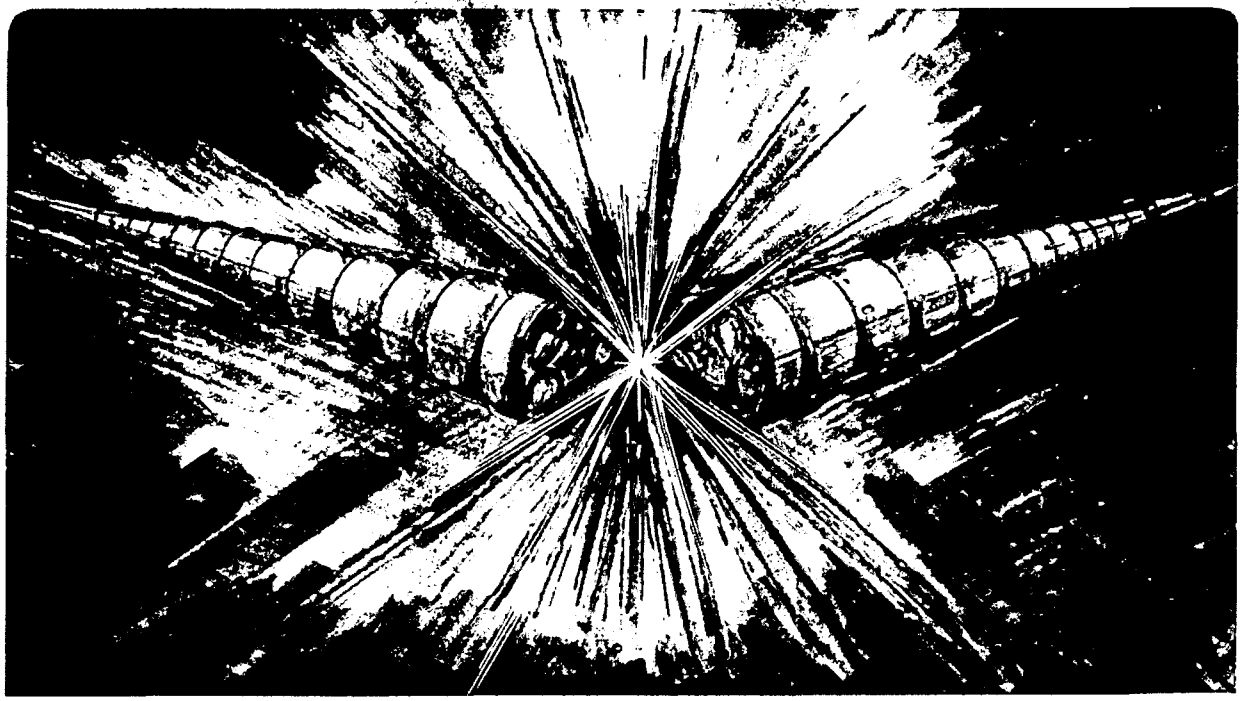

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A PHASE SPACE EIKONAL METHOD FOR TREATING WAVE EQUATIONS*

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ABSTRACT

We present a new method for treating classical (or quantal) wave equations in the short wavelength (semiclassical) regime based on a description of the wave in the ray phase space. The coherent state representation is defined, the equation which it obeys is given and solved under assumptions similar to those of conventional eikonal theory. As indicated by an example, the result is a smooth distribution on phase space which, when "projected" onto configuration space, yields a wave field with no caustic singularities.

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The concept and utility of a phase space (or joint coordinate x, wavenumber k) representation of a wave field is an old idea which has recently received much attention. The Wigner function[1] has been the subject of renewed interest in quantum mechanics[2] and optics[3] and has been a central issue in the study of semiclassical mechanics.[4,5,6] Symbols of pseudodifferential operators have become a cornerstone of modern eikonal theory with a growing mathematical literature.[7,8] The coherent state (or Glauber) representation[9,10] has been used in the study of molecular wave functions[11] and has also provided a basis for semiclassical theories.[11,12] In this Letter we consider a phase space description for application to both classical and quantal wave equations.

In the short wavelength (or semiclassical) regime, the analysis of the structure of the ray phase space and its relationship to the asymptotic eikonal form of a wave $\psi(x)$ has illuminated the reasons for two major shortcomings of the conventional eikonal method: (1) singularities in the projection of the ray manifold in phase space onto x- (or k-) space produces caustic singularities in $\psi(x)$ (or $\hat{\psi}(k)$), and (2) the existence of chaotic rays precludes the application of modern semiclassical quantization techniques to nonintegrable classical Hamiltonians. While many authors have attempted to make use of phase space representations to understand and overcome these difficulties, their approaches have been primarily *deductive* in nature: either a phase space representation of a wave field $\Psi(x,k)$ is studied[4,5,6] in terms of its relationship to the configuration space description $\psi(x)$, or vice versa. In the present paper, we present a *constructive* method: a phase space representation with reasonable properties is defined, the equation which it obeys in phase space is given, and then this equation is solved with assumptions similar to those of conventional eikonal theory. As indicated by an example, the result produces a smooth distribution on phase space which, when "projected" onto configuration space, yields an asymptotic wave field $\psi(x)$ with no

caustic singularities.

We consider the coherent state representation $\Psi(x,k)$ associated with a wave $\psi(x)$:[13]

$$\Psi(x,k) \equiv (\pi\sigma^2)^{-1/4} \int dx' \ \psi(x') \exp[-(x'-x)^2/2\sigma^2 - ik(x'-x)] \tag{1}$$

This phase space representation can be interpreted as a "smoothed local Fourier transform" of $\psi(x)$, with the averaging weighted by a gaussian of arbitrary width σ. Despite this smoothing, one has the exact inversion or "projection"

$$\psi(x) = (\pi\sigma^2)^{1/4} \int \frac{dk}{2\pi} \ \Psi(x,k) \tag{2}$$

Expressions similar to (1) and (2) can be given in terms of $\hat{\psi}(k)$. While this complex-valued quantity $\Psi(x,k)$, linear in the field ψ, will be the primary object of the following development, it induces a real non-negative phase space density $P(x,k) \equiv |\Psi(x,k)|^2$. This density is normalized on phase space when $\psi(x)$ is normalized in x-space and has the following desirable properties: $P(x,k)$ may also be obtained by locally smoothing the Wigner function $W(x,k)$ associated with ψ with a gaussian weight over a region $\Delta x \Delta k \sim 1$ in phase space

$$P(x,k) = 2 \int dx' \frac{dk'}{2\pi} \ W(x',k') \exp[-\sigma^2(k'-k)^2 - (x'-x)^2/\sigma^2].$$

Furthermore, when $P(x,k)$ is projected onto x-space, the gaussian-smoothed wave intensity is obtained

$$\langle |\psi(x)|^2 \rangle_\sigma \equiv \int \frac{dx'}{\sigma\sqrt{\pi}} \ |\psi(x')|^2 \exp[-(x'-x)^2/\sigma^2] = \int \frac{dk}{2\pi} \ P(x,k) \tag{3}$$

As will be seen, these smoothed or average properties are to a large extent responsible for the success of the method and its potential utility.

We now assume that the field ψ obeys a general linear wave equation in one dimension

$$\int dx' \ D(x,x';\omega)\psi(x') = 0 \tag{4}$$

where the kernel $\mathcal{D}(x,x';\omega)$ is taken to be Hermitian and has been Fourier-transformed in time: we thus treat the problem of normal modes or wave propagation in an inhomogeneous stationary medium, or eigenstates of the Schrödinger equation (with energy $E=\hbar\omega$, and $p=\hbar k$). Defining the phase space representation $D(x,k;\omega)$ corresponding to the kernel $\mathcal{D}$ with the Weyl rule

$$D(x,k;\omega) \equiv \int ds\ \mathcal{D}(x+\tfrac{1}{2}s, x-\tfrac{1}{2}s;\omega)\exp(-iks)$$

it can be shown[14] that $\Psi(x,k)$ satisfies the exact phase space equations

$$D(x,k;\omega)\ \exp(i\overleftrightarrow{\mathcal{L}}/2)\ \Psi(2x,2k)\exp(-2ikx) = 0 \tag{5a}$$

$$\Psi(2x,2k)\exp(-2ikx)\ \exp(i\overleftrightarrow{\mathcal{L}}/2)\ [(x/\sigma) - i\sigma k] = 0 \tag{5b}$$

where the bi-directional differential operator is $\overleftrightarrow{\mathcal{L}} \equiv \overleftarrow{\partial_x}\overrightarrow{\partial_k} - \overleftarrow{\partial_k}\overrightarrow{\partial_x}$. The ingredients of these expressions are similar to those which appear in the equations which govern the evolution of the Wigner function[1] (and indeed are most directly obtained by appealing to the calculus of Weyl symbols[14]). An equation for Ψ has been previously given[15] in terms of the Bargmann representation of the abstract operator D expressed as a normally-ordered series of creation and annihilation operators. The present formalism, however, is directly applicable to *classical* wave problems where the immediate description of D is either the kernel (as in (4)) or $D(x,k)$ (from the classical ray problem). We also note that these equations differ from those previously derived[16,17] which govern $P(x,k)$.

We now cast these equations in a form which is convenient for analysis by first transforming to complex conjugate dimensionless variables $(x,k) \to (z,\bar{z}), z \equiv (x/\sigma + i\sigma k)/\sqrt{2}$. This is a complex canonical transformation on phase space in which the Poisson bracket operator $\overleftrightarrow{\mathcal{L}}$ becomes $\overleftrightarrow{\mathcal{L}} = i(\overleftarrow{\partial_z}\overrightarrow{\partial_z} - \overleftarrow{\partial_z}\overrightarrow{\partial_z})$. Now Ψ is a function of both z and $\bar{z}$, but with (1) it can be shown that the z-dependence is particularly simple. For purposes of application

to (5), one can define[10]

$$\Psi(x,k)\exp(-ikx/2) \equiv \Phi(\bar{z})\exp(-z\bar{z}/2) \tag{6}$$

Furthermore, in these variables we have $\tilde{D}(z,\bar{z};\omega) \equiv D(x,k;\omega)$. With these changes in (5), we note that the form (6) identically satisfies (5b). Therefore, we focus our attention on the remaining equation

$$\tilde{D}(z,\bar{z};\omega)\ \exp(i\overleftrightarrow{\mathcal{L}}/2)\ \Phi(2\bar{z})\exp(-2z\bar{z}) = 0 \tag{7}$$

For short wavelength waves in a weakly inhomogeneous medium (or a semiclassical treatment of the Schrödinger equation) we now assume a solution to (7) of the form

$$\Phi(\bar{z}) \equiv A(\bar{z})\exp[i\Theta(\bar{z})] \tag{8}$$

That such a representation is appropriate for this equation can be verified with exact construction of $\Psi(x,k)$ from exact short wavelength wave fields ψ by (1). In that way, one also sees that the following eikonal-like approximations are justified in this asymptotic regime:[14]

(a) We choose our smoothing length σ to be intermediate between a typical wavelength λ of the field $\psi(x)$ and the scalelength of variation of the medium L: $\lambda \ll \sigma \ll L$.

(b) We define the "local phase space wavenumber"

$$K(\bar{z}) \equiv \frac{d\Theta(\bar{z})}{d\bar{z}}$$

(c) We assume that the (dimensionless) magnitudes of both K and $\bar{z}$ are comparable and large

$$K(\bar{z}) \sim \bar{z} \sim (\sigma/\lambda) \sim (L/\sigma) \equiv \epsilon^{-1}$$

(d) We assume the variation of the medium, the amplitude $A(\bar{z})$ and the wavenumber $K(\bar{z})$ satisfy

$$\left|\partial_z^n \tilde{D}\right| \sim \left|\partial_{\bar{z}}^n \tilde{D}\right| \sim \left|\partial_{\bar{z}}^{n+1} K\right| \sim \left|A^{-1}\partial_{\bar{z}}^n A\right| \sim \epsilon^n \qquad n \geq 0$$

Under these approximations, Eq.(7) can be expanded and analyzed order by order in ϵ. We note only one important difference between this method and the traditional eikonal procedure: low-order terms appear at all powers in the expansion of the exponential operator and subsequent differentiation. The terms can be rearranged, however, and the expression for each order can be resummed. The lowest two orders are

$$\tilde{D}(i\mathcal{K}(\bar{z}),\bar{z};\omega) = 0 \tag{9a}$$

$$\frac{d}{d\bar{z}}\left[A^2(\bar{z})\left(\frac{\partial\tilde{D}}{\partial z}\right)(i\mathcal{K}(\bar{z}),\bar{z};\omega)\right] = 0 \tag{9b}$$

These phase space dispersion and amplitude equations are analogous to similar equations obtained at lowest orders in conventional eikonal methods.[7] Equation (9a) is to be solved for $\mathcal{K}(\bar{z})$ and then the phase $\Theta(\bar{z})$ is computed by integration; the phase in this theory may be complex-valued. This equation may also be shown to induce the characteristic ray trajectories in phase space, so that in principle $\Theta(\bar{z})$ can be constructed along rays in phase space. The amplitude $A(\bar{z})$ is also transported along trajectories, although the conservative form of (9b) can be shown to imply that A has singularities only at *fixed points* in phase space (*i.e.*, where $\dot{\bar{z}} = \dot{x} = \dot{k} = 0$).

The full structure and implications of this procedure will be reported elsewhere. We conclude with a simple illustration of the implementation of these ideas. We take the wave equation (4) to be the Schrödinger equation for the quantum mechanical harmonic oscillator of frequency ω_0. For this problem the dispersion function is simply the classical Hamiltonian $D(x,k;E) = \frac{1}{2}\hbar\omega_0(\alpha^2x^2 + k^2/\alpha^2) - E$. It can be shown that the natural quantum oscillator length parameter $\alpha^{-1} \equiv \sqrt{\hbar/m\omega_0}$ satisfies the size restrictions in (a) above for the smoothing length σ, so we set $\sigma = \alpha^{-1}$. In complex variables we then have $\tilde{D}(z,\bar{z};E) = \hbar\omega_0 z\bar{z} - E$. The lowest order equation (9a) reduces to $E = i\hbar\omega_0\mathcal{K}\bar{z}$, so that one obtains $\mathcal{K}(\bar{z}) = -(iE/\hbar\omega_0)\bar{z}^{-1}$. The complex phase is therefore $\Theta(\bar{z}) = -(iE/\hbar\omega_0)\ln\bar{z}$;

the amplitude is simply $A(\bar{z}) \sim \bar{z}^{-1/2}$. Finally, inserting these solutions into (8), we find

$$\Phi(\bar{z}) \sim \bar{z}^{p} \qquad p = (E/\hbar\omega_0) - 1/2 \tag{10}$$

As has been previously noted,[15] this expression has an interesting consequence: in order for $\Phi(\bar{z})$ to be single-valued in the complex $\bar{z}$-plane, the exponent p must be a non-negative integer. Thus we obtain the exact quantization rule for the harmonic oscillator. (Note that if we neglected the higher order contribution from the amplitude, a satisfactory asymptotic quantization condition $E = n\hbar\omega_0$ would have resulted).

Of course, the harmonic oscillator spectrum is also correctly given by conventional eikonal methods; the defect in the usual theory is in the construction of the eigenfunctions. There, the amplitude suffers singularities at the turning points (caustics) and various techniques of matching piecewise solutions have been devised. In this phase space approach, however, we substitute (10) into (6) to find

$$\Psi_n(x,k) = C_n \exp[-(\alpha^2 x^2 + k^2/\alpha^2)/4 + ikx/2](\alpha x - ik/\alpha)^n \tag{11}$$

The associated normalized phase space density $P(x,k)$ in dimensionless polar coordinates is

$$P_n(x,k) = |\Psi(x,k)|^2 = 2^{-n}(n!)^{-1} r^{2n} \exp(-r^2/2) \tag{12}$$

$$r^2 \equiv \alpha^2 x^2 + k^2/\alpha^2$$

a form which is peaked at the radius of the classical torus $r_n \sim \sqrt{2n}$ (yet is nonsingular there, an artifact of the broadening in the wave problem). The remarkable feature of this result is that when (11) is projected by (2) onto x-space, the *exact* eigenfunctions are obtained. Furthermore, projecting (12) with (3) produces a smoothed wave intensity (see Fig.1) which compares favorably with the classical probability density almost everywhere; in the vicinity of the turning points, however, this intensity remains finite as it deviates from the classical

behavior (which is singular). This result is due to the fact that the asymptotic phase space density (12) incorporates the wave broadening of the classical torus. (One should compare this with the asymptotic form of the Wigner function[4] in this case, which becomes singular like the classical density on the classical torus.) In some experimental applications, this result is preferable to *either* the purely wave solution (which exhibits a rapidly oscillating phase) or the purely classical solution (which is singular at caustics). The phase may be obtained from (2) if desired.

Naturally, one should not place too much emphasis on the success of a method when applied to the harmonic oscillator problem. Nevertheless, we suggest that the structure of this theory, which is based on the asymptotic analysis of a wave equation in phase space (where caustics are absent), holds the promise of producing a nonsingular uniform approximation to $\psi(x)$ in a typical problem. In this regard, we note that a similar result has been obtained (also for the harmonic oscillator) from the study of canonical transformation theory of the coherent state formalism by Weissman.[12] Another advantage of this approach is that k is treated as an independent variable (rather than the gradient of the phase as in conventional eikonal methods); this may provide a basis for treating waves associated with chaotic rays (where $k(x)$ is not defined). The procedure given can be easily extended to N dimensions; although this method doubles the number of independent variables, the problem is ultimately reduced to N complex dimensions.

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Figure Captions

FIG. 1. Comparison of configuration space probability densities (wave intensities) for the harmonic oscillator state $n = 60$. Solid oscillatory curve is exact $|\psi_{60}(x)|^2$, dotted singular curve is exact classical ray probability density, and solid non-oscillatory curve is $\langle|\psi_{60}(x)|^2\rangle$, the gaussian-smoothed wave intensity obtained by projecting $P_{60}(x,k)$ (with $\sigma = \alpha^{-1}$) from phase space onto x-space.

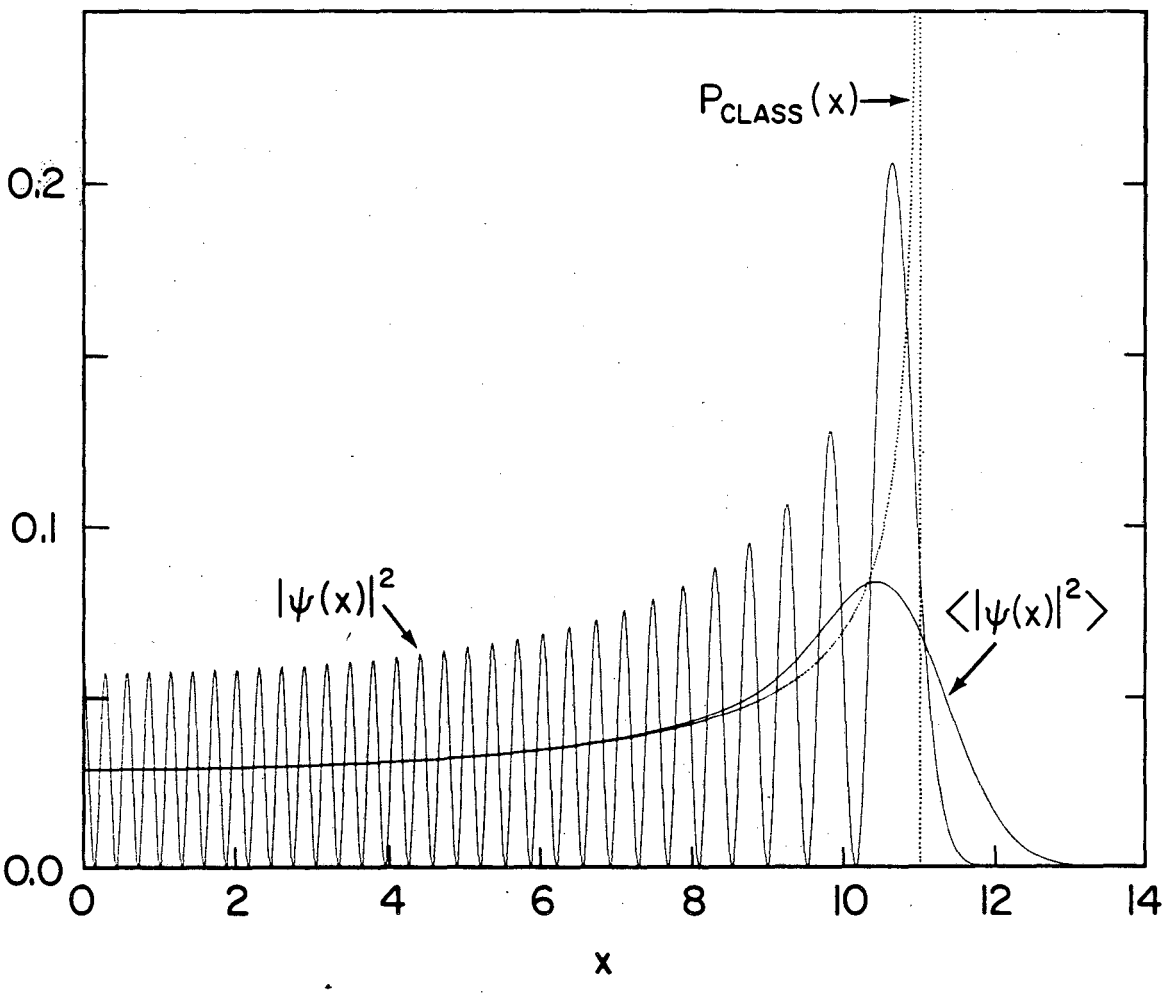

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Fig. 1

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