# Semiclassical perturbation approach to quantum reflection

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We consider the problem of quantum ''reflection above the barrier,'' introducing a distorted-wave Born approximation based on the primitive semiclassical Wentzel-Kramers-Brillouin wave function. The idea generalizes to the concept of an unperturbed Hamiltonian defined as the exact Hamiltonian plus small parts which ''turn off'' nonclassical processes such as barrier reflection and barrier tunneling. [S1050-2947(96)06012-X]

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## I. INTRODUCTION

The difficulty in exactly solving realistic quantum-mechanical problems, and the quest for physical insight, often drive us to consider approximation methods. Two of the most well known are a perturbative approach, where the difference between the real problem and a solvable problem is in some sense ''small,'' and a semiclassical approach, which takes advantage of the smallness of $\hbar$ relative to the actions in the problem. Clearly the two methods have different regions of validity and there are parameter ranges where neither works well. Here we introduce a technique which combines perturbation theory with a semiclassical approach and in fact bridges a gap between the parameter domains where the individual approaches give good results. We consider the problem of ''reflection above the barrier'': scattering from a potential in one dimension when the energy of the particle is greater than the potential maximum. In Sec. II, we briefly review the two standard approximations mentioned above and introduce our technique which combines ideas from both. Section III presents the results of the three techniques as applied to two types of potentials: a barrier and a ramp. In Sec. IV we discuss a fourth approximate method, the multiple-scattering Bremmer result for above-barrier reflection. We discuss possible generalizations of our technique to calculate tunneling coefficients in Sec. V and multidimensional cases in Sec. VI. Finally, we conclude in Sec. VII and discuss some prospects for the ideas introduced in this paper.

## II. A SEMICLASSICALLY MODIFIED BORN RESULT

We address here the problem of scattering from a localized potential. Specifically, we consider the reflection coefficient in one dimension of a particle of energy $E$ incident from the left on an interaction region. In the typical perturbative (Born) approach to scattering theory [1], we start with a plane-wave basis representing free particle motion; the effect of the potential is to induce transitions among these states. For transitions between two degenerate states in a continuum, Fermi's golden rule tells us the probability amplitude is proportional to the matrix element of the potential between the initial and final states. In our case, the initial (final) state is a plane wave moving to the right (left) with energy $E$:$e^{+(-)i/\hbar px}$, where $p=\sqrt{2mE}$. Choosing states normalized to unit flux, we obtain the reflection coefficient

$$\mathcal{R}=\frac{m^2}{\hbar^2 p^2}\left|\int_{-\infty}^{\infty} V(x)e^{\frac{2i}{\hbar}px}dx\right|^2, \tag{1}$$

which is the Born scattering result [1]. This formula is valid under certain ''smallness'' conditions of the potential: we need

$$\left|\frac{V(x)a}{\hbar v}\right| \ll 1, \tag{2}$$

where $v=p\hbar/m$ is the classical velocity of the particle and $a$ is the width of the potential, which essentially requires the scattering potential to be weak compared to the kinetic energy of the incoming particle [1]. For large potentials and for potentials which do not have a finite extent (for example, step potentials rather than barriers), such a perturbative approach is expected to fail.

There are two well-known semiclassical methods, one based on the stationary phase approximation to Feynman's path integral [2], the other on WKB wave functions. The equivalence of the two approaches is shown in [3]. Below we very briefly outline the methods; the reader is referred to the literature, for example, [3–7] for details. The probability amplitude that a state of positive momentum and definite energy evolves into a state of negative momentum is obtained from the energy domain Green's function in momentum representation:

$$G(-p,p,E)=\int G(-p,t;p,0)e^{iEt/\hbar}dt$$

$$=\int \langle -p|e^{-iHt/\hbar}|p\rangle e^{iEt/\hbar}dt, \tag{3}$$

$$=\int dt\int \mathcal{D}[p(\tau)]e^{i\{S(p[\tau])+Et\}/\hbar}, \tag{4}$$

where $\mathcal{D}[p(\tau)]$ implies a summation over all paths in momentum space $p(\tau)$ which starts with momentum $p$ and ends at time $t$ with momentum $-p$, and $S(p[\tau])$ is the classical action $\int_0^t \mathcal{L}(p[\tau])d\tau$ along the (not necessarily classical) path $p[\tau]$, $\mathcal{L}$ being the Lagrangian. This latter expression is a Feynman path integral [2] in momentum space, the position space version of which is perhaps more familiar. In the

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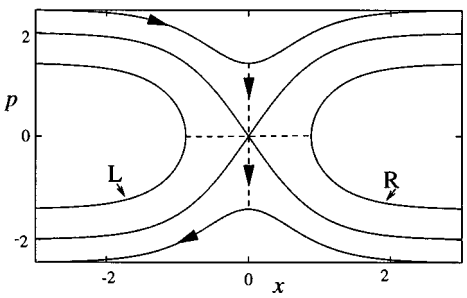


FIG. 1. Classical phase-space contours for a $\mathrm{sech}^2$ barrier (solid line). The horizontal dashed line shows the classically forbidden quantum tunneling process from the left side of the barrier (L) to the right (R) at energy below the barrier. The vertical dashed line connecting contours at energy above the barrier is what this paper addresses, the classically forbidden quantum reflection process.

limit $\hbar \to 0$, we may perform both the time integral and the path integral by stationary phase, which is justified as the integrand oscillates rapidly and cancels itself out everywhere except at stationary points of the integrand. This reduces the sum over all paths that begin with momentum $p$ and end with $-p$ and have energy $E$ to a vastly smaller sum only over paths satisfying the classical equations of motion. However for energies greater than the maximum potential there are no such classical paths for real initial conditions and real time. We nonetheless find an approximation for the quantum reflection coefficient by picking up contributions from complex stationary phase points [3]. The uniformized semiclassical reflection coefficient derived in this way is

$$\mathcal{R} = \frac{e^{-(2/\hbar)\mathrm{Im}\int_{-p_o}^{p_o} x(p')dp'}}{1+e^{-(2/\hbar)\mathrm{Im}\int_{-p_o}^{p_o} x(p')dp'}}, \tag{5}$$

where $p_o$ is the classical value for momentum at the center of the potential, $x(p)$ is the classical solution for the position in terms of momentum, and Im stands for the imaginary part. We note that this is a uniformized expression in the sense that Eq. (5) connects smoothly at $E = V_{max}$ to the reflection coefficient for energies just above the barrier top. The barrier penetration formula may be more familiar, which is of the form Eq. (5) with the exchange of the roles of position and momentum: the transmission probability at energy $E$ is

$$\mathcal{T} = \frac{e^{-(2/\hbar)\mathrm{Im}\int_{-x_o}^{x_o} p(x')dx'}}{1+e^{-(2/\hbar)\mathrm{Im}\int_{-x_o}^{x_o} p(x')dx'}}, \tag{6}$$

where $\pm x_o$ are the classical turning points and $p(x') = \sqrt{2m[E-V(x)]}$ (see also Fig. 1). Formula (5) in fact gives the exact reflection coefficient for the inverse harmonic oscillator. This result may also be seen to arise from a semiclassical analysis by Zwaan which is based on WKB wave functions and Stokes line discontinuities in the complex plane (see [4] for many references and a review). We may also derive semiclassical reflection coefficients starting with the well-known Airy connection method for tunneling, which addresses the problem of barrier penetration and involves matching WKB solutions at turning points. The result may then be generalized to the problem of above-barrier reflection, either through extension to complex turning points or by working with analogous formulas in momentum space.

It is well known that the WKB formulas break down for energies near the top of the barrier. What is mentioned much less often is that they fail completely if the barrier is too low in the sense discussed below. However a low barrier is just the case that can be treated perturbatively, so one might imagine that most cases can be handled by one of the two methods. However, it can easily happen that the potential barrier is too high to be treated perturbatively, yet the action $\int^p x(p')dp'$ is too small compared to $\hbar$ for a semiclassical approach to be reasonably applied. Bridging the gap between the regimes of validity of perturbative and semiclassical approaches is one of the main results of this paper.

In the perturbative approach a transition from a right-going plane wave to a left-going plane wave is considered. For stronger potentials, this is clearly not an ideal choice for zeroth-order states in perturbation theory. We should attempt to use states which incorporate some of the potential, as in the distorted-wave Born approximation. This leads us to ask whether the WKB wave functions may play the role of the distorted-wave basis, although it is not immediately obvious what Hamiltonian they solve exactly and therefore what perturbation to use. We investigate this next. Perhaps surprisingly, we shall find that the WKB wave functions are *exact* solutions to a well behaved, Hermitian Hamiltonian.

As is well known [1], semiclassical solutions to Schrödinger's equation for a potential $V(x)$ may be written as linear combinations of wave functions of the form

$$\psi_{WKB}^{\pm}(x) = \frac{1}{\sqrt{p(x)}} e^{\pm(i/\hbar)\int^x p(x)dx}, \tag{7}$$

where $p(x) = \sqrt{2m[E-V(x)]}$ is the classical momentum and $+(-)$ represents the right- (left-)going wave. As they satisfy Schrödinger's equation to first order in $\hbar$, we may expect that any ''quantum'' behavior shows up $O(\hbar^2)$. Indeed, with $E = p(x)^2/2 + V(x)$, it is readily shown that $\psi_{WKB}^{\pm}(x)$ exactly solves the Schrödinger equation with an additional ''potential'' of order $\hbar^2$:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right)\psi_{WKB}^{\pm}(x) = \hbar^2\left(\frac{-3p'(x)^2}{8mp(x)^2} + \frac{p''(x)}{4mp(x)}\right)\psi_{WKB}^{\pm}(x). \tag{8}$$

Casting the momentum derivatives onto potential derivatives and defining an effective potential for the WKB states as

$$V_{eff}(x,E) = V(x) - \hbar^2\left[\frac{5}{32m}\left(\frac{V'(x)}{E-V(x)}\right)^2 + \frac{V''(x)}{8m[E-V(x)]}\right], \tag{9}$$

we have

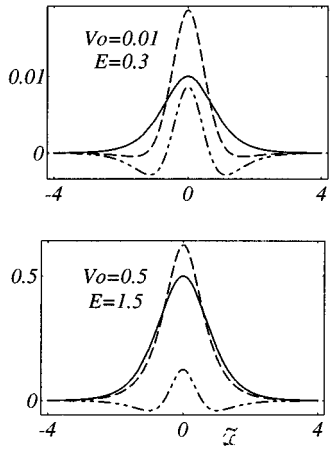


FIG. 2. Effective potentials for the sech$^2$ barrier as a function of the dimensionless length $\tilde{x}$: the solid line represents $V(x)$, the dashed line $V_{eff}(x,E)$, and the dashed-dotted-dotted line $W(x,E)$.

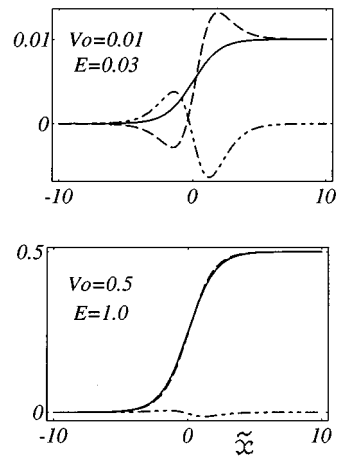


FIG. 3. Effective potentials for the ramp: the solid line represents $V(x)$, the dashed line $V_{eff}(x,E)$, and the dashed-dotted-dotted line $W(x,E)$.

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_{eff}(x,E)-E\right)\psi^{\pm}_{WKB}(x) \equiv (H_{WKB}-E)\psi^{\pm}_{WKB}=0. \quad (10)$$

Thus the WKB wave function exactly solves a quantum-mechanical Hamiltonian problem with real potential which is smooth for energies above any potential maximum. We may think of the difference between the effective and exact potentials $W(x,E)=V_{eff}(x,E)-V(x)$ as a perturbation which ''turns off'' quantum reflection: a wave sent in from the left has no reflected component at energy $E$; it is perfectly ''impedance matched.'' We note that $V_{eff}(x,E)$ is energy dependent and blows up at classical turning points, as does the WKB wave function. At energies above the potential maximum both the WKB wave function and effective potential are well behaved. In Fig. 2, we have plotted the potential $V(x)$, the effective potential $V_{eff}(x,E)$ and the difference potential $W(x,E)$ for a range of energies and potential heights for a typical barrier $V(x)=V_o\text{sech}^2(\alpha x)$. We scale $x$ as $\tilde{x}=\alpha x$, then

$$W(\tilde{x},E)=-\frac{\hbar^2\alpha^2}{m}\left[\frac{5}{32m}\left(\frac{V'(\tilde{x})}{E-V(\tilde{x})}\right)^2+\frac{V''(\tilde{x})}{8m[E-V(\tilde{x})]}\right], \quad (11)$$

thus we choose as independent parameters $V_o$ and $E$. In the figures we vary $V_o$ and $E$ and take $\hbar^2\alpha^2/m$ to be 1.

We observe that the effective perturbation has two valleys as well as a central peak, and this is what enables the quantum reflection of the semiclassical states to be turned off: loosely speaking, reflection from these valleys interferes destructively with the reflection from the original potential. At energies close to the barrier top, the difference potential is quite large. As we increase the energy, the effective potential approaches the original, and we expect that a perturbative approach using the correspondingly small difference potential would yield better results. The difference potential can be small even if the barrier is large.

Figure 3 shows $V(x)$, $V_{eff}(x,E)$, and $W(x,E)$ for the ramp $V(x)=V_o/(1+e^{-\alpha x})$. We see that although the original potential had infinite extent in space, the effective perturbation is localized, and is thus now able to satisfy requirements for the perturbation theory. Similar comments may be made for the unbounded inverse harmonic oscillator, where the effective potential is also localized and finite.

Some insight may be gained by considering a classical phase-space picture for this problem. In Fig. 1, we showed typical phase-space contours for a barrier. The quantum reflection process is indicated by the dashed line from the top curve to the bottom, forbidden in classical mechanics. Conventional perturbation theory based on plane waves used the horizontal $p=\text{const}$ asymptotes as contours to connect; in our modified perturbation approach using WKB wave functions, we take states associated with the curved, constant energy phase-space contours.

## III. REFLECTION COEFFICIENTS

To calculate the reflection coefficient we use a perturbative approach with the WKB states as the unperturbed basis, and so calculate the matrix element of $-W=V-V_{eff}$ between the $\psi^+$ and $\psi^-$:

$$\mathcal{R}=\frac{m^2}{\hbar^2}\left|\int_{-\infty}^{\infty}[V(x)-V_{eff}(x)]\frac{e^{(2i/\hbar)\int^x p(x')dx'}dx}{p(x)}\right|^2. \quad (12)$$

In Figs. 4 and 5 we graph the results of our combined semiclassical perturbation technique together with the known exact quantum reflection coefficient (see [1], for example), the semiclassical result, and the Born result (where applicable) for the two potentials: a sech$^2$ barrier $V(x)=V_o\text{sech}^2(\alpha x)$, and a ramp $V(x)=V_o/(1+e^{-\alpha x})$, where $\alpha=1$. Energy and potential are measured in units of $\hbar^2\alpha^2/m$.

For the sech$^2$ barrier, we see that ordinary perturbation (Born) theory is only good for small potentials and high enough energies. The semiclassical approach is reasonable for large potentials and energy well away from the barrier top. Our combined approach works in the intermediate parameter region, as we expected.

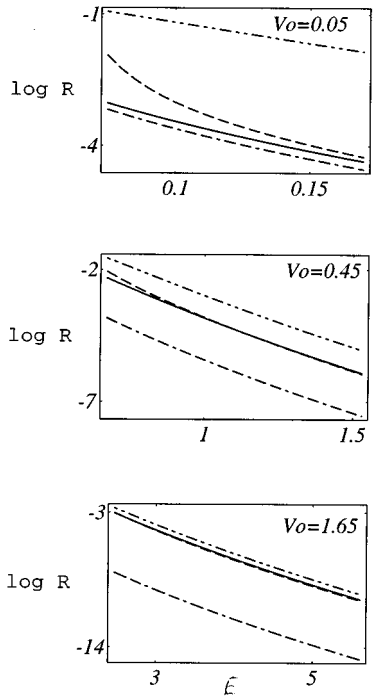


FIG. 4. Natural logarithm of reflection coefficients from the sech$^2$ barrier: solid line is the exact, dashed-dashed-dotted line is the perturbative formula (1), dotted-dotted-dashed line is the semiclassical formula (5), and the dashed line represents our semiclassical-perturbation formula (12).

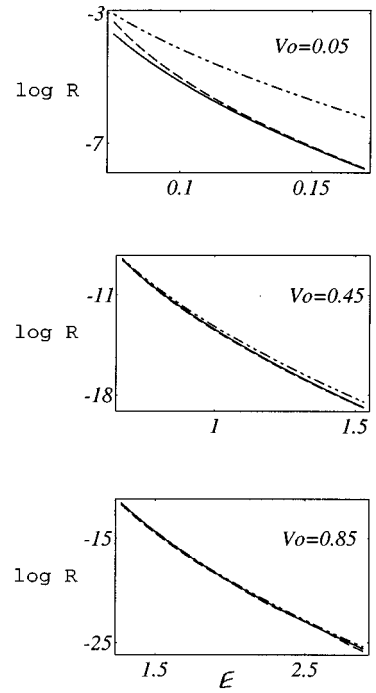


FIG. 5. Reflection from the ramp potential: solid line is the exact, dashed-dashed-dotted line is the perturbative formula (1), dotted-dotted-dashed line is the semiclassical formula (5), and the dashed line represents our semiclassical-perturbation formula (12).

In the case of the ramp, where perturbation theory cannot be applied sensibly due to the infinite extent of the potential, we see that our technique of combining a semiclassical approach with perturbation theory still works well and is better than the semiclassical approximation, provided the energy is not too close to the potential top. In Fig. 6, the typical $\hbar$ dependence of the coefficients is plotted. We observe that for very small $\hbar$, the semiclassical result is a very good approximation as expected, whereas for large $\hbar$ perturbation theory does a better job. The combined semiclassical-perturbation method interpolates between. We notice that corrections to the semiclassical approach depend on $\hbar$ roughly as $e^{-O(\hbar)}$, indicating $\hbar^2$ (and higher) corrections to the action, as is expected in semiclassics.

## IV. THE BREMMER METHOD

We mention briefly another technique for computing quantum reflection coefficients, without which this study would be incomplete. The Bremmer method results from a multiple-scattering approach, where a smooth potential is approximated by a series of $N$ sharp steps, $N$ being large. The wave function at some position $x$ can be expressed as

$$\frac{b_+(x)}{\sqrt{p(x)}}e^{(i/\hbar)\int^x p(x')dx'}+\frac{b_-(x)}{\sqrt{p(x)}}e^{-(i/\hbar)\int^x p(x')dx'}, \qquad (13)$$

where $b_\pm(x)$ are coefficients to be determined. An incoming wave partially reflects and partially transmits at each sharp step for which the fully quantum coefficients are known. Thus we calculate the wave function cumulatively and take the limit of a continuously varying potential. This gives two iterative equations for $b_\pm(x)$ and we take the first iteration to obtain

$$\mathcal{R}=\int\frac{p'(x)}{2p(x)}e^{(-2i/\hbar)\int^x p(x')dx'}. \qquad (14)$$

The Bremmer approach is very much in the spirit of the semiclassical-perturbation results in that a semiclassical foundation is used to build quantum corrections. In the Bremmer case, the WKB wave function with no reflection results if the zeroth approximation is used, and Eq. (14) is the single-scattering correction.

A numerical evaluation of Eq. (14) is in fact very close to the exact result as is shown in Fig. 7, providing in general a

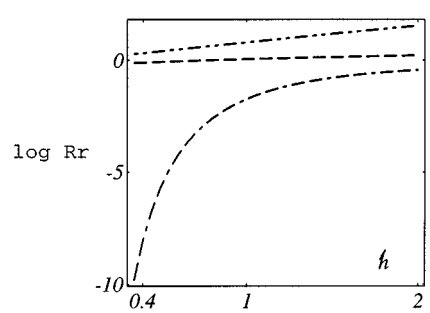


FIG. 6. $\hbar$ dependence of the reflection coefficients $R_r=R/R_{exact}$. Here we have taken the sech$^2$ barrier with $V_o=0.5$ and $E=1.0$: dashed-dashed-dotted line is the perturbative result, dashed-dotted-dotted line is semiclassical, and the dashed line is our semiclassical-perturbation theory.

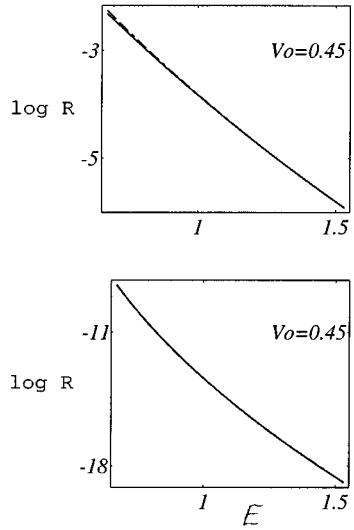


FIG. 7. The Bremmer result (dashed line) for the reflection coefficient for the $\mathrm{sech}^2$ (top figure) and ramp (bottom figure) potentials is very close to the exact result (solid line).

much better estimate than the three approaches discussed in the preceding section. It is, however, challenging to apply the Bremmer approach to more general problems (see below).

Berry and Mount's discussion of the Bremmer approach [4] includes an analytic evaluation of the integral Eq. (14) by a contour integration. The semiclassical approach enters by including only the contribution from the pole involving the smallest imaginary action. Their explicit semiclassical calculation for the potential ramp results in a value for $\mathcal{R}$ which overshoots the standard semiclassical result by the factor of $\pi^2/9$. This 10% discrepancy, very minor compared with the differences in the approaches of Sec. III was attributed to taking only the first iteration in the multiple-scattering coupled equations, that is, to formula Eq. (14) itself. Our numerical evaluation of Eq. (14) which indicates how very close it is to the exact result, together with Berry and Mount's semiclassical calculation, suggests that if all the singularities were included in the contour evaluation we would get an analytic result very close to the exact result. However this is not found to be correct. We can motivate why from the following observation: the exact reflection coefficient is $e^{-O(\hbar)}\mathcal{R}_{sc}$ (Fig. 6), yet summing the contributions from all the poles results in the addition of two geometric series (one stemming from complex turning points, the other from complex singularities) which cannot give such a dependence. This problem remains unsolved, but it is not the main point of our paper.

## V. GENERALIZATION TO BARRIER PENETRATION

We are now led to the question of whether the semiclassical-perturbation technique may be used in more general problems. The success in computing the nonclassical transitions between the positive and negative momentum branches in phase space for reflection from a barrier prompts us to ask whether can we compute the nonclassical transition probability between *any* two contours in classical phase space in a similar ''semiclassically modified perturbation theory.'' In particular, we may be concerned with generalizing this to higher dimensions, where there is much interest in calculating couplings and energy splittings between classically degenerate tori [10].

We consider below the issue of tunneling across a potential barrier in one dimension, with energy below the barrier top. We need to find, for the unperturbed basis, wave functions which ''live'' on one side of the barrier only. We may attempt to construct appropriate combinations of the WKB wave functions Eq. (7) which do this. However at the turning point the wave function blows up (as does the effective potential). Uniformizations of WKB wave functions in position representation are well studied [4]. It is, however, not clear how to uniformize at the turning points without inducing tunneling of the wave function to the other side of the barrier, which we want to avoid in order to follow our plan analogous to the above-barrier case treated earlier. Consider the contours labeled $L$ and $R$ in phase-space Fig. 1 again: at the turning points, the projection of the contour on to $x$ is ill-defined; they are coordinate space caustics. We see the tunneling process connects curve $L$ to curve $R$: the picture suggests momentum space is a more natural space to work in for this problem. If we work in coordinate space for barrier reflection (momentum tunneling) then we should expect to work in momentum space for barrier (position space) tunneling. The turning points then pose no problem, as can be seen by the projection on to the vertical axis. Performing a stationary phase Fourier transform of the $x$-space WKB wave functions living on the left(right) side of the barrier:

$$\psi^{+(-)}(x) - i\psi^{-(+)}(x) \tag{15}$$

we obtain the momentum-space wave function

$$\phi^{\pm}(p) = \frac{1}{\sqrt{-V'(x(p))}} e^{\mp(i/\hbar)\int^{p} x(p')dp'}, \tag{16}$$

where $+(-)$ represents the wave on the left (right) of the barrier. We may calculate the behavior under Schrödinger's equation:

$$\left[\frac{p^2}{2m} + V\left(i\hbar\frac{d}{dp}\right) - E\right]\phi^{\pm}(p) = \hbar^2 h(p)\phi^{\pm}(p) + O(\hbar^3), \tag{17}$$

$$\begin{aligned} h(p) = &-\frac{x'(p)^2 V''''(x(p))}{8} - \frac{x''(p)V'''(x(p))}{6} \\ &- \frac{3V''(x(p))^3 x'(p)^2}{8V'(x(p))^2} + \frac{V''(x(p))^2 x''(p)}{4V'(x(p))} \\ &+ \frac{V''(x(p))V'''(x(p))x'(p)^2}{2V'(x(p))}, \end{aligned} \tag{18}$$

where $V(i\hbar(d/dp))$ was calculated by an expansion-resummation technique, as follows: We consider the operation of the first few terms of a Taylor series expansion around zero for $V(i\hbar(d/dp))$ on $\phi^{\pm}(p)$, collect terms in orders of $\hbar$ and find that to each order in $\hbar$ we have a Taylor series which we then resum. This leads to the results above,

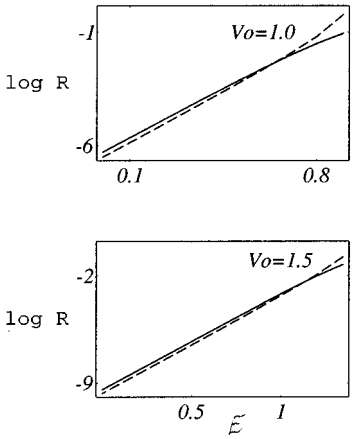


FIG. 8. Transmission through the inverse harmonic oscillator $V(x)=Vo-\frac{1}{2}x^2$: the solid line represents the exact result, which in this case is also the semiclassical result formula (5), and the dashed line is the result of our semiclassical-perturbative approach.

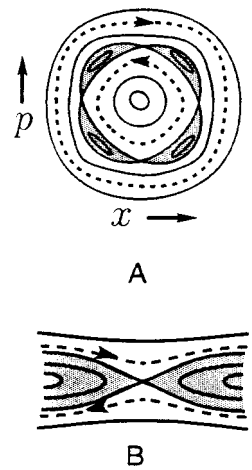


FIG. 9. A. Poincare surface of section plot for a typical interacting system of two degrees of freedom in the nearly integrable regime. Resonance zones which divide regions of phase space are evident. The contours on this $(x,p_x)$ surface are of the same fixed energy $E$. Tunneling across the resonance zones is analogous to the barrier reflection: These resonance islands are to be compared to the phase-space plot for the barrier $B$, which shows the similarity of the tunneling across the separatrix in the two cases.

where in a semiclassical vein, we write down explicitly the lowest order (i.e., $\hbar^2$) correction (see [8] for more detail). Unfortunately the Hamiltonian is more complicated in its position dependence than in its momentum dependence $[V(x)$ as opposed to $p^2/2]$ and the price we pay is a more complicated effective Hamiltonian. In addition, we observe from Eq. (16) and Eq. (17), that at the expense of eliminating the turning point caustic, we have introduced a new type of caustic, caused by the asymptotic constancy of the potential (see Fig. 1).

Before discussing this problem further, we present the results for the inverted harmonic oscillator, for which this new type of caustic is not a problem [in momentum space, with $E>V_{max}$, the top of the barrier plays no role, as it is outside the relevant (i.e., real) domain for $p$]. The analysis follows closely the case of above-barrier reflection from this potential due to the symmetry of the harmonic-oscillator Hamiltonian under the substitution $x\leftrightarrow p$. The series in $\hbar$ in Eq. (17) ends at $\hbar^2$ for this potential, so in fact $H-\hbar^2 h(p)$ is the effective Hamiltonian for which the WKB solutions Eq. (16) are exact eigenstates to any order in $\hbar$. The results are given in Fig. 8 and provide a good approximation to the exact result provided the energy is not too close to the barrier top.

For a generic barrier, which flattens out away from the interaction region, we encounter what we shall call a ''supercaustic'' [8]: as $p\rightarrow\pm\sqrt{2E}$, the WKB wave function blows up. The *exact* momentum-space solution *also* is singular for flat regions of potential, however the WKB behavior is still incorrect, as can be seen by the divergence of the effective perturbation in Eq. (17). Thus the WKB wave function is a poor approximation of the true wave function as $p\rightarrow\pm\sqrt{2E}$. It is possible however, to uniformize the supercaustic, and this process is described in [8] for a barrier whose asymptotic behavior is exponential. This involves exactly solving the case of a potential which tends to the desired potential at large $x$, then adjusting by well-behaved WKB factors, to find a wave function $\phi_{unif}(p)$ which reduces to WKB in the $\hbar\rightarrow 0$ limit, and yet has the correct blowup as $p\rightarrow\pm\sqrt{2E}$. Applying Schrödinger's equation in momentum space to the uniformized wave function we find that the difference between the Hamiltonian for which $\phi_{unif}(p)$ is an eigenstate and the original Hamiltonian does give a finite perturbation and we find this explicitly up to order $\hbar^2$. However the application of our semiclassical-perturbation theory to calculate the tunneling probability from one side of the barrier to the other using the uniformized states as the zeroth-order basis, has not been successful in yielding a good approximation, despite the effective perturbation being small and finite everywhere. Perhaps the neglect of the terms $O(\hbar^3)$ and higher may be partly responsible for this, but as yet this problem is unresolved.

## VI. MULTIDIMENSIONAL CASES

Of course the one-dimensional problems addressed in this paper are of limited utility. However, it is easy to see that as long as there are no position space turning points one can use the same methods in two, three, or more dimensions. For example, backscattering from a three-dimensional potential which has no classical backscattering can be computed. We leave this for future work.

The situation we have discussed here is related to an established technique used to estimate *dynamical tunneling* [9,10] interactions in two or more degree of freedom bound-state systems [11–14]. Dynamical tunneling occurs when (1) there are good classical actions partitioning phase space, giving classical trajectories which fail to flow from one set of actions to another, even over infinite time and (2) tunneling (with associated tunnel splittings and mixing of wave functions otherwise localized to the vicinity of the tori) is observed quantum mechanically. It can be shown that classical resonance island chains which always can be found between the invariant tori control the tunneling between the states localized on the tori. This is most easily seen by analogy

with the barrier reflection problem discussed in this paper. In Fig. 9 we show the phase-space plot for barrier reflection and for a mostly integrable two-dimensional system (on a Poincare surface of section). The two tori involved in the tunneling are indicated; note that between them sits a resonance island chain which has the right Fourier components to give a nonvanishing tunneling (perturbative) integral connecting the two tori. Locally, the resonance zone has exactly the structure of the barrier reflection problem, as indicated in the figure. In the very common case that the islands are narrow (as drawn) the problem can be handled in a manner similiar in spirit to this paper. If a single pair of torus-localized levels is interacting, the resonant zone coupling two tori is removed from the Hamiltonian, thus turning off the tunneling. The tunnel splitting is then estimated by perturbation theory, using the WKB-like wave functions residing on the invariant tori. This program works very well in many cases. Its generalization to stronger resonances and many interacting levels was given by Carioli, Møller, and Heller [15].

## VII. CONCLUSION AND PROSPECTS

We have shown that the WKB wave function for a scattering problem with no turning points solves a Hamiltonian problem close to the original problem. It can thus be used for perturbative calculations for reflection amplitudes. The resulting WKB-distorted-wave Born approximation yields accurate results in parameter regions where neither WKB nor perturbation works alone.

The generalization of the coordinate space reflection problem to barrier tunneling was given. It is more complicated in form due to the need to work in momentum space and the relative functional complexity of $V(x)$ as opposed to $p^2/2$.

Further generalization leads us to the intriguing idea of finding a Hamiltonian which is very close to the exact one, but which is constructed to turn off certain nonclassical processes. Whenever such a Hamiltonian can be found and the perturbative matrix elements evaluated we may have a powerful tool. The reason is that the eigenstates of the unconventional Hamiltonian $H_{WKB}$ can be constructed from classical mechanics, and the remaining quantum effects calculated by perturbation theory. We actually accomplished all the desired features of this plan, including simplicity of the integrals, in the case of reflection above a barrier top or a ramp. We described the analogous situation governing dynamical tunneling between invariant tori. Whether ''turning off the tunneling,'' as it might be termed, will prove practicable in wider circumstances remains to be seen, but the idea is appealing.

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[1] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics (Nonrelativistic Theory)* (Pergamon, New York, 1977).
[2] R. Feynman and A. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[3] B.R. Holstein and A.R. Swift, Am. J. Phys. **50**(9), 829 (1982).
[4] M.V. Berry and K.E. Mount, Rep. Prog. Phys. **35**, 315 (1972); M.V. Berry, J. Phys. A **15**, 3693 (1982).
[5] L.S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
[6] M.C. Gutzwiller, J. Math. Phys. **8**(10), 1979 (1967).
[7] N.T. Maitra and E.J. Heller (unpublished).
[8] N.T. Maitra and E.J. Heller (unpublished).
[9] M.J. Davis and E.J. Heller, J. Chem. Phys. **75**, 246 (1981).
[10] E.J. Heller. J. Phys. Chem. **99**, 2625 (1995).
[11] A.M. Ozorio de Almeida, J. Phys. Chem. **88**, 6139 (1984).
[12] F.L. Roberts and C. Jaffé, J. Chem. Phys. **99**, 2495 (1993).
[13] T. Uzer and R.A. Marcus, J. Chem. Phys. **81**, 5013 (1984).
[14] T. Uzer, D.W. Noid, and R.A. Marcus, J. Chem. Phys. **79**, 4412 (1983).
[15] M. Carioli, K. Møller, and E.J. Heller (unpublished).