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Semiclassical techniques for treating the one-dimensional Schrödinger equation: uniform approximations and oscillatory integrals

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Abstract. A semiclassical theory based upon the oscillatory integral representation of the quantal wavefunction is applied to the one-dimensional Schrödinger equations describing motion in linear and parabolic potentials. It is demonstrated that the method yields exact solutions in both these cases. For more general one and two turning point problems, the oscillatory integral approach would seem to be equivalent to the method of uniform approximation using linear or parabolic comparison functions. The technique yields both continuum and discrete solutions for the parabolic potential—the former corresponding to scattering states (barrier problem) and the latter to resonances or bound states (harmonic oscillator). Precise conditions for the existence of solutions of either type are derived.

Of importance is the fact that oscillatory integral type solutions are globally valid not only in coordinate space but also in parameter space. This enables us to derive the general parabolic connection formula relating the asymptotic wavefunction in different parts of the complex coordinate plane. This formula is applicable to cases when both the potential and the energy may be complex.

1. Introduction

It has long been established (e.g. Kemble 1935, 1937) that the semiclassical method yields exact asymptotic forms for the wavefunction in the case of real linear or parabolic potentials. The technique and results are important in that they are immediately generalisable by the technique of uniform approximation (Miller and Good 1953, Dingle 1956, Berry and Mount 1972) to the connection problem(s) arising in the context of potentials of more general shape. Thus, formulae are provided for all cases when the potential is locally either linear or parabolic in form at a classical turning point. More recently, Knoll and Schaeffer (1976) and Brink and Takigawa (1977) have extended the results to complex potentials (such as are commonly employed in the treatment of nuclear collisions). The derivation, by Brink and Takigawa, of the parabolic-barrier s matrix as an analytic function of the potential parameters constitutes the crucial step in their derivation of a useful closed-form expression for the semiclassical s matrix for scattering by a central field. Their result†, which is valid for a general 'three-turning-point' scattering problem in which the effective radial potential is assumed to behave linearly at the innermost (left-hand) turning point, has found

† It should perhaps be pointed out that Brink and Takigawa's result is essentially equivalent to formulae given in Connor (1973) and Connor *et al* (1976) where they are derived and applied albeit in a more limited context.

important application in the field of nuclear interactions (Lee *et al* 1978, Takigawa 1978, Takigawa *et al* 1978, Delbar *et al* 1978).

The purpose of this paper is to demonstrate that the semiclassical method is capable of providing globally *exact* wavefunctions for linear and parabolic potentials. Furthermore, these wavefunctions are analytically continuable into the domains of complex energy and potential parameters. In the case of a parabolic potential, the method yields not only the scattering solutions, providing a clearer derivation of the s matrix than that of Brink and Takigawa (1977), but also solutions corresponding to bound states (harmonic oscillator) and resonances.

2. Global uniform semiclassical approximation of the wavefunction in one dimension

The basic method, believed to have been originally suggested by Maslov (1972) and which has been since discussed and extended by several others (including Duistermaat (1974), Berry (1976), Poston and Stewart (1978) and Crowley (1979, 1980a))†, involves expressing the semiclassical wavefunction ψ as an oscillatory or generalised diffraction integral. In a one-dimensional Euclidean configuration space $\mathbb{E}^{(1)}\{q\}$, this takes the form:

$$\psi_\alpha(q) = (2\pi\hbar)^{-1/2}C(\alpha)\int_{-\infty}^{\infty}\left(\frac{\partial^2 F(q,\gamma;\alpha)}{\partial q\,\partial\gamma}\right)^{1/2}\exp[(\mathrm{i}/\hbar)F(q,\gamma;\alpha)]\,\mathrm{d}\gamma \tag{1}$$

which, in general, represents a uniformly valid approximate global solution of the Schrödinger equation:

$$\mathscr{H}\left(-\mathrm{i}\frac{\partial}{\partial q}, q\right)\psi = E\psi \tag{2}$$

for a smooth integrable Hamiltonian $\mathscr{H}(p,q)$ and energy $E(\alpha)$, in the semiclassical limit when Planck's constant $\hbar$ is a vanishingly small parameter of the problem (Berry and Mount 1972). In certain cases, as will be demonstrated, the wavefunction (1) represents an exact solution of (2). The function $F(q,\gamma;\alpha)$, which is the main ingredient of the right-hand side of (1), is provided by classical mechanics as follows.

† There are also connections with other semiclassical theories employing the Feynman path integral approach (see, for example, Feynman 1948, Feynman and Hibbs 1965, Berry and Mount 1972 § 7, Voros 1977). In particular, Balian and Bloch (1974) show that the quantal propagator (and hence wavefunction) may be expressed as a Fourier (or Laplace) transform, with $1/\hbar$ as the new transform-variable, of a function Ω which may be defined entirely in terms of the corresponding classical problem. Since F above is a single-valued function of γ, the integral (1) may be transformed to one over F along a contour defined by $F(\gamma)$. This yields the result:

$$\psi_\alpha(q) = (2\pi\hbar)^{-1/2}\int \Omega(q,F;\alpha)\exp[(\mathrm{i}/\hbar)F]\,\mathrm{d}F$$

where $\Omega(q,F;\alpha) = C(\alpha)(-\partial^2\gamma/\partial F\,\partial q)^{1/2}$, which strongly resembles the form proposed by Balian and Bloch. Whereas the integral (1) is dominated by the critical manifold $\mathscr{K}$ (saddle points corresponding to classical trajectories), the integral above is dominated by the branch points of Ω. These occur where $(\partial\gamma/\partial F)^{-1}$ vanishes (i.e. on $\mathscr{K}$) and thus also correspond to classical trajectories. An interesting point is that Balian and Bloch propose their result for the propagator as being exact (though not necessarily with Ω given as above) for integrable systems.

The characteristic function $W(q, \alpha)$ is first obtained by solving the Hamilton–Jacobi equation (Goldstein 1950):

$$\mathcal{H}\left(\frac{\partial W}{\partial q}, q\right) = E(\alpha) \tag{3}$$

with boundary conditions appropriate to the problem under consideration. The function $W(q, \alpha)$, thus obtained, is the generator of a canonical transformation through $p = \partial W/\partial q$, $\gamma = \partial W/\partial \alpha$, whereby the Hamiltonian $\mathcal{H}(p, q)$ is transformed to $K(\alpha, \gamma) \equiv E(\alpha)$ which is cyclic in γ. In a one-dimensional problem for which $\mathcal{H}(p, q)$ is independent of time t there is a one-to-one correspondence between γ and t.

The function $F(q, \gamma; \alpha)$ is a single-valued extension of the classical action $W(q, \alpha)$ (W is not, in general, single-valued) defined to have the following properties:

$$\frac{\partial F}{\partial \gamma} = 0 \Leftrightarrow \frac{\partial W}{\partial \alpha} = \gamma \tag{4}$$

$$F\left(q, \frac{\partial W}{\partial \alpha}; \alpha\right) = W(q, \alpha). \tag{5}$$

Equations (4) define a critical manifold $\mathcal{K}$, in this case a line in $\mathbb{E}^{(1)}\{q\} \otimes \mathbb{E}^{(1)}\{\gamma\}$ commonly known as the classical trajectory, to which the classical motion is confined, and on which $W = F$. With the added constraints that $(\partial^2 F/\partial \gamma\, \partial q)^{1/2}$ be non-vanishing everywhere on $\mathcal{K}$ (except perhaps at $|\gamma| = \infty$) and contain only integrable singularities in $\mathbb{E}^{(1)}\{\gamma\}$, the above are generally sufficient to determine uniquely a universal analytic function F, provided that $W(q, \alpha)$ and its derivatives are *not* everywhere single-valued. The analyticity of F is an indication that the first of equations (4) yields classical dynamical solutions in *complex* q-space. These are associated with *complex trajectories* (Keller 1958, Knoll and Schaeffer 1976, Koeling and Malfliet 1976, Balian *et al* 1978).

Multivaluedness of the classical action can be associated with the presence of caustics in $\mathbb{E}^{(1)}\{q\}$. In terms of F, the caustic set $\mathscr{C}$ is given by

$$\mathscr{C} = \{q | \partial F/\partial \gamma = \partial^2 F/\partial \gamma^2 = 0\} \tag{6}$$

(see, for example, Connor 1976) which, in one dimension, turns out to be just the classical turning points. A useful description of the local properties of caustics is provided by *catastrophe theory* (Poston and Stewart 1978, see also Berry 1976, Connor 1976), the basis of which is a celebrated theorem due to Thom (1969, 1972, 1975). One of the implications of this theorem is that, in $\mathbb{E}^{(1)}\{q\}$, the only structurally stable caustics (Berry 1976) that can occur are those associated with the *fold catastrophe.*

The connection between (1) and the JWKB approximation is provided by approximately evaluating the integral (1) by means of the saddle-point method (Matthews and Walker 1970, Connor 1976). This results in *local* approximations to $\psi(q)$, in the form of superpositions of JWKB approximants (e.g. Crowley 1979). Such local asymptotic approximations to $\psi(q)$ are not valid at or near caustics but do yield *reversible* connection formulae relating the multipliers of the JWKB approximants on either side of a turning point. This is because $\psi(q)$ as defined by (1) is uniformly valid across a caustic.

Furthermore, equation (4) reveals the direct correspondence between the saddle points that dominate the integral (1) and classical trajectories. In event of the saddle-point approximation breaking down (for reasons that are unconnected with ordinary (catastrophe-type) singularities) one is unable to speak of classical trajectories—at least in the global sense. Such a breakdown occurs typically when a classical action characteristic of the problem becomes vanishingly small in some locality of parameter space. For example, in the case of the parabolic potential discussed in § 2.2, the large parameter on which the validity of the saddle-point approximation depends is $\epsilon = -\alpha/\hbar$ (equation (22a)) where α is proportional to the action integrated between the classical turning points. In the semiclassical limit, ϵ is typically very large except in the immediate vicinity of $\alpha = 0$ where the saddle-point approximation fails. The nature of the singularity at $\alpha = 0$ is beyond the scope of catastrophe theory. It has been pointed out by M V Berry (private communication) that this is probably due to the fact that any analytic continuation through the singularity necessarily involves going into complex coordinates and time, whereas catastrophe theory is applicable only to problems for which the critical manifold can be smoothly and reversibly mapped onto a real Euclidean manifold. Thus complex analytic continuation is not necessarily incompatible with catastrophe theory (as has been pointed out, for example, by Connor (1976)) and is permitted, for example, in all cases involving linear potentials (§ 2.1) and, as an approximation, in cases where the potential behaves linearly at all turning points. Nonetheless the orbiting or barrier-top singularity ($\epsilon = 0$) encountered in § 2.2 is a generic feature of wavefunctions resembling (1). The inability of catastrophe theory to describe such a feature represents a serious deficiency to the extent that the general usefulness of catastrophe theory in such applications is questionable (see note added in proof).

In (1), $C(\alpha)$ is just a normalisation constant. Here we adopt the standard form appropriate to a scattering wavefunction and put

$$C(\alpha) = (\mathrm{d}P/\mathrm{d}\alpha)^{-1/2}$$

where $P(\alpha) = (2mE(\alpha))^{1/2}$. Henceforth, we shall work in units in which the particle's mass m is equal to unity.

2.1. *Application to the linear potential*

Because it provides a clear illustration of the above method, we briefly review the application of the above to motion in a linear potential. This is the simplest non-trivial example to which the method may be applied.

Consider the Hamiltonian $\mathscr{H}(p, q) = \frac{1}{2}p^2 - \frac{1}{2}q$ in which the potential energy is represented by $-\frac{1}{2}q$. Solving the Hamilton–Jacobi equation

$$(\partial W/\partial q)^2 = \alpha + q,$$

where $\frac{1}{2}\alpha \equiv E(\alpha)$ is the energy, yields

$$W(q, \alpha) = \tfrac{2}{3}(q + \alpha)^{3/2}.$$

Hence

$$\gamma \equiv t = \partial W/\partial\alpha = (q + \alpha)^{1/2}. \tag{7}$$

The critical manifold defined by (7) has two branches corresponding to the two branches of the square root. For real q these correspond to $t < 0$ and $t > 0$. By equations (4) and (5) the above leads directly to the generating function:

$$F(q, t; \alpha) = (q + \alpha)t - \tfrac{1}{3}t^3 \tag{8}$$

which is a perfect example of a fold catastrophe that is associated with the caustic (classical turning point) at $q=-\alpha$. Application of equation (1) yields the wavefunction as

$$\psi_\alpha(q)=(2\pi\hbar)^{-1/2}(4\alpha)^{1/4}\int_{-\infty}^{\infty}\exp\{(\mathrm{i}/\hbar)[(q+\alpha)t-\tfrac{1}{3}t^3]\}\mathrm{d}t \tag{9a}$$

$$=2\pi^{1/2}\alpha^{1/4}\hbar^{-1/6}\,\mathrm{Ai}\left(-\frac{q+\alpha}{\hbar^{2/3}}\right) \tag{9b}$$

(using Abramowitz and Stegun (1965, equation (10.4.32))) by which one obtains an exact solution of the Schrödinger equation, $-\hbar^2(\partial^2\psi/\partial q^2)-q\psi=\alpha\psi$ (see Abramowitz and Stegun 1965, § 10.4).

In the semiclassical limit ('$\hbar\to 0$') the argument of the Airy function becomes large for $q+\alpha\neq 0$. In the asymptotic limit of large $|x|$, the function $\mathrm{Ai}(x)$ exhibits the well-known Stokes phenomenon (Stokes 1904, 1905, Kemble 1937, Berry and Mount 1972, Dingle 1973) which also arises in the evaluation of the integral (9a) by the saddle-point method. The result is, for $x=q+\alpha$,

$$\psi(x)\underset{'\hbar\to 0'}{\sim}\left(\frac{\alpha}{x}\right)^{1/4}(a_+\,\mathrm{e}^{-\pi\mathrm{i}/4}\,\mathrm{e}^{\mathrm{i}W/\hbar}+a_-\,\mathrm{e}^{\pi\mathrm{i}/4}\,\mathrm{e}^{-\mathrm{i}W/\hbar})\qquad -\pi<\arg x\leqslant\pi,\ |x|>0 \tag{10}$$

where $W=\frac{2}{3}x^{3/2}$ and

$$\begin{aligned} a_+&=1, & -\pi&<\arg x<\pi/3 & \qquad a_-&=1, & -\pi/3&<\arg x\leqslant\pi\\ &=0, & \pi/3&<\arg x\leqslant\pi & &=0, & -\pi&<\arg x<-\pi/3. \end{aligned}$$

This yields the well-known connection formula:

$$\begin{array}{ccc} \left(\dfrac{\alpha\,\mathrm{e}^{\pi\mathrm{i}}}{x}\right)^{1/4}\mathrm{e}^{-\bar{W}/\hbar} & \leftarrow\psi(x)\rightarrow & 2\left(\dfrac{\alpha}{x}\right)^{1/4}\cos\left(\dfrac{1}{\hbar}W-\dfrac{\pi}{4}\right)\\ \pi/3<\arg x<5\pi/3 & & -\pi/3<\arg x<\pi/3 \end{array} \tag{11}$$

where $\bar{W}=\frac{2}{3}(-x)^{3/2}$, $|\arg\bar{W}|<\pi/2$. This formula is reversible only in the sense that the left- and right-hand sides of the formula represent limiting asymptotic forms of the wavefunction† (see discussion by Berry and Mount (1972)).

In more general cases, the fold catastrophe provides a valid *local* description of behaviour near an isolated turning point where the potential is locally linear with non-vanishing slope. In this way one obtains the local Airy function approximation which provides a confined local analytic continuation of the semiclassical wavefunction around a turning point. This is the basis of the complex trajectory formalism of Knoll and Schaeffer (1976).

For the purposes of treating transmission through a thick barrier (for which the potential may be assumed to vary linearly at each of a pair of well-separated turning

† If ψ is such that

$$\lim_{x\to-\infty}\psi(x)\times(-(x)^{-1/4}\,\mathrm{e}^{-\mathrm{i}\bar{W}/\hbar})^{-1}=\text{constant}=A$$

then

$$\lim_{x\to+\infty}\psi(x)\times\left[x^{-1/4}\cos\left(\frac{1}{\hbar}W-\frac{\pi}{4}\right)\right]^{-1}=\text{constant}=2A$$

and conversely.

points), the second connection formula which corresponds to a (globally) unphysical solution of (2) is sometimes useful. This solution arises when the integral (9*a*), instead of being carried out along the contour $\operatorname{Im} t = \epsilon < 0$, is carried out along $\operatorname{Re} t = 0$, $\operatorname{Im} t > \epsilon$; $\operatorname{Im} t = \epsilon < 0$, $\operatorname{Re} t > 0$ between $t = i\infty$ and $t = \infty + i\epsilon$. In this way we obtain the solution

$$\psi(x) \propto \operatorname{Ai}(-x/\hbar^{2/3}) - \mathrm{i}\,\operatorname{Bi}(-x/\hbar^{2/3})$$

(Abramowitz and Stegun 1965, equations (10.4.32-3)) and hence (e.g. Dingle 1973) the second connection formula which is characterised by the presence of an exponentially growing term in the classically forbidden region:

$$\left(\frac{\alpha\, \mathrm{e}^{\pi \mathrm{i}}}{x}\right)^{1/4} \mathrm{e}^{\bar{W}/\hbar} \leftarrow \psi(x) \rightarrow \left(\frac{\alpha}{x}\right)^{1/4} \exp\left[\mathrm{i}\left(\frac{1}{\hbar}W - \frac{\pi}{4}\right)\right]$$

$$\pi/3 < \arg x < 5\pi/3 \qquad\qquad -\pi/3 < \arg x < \pi/3.$$

The solution therefore describes unidirectional propagation of a particle emerging from the forbidden region into the allowed region. Such a solution may be used to describe the transmitted wave in a treatment of barrier penetration. The manner of derivation shows that this solution corresponds to a classical dynamical solution that has been analytically continued into the domain of *complex time*. In this sense we can think of tunnelling as being associated generally with a complex trajectory (Miller and George 1972). In § 2.2 we consider explicitly the problem of penetration through a parabolic barrier in a manner which illustrates the role of trajectories in complex coordinates and time.

2.2. *Application to the parabolic potential*

The simplest situation in which the Airy function approximation breaks down is when the potential is dominated at a turning point by a quadratic dependence on position. An example of such a situation occurs in connection with classical orbiting in a spherically symmetric attractive potential. One finds that, for a certain range of energy and angular momentum, two turning points of the radial motion associated with the angular momentum barrier may occur close together, giving rise to significant barrier penetration effects. As shall eventually become evident, at the classical orbiting situation when the two turning points are coincident, the concept of a classical trajectory breaks down.

We consider the related problem of motion in a one-dimensional parabolic potential. We take the Hamiltonian to be

$$\mathscr{H} = \tfrac{1}{2}p^2 - \tfrac{1}{2}\omega^2 q^2 \qquad \omega \neq 0$$

and consider solutions of the Schrödinger equation:

$$-\hbar^2 \frac{\partial^2 \psi}{\partial q^2} - \omega^2 q^2 \psi = 2\omega\alpha\psi \tag{12}$$

for energy $E = \omega\alpha$, that have the form of (1). It is convenient to define ω so that

$$-\pi/2 < \arg \omega \leqslant \pi/2 \tag{13a}$$

which results in no loss of generality since the original physical problem is specified in terms of ω^2 alone. The parameter α may now be defined to be in the range

$$-\pi/2 \leqslant \arg \alpha < 3\pi/2 \tag{13b}$$

which, for given ω, permits all complex values of E.

A particular integral of the Hamilton–Jacobi equation

$$\left(\frac{\partial W(q, \alpha)}{\partial q}\right)^2 = \omega^2 q^2 + 2\omega\alpha \tag{14}$$

is

$$W(q, \alpha) = -\tfrac{1}{2}\omega\left[q\xi + \eta^2 \ln\left(\frac{q+\xi}{\eta}\right)\right] \tag{15}$$

where $\xi = (q^2+\eta^2)^{1/2}$ and $\eta^2 = 2\alpha/\omega$ with

$$-\pi \leqslant \arg \eta^2 < 2\pi.$$

The functions $\xi(q)$ and $\ln((q+\xi)/\eta)$ are multivalued functions of q and it is necessary to take account of all branches of these functions. The function W given by (15) thus possesses a complicated multivaluedness.

Differentiating (15) with respect to α yields

$$\gamma \equiv \omega t = -\ln\left(\frac{q+\xi}{\eta}\right). \tag{16}$$

For Im $\omega = 0$, the characteristic function (15) leads to the retarded 'scattering' solution in which incident waves propagate from the right ($q > 0$). This can be seen from the following: that $-\xi = \omega^{-1}\partial W/\partial q < 0$ for Im $q = 0$, Re $q \to \infty$ on a branch of $\mathscr{K}$ on which $\gamma \to -\infty$; $-\xi q > 0$ as $|q| \to \infty$ (Im $q = 0$) on a branch of $\mathscr{K}$ on which Re $\gamma \to +\infty$; for $\alpha > 0$, the incident and transmitted components of the wavefunction correspond to real γ; for $\alpha < 0$, γ is real for the incident and reflected components. For Re $\omega > 0$, the solution (15) therefore describes incoming waves ($\xi q > 0$) at $q \to \infty$ for Re $\gamma \to -\infty$, and outgoing waves ($\xi q < 0$) at $|q| \to \infty$ for Re $\gamma \to +\infty$. The advanced solution corresponds to $-W$, while solutions describing an incident wave propagating from the left ($q < 0$) are obtained by replacing q by $-q$.

The generating function F by which the complicated multivaluedness of (15) is tamed is, for $x = q/\eta$,

$$F(\gamma, x; \eta) = -\omega\eta^2[x\,\mathrm{e}^{-\gamma} - \tfrac{1}{4}\mathrm{e}^{-2\gamma} - \tfrac{1}{2}\gamma - \tfrac{1}{2}(x^2 - \tfrac{1}{2})] \tag{17}$$

which is valid for all $\eta \neq 0$. Differentiation of (17) yields

$$\frac{\partial F}{\partial \gamma} = \tfrac{1}{2}\omega\eta^2(2x\,\mathrm{e}^{-\gamma} - \mathrm{e}^{-2\gamma} + 1) \tag{18}$$

$$\frac{\partial^2 F}{\partial x\,\partial \gamma} = \omega\eta^2\,\mathrm{e}^{-\gamma} \tag{19}$$

$$\frac{\partial^2 F}{\partial \gamma^2} = -\omega\eta^2(x - \mathrm{e}^{-\gamma})\,\mathrm{e}^{-\gamma}. \tag{20}$$

It is evident from the above that $\partial F/\partial\gamma = 0$ both implies and is implied by (16), while $F = W$ on the critical manifold $\mathscr{K} = \{x, \gamma | \partial F/\partial \gamma = 0\}$. The caustic set, from the definition (6), comprises the turning points $x = \pm \mathrm{i}$.

A uniformly valid semiclassical wavefunction that follows from the above in the manner of (1) is

$$\psi = C(\alpha)(2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty}[\omega\eta^2\,\mathrm{e}^{-\gamma}]^{1/2}\,\mathrm{e}^{(\mathrm{i}/\hbar)F(\gamma,x;\eta)}\,\mathrm{d}\gamma$$
$$= C(\alpha)\left(\frac{\omega\eta^2}{2\pi\hbar}\right)^{1/2}\exp[(\mathrm{i}/2\hbar)\omega\eta^2(x^2-\tfrac{1}{2})]$$
$$\times\int_{-\infty}^{\infty}\mathrm{e}^{-\gamma/2}\exp\left(-\frac{\mathrm{i}\omega\eta^2}{\hbar}(x\,\mathrm{e}^{-\gamma}-\tfrac{1}{4}\,\mathrm{e}^{-2\gamma}-\tfrac{1}{2}\gamma)\right)\mathrm{d}\gamma. \tag{21}$$

The integrand of (21) is an entire function of γ, and convergence of the integral is guaranteed if the integral is carried out along a contour such that

$$\mathrm{Im}\,(\omega\eta^2\,\mathrm{e}^{-2\gamma})\to\infty \qquad \text{as} \qquad \mathrm{Re}\,\gamma\to-\infty$$

and

$$\mathrm{Re}\,[\gamma(1-\mathrm{i}\omega\eta^2/\hbar)]\to\infty \qquad \text{as} \qquad \mathrm{Re}\,\gamma\to+\infty.$$

It may be verified by direct substitution that the result (21) is an exact solution of the differential equation, $\hbar^2\,\mathrm{d}^2\psi/\mathrm{d}x^2+\omega^2\eta^4(x^2-1)\psi=0$, which is just the transformed form of (12). The semiclassical method outlined in § 2 thus yields an exact solution of the quantum-mechanical problem of motion in a parabolic barrier. To confirm that it is the correct solution, it is necessary to proceed further.

The integral (21) may be transformed by the substitutions:

$$\epsilon=\frac{\omega\eta^2}{2\hbar}\,\mathrm{e}^{-\pi\mathrm{i}}=\frac{\alpha}{\hbar}\,\mathrm{e}^{-\pi\mathrm{i}} \tag{22a}$$

$$X=2\mathrm{i}\epsilon^{1/2}x=\left(\frac{2\omega}{\hbar}\right)^{1/2}q \tag{22b}$$

$$z=\mathrm{e}^{\pi\mathrm{i}/4}\epsilon^{1/2}\,\mathrm{e}^{-\gamma}=(\mathrm{i}\epsilon)^{1/2}\,\mathrm{e}^{-\gamma}. \tag{22c}$$

In accordance with (13*b*), (22*a*) implies

$$-\pi\leqslant\arg\mathrm{i}\epsilon<\pi \tag{22d}$$

which is the same convention as that adopted by Brink and Takigawa (1977). Application of (22) transforms (21) into

$$\psi(X)=C(\alpha)(\mathrm{i}/\pi)^{1/2}(\mathrm{i}\epsilon)^{1/4}\exp[-\tfrac{1}{2}\mathrm{i}\epsilon\,\ln(\mathrm{i}\epsilon/\mathrm{e})]\,\mathrm{e}^{\frac{1}{4}\mathrm{i}X^2}\int_0^{\infty}z^{-\frac{1}{2}+\mathrm{i}\epsilon}\exp(zX\,\mathrm{e}^{-\pi\mathrm{i}/4}-\tfrac{1}{2}z^2)\,\mathrm{d}z \tag{23}$$

for $\mathrm{Im}(\epsilon)<\frac{1}{2}$, when the integral may be carried out along the positive z axis.

Using the integral representation of the Whittaker function $D_\nu(z)$ given by Erdélyi *et al* (1953, equation (8.3(3))) whence

$$D_{-\frac{1}{2}-a}(x)=\frac{\mathrm{e}^{-\frac{1}{4}x^2}}{\Gamma(\frac{1}{2}+a)}\int_0^{\infty}z^{-\frac{1}{2}+a}\exp(-zx-\tfrac{1}{2}z^2)\,\mathrm{d}z \qquad \mathrm{Re}(a)>-\tfrac{1}{2}$$

we are able to express (23) in the form

$$\psi(X)=C(\alpha)(\mathrm{i}/\pi)^{1/2}(\mathrm{i}\epsilon)^{1/4}\Gamma(\tfrac{1}{2}+\mathrm{i}\epsilon)\exp[-\tfrac{1}{2}\mathrm{i}\epsilon\,\ln(\mathrm{i}\epsilon/\mathrm{e})]D_{-\frac{1}{2}-\mathrm{i}\epsilon}(-X\,\mathrm{e}^{-\pi\mathrm{i}/4}). \tag{24}$$

It is convenient to express the wavefunction $\psi(X)$ in terms of the functions $E^+(\epsilon, X)$, $E^-(\epsilon, X)$ defined as follows:

$$E^+(\epsilon, x) = e^{-3\pi i/8}\, e^{\pi\epsilon/4} D_{-\frac{1}{2}-i\epsilon}(x\, e^{-\pi i/4}) \tag{25a}$$

$$E^-(\epsilon, x) = e^{3\pi i/8}\, e^{\pi\epsilon/4} D_{-\frac{1}{2}+i\epsilon}(x\, e^{\pi i/4}) \tag{25b}$$

and which have the following asymptotic forms (Erdélyi *et al* 1953, equation (8.4(1))) for $|x| \to \infty$ in $|\arg(x) - (\pm\pi/4)| \leqslant \pi/2$†:

$$E^{\pm}(\epsilon, x) \sim x^{-1/2} \exp[\pm i(\tfrac{1}{4}x^2 - \epsilon \ln x - \tfrac{1}{4}\pi)] \tag{26}$$

describing outgoing (+) and ingoing (−) waves. With the aid of Erdélyi *et al* (1953, equation (8.2(6))) we are able to deduce the following identity:

$$(2\pi)^{1/2} E^-(\epsilon, x) = -\Gamma(\tfrac{1}{2} + i\epsilon)[e^{\frac{1}{2}\pi\epsilon} E^+(\epsilon, x) - i\, e^{-\frac{1}{2}\pi\epsilon} E^+(\epsilon, -x)]. \tag{27}$$

The functions $E^{\pm}(\epsilon, X)$ may be used to define standard ingoing (−) and outgoing (+) wave solutions as follows:

$$\phi^{\pm}(X) = 2^{1/2} E^{\pm}(\epsilon, X) \exp[\pm \tfrac{1}{2} i\epsilon \ln(i\epsilon/e)]\, e^{\pm\frac{1}{4}\pi\epsilon} \tag{28}$$

in terms of which we can define standard solutions, ϕ_{IW}, ϕ_{RW} and ϕ_{TW}, whose asymptotic forms (in appropriate argument ranges) describe incident, reflected and transmitted waves respectively, according to

$$\phi_{\mathrm{IW}}(X) = \phi^-(X) \qquad \phi_{\mathrm{RW}}(X) = \phi^+(X) \qquad \phi_{\mathrm{TW}}(X) = i\phi^+(-X) \tag{29}$$

(which are in accordance with standard phase conventions). Using (26), the asymptotic forms, for $|X| \to \infty$, of these standard solutions may be verified as being as follows:

$$\phi_{\mathrm{IW}}(X) \sim (\tfrac{1}{2}X)^{-1/2}\, e^{-\frac{1}{4}\pi\epsilon} \exp\{-i[\tfrac{1}{4}X^2 - \epsilon \ln X + \tfrac{1}{2}\epsilon \ln(i\epsilon/e) - \tfrac{1}{4}\pi]\}$$
$$-3\pi/4 \leqslant \arg X \leqslant \pi/4 \tag{30a}$$

$$\phi_{\mathrm{RW}}(X) \sim (\tfrac{1}{2}X)^{-1/2}\, e^{\frac{1}{4}\pi\epsilon} \exp\{i[\tfrac{1}{4}X^2 - \epsilon \ln X + \tfrac{1}{2}\epsilon \ln(i\epsilon/e) - \tfrac{1}{4}\pi]\}$$
$$-\pi/4 \leqslant \arg X \leqslant 3\pi/4 \tag{30b}$$

$$\phi_{\mathrm{TW}}(X) \sim (-\tfrac{1}{2}X)^{-1/2}\, e^{\frac{1}{4}\pi\epsilon} \exp\{i[\tfrac{1}{4}X^2 - \epsilon \ln(-X) + \tfrac{1}{2}\epsilon \ln(i\epsilon/e) + \tfrac{1}{4}\pi]\}$$
$$-\pi/4 \leqslant \arg(-X) \leqslant 3\pi/4$$
$$= (\tfrac{1}{2}X)^{-1/2}\, e^{\frac{5}{4}\pi\epsilon} \exp\{i[\tfrac{1}{4}X^2 - \epsilon \ln X + \tfrac{1}{2}\epsilon \ln(i\epsilon/e) - \tfrac{1}{4}\pi]\}$$
$$-5\pi/4 \leqslant \arg X \leqslant -\pi/4. \tag{30c}$$

† Here we are specifying the boundaries of the domains of validity of the asymptotic expansions to be Stokes lines (e.g. see Berry and Mount 1972) with which one may associate changes in the multiplier of an exponentially subdominant term. However, as such a term remains subdominant upon crossing a Stokes line, the expansion in fact remains valid (in the usual Poincaré sense) in an open domain whose limiting boundaries are antiStokes lines beyond which the term becomes dominant. In this way the asymptotic forms given may be extended into overlapping domains of validity. However, for the purposes of constructing connection formulae, in the semiclassical limit, it is convenient to confine the asymptotic expansion to regions bounded by Stokes lines by requiring that the expansion be valid in the complete sense of Watson (1911). This yields the most accurate representation in that errors arising from exponentially subdominant terms are kept to a minimum. The importance of such considerations has been recently stressed by Balian *et al* (1978).

The following identities are implied by (27):

$$\mathrm{e}^{-\pi\epsilon}\phi_{\mathrm{TW}}(X)=\phi_{\mathrm{RW}}(X)+\frac{1}{R(\epsilon)}\phi_{\mathrm{IW}}(X) \tag{31a}$$

$$-\phi_{\mathrm{TW}}(X)=\mathrm{e}^{-\pi\epsilon}\phi_{\mathrm{RW}}(X)+\frac{\mathrm{i}}{R(\epsilon)}\phi_{\mathrm{IW}}(-X) \tag{31b}$$

where

$$R(\epsilon)=(2\pi)^{-1/2}\Gamma(\tfrac{1}{2}+\mathrm{i}\epsilon)\exp[-\mathrm{i}\epsilon\ \ln(\mathrm{i}\epsilon/\mathrm{e})]. \tag{32}$$

Thus, by combining equations (24), (25), (28) and (29) and making use of (31), one can express the wavefunction $\psi(X)$ in the following ways:

$$\psi(X)=A(\epsilon)R(\epsilon)\,\mathrm{e}^{-\pi\epsilon}\phi_{\mathrm{TW}}(X) \tag{33a}$$

$$=A(\epsilon)[\phi_{\mathrm{IW}}(X)+R(\epsilon)\phi_{\mathrm{RW}}(X)] \tag{33b}$$

$$=-A(\epsilon)\,\mathrm{e}^{-\pi\epsilon}[\mathrm{e}^{-\pi\epsilon}R(\epsilon)\phi_{\mathrm{RW}}(X)+\mathrm{i}\phi_{\mathrm{IW}}(-X)] \tag{33c}$$

where

$$A(\epsilon)=C(\alpha)\,\mathrm{e}^{\pi\mathrm{i}/4}(\epsilon\,\mathrm{e}^{2\pi\epsilon})^{1/4}=\left(\frac{2\hbar}{\omega}\right)^{1/4}(-\epsilon)^{1/2}\,\mathrm{e}^{\pi\epsilon/2}.$$

It is now easily verifiable, with the aid of (29), that the wavefunction (33) is that which satisfies the boundary conditions of the physical problem (as imposed in selecting the particular solution (15) of the Hamilton–Jacobi equation).

Equations (30) and (33) yield the asymptotic forms of $\psi(X)$ as $|X|\to\infty$ for $-5\pi/4\leqslant\arg X\leqslant 3\pi/4$. The required asymptotic form must be obtained by a suitable combination of one or more of equations (30) with one of (33) according to the range of the argument of X. This leads to a manifestation of the Stokes phenomenon such as was encountered with the asymptotic forms of the Airy function in connection with the solution of the linear potential problem. Here the phenomenon is characterised by Stokes lines whose asymptotes lie along $\arg X=\pm\pi/4, \pm3\pi/4, -5\pi/4$. The X plane for $-5\pi/4\leqslant\arg X\leqslant 3\pi/4$ is now divided into three distinct domains corresponding to $-5\pi/4\leqslant\arg X\leqslant-\pi/4$, $-\pi/4\leqslant\arg X\leqslant+\pi/4$, $+\pi/4\leqslant\arg X\leqslant 3\pi/4$ at $|X|\to\infty$. This is reflected by the more complicated nature of the connection formula:

$$\begin{tikzcd}[column sep=small]
 & X^{-1/2}(-\mathrm{e}^{-2\pi\epsilon}R(\epsilon)\,\mathrm{e}^{\mathrm{i}\zeta}+\mathrm{e}^{-\mathrm{i}\zeta}) & \\
 & \psi(X) \arrow[u, "\pi/4\leqslant\arg X\leqslant3\pi/4"'] \arrow[dl, "-5\pi/4\leqslant\arg X\leqslant-\pi/4"'] \arrow[dr, "-\pi/4\leqslant\arg X\leqslant\pi/4"] & \\
X^{-1/2}R(\epsilon)\,\mathrm{e}^{\mathrm{i}\zeta} & & X^{-1/2}(\mathrm{e}^{-\mathrm{i}\zeta}+R(\epsilon)\,\mathrm{e}^{\mathrm{i}\zeta})
\end{tikzcd} \tag{34}$$

where $\zeta=\frac{1}{4}X^2-\epsilon\ln X+\frac{1}{2}\epsilon\ln(\epsilon/\mathrm{e})-\pi/4$. Previous statements of this formula assume either a real potential barrier and real energy (e.g. Miller and Good 1953, Connor 1968, Berry and Mount 1972, Child 1976) or a real potential barrier and complex energy (Connor 1973). In both these cases X can be assumed to be real and the above reduces to a simpler bilateral form. The bilateral connection formula can be applied when X is complex and interest is confined to the domains $|\arg \pm X| < \pi/4$, e.g. Connor *et al* (1976).

By uniform approximation (Miller and Good 1953, Connor 1968, 1973, Berry and Mount 1972, Brink and Takigawa 1977) using the comparison equation,

$$\frac{d^2\psi}{dX^2} + (\tfrac{1}{4}X^2 - \epsilon)\psi = 0, \tag{35}$$

the connection formula (34) is generalisable to the problem of scattering by a general barrier that has associated with it just two turning points, $\{q_+, q_-\}$. The wavefunction $\Psi(q)$ describing this more general system is given approximately in terms of the solution $\psi(X)$ of (35), as given by (33), by

$$\Psi(q) \simeq \left(\frac{\partial X}{\partial q}\right)^{-1/2} \psi(X) \tag{36}$$

where the transformation relating X and q is defined by the mapping:

$$\int_{2\epsilon^{1/2}}^{X} (\tfrac{1}{4}X^2 - \epsilon)^{1/2}\, dX = \frac{1}{\hbar} S_+(q) \tag{37}$$

where

$$S_\pm(q) = 2^{1/2} \int_{q_\pm}^{q} (E - V(q))^{1/2}\, dq \tag{38}$$

integrated on a branch such that $\mathrm{Re}\, \partial S_\pm/\partial q > 0$ as $q \to \infty$. The turning points $q_\pm$ correspond, respectively, to the turning points $X = \pm 2\epsilon^{1/2}$ of the comparison equation. The mapping (37) is one-to-one provided that ϵ and the integration contour of (38) are defined so that

$$\begin{aligned} \epsilon &= \frac{1}{\pi i \hbar}[S_-(q) - S_+(q)] = \frac{2^{1/2}}{\pi i \hbar} \int_{q_-}^{q_+} [E - V(q)]^{1/2}\, dq \\ &= \frac{1}{2^{1/2}\pi i \hbar} \oint [E - V(q)]^{1/2}\, dq \end{aligned} \tag{39}$$

integrated in a clockwise sense around a cut joining $q_\pm$, which ensures that the zeros of $E - V(q)$ map onto the zeros of $\frac{1}{4}X^2 - \epsilon$. The above lead to the standard solutions $\Phi^\pm$, which correspond to $\phi^\pm$, and which describe ingoing and outgoing wave solutions in $|\arg(X) - (\pm\pi/4)| \leq \pi/2$, being given, in these argument ranges, as follows†:

$$\Phi^\pm(q) \simeq \left(\frac{\hbar}{P}\right)^{1/2} \left(\pm \frac{\partial^2 S_+}{\partial q\, \partial P}\right)^{1/2} \exp(\pm (i/\hbar) S_+(q))\, e^{-\pi i/4} \tag{40a}$$

† Equations (40) represent the so-called strong-coupling limits of the semiclassical approximants $\Phi^\pm$ and, as such, are not exactly equivalent to the weak coupling forms, such as are provided by (26) and (30) when $V(q)$ is parabolic, except in the limit of $X^2 \gg 4\epsilon$ (see discussions by Crothers (1976, 1978), and Lozano and Olver (1978)). For a parabolic potential, $V(X) = -\frac{1}{8}\hbar^2/X^2$, equation (37) gives

$$(1/\hbar)S_+(X) = \tfrac{1}{4}X(X^2 - 4\epsilon)^{1/2} - \epsilon \ln[(X + (X^2 - 4\epsilon)^{1/2})/2] + \tfrac{1}{2}\epsilon \ln \epsilon$$

which reduces to $\zeta + \pi/4$ (equation (34)) only in the limit $X \to \infty$. We note that, in general, the JWKB approximation (see Crowley 1979) supplies the strong-coupling limit as, for example, in the case of equations (40), while the weak-coupling limit, from which one obtains the S matrix, corresponds to the limit $X \to \infty$. In particular, we observe that the wave propagation matrix method of Lee and Takigawa (1978) provides a weak-coupling limit of the semiclassical wavefunction and, for this reason, should be used with some caution.

$$= \left(\frac{1}{\hbar}\frac{\partial S_+}{\partial q}\right)^{-1/2} \exp\left[\pm i\left(\frac{1}{\hbar}S_+(q) - \frac{\pi}{4}\right)\right] \tag{40b}$$

which have the structure of local JWKB approximants (e.g. Crowley 1979). Hence the (strong-coupling†) generalisation of (34) may be deduced by transforming the asymptotic wavefunctions according to

$$\zeta \to \frac{1}{\hbar}S_+(q) - \pi/4 \tag{41a}$$

$$X \to \frac{1}{\hbar}\frac{\partial S_+}{\partial q}. \tag{41b}$$

The boundaries between the regions defined for $|X| \to \infty$ by $\arg X = (-5\pi/4, -\pi/4)$, $(-\pi/4, \pi/4)$, $(\pi/4, 3\pi/4)$ are the mappings of the Stokes lines in $\{X\}$ onto $\{q\}$. The correspondence between the Stokes lines in $\{X\}$ and those in $\{q\}$ may be determined from the local behaviour in the vicinities of the turning points.

In cases for which the physically accessible points X lie in the domains $|\arg(\pm X)| \leqslant \pi/4$, the results expressed by (33) and (34) clearly define $R(\epsilon)$, equation (32), as the *barrier reflection coefficient*, and

$$T(\epsilon) = R(\epsilon)\,e^{-\pi\epsilon} \tag{42}$$

as the *barrier transmission coefficient*. These results form the basis of the barrier s matrix of Brink and Takigawa (1977), the connection being provided through the following expression for the barrier matrix $\mathbf{B}$ (Lee and Takigawa 1978):

$$\mathbf{B} = \frac{1}{T}\begin{pmatrix} 1 & R \\ R & R^2 + T^2 \end{pmatrix} \tag{43}$$

with ϵ given by (39) (see also Crowley 1980a, b).

For $|\epsilon| \gg 1 \equiv |\omega\eta^2| \gg \hbar$, the *classical trajectories* correspond to *saddle points* of the integral (21) which give rise to the various exponential terms in the asymptotic forms of ψ. A treatment of the Stokes phenomenon is a feature of the saddle-point approximation. The procedure (Fröman and Fröman 1965, Berry and Mount 1972) involves invoking the principles of reality (or, alternatively, single-valuedness (Furry 1947)) and of exponential dominance. The connection formula (34) provides a clear illustration of the latter—the multipliers associated with each of the approximants $X^{1/2}\,e^{\pm i\zeta}$ change only at a Stokes line where the term is subdominant. Note that in the case of $|\epsilon| \gg 1$, Airy function approximations provide a good *local* description of the wavefunction near a turning point and correspond to approximating the potential near a turning point by a linear function (§ 2.1) (Knoll and Schaeffer 1976). However, when $|\epsilon| \leqslant 1$, the saddle-point approximation breaks down and the concept of classical trajectories is no longer globally valid. This situation corresponds to energies close to the barrier top. The presence of resonances in this region can lead to important effects, even in the semiclassical limit (Brink and Takigawa 1977, Lee *et al* 1978). The derivation of the result (33) and the connection formula (34) does not depend upon the validity of the saddle-point approximation and holds for all ϵ such that $\mathrm{Im}\,\epsilon < \frac{1}{2}$.

We now compare the result of applying the saddle-point approximation to the evaluation of the oscillatory integral (1), for the general barrier problem, with the uniform approximation wavefunction (36). We note that the latter is equivalent to (33)

† See footnote p 1237.

when $\phi^{(\pm)}$ are replaced by $\Phi^{\pm}$ (equation (40*a*)) and that this is the result that one would have obtained from the oscillatory integral in the saddle-point approximation (Crowley 1979) in the presence of only two turning points in the active region. The absence of any other nearby turning points is an indication of the validity of a local analytic continuation based upon the parabolic connection formula (analogous to the Knoll and Schaeffer (1976) approximation as applied to single isolated turning points). Thus, in the semiclassical limit the oscillatory integral and uniform approximation methods are effectively equivalent, at least in so far as their application to one and two turning point problems is concerned. Both methods give exact results for linear and parabolic potentials.

2.2.1. Bound states and resonances. The foregoing provides solutions to (12) for $|\arg\omega|<\pi/2$ and $\mathrm{Re}(-\mathrm{i}\epsilon)<\frac{1}{2}$. In order to investigate solutions for which $\arg\omega\leqslant\pi/2$ and $\mathrm{Re}(-\mathrm{i}\epsilon)\geqslant\frac{1}{2}$, we first make the substitutions

$$\omega=\tilde{\omega}\,\mathrm{e}^{\pi\mathrm{i}/2}\qquad\alpha=\tilde{\alpha}\,\mathrm{e}^{-\pi\mathrm{i}/2}\tag{44a}$$

where

$$-\pi<\arg\tilde{\omega}\leqslant 0\qquad 0\leqslant\arg\tilde{\alpha}<2\pi\tag{44b}$$

thereby transforming (12) to

$$-\hbar^2\frac{\partial^2\psi}{\partial q^2}+\tilde{\omega}^2q^2\psi=2\tilde{\omega}\tilde{\alpha}\psi.\tag{45}$$

It follows from (16) that the solution of (45) provided by (21) corresponds, for real $\tilde{\omega}$, to motion in imaginary time. This observation enables us to identify another set of possible solutions (valid for $\mathrm{Re}\,\tilde{\omega}>0$) for which such motion takes place in real time. These are given by

$$\psi=\left(-\frac{\mathrm{i}\tilde{\omega}\eta^2}{2\pi\hbar}\right)^{1/2}\exp\left(-\frac{\tilde{\omega}}{2\hbar}\eta^2(x^2-\tfrac{1}{2})\right)\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\mathrm{e}^{\gamma/2}\exp\left(\frac{\tilde{\omega}\eta^2}{\hbar}(x\,\mathrm{e}^{\gamma}-\tfrac{1}{4}\,\mathrm{e}^{2\gamma}+\tfrac{1}{2}\gamma)\right)\mathrm{d}\gamma$$

(cf equation (21))

$$=\mathrm{i}\left(\frac{\mathrm{i}\nu}{\pi}\right)^{1/2}\mathrm{e}^{\nu(x^2-\frac{1}{2})}\int_{-\infty}^{\infty}\mathrm{e}^{\frac{1}{2}\mathrm{i}\tau}\exp[-2\nu(x\,\mathrm{e}^{\mathrm{i}\tau}-\tfrac{1}{4}\,\mathrm{e}^{2\mathrm{i}\tau}+\tfrac{1}{2}\mathrm{i}\tau)]\,\mathrm{d}\tau\tag{46}$$

where

$$\nu=\tilde{\alpha}/\hbar=\mathrm{e}^{3\pi\mathrm{i}/2}\epsilon.\tag{47}$$

Transforming the integral (46) by means of the substitutions:

$$X=-2\mathrm{i}\nu^{1/2}x=\left(\frac{2\tilde{\omega}}{\hbar}\right)^{1/2}q\tag{48a}$$

$$z=-\mathrm{i}\nu^{1/2}\,\mathrm{e}^{\mathrm{i}\tau}\tag{48b}$$

leads to

$$\psi(X)=\sum_{\mathrm{C}}\frac{\Gamma(\nu+\frac{1}{2})}{2\pi\mathrm{i}}\,\mathrm{e}^{-\frac{1}{4}X^2}\oint_{\mathrm{C}}\mathrm{e}^{zX-\frac{1}{2}z^2}z^{-\nu-\frac{1}{2}}\,\mathrm{d}z\tag{49}$$

where C denotes the contour $|z/\nu^{\frac{1}{2}}|=1$ in the complex z plane. The wavefunction (49) consists of a sum over integrals corresponding to all branches of the function

$e^{zX-\frac{1}{2}z^2}z^{-\nu-\frac{1}{2}}$. The wavefunction defined by (49) is finite, single-valued and $\mathscr{L}^2$ in $-\infty \leqslant X \leqslant \infty$ only if $\nu+\frac{1}{2}$ is a positive integer. With

$$\nu = n+\tfrac{1}{2} \qquad n = 0, 1, 2, 3, \ldots \tag{50}$$

the integrand becomes single-valued and, by means of the expansion (Abramowitz and Stegun 1965, equation (22.9.17))

$$e^{zX-\frac{1}{2}z^2} = \sum_{m=0}^{\infty} z^m \frac{2^{-\frac{1}{2}m}}{\Gamma(m+1)} H_m(X/\sqrt{2})$$

and use of Cauchy's theorem, reduces to

$$\psi(X) \propto \frac{1}{2\pi i}\Gamma(n+1)\, e^{-\frac{1}{4}X^2} \oint_C z^{-n-1}\, e^{zX-\frac{1}{2}z^2}\, dz = 2^{-\frac{1}{2}n}\, e^{-\frac{1}{4}X^2} H_n(X/\sqrt{2}) \equiv D_n(X) \tag{51}$$

where $H_n(x)$ denotes a Hermite polynomial of degree n. Thus we obtain the well-known bound-state solutions of the harmonic oscillator together with the energy quantisation rule (50). The wavefunction (51) is $\mathscr{L}^2$ only if Re $\tilde{\omega} > 0$. Similar solutions valid for Re $\tilde{\omega} < 0$ may be derived by using $-F$ in place of F (corresponding to the advanced scattering solution instead of the retarded solution) in deriving (46). These discrete solutions describe states with energies

$$E_n = (n+\tfrac{1}{2})\hbar\tilde{\omega}.$$

From (44), Im $\tilde{\omega} \leqslant 0 \Rightarrow$ Im $E_n \leqslant 0$. Therefore, for Im $\tilde{\omega} \neq 0$, these states possess finite lifetimes given by

$$T_n = [(n+\tfrac{1}{2})|\mathrm{Im}\,\tilde{\omega}|]^{-1}$$

and are therefore analogous to resonances. It is perhaps surprising that the presence of such solutions does not seem to depend upon the relative magnitudes of the real and imaginary parts of $\tilde{\omega}$.

Thus, to summarise, the Schrödinger equation (12) possesses continuum solutions for $\mathrm{Re}(-i\epsilon) < \frac{1}{2}$ and $|\arg \omega| < \pi/2$ (where $-i\epsilon = i\alpha/\hbar$), and discrete solutions for $-i\epsilon = n+\frac{1}{2}$ and $0 < |\arg \omega| \leqslant \pi/2$. Note that the discrete eigenvalues correspond to the poles of the reflection coefficient $R(\epsilon)$ given by equation (32).

3. Conclusions

The semiclassical method based on the oscillatory integral yields globally exact analytic solutions of the one-dimensional Schrödinger equation for linear and parabolic potentials. For more general one-turning-point and two-turning-point problems the method is apparently equivalent to the uniform approximation involving the method of comparison equations.

The same technique also yields the bound-state solutions of the one-dimensional harmonic oscillator and, for complex ω, discrete solutions analogous to resonances whose presence in all parabolic potentials, with the exception of the real barrier, is independent of the relative magnitudes of the real and imaginary parts of ω.

The wavefunction (1) possesses all the usual features normally attributed to an exact quantal wavefunction, such as single-valuedness and continuity, and the ability to describe specifically wave-mechanical phenomena such as diffraction and tunnelling.

Applying the saddle-point approximation (in the short-wavelength limit) leads directly to a description of the same wave field in terms of trajectories which, when real, yield a description in terms of classical particle dynamics. Complex trajectories are also a possibility and these provide a dynamical (or geometrical) description of diffraction and tunnelling. The superposition principle is retained and this leads to the possibility of interference between trajectories on different sheets of the critical manifold.

Having shown that (1) represents the exact solution of the quantal problem for two exactly soluble cases, we are led to speculate as to whether a superposition of wavefunctions of type (1) represents the general exact solution of (2). There is no obvious *a priori* reason why this should be so. It is nevertheless an interesting possibility which, given that the only dependence of the integrand on $\hbar$ is provided through the $1/\hbar$ appearing in the exponent, would be consistent with the claims of Balian and Bloch.

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Note added in proof. According to catastrophe theory, the only structurally stable point singularity that can occur in the two-dimensional parameter space $\{\alpha, q\}$ is the cusp. While the barrier-top singularity of § 2.2 is not a cusp, the wavefunction $\psi_{\alpha=0}(q)$ is *exactly* a section through the cusp diffraction catastrophe. In other words, the most singular point is correctly described with the correct singularity index, in spite of the non-catastrophic nature of the (logarithmic) singularity in the extended action F. Although the orbiting singularity represents a limitation of catastrophe theory in its current form, it does not follow that catastrophe theory is therefore without application in such situations. Whereas there is need to exercise caution when applying Thom's theorem to the singularities of wave-fields in the short-wavelength limit—in view of the possible presence of singularities that are beyond the scope of the theorem—the local descriptions of catastrophe-type singularities (those that are covered by the theorem) remain valid.

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