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A new semi-classical approach to the treatment of elastic scattering and direct reactions

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Abstract. In this paper we consider the short wavelength (semi-classical) limits of the s -matrix for elastic scattering, and the distorted wave Born approximation (DWBA) t -matrix for a direct reaction, and derive some interesting and useful formulae. One result takes the form of an integral representation of the elastic s -matrix which resembles the Poisson sum representation of the exact elastic s -matrix.

The main result of this paper is a new approximate expression for the DWBA t -matrix in which the main effects of the distorting potentials are described in terms of average elastic phase shifts. This approximation is applicable in various forms to the treatment of a wide range of direct nuclear and atomic reactions. It possesses a number of attractive and useful features offering some practical advantages over the original quantal expression. In particular the formulae are easy to evaluate and are amenable to detailed interpretation and further analytical approximation. Conditions for their validity are stated and demonstrate their wide range of applicability. More detailed discussion is given of application to peripheral reactions and to Coulomb excitation.

1. Introduction

Semi-classical techniques provide powerful approximations to quantum mechanical theories, and are applicable to a wide variety of problems in molecular, atomic and nuclear physics. They are a valuable aid to the understanding and interpretation of both theories and experimental data. This is only partly because semi-classical theories can often provide a more intuitive description of the system. In performing a detailed analysis of experimental data, semi-classical methods enable attention to be focused on features that may not be (easily) described by quantal calculations constrained to fit the remainder of the data. This can sometimes lead to important conclusions that may otherwise be missed.

In this paper we report the results of a study of the semi-classical limits of the elastic s -matrix and the distorted wave Born approximation (DWBA) t -matrix for a direct reaction. Some of these results are of practical importance, being directly applicable to the treatment of direct reactions. The results concerning elastic scattering are given mainly by way of illustration, and because they have some relevance to the inelastic case. The methods used in their derivation are outlined in this paper in order to illustrate the ideas involved rather than to rigorously justify the final formulae. The plausibility of these formulae is apparent without the need to understand their derivation. The inelastic scattering calculation, though more complicated,

follows similar lines to those for elastic scattering. It is intended that full accounts of the derivations be published separately in due course.

The definition of the semi-classical limit referred to is that adopted by Berry and Mount (1972), Koeling and Malfliet (1975) and others (e.g. Miller 1974, Connor 1976). Semi-classical approximations to quantum theory are applicable when Planck's constant \hbar is small in the corresponding classical problem. (Following Berry and Mount, I shall abbreviate such statements by ' $\hbar \rightarrow 0$ ' or ' $\hbar \sim 0$ '). The *semi-classical limit*, ' $\hbar \sim 0$ ', is the lowest-order semi-classical approximation which takes full account of the various types of singularity at ' $\hbar = 0$ '. Such a theory provides a complete short wavelength description of the wave field, and thus not only describes classical particle dynamics in a real (or weakly absorbing) potential, but also wavelike phenomena such as interference, diffraction (such as may be due to strong absorption), reflection at an under-dense barrier and tunnelling through an over-dense barrier. In order to do so the theory must retain the *superposition principle* and take into account *complex paths* as well as real paths when dealing with the solutions (Keller 1958).

In a real potential, consideration of just the real paths gives a full account of classical particle motion. Complex solutions of the classical equations of motion are often disregarded. These describe tunnelling and phenomena associated with wave-like behaviour which may be important in atomic and subatomic systems (Miller and George 1972, Miller 1974). Weak absorption gives rise to attenuation of particle flux along the various (real) trajectories and has little effect on the dynamics. Strong absorption, however, does affect the dynamics and may give rise to strong diffraction. In this case the complex nature of the assumed potential makes the consideration of complex paths obligatory. The treatment of complex trajectories in semi-classical scattering by strongly absorbing potentials is described in recent work by Knoll and Schaeffer (1975, 1976) and by Koeling and Malfliet (1975).

In this paper several references are made to 'classical solutions'. These are solutions which involve only a single turning-point (at the distance-of-closest-approach) and which do not require or imply solution of the *connection problem* in one dimension. For a real potential such solutions correspond to real classical trajectories. In the case of a complex potential the concept of a single classical turning-point, and hence of a 'classical trajectory', can be retained using the procedure of Crowley (1976). Such classical solutions are incomplete in that complex branches associated with reflections and multiple reflections involving other turning-points are ignored. Implications of this are discussed later.

The reader should note that many discussions of the validity of semi-classical theories given in the literature (e.g. Frahn 1975, Harney *et al* 1974) are relevant only to those approximations applicable to situations involving weak absorption when complex paths can be and are ignored.

My investigations concern the semi-classical limits of the following: (i) the elastic scattering s -matrix,

$$S_{\beta\alpha}(0) = \int \bar{\psi}_{\beta}^{(-)*}(\mathbf{r}) \psi_{\alpha}^{(+)}(\mathbf{r}) d^3\mathbf{r}, \quad (1)$$

and (ii) the DWBA t -matrix describing a direct reaction (e.g. Austern 1970),

$$t_{\gamma\alpha} = \int \bar{\psi}_{\gamma}^{(-)*}(\mathbf{r}) U_{\gamma\alpha}(\mathbf{r}) \psi_{\alpha}^{(+)}(\mathbf{r}) d^3\mathbf{r}, \quad (2)$$

where $U_{\gamma\alpha}(\mathbf{r})$ is the form-factor which includes information about the internal states

of the system. In the latter only the distorted waves, $\psi_\alpha^{(+)}$ and $\bar{\psi}_\gamma^{(-)}$, are treated semi-classically. The discussion is therefore equally applicable to other distorted wave theories such as the distorted wave impulse approximation (DWIA) and coupled channels theories (CCBA).

2. The semi-classical wavefunction

In the above equations, $\psi_\alpha^{(+)}$ (\mathbf{r}) is an elastic scattering wavefunction, with outgoing wave boundary conditions, describing scattering by a spherically symmetric (optical) potential $V_\alpha(\mathbf{r})$, from the entrance channel (denoted by the subscript α). The elastic scattering wavefunctions, $\bar{\psi}_\beta^{(-)}$ (\mathbf{r}) and $\bar{\psi}_\gamma^{(-)}$ (\mathbf{r}), both have ingoing wave boundary conditions and describe scattering by potentials $V_\beta^*(\mathbf{r}) = V_\alpha^*(\mathbf{r})$ and $V_\gamma^*(\mathbf{r})$, into the exit channels β and γ respectively. In the notation used here, β denotes an elastic scattering channel, and γ denotes a reaction channel. Scattering *states* described by the wavefunctions $\psi_\alpha^{(+)}$, $\psi_\beta^{(-)}$ and $\psi_\gamma^{(-)}$ may be denoted by $\alpha^{(+)}$, $\beta^{(-)}$ and $\gamma^{(-)}$ respectively. These wavefunctions are solutions of Schrödinger equations as follows:

$$-\frac{\hbar^2}{2M} \nabla^2 \psi_\alpha^{(+)} + V_\alpha \psi_\alpha^{(+)} = \frac{\hbar^2 k_\alpha^2}{2M} \psi_\alpha^{(+)}; \quad (3a)$$

$$-\frac{\hbar^2}{2M} \nabla^2 \bar{\psi}_\nu^{(-)} + V_\nu^* \bar{\psi}_\nu^{(-)} = \frac{\hbar^2 k_\nu^2}{2M} \bar{\psi}_\nu^{(-)}, \quad \nu \in \{\beta, \gamma\}, \quad (3b)$$

where M and $\hbar^2 k_\nu^2/2M$ are respectively the particle's mass and energy.

The first step in deriving the semi-classical limits of (1) and (2) consists of replacing the exact wavefunctions $\psi_\alpha^{(+)}$, $\bar{\psi}_\beta^{(-)*}$ and $\bar{\psi}_\gamma^{(-)*}$ by the corresponding semi-classical wavefunctions which are approximate solutions of (3). These are

$$\left. \begin{matrix} \psi_\alpha^{(+)} \\ \bar{\psi}_\beta^{(-)*} \\ \bar{\psi}_\gamma^{(-)*} \end{matrix} \right\} = \sum_n (g_n^{(\pm)}(\mathbf{r}))^{1/2} \exp\left(\pm \frac{i}{\hbar} W_n^{(\pm)}(\mathbf{r}, \hbar \mathbf{k}_\nu)\right), \quad (4)$$

where $\dagger \nu \in \{\alpha, \beta, \gamma\}$ and $n \in \{n\} \in \{\{a\}, \{b\}, \{c\}\}$. The label $n \in \{a, b, c\}$ denotes classical trajectories passing through the point \mathbf{r} . These trajectories may be complex. The presence of the sum over n to include all such trajectories reflects the multi-valuedness of the solutions of the classical problem. The functions $W_n^{(\pm)}$ are the *characteristic functions* and are solutions of classical Hamilton-Jacobi equations (Goldstein 1969). Expressions for these and other quantities appearing in (4) are as follows (Crowley 1976, and to appear, Van Vleck 1928):

$$\frac{1}{\hbar} W_n^{(\pm)}(\mathbf{r}; \hbar \mathbf{k}_\nu) = \pm [\delta_\nu(L_n) - \frac{1}{2} L_n \Theta_\nu(L_n) - \pi \mu_n^{(\pm)}(\mathbf{r})] + \int_{r_n}^{\mathbf{r}} \mathbf{p}_n \cdot d\mathbf{s}_n, \quad (5)$$

$$g_n^{(+)} = \det \left[\frac{1}{\hbar} \frac{\partial^2 W_n^{(+)}}{\partial r_i \partial k_{\nu j}} \right] = \exp \left(- \int_{-\infty}^{\mathbf{r}} \nabla \cdot \mathbf{p}_n \frac{1}{p_n^2} \mathbf{p}_n \cdot d\mathbf{s}_n \right), \quad (6a)$$

\dagger The notation is that (lower case) Latin letters are used to label trajectories while (lower case) Greek letters are used to label channels. The dummy label n denotes a general element of a set of labels $\{n\}$ which may be $\{a\}$, $\{b\}$ or $\{c\}$. In usage dummy labels, a , b and c , correspond respectively to channel labels, α , β and γ , thus removing the necessity to simultaneously label both channel and trajectory.

$$g_n^{(-)} = \det \left[\frac{1}{\hbar} \frac{\partial^2 W_n^{(-)}}{\partial r_i \partial k_{vj}} \right] = \exp \left(\int_r^\infty \nabla \cdot \frac{\mathbf{p}_n}{p_n} \cdot \mathbf{p}_n \cdot d\mathbf{s}_n \right), \quad (6b)$$

where subscripts i, j denote components of a vector; and where \mathbf{p}_n denotes a local wavenumber according to: $\mathbf{p}_a = (1/\hbar)\nabla W_a^{(+)}$, or $\mathbf{p}_b = (1/\hbar)\nabla W_b^{(-)}$, or $\mathbf{p}_c = (1/\hbar)\nabla W_c^{(-)}$; L_n is the angular momentum associated with the trajectory, namely

$$L_n = |\mathbf{r} \times \mathbf{p}_n| = r_n p_\nu(r_n)$$

with

$$p_\nu^2(r) = k_\nu^2 - (2M/\hbar)^2 V_\nu(r),$$

$r_n = |\mathbf{r}_n|$ where \mathbf{r}_n is the point-of-closest approach; $\delta_\nu(L)$ is the JWKB *phase shift*,

$$\delta_\nu(L) = \lim_{R \rightarrow \infty} \left[\int_{r_0}^R \left(p_\nu^2 - \frac{L^2}{r^2} \right)^{1/2} dr - \int_{L/k_\nu}^R \left(k_\nu^2 - \frac{L^2}{r^2} \right)^{1/2} dr \right], \quad (7)$$

(with r_0 given by: $L = r_0 p_\nu(r_0)$) which may be replaced by a more exact expression if so desired; and $\Theta_\nu(L)$ is the *deflection function* defined by

$$\Theta_\nu(L) = 2 \frac{\partial}{\partial L} \delta_\nu(L). \quad (8)$$

The path integrals $\int d\mathbf{s}_n$ are taken along the classical trajectories with the limits '+ ∞ ' and '- ∞ ' indicating points at large distances away from the scattering centre and lying respectively on the outgoing and ingoing branches of the trajectory. The term $-\pi\mu_n^{(\pm)}(\mathbf{r})$ appearing in the phase ensures that the quantal wavefunction is single-valued for all values of \mathbf{r} , provided that angular momentum is quantised according to the Bohr-Sommerfeld rule†,

$$\oint L d\psi = 2\pi(l + \frac{1}{2}),$$

where l is an integer, and ψ is here the angular coordinate conjugate to L . The path integral $\oint d\psi$ is taken once around the origin along a classical trajectory. The index $\mu_n^{(+)}(\mathbf{r})$ is an integer function of \mathbf{r} and is equal to the number of complete times the trajectory n has encircled the origin in connecting $-\infty$ to \mathbf{r} ; $\mu_n^{(-)}(\mathbf{r})$ is given by $\mu_n^{(-)}(\mathbf{r}) = m_n - \mu_n^{(+)}(\mathbf{r})$ where m_n is an integer specifying the total number of complete times the trajectory encircles the origin in connecting $-\infty$ to $+\infty$. The $\mu_n^{(\pm)}$ define various branches of an orbiting trajectory in such a way that $W_n^{(\pm)}$ (and hence the wavefunction) is a single-valued function of position on the trajectory, n . In this way we cope with multi-valuedness associated with *orbiting*. However the functions are non-analytic near the discontinuities of $\mu_n^{(\pm)}$. (Note that $\mu_n^{(\pm)}$ appeared originally as *constants* of integration when solving the Hamilton-Jacobi equation.) The problem is much the same as the one faced when dealing with a multi-valued function in the complex plane by the introduction of *cuts*. The various $\mu_n^{(\pm)}$ define a series of Riemann sheets in coordinate space, and the rule is, as in the complex plane, to stay on the same sheet wherever possible. The particular way the μ 's and m 's have been defined here has the effect of introducing cuts in L -space at $\Theta(L) = \pm(2n+1)\pi$, for integral values of n .

† Which implies the Langer relation, $L \rightleftharpoons l + \frac{1}{2}$.

The multi-valuedness of the classical solutions for fixed μ may be represented by defining a single continuous folded surface (cf Riemann sheet) in such a way that the functions W and g are continuous and single valued on the sheet. The projection of this sheet onto ordinary coordinate space gives rise to regions of different multiplicity separated by caustics. Features of such a surface can be described in terms of *catastrophes* (Connor 1976, Zeeman 1976) which may be associated with folds in the surface. The projections of these folds onto coordinate space indicate *caustic* surfaces—surfaces generated by *rainbow* trajectories or envelopes of many trajectories—across which the multiplicity of the classical solutions change. It is the presence of caustics associated with the variable multi-valuedness of the classical solutions determining W and g which makes integrals such as (1) and (2) involving semi-classical wavefunctions difficult to handle.

The first step in overcoming this problem consists of finding a transformation which maps the classical solutions into a space in which they are defined and single valued for all values of the new coordinates. Such a transformation effectively ‘unfolds’ the ‘Riemann’ surface and, for this reason, I refer to such a transformation of variable as an ‘*unfolding*’.

The new coordinates, in the case of motion in a spherically symmetric potential, are easily found. They may be taken to be (\mathbf{L}, τ) where \mathbf{L} is the angular momentum (in units of \hbar) specifying a classical trajectory, and τ is a coordinate related to time (in a parametric sense) uniquely specifying the position of a point on such a trajectory. A set of coordinates (\mathbf{L}, τ) may thus specify, not only a unique point in the space of coordinates \mathbf{r} , but also a unique trajectory through it.

The second step involved in obtaining the results given in §§ 3–4, which permits simultaneous unfolding for both sets of functions W and g appearing in the integrals, is to make use of the fact that, in the semi-classical limit, contributions to the integrals come only from the neighbourhood of classical trajectories connecting the incoming channel α to the outgoing channel, β or γ . The complete procedure for thus carrying out the transformation $(\mathbf{r}, n) \rightarrow (\mathbf{L}, \tau)$ for integrals such as (1) and (2) is, in general, non-trivial.

Whereas the transformation to (\mathbf{L}, τ) constitutes an unfolding for classical solutions, extending the theory to include complex paths may lead to trajectories having complex branches, in which case the simple unfolding procedure outlined breaks down. However, the method may be generalised by noting that the transformation to (\mathbf{L}, τ) is an unfolding for each branch (which we label by Γ). The complete unfolding will therefore include a sum over Γ . The generalisation, $\delta^{(\Gamma)}(\mathbf{L})$, of the phase shift (7) includes a dependence on the pattern of reflections from several turning-points in one dimension. This is discussed in some detail by Knoll and Schaeffer (1976). The possible reflection patterns, Γ , correspond to different branches of the complete three-dimensional trajectory. The final sum over Γ thus constitutes a multiple-reflection series which may be summed to yield more manageable expressions for the s -matrix in the forms given by Brink and Takigawa (1977) and Lee and Takigawa (1977).

In the elastic-scattering treatment which follows, the sum over Γ is omitted. Including it is equivalent to replacing the phase shift, as given by (7), by the exact JWKB expression which includes all multiple-reflection contributions. The exact quantal expression would also suffice.

The discussion, as given, for the inelastic case is applicable to classical trajectories without complex branches. (This is equivalent to using a single-reflection approxima-

tion in one dimension (e.g. Crowley 1976.) It may be possible to generalise the result to include contributions from *some* complex branches such as those which correspond to a single reflection from one complex turning-point or to a single reflection from an interior turning-point preceded and followed by barrier penetration. Nevertheless the results of § 4 are expected to be valid only for scattering in non-resonant situations such as one finds in the presence of strong absorption.

3. The semi-classical s -matrix

Substituting the semi-classical wavefunctions (4) into (1) leads to the following expression for the semi-classical s -matrix:

$$S_{\beta\alpha}(0) = \int \sum_{a,b} (g_a^{(+)} g_b^{(-)})^{1/2} \exp\left(\frac{i}{\hbar} (W_a^{(+)}(r, \hbar k_\alpha) - W_b^{(-)}(r, \hbar k_\beta))\right) d^3 r.$$

A semi-classical unfolding of this integral carried out as outlined in the appendix leads to:

$$S_{\beta\alpha}(0) = \frac{1}{k_\alpha^2} \sum_{m=-\infty}^{+\infty} \int \exp\{i[(k_\alpha - k_\beta)\tau + \Omega_m(L, \phi; \theta)]\} d\tau L dL d\phi, \quad 0 \leq \theta \leq \pi, \quad (9)$$

where

$$\Omega_m(L, \phi; \theta) = 2\delta(L) - L\Theta(L) - m\pi + 2L[\cos(\frac{1}{2}\theta)\sin(\frac{1}{2}\Theta + m\pi) - \sin(\frac{1}{2}\theta)\cos(\frac{1}{2}\Theta + m\pi)\cos\phi], \quad (10)$$

where $\delta(L) = \delta_\alpha(L) = \delta_\beta(L)$ is the phase shift; $\Theta = \Theta(L) = \Theta_\alpha(L) = \Theta_\beta(L)$ is the deflection; and θ is the *scattering angle* which is the angle between the wavevectors k_α and k_β defined in the range $0 \leq \theta \leq \pi$. The integer m labels the orbiting surfaces of the 'Riemann' sheet and was introduced so that, at a saddle-point of the phase,

$$-\pi \leq \Theta + 2m\pi \leq \pi.$$

The expression on the right-hand side of (9) contains a sum over all values of m and the above property of the index m is implicit because of the restriction on the range of values permitted to θ . The range of integration over the angular momentum variables, L and ϕ , in (9) is restricted to values in the vicinity of classical trajectories defined by:

$$\Theta + 2m\pi = \pm \theta$$

and, if $\theta \neq 0$ or π , $\cos \phi = \pm 1$.

From (9) it follows immediately that

$$S_{\beta\alpha}(0) = \frac{2\pi}{k_\alpha^2} \delta(k_\alpha - k_\beta) \sum_{m=-\infty}^{\infty} \int \exp(i\Omega_m(L, \phi; \theta)) L dL d\phi. \quad (11)$$

Since Ω is $O(1/\hbar)$, the remaining two-dimensional integrals on the right-hand side of (11) may be evaluated directly, in the semi-classical limit, by a method of stationary phase (or saddle-point method for complex Ω). The stationary points occur where

$$\frac{\partial \Omega}{\partial L} = \frac{\partial \Omega}{\partial \phi} = 0,$$

for values of L and ϕ such that the following are true.

(i) If $\theta \neq 0, \theta \neq \pi$:

$$\phi = 0, \quad \Theta + 2m\pi = \theta \tag{12a}$$

$$\phi = \pi, \quad \Theta + 2m\pi = -\theta. \tag{12b}$$

(ii) If $\theta = 0$:

$$\Theta + 2m\pi = 0. \tag{12c}$$

(iii) If $\theta = \pi$:

$$\Theta + 2m\pi = \pm \pi. \tag{12d}$$

(Note that at least two different values of m contribute to $\theta = \pi$; and that real values of $\theta > \pi$ are dynamically forbidden.)

(iv) Other saddle points are explicitly excluded.

Confining integration over L to the vicinity of classical trajectories is equivalent, in the semi-classical limit, to integrating over all possible values of L , ($0 \leq L \leq \infty, 0 \leq \phi < 2\pi$), and subtracting from the result contributions arising from ‘spurious’ saddle-points.

Since $\partial^2 \Omega / \partial L \partial \phi$ vanishes at any of the stationary points given by (12a)–(12d), a two-variable Taylor series expansion of Ω about a stationary point renders the integrals (11) separable when taken to second order. In the case of an isolated stationary point at $L = L_i$ and $\phi = \frac{1}{2}\pi \pm \frac{1}{2}\pi$, where $\Theta(L_i) + 2m_i\pi = \pm \theta$, the result is

$$S_{\beta\alpha}(0) \sim \frac{2\pi}{k_\alpha^2} \delta(k_\alpha - k_\beta) \left(\frac{2\pi L_i}{\Theta'(L_i) \sin \theta} \right)^{\frac{1}{2}} \exp[i(2\delta(L_i) \pm L_i \theta - m_i \pi + \frac{1}{4}\pi)]. \tag{13}$$

provided that θ is not near 0 or π and $\Theta'(L_i) \neq 0$. (The correct branch of the square-root depends upon the directions of the paths of steepest descent.) This leads directly to the following expression for the differential cross section (where $d\Omega$ represents an element of solid angle):

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{k_\alpha^2 \sin \theta} \left| \frac{L_i}{\Theta'(L_i)} \right|$$

which is equivalent to the classical expression. More generally $S_{\beta\alpha}$ is a sum of contributions from several isolated stationary points (for which $\Theta'(L) \neq 0$) which, by the superposition principle, may lead to a cross-section containing oscillatory interference terms. The treatment of *Glory scattering* ($\theta \approx 0$ or π)† and *rainbow scattering* ($\Theta' \approx 0$) requires the use of different techniques (Ford and Wheeler 1959, Berry 1966, 1969, Connor and Marcus 1971, Gross 1975, Frahn 1975).

An s -matrix given as a sum of terms of the form of (13) is identical with that obtainable in the semi-classical limit of the analytic quantal s -matrix. Making use of the Poisson summation formula (Berry and Mount 1972, § 6, Morse and Feshbach 1953, p 467), the latter can be expressed in the following form:

$$S_{\beta\alpha} = \left(\frac{2\pi}{k_\alpha} \right)^2 \delta(k_\beta - k_\alpha) \sum_{m=-\infty}^{+\infty} e^{-im\pi} \int_0^\infty e^{2\pi imL} P_{L-1/2}(\cos \theta) e^{2i\delta(L)} L dL, \tag{14}$$

† The treatment of the $\theta = \pi$ Glory requires that the $\Theta = \pm(2n+1)\pi$ cuts be removed to $\Theta = \pm 2n\pi$. This may be achieved by the transformation $\theta \rightarrow \pi - \theta, m \rightarrow m - \frac{1}{2}$ which leaves $S_{\beta\alpha}$ (equation (14)) invariant.

which is an exact representation of the more familiar partial-wave sum,

$$S_{\beta\alpha} = \frac{2\pi^2}{k_\alpha^2} \delta(k_\beta - k_\alpha) \sum_{l=0}^{\infty} (2l+1) e^{2i\delta(l+1/2)} P_l(\cos \theta), \quad (15)$$

where $P_\nu(x)$ is a Legendre function defined for $-1 \leq x \leq 1$. In the semi-classical limit the sum (15) is dominated by large values of l . The Legendre function in each of the integrals in the Poisson sum (14) may therefore be replaced by one of its Bessel function approximations (Szëgo 1934, Berry and Mount 1972, equations (6.18)–(6.20)) which are very accurate representations of the Legendre function for $l \geq 10$. Thus, for example, one can derive the short wavelength representation,

$$S_{\beta\alpha} \approx \frac{2\pi}{k_\alpha^2} \delta(k_\beta - k_\alpha) \left(\frac{\theta}{\sin \theta} \right)^{1/2} \sum_{m=-\infty}^{m=\infty} e^{-im\pi} \int \exp [i(2\delta(L) + 2\pi mL - L\theta \cos \phi)] L \, dL \, d\phi, \quad (16)$$

valid for $\pi - O(1/L) > \theta \geq 0$, which bears a close resemblance to (11). In the above the Bessel function has been replaced by one of its integral representations; L and ϕ are plane polar coordinates, $0 \leq L \leq \infty$, $0 \leq \phi < 2\pi$. Evaluation of the integrals by the stationary phase method described leads to an expression for $S_{\beta\alpha}$ involving terms of the form of (13).

A problem with (11) is the presence of spurious saddle-points which necessitates limiting the range of integration over L to the vicinity of those saddle-points representing classical trajectories. For θ not too close to π it is possible to remove the spurious saddles by linearising the dependence of Ω on $\Theta + 2m\pi \pm \theta$. This is done by 'approximating' $\sin[\frac{1}{2}(\Theta + 2m\pi \pm \theta)]$ and $\cos(\frac{1}{2}\Theta + m\pi)$ ($1 \pm \cos \phi$) by $\frac{1}{2}(\Theta + 2m\pi \pm \theta)$ and $\cos(\frac{1}{2}\theta)$ ($1 \pm \cos \phi$) respectively for $\phi \approx 0$ (when the lower sign is taken) and $\phi \approx \pi$ (when the upper sign is taken). This is equivalent to 'approximating' Ω as follows:

$$\Omega_m(L, \phi; \theta) \approx \begin{cases} 2\delta(L) - L\theta + 2m\pi(L - \frac{1}{2}) + L \sin \theta(1 - \cos \phi), & -\frac{1}{2}\pi < \phi < \frac{1}{2}\pi, \\ 2\delta(L) + L\theta + 2m\pi(L - \frac{1}{2}) - L \sin \theta(1 + \cos \phi), & \frac{1}{2}\pi < \phi < \frac{3}{2}\pi, \end{cases}$$

and taking ϕ to be in the range $-\frac{1}{2}\pi \leq \phi < \frac{3}{2}\pi$. Hence

$$S_{\beta\alpha}(0) = \frac{4\pi}{k_\alpha^2} \delta(k_\alpha - k_\beta) \sum_{m=-\infty}^{\infty} e^{-im\pi} \int_{\phi=-\pi/2}^{\phi=\pi/2} d\phi \int_0^{\infty} dL \exp[2i(\delta(L) - \pi mL)] \\ \times \cos[L(\theta - \sin \theta(1 - \cos \phi))].$$

The integral

$$\frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \cos[L(\theta - \sin \theta(1 - \cos \phi))] \, d\phi$$

may be evaluated exactly to yield

$$\cos(L(\theta - \sin \theta)) J_0(L \sin \theta) - \sin(L(\theta - \sin \theta)) H_0(L \sin \theta),$$

which is recognised[†] as a large- L asymptotic form of $P_{L-1/2}(\cos \theta)$ for $0 \leq \theta < \pi - O(1/L)$. Replacing this integral by $P_{L-1/2}(\cos \theta)$ yields the exact formula (14) for $S_{\beta\alpha}$.

[†] By comparison with the Szëgo (1934) formulae (Berry and Mount 1972, equations (6.18)–(6.20)) for $L \gg 1$ and θ such that $L \sin \theta \gg 1$ or $L\theta \ll O(1)$ (see also Abramowitz and Stegun 1965, chaps 8, 9 and 12).

This result may be shown more clearly, though less generally, by performing the ϕ -integration for $L \sin \theta \gg 1$ (either by using the saddle-point method, or exactly and subsequently replacing the Bessel function by its asymptotic form). The spurious saddle-points may then be removed by linearising the phase as described, and one recovers just the Poisson summation formula (14) in which the Legendre polynomial has been replaced by its asymptotic form.

These observations lead us to stating the following correspondence-principle theorem which will be of use later.

If $f(L)$ is a function of L that is regular on $0 \leq L \leq \infty$ and if $f(L) P_{L-1/2}(\cos \theta) \times (e^{2i\delta(L)} - 1)$ is $\mathcal{L}^{(2)}$ for all θ such that $\pi \geq \theta \geq 0$; and $|f'(L)/f(L)| \leq O(L^{-1})$ for all $L \gg 1$, then

$$\frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \int f(L) \exp(i\Omega_m(L, \phi; \theta)) dL d\phi \underset{\hbar \rightarrow 0}{\rightleftharpoons} \sum_{l=0}^{\infty} f(l+1/2) e^{2i\delta(l+1/2)} P_l(\cos \theta), \quad (17)$$

when the integral $\int L dL d\phi = \int d^2L$ is confined to the vicinity of classical trajectories defined by (12a)–(12d).

When the right-hand side of (17) is expressed as a sum of integrals using the Poisson summation formula, integrands on both sides contain the same contributing saddle points giving rise to the same asymptotic forms in the semi-classical limit.

This theorem and the techniques used to obtain (9) have been applied to the treatment of inelastic scattering yielding important results as described in the next section.

4. The semi-classical limit of the DWBA

The DWBA t -matrix element (2) may be expressed as a momentum-space integral of the form:

$$t_{\gamma\alpha} = \int S_{\gamma\alpha}(\mathbf{q}) F_{\gamma\alpha}(\mathbf{q}) d^3\mathbf{q}, \quad (18)$$

where

$$F_{\gamma\alpha}(\mathbf{q}) = \frac{1}{(2\pi)^3} \int U_{\gamma\alpha}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r}, \quad (19)$$

and

$$S_{\gamma\alpha}(\mathbf{q}) = \int \bar{\psi}_{\gamma}^{(-)*}(\mathbf{r}) \psi_{\alpha}^{(+)}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r}. \quad (20)$$

Equation (20) is just a generalisation of (1) and techniques similar to those leading to (9) may be applied.

Substituting the semi-classical wavefunctions (4) into (20) leads to

$$S_{\gamma\alpha}(\mathbf{q}) = \int \sum_{a,c} (g_a^{(+)} g_c^{(-)})^{1/2} \exp\left(\frac{i}{\hbar} (W_a^{(+)}(\mathbf{r}, \hbar\mathbf{k}_a) - W_c^{(-)}(\mathbf{r}, \hbar\mathbf{k}_c)) + i\mathbf{q}\cdot\mathbf{r}\right) d^3\mathbf{r}. \quad (21)$$

The points of stationary phase (saddle-points) for this integral occur where

$$\mathbf{p}_c(\mathbf{r}) - \mathbf{p}_a(\mathbf{r}) = \mathbf{q},$$

so that \mathbf{q} can be interpreted as the *impulse* which connects the incoming trajectory, a , to the outgoing one, c . The function $S_{\gamma\alpha}(\mathbf{q})$ is the amplitude for a process in which an

applied impulse \mathbf{q} leads to a transition from the scattering state $\alpha^{(+)}$ to the scattering state $\gamma^{(-)}$. Folding $S_{\gamma\alpha}(\mathbf{q})$ with the *impulse spectrum* $F_{\gamma\alpha}(\mathbf{q})$ yields the t -matrix element $t_{\gamma\alpha}$ according to (14).

An *approximate* unfolding of the integral (21) may be achieved by assuming that \mathbf{q} is restricted to values such that $q/p \ll 1$; and that the reaction is effectively localised to the vicinity of points-of-closest-approach on the incoming and outgoing trajectories, where the potentials are sufficiently smoothly varying for motion to be *locally rectilinear*. This last assumption justifies *local momentum* approximations of the wavefunctions (4) which involve approximating

$$\int_{r_n}^r \mathbf{p}_n \cdot d\mathbf{s}_n \quad \text{by} \quad \mathbf{p}_n \cdot \mathbf{r}, \quad n \in \{a, c\},$$

in the expressions for $W_n^{(\pm)}$. In general, this approximation is likely to be poor for scattering into large angles. Conditions on the magnitude of θ are made explicit in (27). A further assumption is that the potentials V_α and V_γ are everywhere (except where obscured by strong absorption in both channels) similar in magnitude (of both real and imaginary parts), and do not give rise to significantly different scattering in the respective elastic channels. A treatment of all small quantities to at least first order leads to an approximate unfolding of (21) giving:

$$S_{\gamma\alpha}(\mathbf{q}) \approx \frac{1}{k^2} \int \exp \left[\frac{i}{k} \left(\mathbf{p} \cdot \mathbf{q} + \frac{M}{\hbar^2} (\Delta V - Q) \right) \tau + i\Omega_0(L, \phi; \chi) \right] L \, dL \, d\phi \, d\tau, \quad (22)$$

where

$$\begin{aligned} k &= \frac{1}{2}(k_\alpha + k_\gamma), \\ \mathbf{p} &= \frac{1}{2}(\mathbf{p}_\alpha + \mathbf{p}_\gamma) \approx \frac{1}{4}(p_\alpha(r) + p_\gamma(r)) (\hat{\mathbf{k}}_\alpha + \hat{\mathbf{k}}_\gamma) \sec\left(\frac{1}{2}\theta\right), \\ \Delta V &= V_\gamma - V_\alpha, \\ Q &= \frac{\hbar^2}{2M} (k_\gamma^2 - k_\alpha^2) = \frac{\hbar^2 k}{M} (k_\gamma - k_\alpha), \\ \mathbf{L} &= \mathbf{r} \times \mathbf{p}, \end{aligned}$$

$\Omega_0(L, \phi; \chi)$ is given by (10) (we note that large Θ is not consistent with the assumptions involved in making the local momentum approximations so there is no need to include $m \neq 0$ terms) with

$$\begin{aligned} \delta(L) &= \frac{1}{2}(\delta_\alpha(L) + \delta_\gamma(L)), \\ \Theta(L) &= \frac{1}{2}(\Theta_\alpha(L) + \Theta_\gamma(L)) = 2 \frac{\partial \delta(L)}{\partial L}, \end{aligned}$$

and where

$$\cos \chi = \left(\frac{k}{p} \cos \frac{1}{2}\theta \right) \cos \xi + \left(1 - \frac{k}{p} \cos \frac{1}{2}\theta \right) \cos \theta, \quad (23a)$$

where

$$\cos \xi = 1 - \frac{1}{2k^2} (\mathbf{k}_\gamma - \mathbf{k}_\alpha - \mathbf{q})^2. \quad (23b)$$

Note that when $\mathbf{q} = \mathbf{0}$ and $\Delta V \equiv 0$, the right-hand side of (22) reduces to the $m = 0$ term in (9) when β replaces γ .

The derivation of equation (22) follows precisely similar lines to that used in the elastic case. Small quantities such as \mathbf{q}/p , $(\mathbf{r} \times \mathbf{q})/L$, $\Theta_\gamma(L) - \Theta_\alpha(L)$ (all identically zero for elastic scattering) are treated only in lowest order. Nevertheless the algebraic manipulations become considerably more arduous.

An approximate evaluation of the integral over τ in (22) yields

$$S_{\gamma\alpha}(\mathbf{q}) \approx \frac{2\pi}{k^2} \int \delta\left(\frac{\mathbf{p}_0 \cdot \mathbf{q}}{k} + \frac{\Delta V_0 - Q}{\hbar v}\right) e^{i\Omega_0(L, \phi; \chi_0)} L \, dL \, d\phi, \quad (24)$$

where

$$\mathbf{p}_0 = \frac{1}{2} p_0 \sec\left(\frac{1}{2}\theta\right) (\hat{\mathbf{k}}_\alpha + \hat{\mathbf{k}}_\gamma) = p_0 \hat{\mathbf{k}},$$

$$p_0 = \frac{1}{2}(p_\alpha(r_0) + p_\gamma(r_0)),$$

$$r_0 = L/p_0,$$

$$v = \hbar k/M,$$

$$\Delta V_0 = V_\gamma(r_0) - V_\alpha(r_0),$$

and χ_0 is given by (23) with p_0 replacing p . The function $\tilde{\delta}(z)$ is sharply peaked in energy or momentum space where it resembles the Dirac δ -function. It does, however, have a small finite width,

$$\Delta E \sim E \frac{|p_0|}{k} \left(\frac{1}{ELk} \left| \frac{\partial}{\partial r} (\Delta V) - \frac{\mathbf{q} \cdot \hat{\mathbf{k}}}{p_0} \frac{\partial V}{\partial r} \right|_{r=r_0} \right)^{1/3}, \quad (25a)$$

evaluated for L and \mathbf{q} such that the argument of $\tilde{\delta}$ vanishes. (In the above: $E = \hbar^2 k^2/2M$; $V = E - \hbar^2 p^2/2M$.) The corresponding width in L -space may, however, be large, being given by

$$\Delta L \sim \frac{1}{L} \left(\frac{E}{\Delta E} \right)^2. \quad (25b)$$

This finite width arises because the coefficient of τ in the phase of (22) is itself a (slowly varying) function of τ . As a result, contributions to the τ integral come from a limited region of τ -space, as has already been implied by the condition $\mathbf{p}_c - \mathbf{p}_a = \mathbf{q}$ (for non-vanishing \mathbf{q} or ΔV). In accordance with the second assumption we confine our attention only to contributions from the vicinity of points-of-closest-approach ($\tau = \tau_0$). This is done by expanding the phase in powers of $(\tau - \tau_0)$ about a point-of-closest-approach and continuing the expansion up to third order. A significant contribution then only arises if the coefficient of $(\tau - \tau_0)$, the argument of the $\tilde{\delta}$ -function, is close to zero. This is so because our assumptions imply that the region of contribution should be large compared with the local wavelength. The width of the $\tilde{\delta}$ -function arises because of variation in the functions V and ΔV over the contributing region.

In what follows it is assumed that $F_{\gamma\alpha}(\mathbf{q})$ is a sufficiently slowly varying function of $q_z = \mathbf{q} \cdot \hat{\mathbf{k}}$ to enable the $\tilde{\delta}$ -function to be treated like a true δ -function in q -space. This requires that terms of order $\Delta q_z \partial F_{\gamma\alpha}/\partial q_z$ and $(\Delta q_z)^2 \partial^2 F_{\gamma\alpha}/\partial q_z^2$, where $\Delta q_z = 2M\Delta E/\hbar^2|p_0|$, can be considered to be negligible.

After performing the integration over q_z as in (18) the product $\tilde{\delta}F_{\gamma\alpha}$ is replaced by a very slowly varying function of L . This permits application of the theorem expressed by (17)—bearing in mind that previously made assumptions imply negligible

contribution from $m \neq 0$ terms—leading to the following result for an effective $S_{\nu\alpha}(\mathbf{q})$ in the form of a partial-wave series:

$$S_{\nu\alpha}^{\text{eff}}(\mathbf{q}) = \frac{2\pi^2}{k^2} \sum_{l=0}^{\infty} \delta\left(\frac{\mathbf{p}_0 \cdot \mathbf{q}}{k} + \frac{\Delta V_0 - Q}{\hbar v}\right) (2l+1) e^{2i\delta(l+1/2)} P_l(\cos \chi). \quad (26)$$

Other conditions for the validity of (26) are given below.

(i) Values of q are restricted to values such that

$$\left|\frac{q}{p_0}\right|^2 \ll 1, \quad (27a)$$

$$\left|\frac{q}{p_0}\right|^2 \left|1 - \frac{k}{p_0} \cos \frac{1}{2}\theta\right| \ll \frac{\pi}{l}, \quad (27b)$$

$$\left|\frac{q}{p_0}\right| \left|r \frac{\partial p}{\partial r}\right|_{r=r_0} \ll \left|p_0 + r_0 \frac{\partial p}{\partial r}\right|_{r=r_0}; \quad (27c)$$

—the last of these conditions follows from the requirement that

$$l \left|\frac{\partial \chi}{\partial l}\right| \ll 1, \quad (27d)$$

which also implies

$$l \left|\frac{\partial}{\partial l} \cos \chi\right| \ll \sin \chi \sim \sin \theta. \quad (27e)$$

(ii) The potentials V_α and V_ν give rise to similar scattering at energies E_α and E_ν respectively. Stated more precisely:

$$\cos\left(\frac{1}{2}(\Theta_c - \Theta_a)\right) \approx 1; \quad (27f)$$

(iii)

$$\left|\frac{Q}{E} - \frac{2M(Q - \Delta V_0)}{\hbar^2 p_0^2}\right| \ll \frac{\pi}{l}; \quad (27g)$$

(iv)

$$d \left|\frac{\partial p}{\partial r}\right|_{r=r_0} \ll |p_0|, \quad (27h)$$

which is the condition for the validity of the local momentum approximation. The length scale d is the smaller of r_0 and the absorption free-path at $r = r_0$. Condition (27h) need not be very strictly satisfied. Since higher-order terms are of second order in $\partial p/\partial r$, the local momentum approximation should be good for

$$d \left|\frac{\partial p}{\partial r}\right|_{r=r_0} \leq 3|p_0|$$

and is still apparently reasonable if

$$d \left|\frac{\partial p}{\partial r}\right|_{r=r_0} \sim |p_0|$$

(as for Coulomb excitation when $d \sim r_0$).

All of the above conditions apply to the principal partial waves contributing to the reaction, for which $l \gg 1$.

The plausibility of (26) and results following from there may be established by noting that: (a) it yields the correct limit at high energy (Crowley 1976, 1977 Crowley and Buck 1978); (b) it correctly yields the elastic-scattering limit for $\mathbf{q} = \mathbf{0}$; (c) in the plane-wave limit, $V = \Delta V \equiv 0$, the formulae yield good approximations to the plane-wave Born approximation in the forward angle region; (d) energy conservation near a point-of-closest-approach is correctly described by the condition,

$$p_0 \cdot \mathbf{q}/k \approx (Q - \Delta V_0)/\hbar v.$$

Further approximations to (26) may be usefully made when ΔL is sufficiently large for the argument of the δ -functions to be considered independent of L . The additional sufficient condition for this to be so is that ΔL is greater than or approximately equal to the number of contributing partial waves. We shall consider the validity of such an approximation when the result is to be applied to a peripheral reaction (e.g. nuclear heavy-ion scattering) or to (pure) Coulomb excitation. In either case the approximation involves the replacement of r_0 , within the δ -function argument, by a constant, R , which may be given in terms of a particular value, Λ , of the angular momentum (as is appropriate in the treatment of a peripheral reaction when contributions come only from a limited range ($\sim \Delta\Lambda$) of angular momenta centred about $\sim \Lambda \gg \Delta\Lambda$); or in terms of the scattering angle, θ , as expressed by the unperturbed-orbit equation (as is usually considered appropriate in the treatment of Coulomb scattering).

Such an approximation is valid in the treatment of a peripheral reaction if $\Delta L \geq \Delta\Lambda$. Taking Λ to be of the order of the orbiting value (neglecting absorption) provides the following upper-limit estimate of $(\partial V/\partial r)|_{r=R}$:

$$\left. \frac{\partial V}{\partial r} \right|_{r=R} \leq \frac{2(E - V(R))}{R}.$$

Hence, assuming $\partial(\Delta V/V)/\partial r \approx 0$, estimates of ΔE and ΔL are† (with the aid of (25)):

$$\Delta E \approx E \left(\frac{\Lambda}{k^2 R^2} \right)^{2/3} \epsilon^{1/3}, \quad \Delta L \approx \left(\frac{\Lambda}{kR} \right)^{-3} \left(\frac{\Lambda^2}{\epsilon^2 kR} \right)^{1/3},$$

where

$$\frac{\Lambda^2}{k^2 R^2} \approx \frac{E - V(R)}{E},$$

$$\epsilon \approx \left| 2Q \left(\frac{1}{V(R)} - \frac{1}{E} \right) - Q_{\text{eff}} \left(\frac{2}{V(R)} - \frac{1}{E} \right) \right|,$$

and

$$Q_{\text{eff}} = Q - \Delta V(R) \tag{28}$$

is the *effective Q-value*. If $\Lambda \gg 1$, $kR \gg 1$ and $\epsilon \ll 1$ then $\Delta E/E \ll 1$ and $\Delta L \gg 1$ so that the approximation is well justified if $\epsilon \Delta\Lambda \lesssim 1$.

† The arguments ignore the fact that V and ΔV may be complex. However, simple arguments show that $\text{Im}(p_0) \sim \Lambda^{-1}$ for $L \approx \Lambda$, so it may be concluded that, for large Λ , *dynamical* effects of absorption are negligible. The important *diffractive* effects of absorption are largely contained in the phase shifts.

In the case of Coulomb excitation, Λ and R may be taken to be given by the Rutherford formulae:

$$\Lambda = \eta \cot \frac{1}{2}\theta,$$

$$R = (\eta/k) (1 + \operatorname{cosec} \frac{1}{2}\theta),$$

where η is the Coulomb–Sommerfeld parameter, in terms of which $V(r) = 2E\eta/k r$. Taking $\Delta V = 0$, the widths ΔE and ΔL are easily calculated from (25) and found to be:

$$\Delta E = \frac{E}{\Lambda} \left(\frac{\eta Q}{E} \right)^{1/3} = E \tan(\frac{1}{2}\theta) \left(\frac{Q}{\eta^2 E} \right)^{1/3},$$

$$\Delta L = \Lambda \left(\frac{E}{\eta Q} \right)^{2/3}.$$

Unlike the previously described peripheral reaction, Coulomb excitation can involve a large number of partial waves with no definite cut-off in l -space. However, the approximation under consideration is likely to be valid if

$$\Delta L \gg \Lambda,$$

which requires that

$$\frac{\eta Q}{E} \ll 1$$

(i.e. the collision should be non-adiabatic).

Applying the techniques described to direct Coulomb excitation, in the limit of $\eta Q/E = 0$, yields the known (semi-) classical formulae (Huby 1958) for the pure $E\Lambda$ electric multipole transition amplitudes, namely

$$f_{E\lambda}(\theta) \propto \frac{1}{k} \frac{(\sin \frac{1}{2}\theta)^{\lambda-2}}{(1 + \sin \frac{1}{2}\theta)^\lambda}$$

except for terms in low partial waves ($l \leq \lambda$).

Upon approximating (26) as described, the expression for $S_{\gamma\alpha}^{\text{eff}}(\mathbf{q})$ becomes:

$$S_{\gamma\alpha}^{\text{eff}}(\mathbf{q}) \approx \frac{2\pi^2}{k^2} \tilde{\delta} \left(\frac{\mathbf{q} \cdot \mathbf{P}}{k} - \frac{Q_{\text{eff}}}{\hbar v} \right) \sum_{l=0}^{\infty} (2l+1) e^{2i\delta(l+1/2)} P_l(\cos \chi), \quad (29)$$

where $\mathbf{P} = \Lambda \hat{\mathbf{k}}/R = p_0(\Lambda) \hat{\mathbf{k}}$.

This formula for $S_{\gamma\alpha}^{\text{eff}}(\mathbf{q})$ has a very simple structure which is analogous to that of an elastic s -matrix. The partial-wave sum describes an angular distribution in the space of the angle χ (which can be treated as being virtually independent of l , on account of (27*d*)) in terms of average phase shifts. Analytical stationary-phase methods (Ford and Wheeler 1959) may be applied to this sum in order to derive other forms of (29).

Another simplifying feature of the formula is that $\cos \chi$ depends upon \mathbf{q} only through the length of the vector $\mathbf{t} = \mathbf{k}_\gamma - \mathbf{k}_\alpha - \mathbf{q}$. Expressing the result (29) in terms of \mathbf{t} :

$$S_{\gamma\alpha}(s - \mathbf{t}) = \frac{2\pi^2}{k^2} \tilde{\delta} \left(\frac{\mathbf{t} \cdot \mathbf{P}}{k} - \frac{\Delta V_{\text{eff}}}{\hbar v} \right) \sum_{l=0}^{\infty} (2l+1) e^{2i\delta(l+1/2)} P_l(\cos \chi), \quad (30)$$

where

$$s = \mathbf{k}_\gamma - \mathbf{k}_\alpha,$$

$$\Delta V_{\text{eff}} = Q \frac{P}{k} \cos \frac{1}{2}\theta - Q_{\text{eff}} = \Delta V(R) + Q(P \cos \frac{1}{2}\theta - k)/k,$$

and

$$\cos \chi = \left(\frac{k}{p_0} \cos \frac{1}{2}\theta \right) \left(1 - \frac{t^2}{2k^2} \right) + \left(1 - \frac{k}{p_0} \cos \frac{1}{2}\theta \right) \cos \theta.$$

In view of condition (27g) it is often possible, particularly at high energies, to neglect ΔV_{eff} altogether (Crowley 1977).

Treating $\tilde{\delta}(z)$ as a delta-function in the space of the variable $\mathbf{t} \cdot \hat{\mathbf{k}}$ enables the momentum-space integral (19) for the DWBA t -matrix $t_{\gamma\alpha}$ to be expressed in the form

$$t_{\gamma\alpha} = \int A(t) F_{\gamma\alpha}(s - \mathbf{t}) d^2 t, \quad (31)$$

where $S_{\gamma\alpha}(s - \mathbf{t})$ is given by (30) and has been expressed in the form:

$$S_{\gamma\alpha}(s - \mathbf{t}) = \delta(\hat{\mathbf{k}} \cdot \mathbf{t} - M \Delta V_{\text{eff}}/(\hbar P)) A(t).$$

The integral (31) is carried out in the plane

$$\mathbf{t} \cdot \hat{\mathbf{k}} = M \Delta V_{\text{eff}}/(\hbar P)$$

over values of t such that $-1 \leq \cos \chi \leq 1$. A high-energy form of this formula, suggested by the eikonal approximation, has been proposed (Crowley 1976, chap. 2, Crowley and Buck 1978) and applied successfully to the treatment of direct single-nucleon transfer between heavy ions (Crowley 1976, chap. 3, 1977).

The formulae derived in this section provide simple means of approximately evaluating the DWBA t -matrix; and particular advantage can be gained in the treatment of transfer reactions (Crowley 1976, 1977). The formulae offer several other advantages over the original quantal expression (2) in that they are amenable to further analytical approximation as well as clearer interpretation in terms of classical and semi-classical (including diffractive) models.

5. Summary

Section 2 of this paper contains a description of a semi-classical wavefunction proposed as a useful approximation for use in conjunction with distorted-wave theories. In particular, the local-momentum approximation described in §4 can be used to derive a wavefunction whose phase depends almost linearly on \mathbf{r} and is therefore a possible means of treating recoil in transfer and knockout reactions. In this paper we are mainly concerned with semi-classical saddle-point-method approximations as a means of evaluating matrix elements involving these wavefunctions.

In § 3 and in the appendix we describe a technique for evaluating the semi-classical s -matrix and illustrate the connection between the resulting formulae, (11), (13) etc., and the exact quantal s -matrix expressed in the form of (14) with the aid of the Poisson summation formula. The theorem (17) is a statement of a *principle of asymptotic equivalence* based on the connection between the derived semi-classical

formula and the quantal partial-wave sum. The latter leads to more tractable expressions for the semi-classical s -matrix by employing the Poisson formula and Szëgo approximations for $P_\nu(\cos \theta)$. The theorem is therefore useful as a means of introducing a partial wave sum or any of its limiting forms into a semi-classical calculation in which expressions having the form of the left-hand side of (17) arise.

The most important results of this paper are described in § 4. These follow from applying the methods outlined in § 3 and appendix 1 to the treatment of the DWBA t -matrix (2), (18). The general form of the main result is equation (26) in which $S_{\gamma\alpha}(\mathbf{q})$ is related to the DWBA t -matrix by (18). The main assumptions made in obtaining (26) are discussed and subsequently summarised in (27). Additional (weak) assumptions have to be made in order to deduce (29) and (30) and hence (31). These are discussed in detail in the context of peripheral reactions and pure Coulomb excitation. The formulae (26), (29) or (30) used in conjunction with (18) lead to simple expressions for the t -matrix, such as (31) in which $A(t)$ has the form of

$$\frac{2\pi^2}{k^2} \sum_{l=0}^{\infty} (2l+1) e^{2i\delta(l+1/2)} P_l(\cos \chi(t)),$$

and $F_{\gamma\alpha}(\mathbf{q})$ is just the Fourier transform of the form factor. The formulae do, however, contain all the essential physics and are capable of giving an excellent description of a reaction when the assumptions made are valid. They are applicable, for example, to nuclear heavy-ion direct reactions at moderately high energies (≥ 10 MeV/nucleon) (Crowley 1976, 1977). Other important features of these formulae are summarised towards the end of the section.

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Appendix 1. Outline of method leading to result expressed by equation (9)

We begin by considering the asymptotic limit as ' $\hbar \rightarrow 0$ ' of the expression for the semi-classical s -matrix,

$$S_{\beta\alpha}(0) = \int \sum_{a,b} (g_a^{(+)} g_b^{(-)})^{1/2} \exp\left(\frac{i}{\hbar}(W_a^{(+)}(\mathbf{r}, \hbar\mathbf{k}_\alpha) - W_b^{(-)}(\mathbf{r}, \hbar\mathbf{k}_\beta))\right) d^3\mathbf{r} \quad (\text{A.1})$$

obtained at the beginning of § 3. The unfolding of this integral is subsequently achieved in this limit by making use of the property of $W_n(\mathbf{r}, \hbar\mathbf{k}_\nu)$ that it is the generating function of a canonical transformation relating (\mathbf{r}, n) to new 'coordinates' (\mathbf{L}_n, τ) (e.g. Goldstein 1969).

This integral (A.1) is carried out, in the first instance, over real values of \mathbf{r} . This may involve complex values of angular momentum associated with the trajectories a and b , particularly if the potential is complex. Since the wavefunction has been constructed to be an analytic function of \mathbf{r} (except at certain well defined points) we can extend the \mathbf{r} -integration to complex values of \mathbf{r} and apply saddle-point methods to

evaluating the integrals. Therefore, in general, the procedure described here involves complex values of both angular momentum and coordinates. Trajectories relating to observable situations correspond to *real* values of energy and begin and end at *real* points in space (the points of observation). Thus, in a scattering problem, we are interested in real E and θ , while quantities such as \mathbf{p} , \mathbf{L} and $r \neq \pm \infty$, which are not directly observed, are allowed to become complex. See also Knoll and Schaeffer (1976), and Koeling and Malfliet (1975).

In the semi-classical limit the phase of the integrand of (A.1) is $O(1/\hbar)$, so the latter is a rapidly varying function of \mathbf{r} . The only contribution to the integral comes from the vicinity of stationary-phase (or saddle-) points where $\nabla W_a^{(+)} = \nabla W_b^{(-)}$, i.e. where $\mathbf{p}_a = \mathbf{p}_b$. The points of stationary phase therefore lie on a classical trajectory (o) connecting the entrance channel α to the exit channel β .

Let us consider a point \mathbf{r} in the neighbourhood of such a trajectory. The phase $(W_a^{(+)} - W_b^{(-)})/\hbar$ may then be approximated by expanding the functions $W_a^{(+)}$ and $W_b^{(-)}$ about their values on a neighbouring classical trajectory (o') which connects the channels α' and β' chosen so that o' actually passes through \mathbf{r} (see figure 1).

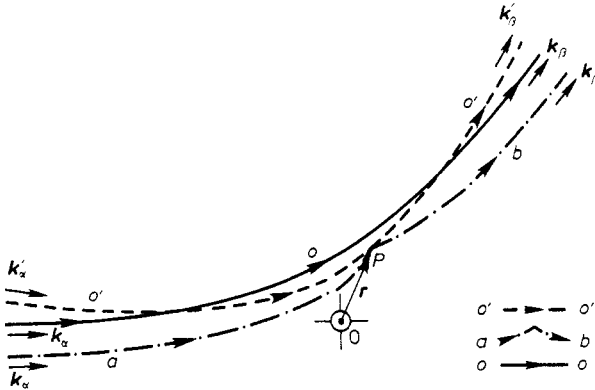


Figure 1. Diagram illustrating various trajectories (a, b, o') through a point P . The trajectory o (full curve) is a nearby classical trajectory for scattering from k_α to k_β . The trajectories a and b (chain curve), are incoming and outgoing branches of trajectories which intersect at P . These trajectories have incoming and outgoing asymptotic wavevectors equal to k_α and k_β respectively. The broken curve is the classical trajectory o' describing scattering from k'_α to k'_β , which is constructed so as to pass through P (see text).

In what follows, when the subscripted trajectory label has been omitted, o' is to be understood.

Expanding $W_a^{(+)}(\mathbf{r}, \hbar \mathbf{k}_\alpha)/\hbar$ and $W_b^{(-)}(\mathbf{r}, \hbar \mathbf{k}_\beta)/\hbar$ as Taylor series in powers of $(\mathbf{k}_\alpha - \mathbf{k}'_\alpha)$ and $(\mathbf{k}_\beta - \mathbf{k}'_\beta)$ yields

$$\frac{1}{\hbar} W_a^{(+)}(\mathbf{r}, \hbar \mathbf{k}_\alpha) = \frac{1}{\hbar} W^{(+)}(\mathbf{r}, \hbar \mathbf{k}'_\alpha) + (\mathbf{k}_\alpha - \mathbf{k}'_\alpha) \cdot \frac{\partial W^{(+)}(\mathbf{r}, \hbar \mathbf{k}'_\alpha)}{\partial (\hbar \mathbf{k}'_\alpha)} + \dots,$$

$$\frac{1}{\hbar} W_b^{(-)}(\mathbf{r}, \hbar \mathbf{k}_\beta) = \frac{1}{\hbar} W^{(-)}(\mathbf{r}, \hbar \mathbf{k}'_\beta) + (\mathbf{k}_\beta - \mathbf{k}'_\beta) \cdot \frac{\partial W^{(-)}(\mathbf{r}, \hbar \mathbf{k}'_\beta)}{\partial (\hbar \mathbf{k}'_\beta)} + \dots$$

If $\Theta'_\alpha(L_\alpha)$ is not too large, we can approximate $W_a^{(+)}$ and $W_b^{(-)}$ by the first two terms in each of these series. However, unlike using a truncated Taylor series in \mathbf{r} , this

procedure may have the effect of introducing 'spurious' saddle-points which have nothing to do with classical trajectories. To avoid picking up contributions from these it is necessary to explicitly restrict the ranges of integration to the vicinity of the classical trajectories. (The restriction on Θ' ensures that the 'spurious' saddles do not lie too close to the classical trajectories.)

Making use of the symmetry properties of the Hamiltonian, namely time independence and spherical symmetry of the interaction, it can be shown (appendix 2) that:

$$\frac{\partial W^{(+)}(\mathbf{r}, \hbar \mathbf{k}'_{\alpha})}{\partial(\hbar \mathbf{k}'_{\alpha})} = \tau \hat{\mathbf{k}}'_{\alpha} + \frac{1}{k}(\mathbf{k}'_{\alpha} \times \mathbf{L}),$$

$$\frac{\partial W^{(-)}(\mathbf{r}, \hbar \mathbf{k}'_{\beta})}{\partial(\hbar \mathbf{k}'_{\beta})} = \tau \hat{\mathbf{k}}'_{\beta} + \frac{1}{k}(\mathbf{k}'_{\beta} \times \mathbf{L}),$$

where \mathbf{L} is the angular momentum associated with o' , and τ is a parametric time coordinate ($-\infty \leq \tau \leq \infty$) specifying the position of \mathbf{r} on o' . With a suitable choice of time origin, τ is related to time, t , during the motion, by $\tau = \hbar k' t / m$, where $k' = k'_{\alpha} = k'_{\beta}$.

The next step is to carry out the transformation from the coordinates \mathbf{r} to the new coordinates (\mathbf{L}, τ) . This is most easily done by choosing the wavevectors \mathbf{k}'_{α} and \mathbf{k}'_{β} so that:

$$\hat{\mathbf{k}} \equiv \frac{\hat{\mathbf{k}}_{\alpha} + \hat{\mathbf{k}}_{\beta}}{|\hat{\mathbf{k}}_{\alpha} + \hat{\mathbf{k}}_{\beta}|} = \frac{\hat{\mathbf{k}}'_{\alpha} + \hat{\mathbf{k}}'_{\beta}}{|\hat{\mathbf{k}}'_{\alpha} + \hat{\mathbf{k}}'_{\beta}|},$$

and $k \equiv \frac{1}{2}(k_{\alpha} + k_{\beta}) = |\mathbf{k}'_{\alpha}| = |\mathbf{k}'_{\beta}|$, in addition to requiring that o' passes through \mathbf{r} . It then follows that, for \mathbf{r} close to o ,

$$(g_a^{(+)} g_b^{(-)})^{1/2} \approx g^{(o)}, \quad \text{where} \quad g^{(o)} = \det \left| \frac{1}{\hbar} \frac{\partial^2 W^{(o)}}{\partial r_i \partial k_j} \right|$$

is the Jacobian of the transformation $\mathbf{r} \rightarrow (\mathbf{L}, \tau)$. The generating function of the transformation is $W^{(o)}(\mathbf{r}; \mathbf{k})$ which is a solution of the Hamilton-Jacobi equation describing an ensemble with energy $\hbar^2 k^2 / 2m$, and having trajectories which are all parallel to $\pm \mathbf{k}$ at their points-of-closest-approach. The transformation is achieved by means of

$$\tau = \frac{\partial W^{(o)}}{\partial k}, \quad \mathbf{L} = \frac{\partial W^{(o)}}{\partial \mathbf{k}} \times \hat{\mathbf{k}}.$$

The above relation between $g_a^{(+)}$, $g_b^{(-)}$ and $g^{(o)}$ can be seen to hold when \mathbf{r} lies on o (when $o \equiv o'$) by referring to equations (6) and noting that

$$\det \left| \frac{1}{\hbar} \frac{\partial^2 W^{(o)}}{\partial r_i \partial k_j} \right| = \det \left| \frac{\partial R_j}{\partial r_i} \right|,$$

with $R_j = \partial W^{(o)} / \hbar \partial k_j$, and that $\mathbf{R} \equiv \partial W^{(o)} / \hbar \partial \mathbf{k}$ is equivalent, by the above, to (\mathbf{L}, τ) . For \mathbf{r} close to o , the particular choice of \mathbf{k}'_{α} and \mathbf{k}'_{β} described above leads to the disappearance of first-order terms in $g^{(o)} - (g_a^{(+)} g_b^{(-)})^{1/2}$. Clearly any other choice of \mathbf{k}'_{α} and \mathbf{k}'_{β} which is equivalent to the above to first order in $(\mathbf{k}_{\alpha} - \mathbf{k}'_{\alpha})$ and $(\mathbf{k}_{\beta} - \mathbf{k}'_{\beta})$ would also have this property.

The construction of the trajectory o' is illustrated in figure 1.

A transformation of variables of integration may therefore be carried out using

$$(g_a^{(+)} g_b^{(-)})^{1/2} d^3 r \approx \frac{1}{k^2} d^2 L d\tau.$$

The τ -dependence of the phase is entirely expressed by the term

$$[(\mathbf{k}_\alpha - \mathbf{k}'_\alpha) \cdot \hat{\mathbf{k}}'_\alpha - (\mathbf{k}_\beta - \mathbf{k}'_\beta) \cdot \hat{\mathbf{k}}'_\beta] \tau = \hat{\mathbf{k}}_\alpha \cdot \hat{\mathbf{k}}'_\alpha (k_\alpha - k_\beta) \tau \approx (k_\alpha - k_\beta) \tau$$

(neglecting terms of $O((\mathbf{k}'_\alpha - \mathbf{k}_\alpha)^2)$). Integrating over τ yields the energy delta-function in the form of $\delta(k_\alpha - k_\beta)$. We therefore need only consider the remainder of the expression for values of the wavenumbers such that $k_\alpha = k_\beta = k$.

Since \mathbf{r} lies on o' we have by substitution of the solutions for $W^{(+)}$ and $W^{(-)}$ in the forms of (4a), that

$$\frac{1}{\hbar} (W^{(+)}(\mathbf{r}, \hbar \mathbf{k}'_\alpha) - W^{(-)}(\mathbf{r}, \hbar \mathbf{k}'_\beta)) = 2\delta(L) - L\Theta(L) - m\pi,$$

where $\delta(L) = \delta_\alpha(L) = \delta_\beta(L)$ is the phase shift and $\Theta(L) = \Theta_\alpha(L) = \Theta_\beta(L) = \Theta$ is the deflection; the integer m specifies the total number of complete circuits of the origin made by o (since o' is constructed by analytic continuation from o , m cannot change in going from o to o') and is given in terms of $\Theta_o = \Theta(L_o)$ by:

$$-\pi \leq \text{Re}(\Theta_o + 2m\pi) \leq \pi$$

(two values of m are possible when $\text{Re} \Theta_o$ is an odd multiple of π).

Hence an approximation of the phase $(W_a^{(+)} - W_b^{(-)})/\hbar$ in the vicinity of a classical trajectory is

$$\begin{aligned} & 2\delta(L) - L\Theta - m\pi - (k_\alpha - k_\beta)\tau + (\hat{\mathbf{k}}_\alpha \times \hat{\mathbf{k}}'_\alpha - \hat{\mathbf{k}}_\beta \times \hat{\mathbf{k}}'_\beta) \cdot \mathbf{L} \\ & = 2\delta(L) - L\Theta - m\pi - (k_\alpha - k_\beta)\tau + 2L(\cos(\frac{1}{2}\theta) \sin(\frac{1}{2}\Theta + m\pi) \\ & \quad - \sin(\frac{1}{2}\theta) \cos(\frac{1}{2}\Theta + m\pi) \cos \phi), \end{aligned} \tag{A.2}$$

where θ is the scattering angle which is the angle between k_α and k_β , defined in the range $\pi \geq \theta \geq 0$; and

$$\cos \phi = \mathbf{L} \cdot (\hat{\mathbf{k}}_\beta \times \hat{\mathbf{k}}_\alpha) / (L \sin \theta).$$

The angle ϕ is thus the angle between the normal to the scattering plane and the angular momentum vector, \mathbf{L} . The well known classical result that $\cos \phi = \pm 1$ when $\theta \neq 0$ and $\theta \neq \pi$ follows from the stationary-phase conditions (12).

Including contributions from all trajectories through each point \mathbf{r} when performing the volume integration over \mathbf{r} leads to the integral $\int d^2 L$ including contributions from all saddle-points given by (12a)–(12d). Each such saddle-point is characterised by an index m which must therefore be summed over. Hence the complete unfolding transformation is

$$\int_{a,b} \sum (g_a^{(+)} g_b^{(-)})^{1/2} d^3 r \rightarrow \frac{1}{k^2} \sum_{m=-\infty}^{\infty} \int d^2 L d\tau. \tag{A.3}$$

It is not necessary for saddle-points to exist for all m in (A.3). Where a term of given m does not contain any saddle-points in the integral its contribution in the semi-classical limit is zero. Since m may be expressed as an integer function of L , the final sum over m corresponds to piecewise integration over L . (Thus, although a sum over m appears in the final expression, m is not an unfolding coordinate.)

Note that the formula breaks down if a saddle-point occurs too close to a cut at $\Theta(L) = \pm(2n + 1)\pi$. (See first footnote in § 3.) Finally we note that d^2L can be represented in plane polar coordinates as $LdLd\phi$. The integrand has a cyclic dependence on ϕ , so ϕ can take on values in any 2π interval.

Combining (A.1), (A.2) and (A.3) leads to the result,

$$S_{\beta\alpha}(0) = \frac{1}{k_\alpha^2} \sum_{m=-\infty}^{\infty} \int \exp\{i[2\delta(L) - L\Theta - m\pi - (k_\alpha - k_\beta)\tau + 2L(\cos(\frac{1}{2}\theta)\sin(\frac{1}{2}\Theta + m\pi) - \sin(\frac{1}{2}\theta)\cos(\frac{1}{2}\Theta + m\pi)\cos\phi)]\} L dL d\phi d\tau.$$

Appendix 2. Proof of the relations $\partial W(r, \hbar k)/\partial(\hbar k) = \tau\hat{k} + (\hat{k} \times L)/k$.

Lemma 1. Proof that $\partial W/\partial k = \hbar\tau$.

If the Hamiltonian is independent of time t then (Goldstein 1969) the principal function $S(r, \hbar k; t)$ is given in terms of $W(r, \hbar k)$ by

$$S(r, \hbar k; t) = W(r, \hbar k) - \frac{\hbar^2 k^2}{2m} t.$$

Differentiating with respect to k gives:

$$\frac{\partial S}{\partial k} = \frac{\partial W}{\partial k} - \frac{\hbar^2 k}{m} t$$

but $\partial S/\partial(\hbar k)$ is just a constant, denoted by a , so that

$$\frac{\partial W}{\partial k} = \hbar \left(a + \frac{\hbar k}{m} t \right) \equiv \hbar\tau. \tag{A.4}$$

This shows that τ is (with suitable choice of units and origin) related to time (in a parametric sense).

The main part of the proof requires that the potential $V(r)$ is spherically symmetric about some origin O so that

$$V(\mathbf{r}) \equiv V(r).$$

We consider the properties of $W(r, \mathbf{P})$ that result from such a symmetry.

Let $\mathbf{R}(\phi)$ be an orthogonal matrix or operator which acts upon a vector rotating it through an angle ϕ in a right-handed sense about an axis, $\hat{\phi}$, so that

$$\mathbf{R}(\phi)\mathbf{P} \approx \mathbf{P} + \phi \times \mathbf{P},$$

for first-order rotations through small angles.

Let $U_{\mathbf{R}}(\phi)$ be the operator which rotates a function through an angle ϕ . Again, for first-order small-angle rotations,

$$U_{\mathbf{R}}(\phi)f(\mathbf{r}) = f(\mathbf{R}(-\phi)\mathbf{r}) \approx f(\mathbf{r} - \phi \times \mathbf{r}) \approx f(\mathbf{r}) - (\phi \times \mathbf{r}) \cdot \nabla f.$$

Therefore

$$U_{\mathbf{R}}(\phi)f(\mathbf{r}) \approx f(\mathbf{r}) - \phi \cdot (\mathbf{r} \times \nabla f). \tag{A.5}$$

The characteristic function $W(\mathbf{r}, \mathbf{P})$ for scattering by a central field $V(r)$ must possess axial symmetry in \mathbf{r} -space about an axis through O parallel to \mathbf{P} . Rotation of \mathbf{P} is therefore equivalent to a similar rotation of $W(\mathbf{r})$, so that

$$W(\mathbf{r}, \mathbf{R}(\phi)\mathbf{P}) \equiv U_{\mathbf{R}(\phi)}W(\mathbf{r}, \mathbf{P}). \tag{A.6}$$

Hence, using (A.5),

$$W(\mathbf{r}, \mathbf{R}(\phi)\mathbf{P}) \approx W(\mathbf{r}, \mathbf{P}) - \phi \cdot (\mathbf{r} \times \nabla W) = W(\mathbf{r}, \mathbf{P}) - \phi \cdot \mathbf{L}, \tag{A.7}$$

where ϕ is a small angle, and

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \equiv \mathbf{r} \times \nabla W$$

is the *angular momentum*.

The general increment of \mathbf{P} may be considered to be a rotation plus a change in magnitude. Since, for $P \neq 0$,

$$\begin{aligned} \delta\mathbf{P} &\equiv \frac{\delta\mathbf{P} \cdot \mathbf{P}}{P^2} \mathbf{P} + \left(\frac{\mathbf{P} \times \delta\mathbf{P}}{P^2} \right) \times \mathbf{P}, \\ \mathbf{P} + \delta\mathbf{P} &= \frac{\delta\mathbf{P} \cdot \mathbf{P}}{P} \hat{\mathbf{P}} + \mathbf{R} \left(\frac{\mathbf{P} \times \delta\mathbf{P}}{P^2} \right) \mathbf{P}. \end{aligned}$$

Therefore, by means of a Taylor expansion of W to first order, and by making use of (A.7):

$$\begin{aligned} W(\mathbf{r}, \mathbf{P} + \delta\mathbf{P}) &= \frac{\mathbf{P} \cdot \delta\mathbf{P}}{P} \frac{\partial W}{\partial P} + W \left(\mathbf{r}, \mathbf{R} \left(\frac{\mathbf{P} \times \delta\mathbf{P}}{P^2} \right) \mathbf{P} \right) \\ &= W(\mathbf{r}, \mathbf{P}) + \frac{\mathbf{P} \cdot \delta\mathbf{P}}{P} \frac{\partial W}{\partial P} - \left(\frac{\mathbf{P} \times \delta\mathbf{P}}{P^2} \right) \cdot \mathbf{L} = W(\mathbf{r}, \mathbf{P}) + \left(\tau \frac{\mathbf{P}}{P} + \frac{\mathbf{P} \times \mathbf{L}}{P^2} \right) \cdot \delta\mathbf{P}, \end{aligned}$$

where $\tau = \partial W / \partial P$ (by lemma 1).

Hence

$$\frac{\partial W}{\partial \mathbf{P}} = \tau \hat{\mathbf{P}} + \frac{1}{P} (\hat{\mathbf{P}} \times \mathbf{L}) \tag{A.8}$$

or, writing $\mathbf{P} = \hbar \mathbf{k}$, and replacing \mathbf{L} by $\hbar \mathbf{L}$,

$$\frac{\partial W}{\partial(\hbar \mathbf{k})} = \tau \hat{\mathbf{k}} + \frac{1}{k} (\hat{\mathbf{k}} \times \mathbf{L}).$$

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