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Interpretation of Interference Structure in Elastic Scattering Using the Semiclassical Action*†

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We show how to interpret the Ford-Wheeler semiclassical expression for the scattering amplitude as a integral, over both positive and negative impact parameters, of a quantity depending on the action. This formulation clarifies the relationship between the action and the phase of the semiclassical expression for the scattering amplitude. Using this formulation, we show that interference processes in both one- and two-channel elastic scattering are analogous to those occurring in the two-slit diffraction of light.

I. INTRODUCTION

In quantum-mechanical treatments of scattering, the impact parameter cannot be known because of the uncertainty principle (the transverse momentum before the collision is fixed by the incident angle and momentum). If the de Broglie wavelength

$$\lambdabar=\hbar/p=\hbar(2mE)^{-1/2} \tag{1}$$

is much smaller than the scale of variation of the potential, however, the impact parameter b becomes physically significant. One can imagine that each portion of the incident wave can be followed through the collision; its deflection being determined only by the impact parameter b (and the reduced potential).

This idea forms the basis of this paper. In Sec. II, we show how the semiclassical scattering amplitude may be expressed as an integral over all impact parameters, and in Sec. III, we show the close relationship between the action and the phase of various contributions to the scattering amplitude. In Sec. IV, we give a simple interpretation of interference phenomena in single-channel (one-potential) scattering, which is extended to two-channel interference phenomena (e.g., resonant exchange) in Sec. V.

II. SCATTERING AMPLITUDE INTEGRAL

Ford and Wheeler[1] have shown that a considerable mathematical simplification in the usual partial-wave treatment of scattering results when the de Broglie wavelength is smaller than the scale of variation of the potential. By making a related set of approximations, collectively called the semiclassical approximation, they show that the scattering amplitude may be written

$$f(\theta) = -\bar{\lambda}(2\pi\sin\theta)^{-1/2}\int_0^\infty (l+\tfrac{1}{2})^{1/2} \times (e^{i\Phi_+} - e^{i\Phi_-})\,dl \ , \quad (2)$$

where $$\Phi_\pm = 2\eta(l) \pm (l+\tfrac{1}{2})\theta \pm \tfrac{1}{4}\pi \ , \quad (3)$$

and the phase shift $\eta(l)$ is to be considered a continuous function of l (and may be found consistently from the JWKB approximation).

We introduce the impact parameter by means of the usual correspondence relationship

$$(l+\tfrac{1}{2}) \longleftrightarrow |L|/\hbar \longleftrightarrow b/\bar{\lambda} \ . \quad (4)$$

The angular momentum L can have either sign, but l (and also b) is restricted to positive values. We rewrite Eqs. (2) and (3) using the impact parameter

$$f(\theta) = -(2\bar{\lambda}\pi\sin\theta)^{-1/2}\int_0^\infty b^{1/2}(e^{i\Phi_+} - e^{i\Phi_-})\,db \ , \quad (5)$$

where $$\Phi_\pm = 2\eta(b) \pm b/\bar{\lambda}\theta \pm \tfrac{1}{4}\pi \ . \quad (6)$$

The function $\eta(b)$ equals $\eta(l)$ when b equals $l\bar{\lambda}$. [This follows naturally from the JWKB expression for $\eta(l)$.] $\eta(b)$ is also closely related to the classical phase.[2]

The expression in Eq. (5) is physically misleading because only regions with $b > 0$ contribute to the scattering amplitude, while it is clear (see Fig. 1) that processes with either a net repulsive interaction and positive impact parameter or a net attractive interaction and negative impact parameter can contribute to the scattering at positive angles. This fact is accounted for by the two terms in Eq. (5): the term Φ_- contributes for repulsive scattering, the Φ_+ for attractive scattering.

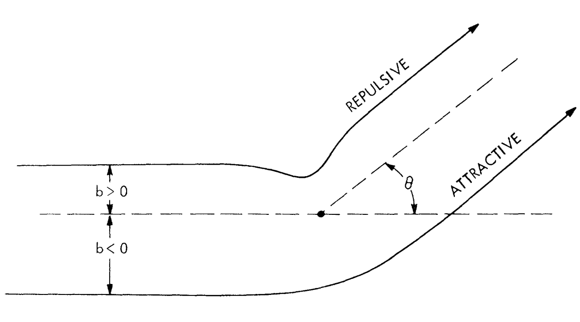

FIG. 1. Trajectories for a collision with attractive interaction (and negative impact parameter) and a collision with dominantly repulsive interaction (and positive impact parameter), which both result in the same deflection χ.

A more meaningful expression may be obtained by changing the variable of integration for the Φ_+ term from b to $-b$, since then the attractive scattering will occur with a negative impact parameter, as it should. We accomplish this by making the substitution $b' = be^{-i\pi}$, so that the integral with Φ_+ in Eq. (5) becomes

$$\int_0^\infty db\, b^{1/2} \exp\{i[2\eta(b) + b\theta/\bar{\lambda} + \tfrac{1}{4}\pi]\}$$
$$= \int_0^{-\infty} db'(e^{-i\pi}b')^{1/2} \exp\{i[2\eta(-b') - b'\theta/\lambda + \tfrac{1}{4}\pi]\}$$
$$= \int_{-\infty}^{0} db' b'^{1/2} \exp\{i[2\eta(-b') - b'\theta/\lambda - \tfrac{1}{4}\pi]\} \ . \quad (7)$$

Note that $\eta(-b) = \eta(b)$, so that the exponent in this expression is the same as the exponent in the Φ_- integral in Eq. (5). We can now write the scattering amplitude as an integral containing Φ_- over the whole range of b:

$$f(\theta) = \bar{\lambda}(2\pi\sin\theta)^{-1/2}\int_{-\infty}^{\infty} db\, b^{1/2} \times \exp\{i\Phi[2\eta(b) - \theta b/\bar{\lambda} - \tfrac{1}{4}\pi]\} \ . \quad (8)$$

III. ACTION AND PHASE

This expression is simpler and more natural than Eq. (5), since all impact parameters now can contribute to the scattering amplitude. An additional simplification results because the exponent is closely related to the action. Smith[2] has defined the collision action A (hereafter called simply the action) to be the difference between the total action with the potential V "on" and with it "off" (in which case the path is straight):

$$A(\theta, b) = \int \vec{p}\cdot d\vec{q} - \int_{V=0} \vec{p}_0 \cdot d\vec{q}_0) \ , \quad (9)$$

where the total energy is fixed. He shows that each term may be broken into radial and tangential components, the radial component being twice the JWKB phase shift, and the tangential component being proportional to the angular momentum and to the scattering angle:

$$A(\theta, b) = 2\hbar\eta(b) - \hbar b\theta/\bar{\lambda} \ . \quad (10)$$

The radial component is independent of the sign of b [that is, $\eta(-b) = \eta(b)$], while the angular term shows more action for collisions with $b < 0$, since this corresponds to the "outside track."

Our expression for the scattering amplitude [Eq. (8)] is simply expressed in terms of the action

$$f(\theta)=(2\pi ƛ \sin\theta)^{-1/2} e^{-i\pi/4} \int_{-\infty}^{\infty} db\, b^{1/2} e^{iA(\theta, b)/\hbar} . \quad (11)$$

This expression is similar to the formulation of quantum mechanics that is due to Feynman,[3] which was extended by Motz[4] and Pechukas[5] (who considered semiclassical scattering theory), in which the amplitude for a particle to move from one place to another is expressed as an integral over all possible trajectories of $\exp(iS/\hbar)$, where S is the action. (In our analogy, the $b^{1/2}$ weights the trajectories with larger b more heavily because there are more of them.)

Our expression for the scattering amplitude may be integrated by the stationary phase technique, since the action is a rapidly changing function of b except at a few impact parameters b_i, where

$$\frac{\partial}{\partial b} A(\theta, b)\Big|_{b_i}=0 , \quad (12)$$

which occurs where

$$2\eta'(b_i)=\theta/ƛ . \quad (13)$$

[$\eta'(b_i)$ is used for $d\eta/db|_{b_i}$.] In the neighborhood of these stationary points the action may be expressed

$$A(\theta, b)\simeq A(\theta, b_i)+\frac{1}{2}\frac{\partial^2 A}{\partial b^2}\Big|_{b=b_i}(b-b_i)^2$$

$$\simeq A(\theta, b_i)+\hbar\eta''(b_i)(b-b_i)^2 . \quad (14)$$

The stationary phase integration must be performed at each impact parameter where the action is stationary, so the scattering amplitude becomes a sum over all impact parameters b_i that satisfy Eq. (13),

$$f(\theta)=\sum_{b_i(\theta)} |b_i|[2b_i ƛ \sin\theta\,\eta''(b_i)]^{-1/2} e^{iA(\theta, b_i)/\hbar} . \quad (15)$$

[This expression fails if $\theta=0$, or π (glory scattering), or $\eta''(b_i)=0$ (rainbow scattering).] All quantities must be treated as complex numbers, so that a factor $e^{-i\pi/2}$ will result if either b_i or $\eta''(b_i)$ is negative. [If $b<0$ in Eq. (11), $b^{1/2}$ must be interpreted as $e^{-i\pi/2}|b|^{1/2}$, because of the transformation used in Eq. (7).]

Equation (15) shows that contributions to the scattering amplitude come from (the neighborhood of) discrete values of the impact parameter. The magnitude of each contribution is determined by the angle, the impact parameter, and the second derivative of the phase. The phase of each contribution is determined solely by the action (apart from a possible constant). This makes our analysis especially enlightening when applied to scattering processes that are sensitive to the phase of the scattering amplitude (or its components).

IV. SINGLE-CHANNEL INTERFERENCE

Let us now consider the application of these results to elastic scattering by a single potential. Since the preceding results are most helpful in simplifying the discussion of scattering when more than one impact parameter contributes to the scattering, we consider a potential that, like most interatomic potentials, is attractive at long distances and repulsive at short distances. The phase function $\eta(b)$ for this potential is shown in Fig. 2. We also show the classical deflection function

$$\chi(b)=2ƛ\eta'(b) , \quad (16)$$

which is the locus of points where the action is stationary [that is, where Eqs. (12) and (13) hold]. The lower half of the deflection function is shown dashed to emphasize that only impact parameters for which $\chi(b)=\theta$ contribute to $f(\theta)$ in Eq. (15) (θ is the angle of observation, and is always positive).[6] Thus, at angle θ_0 (in Fig. 2), three impact parameters contribute to the scattering amplitude, b_1, b_2, and b_3; b_1 and b_2 are both negative and correspond to predominantly attractive scattering, while b is positive and corresponds to predominantly repulsive scattering.

When two (or more) impact parameters contribute to the scattering amplitude in Eq. (15) the differential cross section will contain interference terms whose phase difference varies as $\{A[\theta, b_1(\theta)] - A[\theta, b_2(\theta)]\}/\hbar$. The angular spacing of the resulting maxima and minima in the cross section depends on the total rate of change of the action with θ. This is

$$\frac{d}{d\theta}A[\theta, b_i(\theta)]=\frac{\partial A}{\partial\theta}\Big|_{b_i}+\frac{\partial A}{\partial b}\Big|_{b_i}\frac{db_i}{d\theta}=-\hbar b_i/ƛ \quad (17)$$

from Eq. (10) [the second term is zero from Eq. (13)]. If b_1 and b_2 both contribute to scattering at some angle, the angular spacing of successive maxima and minima in that neighborhood is given by

$$\Delta\theta\frac{d}{d\theta}[A(\theta, b_1)-A(\theta, b_2)]=2\pi\hbar , \quad (18)$$

so that $$\Delta\theta=\frac{2\piƛ}{b_1(\theta)-b_2(\theta)} . \quad (19)$$

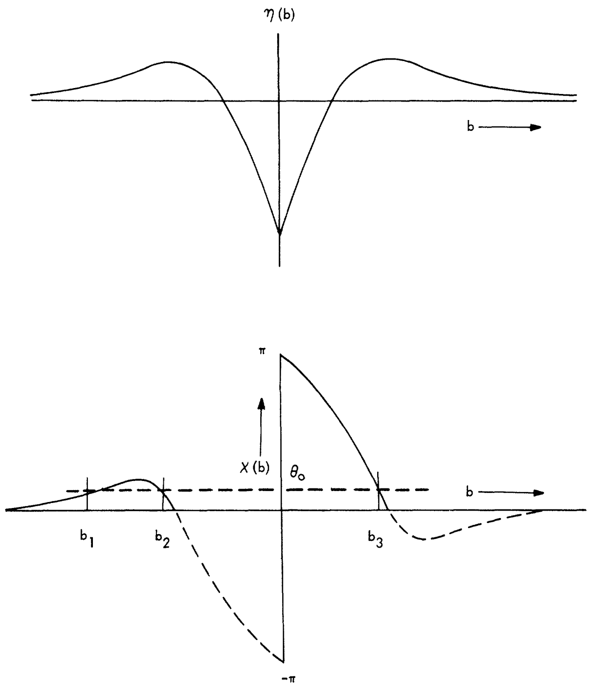

FIG. 2. Phase function $\eta(b)$ and deflection function $\chi(b)$; each shown for both positive and negative values of impact parameter b.

Thus, the *local* spacing of maxima and minima is determined solely by distance between b_1 and b_2; the potential plays no role; once b_1 and b_2 have been determined.[7]

Equation (19) also governs the spacing of intensity maxima in the two-slit diffraction of light (Young's experiment), in which case Eq. (19) can be derived simply by considering the difference in path length caused by changing the angle.[8] This simple derivation works for scattering because the action is stationary so that the variations in $b_1 - b_2$ (analogous to changing the slit separation in Young's experiment) with angle do not affect the phase. These changes of $b_1 - b_2$ with angle account for the fact that the spacing of successive maxima and minima in the scattering section is not constant, as it is in Young's experiment (at small angles where $\sin\theta \sim \theta$).

Equation (10) may be used to determine the distance between the impact parameters that contribute to the scattering amplitude. As an example we consider Hundhausen and Pauly's[9] data for Na-Hg scattering at $v_{\text{rel}} = 1.475\times 10^5$ cm/sec ($\lambda\!\!\!^{-}$ is 0.0208 Å at this velocity). They observe interference between b_1 and b_2 (supernumerary rainbows) with a period of 0.09 rad, which implies that $b_1 - b_2 = 1.5$ Å; and they observe interference between b_1 and b_3 (rapid oscillations) with a period of 0.0127 rad, which implies that $b_1 - b_3 = 10.2$ Å These distances are quite compatible with the size of the potentials which they determined by partial-wave analysis.

V. TWO-CHANNEL INTERFERENCE

Let us now consider a typical exchange cross section

$$\sigma_{\text{ex}}(\theta) = |f_+(\theta) - f_-(\theta)|^2 , \tag{20}$$

where f_+ and f_- are two independent scattering amplitudes. Such expressions arise in spin exchange and in resonant charge exchange; in both processes the expected oscillatory structure has been observed. As in single-channel scattering, the oscillatory behavior is due to interference between the two scattering amplitudes whose phase difference varies as the difference between the two actions times $1/\hbar$. The local change of action with θ depends only upon b [and not on the potential, see Eq. (17)], so we find the angular spacing of successive maxima and minima in the exchange cross section to be

$$\Delta\theta = 2\pi\lambda\!\!\!^{-}/[b_+(\theta) - b_-(\theta)] \tag{21}$$

in the neighborhood of θ.[10]

Frequently, it is possible to infer the phase difference between the two scattering amplitudes exactly, in which case we can measure the relative phase

$$\delta(\theta) = [A_+(\theta, b_+) - A_-(\theta, b_-)]/\hbar . \tag{22}$$

[We assume that the potentials have similar shapes, so the additional $e^{i\pi/4}$ terms in Eq. (15) cancel out.] Although the impact parameters in the plus and minus states are different, the action is stationary for small variations of b, so if b_+ and b_- are approximately equal (as they will be if the potentials for the two states are nearly equal), we can approximate

$$\delta(\theta) \simeq [A_+(\theta, \bar{b}) - A_-(\theta, \bar{b})]/\hbar = 2\eta_+(\bar{b}) - 2\eta_-(\bar{b}) , \tag{23}$$

where $\bar{b} = \frac{1}{2}(b_+ + b_-)$; the second line follows from Eq. (10). Use of the first term of the impact approximation[2] for $\eta_\pm(\bar{b})$ yields the familiar result

$$\delta(\theta) \approx \frac{1}{\hbar v}\int_{b} V_+ dl - \frac{1}{\hbar v}\int_{\bar{b}} V_- dl \equiv \frac{1}{\hbar v}\int_{\bar{b}} \Delta V dl , \tag{24}$$

where ΔV is the difference potential $V_+ - V_-$ and v is the relative velocity of the collision.

The argument frequently used[1] to derive Eq. (24), under the assumption that the impact parameter is the same for collisions in both states, is incorrect; the "particle" in the state with weaker potential must travel closer to the target in order to sustain the deflection θ. In so doing, it travels in a region of deeper potential and picks up some extra phase (η). The phase of the scattering amplitude is governed, however, by the action, which is also affected by the decrease in path length caused by passing closer to the target. These two effects cancel exactly, since the action is stationary, so Eq. (24) is correct. A similar argument also applies for dominantly repulsive potentials.

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