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SEMICLASSICAL THEORY OF DIFFRACTION IN ELASTIC SCATTERING*

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ABSTRACT

It is shown that diffraction from a purely repulsive potential can be described by a simple extension of the Ford and Wheeler semiclassical analysis. The diffraction arises from interference between a "classically allowed" and a "classically forbidden" contribution to the scattering amplitude. A numerical example is presented to show that the semiclassical description is quite quantitative.

I. INTRODUCTION

The semiclassical theory of elastic scattering--the scattering of two atoms, for example, at least one of which is in a ^1S state--is one of the outstanding triumphs of molecular collision theory.[1-3] Quantum effects, such as rainbow structure in the differential cross section and glory oscillations in the energy dependence of the total cross section, can be understood simply as interference between different classical-like contributions to the scattering amplitude. The description of these quantum effects afforded by semiclassical theory is, in addition, quantitatively accurate and thus a useful aid in analyzing experimental results.

One quantum phenomenon for which the usual semiclassical treatment[1,2] fails is diffraction from a monotonically repulsive potential. If the potential $V(r)$ is monotonically repulsive,[4] then the classical deflection function $\Theta(L)$ is also monotonic and there will thus be only one value of orbital angular momentum L which satisfies the classical condition

$$\Theta(L) = \pm\,\theta \quad . \tag{1.1}$$

Figure 1 shows such a monotonic deflection function and indicates the graphical solution of Eq. (1.1). In this situation the usual semiclassical analysis[1,2] gives only one contribution to the semi-classical amplitude and there is thus no interference structure; i.e., for this monotonic case the usual analysis gives

$$\sigma_{SC}(\theta) = \sigma_{CL}(\theta) \quad , \tag{1.2}$$

(SC = semiclassical, CL = classical). It is known, however, that an interference structure can exist in these cases--it is seen experimentally[5] and appears in a fully quantum mechanical calculation[6]--and the usual conclusion is that such diffraction effects simply lie outside the realm of semiclassical theory.

The purpose of this paper is to show that a straight-forward extension of the usual semiclassical treatment[1,2] accounts for these diffraction effects in a completely natural way; it is seen that even for the purely repulsive case they arise from interference of different classical-like contributions to the scattering amplitude. A similar analysis has been carried out by Knoll and Schaeffer,[7] with particular application to the case of a complex optical potential. The main difference between the present work and that of ref. 7 is that here there is no explicit appearance of complex-valued classical trajectories (although such are implicit), and the emphasis is on the ordinary case of a real potential function. The theoretical development is carried out in Section II, and a numerical example is presented in Section III to show that the description which results is also quite quantitative.

II. SEMICLASSICAL ANALYSIS

The differential cross section for elastic scattering is given by

$$\sigma(\theta) = |f(\theta)|^2 \quad , \tag{2.1}$$

and the standard quantum mechanical expression for the scattering amplitude is

$$f(\theta) = (2ik)^{-1} \sum_{\ell=0}^{\infty} (2\ell+1)\,(e^{2i\eta_\ell}-1)\,P_\ell(\cos\theta) \quad . \tag{2.2}$$

With the usual semiclassical approximations:[1,2]

$$\sum_{\ell=0}^{\infty} \rightarrow \int_{-\frac{1}{2}}^{\infty} d\ell \tag{2.3a}$$

$$P_\ell(\cos\theta) \rightarrow \frac{\sin[\frac{\pi}{4} + (\ell+\frac{1}{2})\theta]}{[\frac{\pi}{2}\;(\ell\;\;\frac{1}{2})\sin\theta]^{1/2}} \tag{2.3b}$$

$$\eta_\ell \rightarrow \eta_\ell^{\mathrm{WKB}} \quad , \tag{2.3c}$$

it is easy to show that Eq. (2.2) becomes

$$f(\theta) = k^{-1}(2\pi\sin\theta)^{-1/2}\,[e^{-i\frac{\pi}{4}}\,I_+(\theta) - e^{i\frac{\pi}{4}}\,I_-(\theta)] \quad , \tag{2.4}$$

where

$$I_{\pm}(\theta) = \int_0^{\infty} dL \quad L^{1/2} \exp\{i[2\eta(L) \mp L\theta]\} \quad , \tag{2.5}$$

and where $L \equiv \ell + \frac{1}{2}$ and $\eta(L)$ is now the WKB phase shift. (The approximation in Eq. (2.3b) is valid only for $L\theta > 1$; a semi-classical approximation valid for all θ, $0 < \theta < \frac{\pi}{2}$, is

$$P_{\ell}(\cos\theta) \rightarrow \left(\frac{\theta}{\sin\theta}\right)^{1/2} J_o(L\theta) \quad , \tag{2.6}$$

but this more accurate approximation is not needed for our present purposes.)

The next step in the normal development is to evaluate the integrals $I_+(\theta)$ and $I_-(\theta)$ of Eq. (2.5) via the stationary phase approximation.[8] For $I_+(\theta)$ the stationary phase condition is

$$\Theta(L) = \theta \quad , \tag{2.7}$$

where $\Theta(L)$, the classical deflection function, is related to the WKB phase shift in the usual way:[1,2]

$$\Theta(L) = 2\eta'(L) \quad . \tag{2.8}$$

For the case of a monotonically repulsive deflection function, as shown in Figure 1, it is clear that Eq. (2.7) has one and only one root; let $L_1(\theta)$ denote this root. The stationary phase approximation then gives $I_+(\theta)$ as

$$I_{+}(\theta) \simeq \left[\frac{2\pi i L_1}{\theta'(L_1)}\right]^{1/2} \exp\{i[2\eta(L_1) - L_1\theta]\} \quad . \tag{2.9}$$

The stationary phase condition for the integral $I_{-}(\theta)$ is

$$\Theta(L) = -\theta \quad , \tag{2.10}$$

for which there are clearly no roots in the case of a purely repulsive potential; within the stationary phase approximation one thus has

$$I_{-}(\theta) \simeq 0 \quad , \tag{2.11}$$

and the net amplitude of Eq. (2.4) is simply

$$f(\theta) = f_1(\theta) \quad , \tag{2.12}$$

where

$$f_1(\theta) = k^{-1}\left[\frac{iL_1}{\sin\theta\ \Theta'(L_1)}\right]^{1/2} \exp\{i[2\eta(L_1) - L_1\theta - \tfrac{\pi}{4}]\}. \tag{2.13}$$

This is the usual result for the case of a monotonic deflection function,[4] and the cross section which results is the purely classical expression,

$$\sigma(\theta) \simeq \sigma_{CL}(\theta) \equiv \frac{L_1}{k^2 \sin\theta\ |\Theta'(L_1)|} \quad , \tag{2.14}$$

and thus shows no interference structure.

The necessary extension of this standard analysis is to note that although Eq. (2.10), the stationary phase condition for $I_-(\theta)$, has no real roots, there will in general be complex values of L which satisfy Eq. (2.10), the mathematical meaning of which is the following. Finding no real points of stationary phase for the integral $I_-(\theta)$, one analytically continues the integrand and looks for complex points of stationary phase, i.e., complex roots to Eq. (2.10); finding such a root, call it L_2, the integral over L is deformed into a contour integral in the complex L-plane which passes through L_2 (which is also called a "saddle point"). The saddle point method, or method of deepest descent[9] is then applied to this contour integral, all of which gives the following asymptotic approximation to $I_-(\theta)$:

$$I_-(\theta) \simeq \left[\frac{2\pi i L_2}{\Theta'(L_2)}\right]^{1/2} \exp\{i[2\eta(L_2) + L_2\theta]\} \quad , \tag{2.15}$$

$L_2 \equiv L_2(\theta)$ being the (complex) root of Eq. (2.10). One notes that the result for the asymptotic approximation to $I_-(\theta)$, Eq. (2.15), has exactly the same form as that for $I_+(\theta)$, Eq. (2.9), with L_1 and L_2 being the roots of Eq. (2.7) and (2.10), respectively.

In the language of Miller's "classical S-matrix" theory[10] of molecular collisions one says that $I_+(\theta)$ has a "classically allowed" contribution--i.e., there is a real-valued classical trajectory for which the final scattering angle is $+\theta$--and that $I_-(\theta)$ has only a "classically forbidden" contribution--i.e., no real-valued classical trajectory has a scattering angle $-\theta$, but there are complex-valued ones which do so. If there is more than one complex root to Eq. (2.10), then one chooses the one for which the imaginary part of the phase (the classical action) in Eq. (2.15) is the smallest. (The imaginary part of the phase must always be positive; if L_2 is a root of Eq. (2.10), then it is clear that L_2^*, its complex conjugate, is also a root. If the classical action for the root L_2 has a negative imaginary part, then that for L_2^* will clearly be positive and thus the desired choice of the two roots L_2 and L_2^*.)

With the asymptotic approximation to $I_-(\theta)$ in Eq. (2.15), the scattering amplitude is now given by

$$f(\theta) = f_1(\theta) + f_2(\theta) \quad , \tag{2.16}$$

with $f_1(\theta)$ given by Eq. (2.13), and with

$$f_2(\theta) = -k^{-1}\left[\frac{iL_2}{\sin\theta\ \Theta'(L_2)}\right]^{1/2} \exp\{i[2\eta(L_2) + L_2\theta + \tfrac{\pi}{4}]\}. \tag{2.17}$$

(Note again that the classically allowed term, $f_1(\theta)$, and classically forbidden term, $f_2(\theta)$, have essentially the same structure in terms of their respective stationary phase points L_1 and L_2.) It is now clear that interference effects can appear in the cross section,

$$\sigma_{SC}(\theta) = |f_1(\theta) + f_2(\theta)|^2$$

$$= |f_1(\theta)|^2 + |f_2(\theta)|^2 + 2\,\mathrm{Re}[f_1(\theta)^* f_2(\theta)] \quad , \tag{2.18}$$

and this is the origin of the diffraction effects discussed above. For highly classical-like systems one will have

$$\mathrm{Im}\;[2\eta(L_2) + L_2\theta] \gg 0 \quad , \tag{2.19}$$

and the classically forbidden contribution will be negligible and diffraction thus absent. For light atoms and sufficiently low energy, however, it will survive.

In concluding the Section it is interesting to show qualitatively that Eq. (2.10) will indeed have complex roots for typical atom-atom potential functions. The classical deflection function $\Theta(L)$ has essentially the same algebraic behavior as the potential function $V(r)$. If, for example, the potential is exponentially repulsive, then one will approximately have

$$\Theta(L) \simeq A\, e^{-L/L_o} \quad . \tag{2.20}$$

The roots of Eq. (2.10) in this case are given by

$$\begin{aligned} L_2 &= -L_o\, \ell n(-\theta/A) \\ &= L_o\, \ell n(A/\theta) + i\pi L_o\,(2n+1) \quad , \end{aligned} \tag{2.21}$$

$n = 0, \pm 1, \pm 2, \pm 3, \ldots$; the one for which the imaginary part of the action is positive and smallest corresponds to choosing $n = 0$.

Another repulsive potential function commonly used is an inverse power potential,

$$V(r) \sim 1/r^s \quad ; \tag{2.22}$$

the deflection function in this case will behave approximately as

$$\Theta(L) \sim (L_o/L)^s \quad , \tag{2.23}$$

for L not too small. The roots to Eq. (2.10) in this case are given by

$$L_2 = L_o\, \theta^{-1/s}\, e^{i\frac{\pi}{s}(2n+1)} \quad , \tag{2.24}$$

$n = 0, \pm 1, \pm 2, \ldots$, the dominant contribution again corresponding to the choice $n = 0$; thus

$$\mathrm{Re}\, L_2 = L_o\, \theta^{-1/s} \cos(\pi/s) \tag{2.25a}$$

$$\mathrm{Im}\, L_2 = L_o\, \theta^{-1/s} \sin(\pi/s) \quad . \tag{2.25b}$$

It is interesting to observe that for the Coulomb case, $s = 1$, Eq. (2.25) shows that L_2 is real and negative, i.e., there are no complex roots to Eq. (2.10). This is as it should be, of course, for it is well-known that the classical cross section happens to agree exactly with the quantum result for a Coulomb potential, and there is thus no diffraction in this case; fortunately, this extended semiclassical theory predicts none. Only for $s > 2$ does Eq. (2.25) give a complex value of L_2 with $\mathrm{Re}\, L_2 > 0$. This simply says that diffraction occurs only if the repulsive wall of the potential is sufficiently "hard".

III. NUMERICAL EXAMPLE

To give a numerical illustration of the theory developed in the preceeding section we have chosen a monotonic classical deflection function which shows prominent diffraction:

$$\Theta(L) = \pi \frac{1 + e^{-L_o}}{1 + e^{(L-L_o)}} \quad , \tag{3.1}$$

where L_o is a constant. The particular repulsive potential function to which this corresponds can be determined[11] but it is irrelevant for our present purposes. The one parameter in the model, L_o, is a measure of how quantum-like the system is, small (large) L_o corresponding to a quantum (classical)-like system; roughly speaking, L_o is the number of partial waves which contribute significantly to the partial wave sum in Eq. (2.2).

With the deflection function of Eq. (3.1) one can compare the classical cross section (which is also the usual semiclassical result for this monotonic situation), our semiclassical cross section, and a completely quantum cross section. The phase shift is determined from the deflection function by integrating Eq. (2.8), i.e.,

$$2\eta(L) = -\int_L^\infty dL' \; \Theta(L') \quad , \tag{3.2}$$

and for the deflection function in Eq. (3.1) this gives

$$2\eta(L) = -\pi\ (1 + e^{-L_o})\ \ell n\ [1 + e^{(L_o - L)}] \quad . \qquad (3.3)$$

The quantum cross section can then be computed from the partial wave expression, Eq. (2.2).

The two points of stationary phase L_1 and L_2, the roots of Eq. (2.7) and (2.10), are easily found to be

$$L_1(\theta) = L_o + \ell n\ [\frac{\pi}{\theta}\ (1 + e^{-L_o}) - 1] \qquad (3.4a)$$

$$L_2(\theta) = L_o + \ell n\ [\frac{\pi}{\theta}\ (1 + e^{-L_o}) + 1] + i\pi \quad ; \qquad (3.4b)$$

the classical and semiclassical cross sections can then be computed from Eq. (2.14) and Eqs. (2.13), (2.17)-(2.18), respectively.

Figure 2 shows the classical, semiclassical, and quantum mechanical cross sections for this model problem for $L_o = 20$. The diffraction effects are prominent for this case but the semiclassical theory describes them quite well. The classical result, of course, shows no interference structure. One can conclude, therefore, that the physical origin of diffraction is the interference between the two classical-like contributions to the scattering amplitude discussed in Section II.

IV. CONCLUDING REMARKS

One thus sees that diffraction is also accurately described by semiclassical theory provided one includes the classically forbidden contribution to the scattering amplitude in addition to the usual classically allowed term. The analysis presented in Section II is a simple example of the more general classical S-matrix theory[10] in which one includes complex and real-valued classical trajectories which obey the appropriate boundary conditions.

One usually assumes that classically forbidden contributions are negligible in comparison to classically allowed ones; even though the classically allowed contribution is indeed larger for the example treated in Section III, the classically forbidden contribution is not entirely negligible. One may very well expect this also to be the case in applications of classical S-matrix theory to more complicated collision processes.

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FIGURE CAPTIONS

Figure 1. A typical classical deflection function for a purely repulsive potential; the solution of the equation $\Theta(L) = \theta$ is indicated.

Figure 2. The classical (dotted line), semiclassical (dashed line), and quantum mechanical (full line) cross sections corresponding to the classical deflection function in Eq. (3.1) with $L_o = 20$.

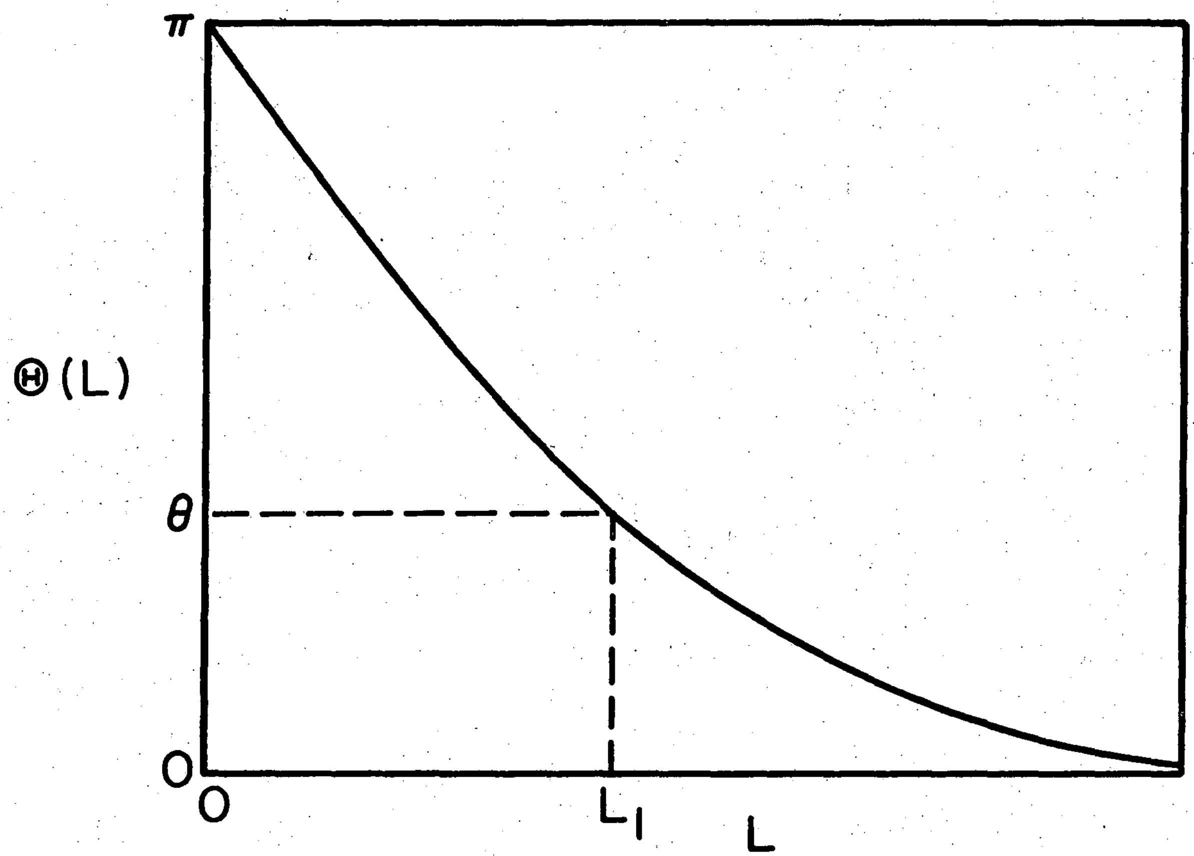

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Fig. 1

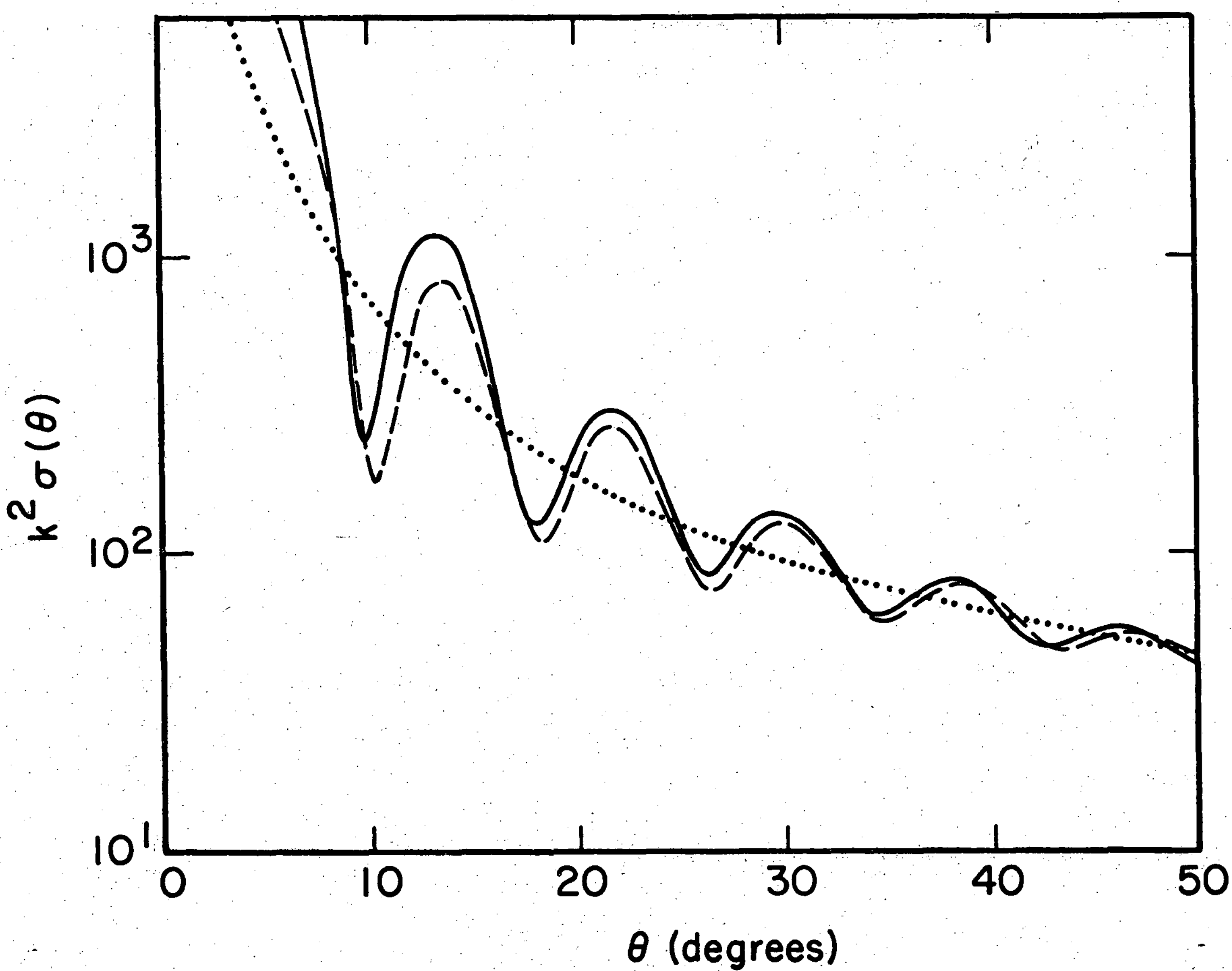

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Fig. 2

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