Transfer-matrix approach to tunneling between Kolmogorov-Arnold-Moser tori

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We consider splittings of the energies of degenerate quasimodes in a two-dimensional channel. This system is a model for splittings of degeneracies due to multidimensional tunneling in a general quasi-integrable system. We formulate a determinant quantization condition in terms of the transfer matrix, which enables us to relate the splittings to elements of the scattering matrix. We find that the splittings can be due to either a single- or a multiple-scattering process. In the former case, the results reduce to an earlier theoretical analysis which used an assumption that the splittings are canonically invariant quantities. We demonstrate a quantitative agreement between semiclassical theory and numerical calculations of the splittings.

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I. INTRODUCTION

A particle moving in a smooth potential well in $d \geqslant 2$ dimensions typically has a mixture of regular trajectories, which explore d dimensional tori in phase space, and irregular trajectories that explore regions of higher dimensionality. Quantum eigenstates can be associated with a subset of the phase space tori which satisfy the Einstein-Brillouin-Keller (EBK) quantization rule: this states that the actions I_j associated with the d independent irreducible circuits Γ_j on these tori satisfy

$$I_j=\frac{1}{2\pi}\int_{\Gamma_j}\mathbf{p}\cdot d\mathbf{q}=\left(n_j+\frac{1}{4}\,\gamma_j\right)\hbar, \tag{1.1}$$

where the n_j are a set of quantum numbers and the γ_j are integers termed Maslov indices. The energies of these torus quantized states are approximately

$$E_{\mathbf{n}}=H(\mathbf{I}), \tag{1.2}$$

where $H(\mathbf{I})$ is the Hamiltonian expressed in terms of the set of actions, $\mathbf{I}=(I_1,I_2,\ldots,I_d)$, and $\mathbf{n}=(n_1,n_2,\ldots,n_d)$ is a vector formed from the quantum numbers n_j. Classical Hamiltonian dynamics, the Kolmogorov-Arnold-Moser (KAM) theorems on the ubiquity of phase space tori, and the EBK quantization scheme are reviewed in a book by Gutzwiller [1].

An interesting feature of the EBK quantization scheme is that it predicts degeneracies in cases where more general arguments indicate that they should not exist. If the system has a geometrical symmetry such as a mirror plane, it is possible for phase space tori to exist in pairs related by the symmetry operation. The EBK quantization scheme predicts the existence of torus-quantized states with exactly the same energy. Because the irreducible representations of this symmetry group are one dimensional, we do not expect any exact degeneracies in the spectrum. Numerical experiments show that the spectrum contains doublets with a small splitting [2,3]. Similarly, if we vary a parameter in the Hamiltonian, the EBK scheme predicts that levels can degenerate for isolated parameter values, whereas the noncrossing rule [4] tells us that this should not happen. Again, numerical experiments show that varying a parameter leads to avoided crossings with very small splittings [5]. The splittings of these doublets and avoided crossings are the subject of this paper.

It has been suggested [2,3] that these splittings result from a tunneling effect, and that they should decrease exponentially in the semiclassical limit (taking $\hbar \to 0$, keeping all the classical parameters of the Hamiltonian fixed):

$$\Delta E \sim A\exp(-W/\hbar). \tag{1.3}$$

Here W is a classical action, and the prefactor A may have a power law dependence on $\hbar$. Theoretical arguments have been advanced to support this hypothesis [6,7], and it is consistent with some numerical experiments [5], although not with others [8,9]. Because the wave functions of the two degenerate quasimodes overlap in coordinate space, an entirely satisfactory solution of this problem will require an analysis of the Stokes phenomenon [10] in two or more dimensions, enabling us to describe exponentially small corrections to the wave function in the classically allowed region. Progress on this problem has been slow.

In this paper we discuss a model in which the tunneling splittings can be related to the S matrix for a scattering problem. Although there is not yet a fully satisfactory theory for the semiclassical S matrix in the classically forbidden region, procedures (pioneered by Miller and George [11,12]) for calculating the exponentially small scattering matrix elements exist which yield satisfactory results (i.e., excellent agreement with numerical experiments). We will show that multidimensional tunneling provides a good description of the splittings of degeneracies in some cases, and that it is described by a formula which is equivalent to that proposed in an earlier paper by one of us [6]. We also show how the simple tunneling picture can fail and be replaced by a multiple scattering process; we indicate how our approach can be extended to the case of multiple scattering.

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We consider the following model. A particle of mass μ moves in a two-dimensional channel, for which the smooth potential $V(x,y)$ is periodic in x, bounded in y, and symmetric:

$$V(x+L,y)=V(x,y), \tag{1.4a}$$

$$\lim_{y\to\pm\infty} V(x,y)=\infty, \tag{1.4b}$$

$$V(-x,y)=V(x,y). \tag{1.4c}$$

We will apply the Bloch boundary condition

$$\Psi(x+L,y)=\exp(iKL)\Psi(x,y) \tag{1.5}$$

and the eigenvalues depend on the Bloch wave vector K.

Consider the classical motion along the channel at energies for which the channel is open, in the sense that there are trajectories connecting $x=0$ and $x=L$. Typically, in a smoothly varying potential we expect that some of these extended classical trajectories will exist on KAM tori in phase space. If $K=0$, the inversion symmetry of the potential implies that these extended KAM tori exist as symmetry related pairs, in which tori with opposite directions of propagation of the particle satisfy the EBK quantization condition at the same energy. For typical values of K there are no symmetry related doublets, but by varying the parameter K avoided crossings can be observed.

Our approach is as follows. In Sec. II we will set up an exact determinantal quantization condition for the energy levels in terms of the transfer matrix $\tilde{M}$ for propagation along the channel. In Sec. III we describe how this quantization condition leads to a simple expression for the splitting ΔE of the degeneracy under certain conditions. When these conditions are not satisfied, we can interpret the splitting as resulting from a multiple scattering process, and discuss an extension of our equation for the splitting to this case. Our equations for the splitting are expressed in terms of elements of the scattering matrix $\tilde{S}$ corresponding to classically forbidden processes: in Sec. IV we use Miller's semiclassical theory [11] to relate these matrix elements to classical trajectories in a complex phase space. We show that the results are in agreement with an earlier prediction by one of us [6], which used an entirely different approach. We mention that we recently received a report by Doron and Frischat [13], which also discusses dynamical tunneling using a determinantal quantization condition. They analyze the billiard model discussed in [8], and their approach is quite specific to that system.

We describe some numerical tests of this theory in Sec. V. For convenience we will confine our numerical studies to potentials of the form

$$V(x,y)=\alpha v(x)+\frac{1}{2}y^2+(\epsilon y+\epsilon' y^2)v(x) \tag{1.6}$$

with $v(x)$ either a periodized sech^2 function

$$v(x)=\sum_{n=-\infty}^{\infty}\mathrm{sech}^2[(x-nL)/\lambda] \tag{1.7}$$

or a Gaussian

$$v(x)=\sum_{n=-\infty}^{\infty}\exp\left[-\frac{1}{2}(x-nL)^2/\lambda^2\right]. \tag{1.8}$$

In many cases, we find good agreement with our formulas for splittings due to single-step scattering. The other splittings must be described by a multiple-scattering theory, which we did not consider in detail. Section VI contains some concluding remarks.

II. THE TRANSFER-MATRIX QUANTIZATION CONDITION

Because the Hamiltonian is periodic in x, we concentrate on a period of the potential $-L/2<x<L/2$. We will consider the case where the period L of the potential is large compared to the length λ of the scattering region, so that the channel approaches a uniform cross section when $|x|\sim L/2\gg\lambda$. We expand the wave function satisfying the time-independent Schrödinger equation in terms of asymptotic modes of propagation,

$$\Psi(x,y)=\frac{1}{\sqrt{k_n}}\sum_{n=1}^{\infty}\{a_n^+(x)\exp(ik_nx) + a_n^-(x)\exp(-ik_nx)\}\varphi_n(y) \tag{2.1}$$

where the asymptotic basis functions $\varphi_n(y)$ satisfy the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2\varphi_n}{dy^2}+V(L/2,y)\varphi_n=E_n\varphi_n \tag{2.2}$$

with the boundary condition $\varphi(y)\to 0$ as $y\to\pm\infty$. The wave vector k_n is given by

$$k_n(E)=\sqrt{2\mu(E-E_n)}/\hbar. \tag{2.3}$$

The expansion coefficients $a_n(x)$ at different values of x are linearly related; we write

$$\begin{pmatrix}\mathbf{a}^+(L/2)\\ \mathbf{a}^-(L/2)\end{pmatrix}=\begin{pmatrix}\tilde{M}_{++} & \tilde{M}_{+-}\\ \tilde{M}_{-+} & \tilde{M}_{--}\end{pmatrix}\begin{pmatrix}\mathbf{a}^+(-L/2)\\ \mathbf{a}^-(-L/2)\end{pmatrix} =\tilde{M}\begin{pmatrix}\mathbf{a}^+(-L/2)\\ \mathbf{a}^-(-L/2)\end{pmatrix} \tag{2.4}$$

where $\mathbf{a}^{\pm}(x)=(a_1^{\pm}(x),a_2^{\pm}(x),\dots)$ are infinite dimensional vectors containing the coefficients $a_n^{\pm}$, and the matrix $\tilde{M}$ is termed the transfer matrix. The subscripts on the four submatrices of $\tilde{M}$ indicate whether, respectively, the initial or final states represent leftgoing or rightgoing waves. Because we are considering the case $L\gg\lambda$, the amplitudes $a_n^{\pm}(x)$ are expected to approach constant values in region $|x|\sim L/2$, which will be denoted by $a_n^{\pm L}$ and $a_n^{\pm R}$ for $x\ll-\lambda$ and $x\gg+\lambda$, respectively. The relationship between these coefficients can be expressed by the asymptotic value of the transfer matrix, or alternatively by means of a scattering matrix $\tilde{S}$, defined as follows:

$$\begin{pmatrix} \mathbf{a}^{+R} \\ \mathbf{a}^{-L} \end{pmatrix} = \begin{pmatrix} \tilde{T}_+ & \tilde{R}_+ \\ \tilde{R}_- & \tilde{T}_- \end{pmatrix} \begin{pmatrix} \mathbf{a}^{+L} \\ \mathbf{a}^{-R} \end{pmatrix} = \tilde{S} \begin{pmatrix} \mathbf{a}^{+L} \\ \mathbf{a}^{-R} \end{pmatrix}. \tag{2.5}$$

The scattering matrix gives the amplitudes of the outgoing waves in terms of the incoming waves incident on the scatterer. The submatrices of the transfer matrix and those of the scattering matrix are related as follows:

$$\tilde{M}_{++} = \tilde{T}_+ - \tilde{R}_+ \tilde{T}_-^{-1} \tilde{R}_-, \quad \tilde{M}_{+-} = \tilde{R}_+ \tilde{T}_-^{-1}$$

$$\tilde{M}_{-+} = -\tilde{T}_-^{-1} \tilde{R}_-, \quad \tilde{M}_{--} = \tilde{T}_-^{-1}. \tag{2.6}$$

Because of the symmetry of our potential represented by (1.4c), the reflection and transmission matrices are the same for each direction, i.e., $\tilde{R}_- = \tilde{R}_+ = \tilde{R}$ and $\tilde{T}_- = \tilde{T}_+ = \tilde{T}$.

Bloch's theorem (1.5) implies that the eigenfunctions in a periodic potential satisfy

$$a_n^{\pm R} = \exp[\mp i k_n L + iKL] a_n^{\pm L}. \tag{2.7}$$

It will be useful to introduce a modified transfer matrix $\tilde{M}'$ by means of a phase transformation of the elements of $\tilde{M}$

$$(\tilde{M}'_{\pm s})_{nm} = \exp[\pm i k_n L] (\tilde{M}_{\pm s})_{nm} \tag{2.8}$$

where $s = \pm$, or in matrix form,

$$\begin{pmatrix} \tilde{M}'_{++} & \tilde{M}'_{+-} \\ \tilde{M}'_{-+} & \tilde{M}'_{--} \end{pmatrix} = \begin{pmatrix} \tilde{\kappa} & 0 \\ 0 & \tilde{\kappa}^{-1} \end{pmatrix} \begin{pmatrix} \tilde{M}_{++} & \tilde{M}_{+-} \\ \tilde{M}_{-+} & \tilde{M}_{--} \end{pmatrix}, \tag{2.9}$$

where a diagonal matrix $\tilde{\kappa}$ is defined by

$$\tilde{\kappa} = \mathrm{diag}(\{\exp[i k_n L]\}). \tag{2.10}$$

The Bloch condition can then be written

$$\det[\tilde{M}'(E) - \exp(iKL)\tilde{I}] = 0 \tag{2.11}$$

where $\tilde{I}$ is the identity matrix. This is a quantization condition on the energy for a state with a given Bloch wave vector K. The matrix $\tilde{M}'$ is infinite dimensional, but we will assume that accurate energy levels can be obtained by truncating this matrix to a large finite dimension $2\mathcal{N}$. The condition can also be written in the form

$$\det[\tilde{M}'^{N}(E) - \exp(iNKL)\tilde{I}] = 0. \tag{2.12}$$

This alternative form of the quantization condition may have spurious additional solutions, but it can be more suitable for further analysis.

III. SIMPLE ESTIMATE FOR THE SPLITTING AND ITS VALIDITY

We will now consider a simple expression for the energy splitting ΔE, which applies when the S matrix is close to diagonal. We will assume that, for the case of interest, the transmission and reflection matrices take the form

$$\tilde{T} = \tilde{d} + \tilde{t}, \quad \tilde{R} = \tilde{r} \tag{3.1}$$

where $\tilde{d}$ is a diagonal matrix which we will write in the form

$$\tilde{d} = \mathrm{diag}(\{\exp[i\phi_n]\}) \tag{3.2}$$

and ϕ_n is real valued (its explicit semiclassical form will be given in Sec. IV). It is assumed that all of the elements of the matrices $\tilde{t}$ and $\tilde{r}$ are small; in the semiclassical limit those off-diagonal matrix elements corresponding to classically forbidden processes are exponentially small in $\hbar$:

$$r_{nm} = A_{nm}^{(r)} \exp(-W_{nm}^{(r)}/\hbar),$$

$$t_{nm} = A_{nm}^{(t)} \exp(-W_{nm}^{(t)}/\hbar). \tag{3.3}$$

Formulas for the tunneling actions W_{nm} and the prefactors A_{nm} will be given in Sec. IV.

We can ensure that the scattering matrix takes this form by making the asymptotic regions ($|x| \gg \lambda$) of the KAM tori coincide with the asymptotic states of the scattering problem. This can be achieved by a perturbative approach, in which the coupling constants ϵ and ϵ' which break the separability of the potential (1.6) are very small; this is the method we adopt in this paper. An alternative approach would be to make $\lambda \gg 1$ as well as $L \gg \lambda$, in which case the transverse mode of the channel varies adiabatically. The classical adiabatic theorem [14] then ensures that the action I of the transverse motion is a good approximate constant of motion as we propagate along the channel.

If both $\tilde{t}$ and $\tilde{r}$ are small but not zero, as we have assumed, we can approximate the transfer matrix $\tilde{M}'$ as follows:

$$\tilde{M}' = \begin{pmatrix} \tilde{\kappa}(\tilde{d} + \tilde{t}) & \tilde{\kappa}\tilde{r}\tilde{d}^{-1} \\ -\tilde{\kappa}^{-1}\tilde{d}^{-1}\tilde{r} & \tilde{\kappa}^{-1}(\tilde{d} + \tilde{t})^{-1} \end{pmatrix}. \tag{3.4}$$

Then, by neglecting the classically forbidden processes ($\tilde{t}$ and $\tilde{r}$) and inserting it into the quantization condition (2.11), we can write the EBK quantization condition in terms of elements of $\tilde{d}$ in the form

$$\Phi_n(E_{n,m}) \equiv \phi_n(E_{n,m}) + k_n(E_{n,m})L = 2\pi m \pm KL. \tag{3.5}$$

Here the $E_{n,m}$ are the EBK quantized energies corresponding to the KAM tori.

Let us assume that the EBK energies of two modes with indices n_1 and n_2 are degenerate at energy E_0. Referring to the EBK quantization condition (3.5), we see that this is realized if

$$\Phi_{n_1}(E_0) - 2\pi m_1 = KL = \Phi_{n_2}(E_0) - 2\pi m_2. \tag{3.6}$$

These two equations can be solved by varying the parameters E_0 and K, implying degeneracy between quasimodes with quantum numbers (n_1, m_1) and (n_2, m_2). When the off-diagonal matrix elements are included in the determinant quantization condition, these apparent degeneracies are split. By permuting rows and columns of the determinant and using the approximation (3.4), we can write the quantization condition (2.11) in the form

$$D(E)=\det\left(\begin{array}{cc|ccc} e^{i\Phi_{n_1}}-e^{iKL} & e^{ik_{n_1}L}t_{n_1n_2} & (M'_{++})_{n_11} & \cdots & (M'_{+-})_{n_1,J} \\ e^{ik_{n_2}L}t_{n_2n_1} & e^{i\Phi_{n_2}}-e^{iKL} & (M'_{++})_{n_21} & \cdots & (M'_{+-})_{n_2,J} \\ \hline (M'_{++})_{1n_1} & (M'_{++})_{1n_2} & (M'_{++})_{11}-e^{iKL} & \cdots & (M'_{+-})_{1,J} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (M'_{-+})_{J,n_1} & (M'_{-+})_{J,n_2} & (M'_{-+})_{J,1} & \cdots & (M'_{--})_{J,J}-e^{iKL} \end{array}\right)=0. \tag{3.7}$$

The determinant $D(E)$ can be written

$$D(E)=D_2(E)D'(E)+R(E), \tag{3.8}$$

where $D_2(E)$ is the determinant of the 2×2 submatrix at the top left of (3.7), $D'(E)$ is the determinant of the lower right hand submatrix, and $R(E)$ is a remainder term. If the elements in the upper right or lower left submatrices are sufficiently small, the remainder term can be neglected, in which case the quantization condition states that either $D'(E)=0$ or else

$$\det\begin{pmatrix} e^{i\Phi_{n_1}}-e^{iKL} & e^{ik_{n_1}L}t_{n_1n_2} \\ e^{ik_{n_2}L}t_{n_2n_1} & e^{i\Phi_{n_2}}-e^{iKL} \end{pmatrix}=0. \tag{3.9}$$

If the off-diagonal matrix element $t_{n_1n_2}$ is small, there will be two solutions of (3.9) close to E_0. Approximating $\exp[i\Phi_{n_1}(E)]-\exp[iKL]$ by the first nonvanishing term of its Taylor expansion about E_0, we can write this condition in the form

$$\det\begin{pmatrix} i\dfrac{d\Phi_{n_1}}{dE}(E-E_0)\,e^{i\Phi_{n_1}} & t_{n_1n_2}e^{ik_{n_1}L} \\ t_{n_2n_1}e^{ik_{n_2}L} & i\dfrac{d\Phi_{n_2}}{dE}(E-E_0)e^{i\Phi_{n_2}} \end{pmatrix}=0. \tag{3.10}$$

This quadratic equation is solved by a pair of energies with separation

$$\Delta E=2|t_{n_1n_2}|\Big/\sqrt{\frac{d\Phi_{n_1}}{dE}\frac{d\Phi_{n_2}}{dE}}. \tag{3.11}$$

If we consider the case in which, at energy E_0, we have

$$\Phi_{n_1}(E_0)-2\pi m_1=KL=-\Phi_{n_2}(E_0)+2\pi m_2 \tag{3.12}$$

instead of (3.6), then the formula (3.11) is replaced by

$$\Delta E=2|r_{n_1n_2}|\Big/\sqrt{\frac{d\Phi_{n_1}}{dE}\frac{d\Phi_{n_2}}{dE}}. \tag{3.13}$$

Equations (3.11) and (3.13) are good approximations for the splitting of the nearly degenerate levels provided that the remainder term in (3.8) can be ignored. Equation (3.11) describes the situation where the dominant contribution to the splitting of modes with indices n_1 and n_2, propagating in the same direction, comes from a single scattering from one mode to the other. Similarly, Eq. (3.13) applies when the degenerate quasimodes are propagating in opposite directions, implying that the scattering matrix element between these modes is a reflection.

It is straightforward to write down sufficient conditions for the neglect of the remainder term, but we will not pursue this here. The neglect of the remainder term cannot always be justified, if the determinant condition is written in the form (2.11). By rewriting this condition in the form (2.12), it may in some circumstances be possible to show that the conditions for the remainder term being neglected are satisfied for some power N. In this case, we can use a modification of the formula (3.11) or (3.13) to calculate the splitting, and we can interpret the splitting as being dominated by an N-fold scattering process.

IV. SEMICLASSICAL APPROXIMATIONS

In order to calculate the energy splittings we require formulas for matrix elements of the S matrix. Miller [11] has given a semiclassical theory for these matrix elements, based on the van Vleck formula [1]: his theory gives expressions for the matrix elements of both classically allowed and classically forbidden transitions. We will begin by describing Miller's theory as it applies to a scatterer in a two-dimensional channel. The asymptotic states of the scattering problem can be described by two classical momenta; one is the momentum p of the particle along the direction of the channel, the other is the action variable I for the transverse oscillations. The transverse action I is quantized and the longitudinal momentum p is determined by conservation of energy: $p=\sqrt{2\mu(E-E_n)}$. The S matrix elements take the form

$$S_{n_2n_1}=\sum_k\left(\frac{i\hbar}{2\pi}\frac{\partial^2W^{(k)}}{\partial I_1\partial I_2}\right)^{1/2}\exp\left[\frac{i}{\hbar}W^{(k)}(I_2,p_2,I_1,p_1;E)\right], \tag{4.1}$$

where the action is

$$W=-\int_{t_1}^{t_2}dt(x\dot{p}+\theta\dot{I}). \tag{4.2}$$

(x and θ are the coordinates conjugate to the canonical momenta p and I, respectively.) The sum runs over all the trajectories which satisfy the appropriate boundary conditions, implying that the incoming and outgoing trajectories satisfy the EBK quantization condition for a transverse mode in the asymptotic regions. These boundary conditions are

$$I_1=\left(n_1+\frac{1}{4}\gamma_1\right)\hbar,\quad \theta_1=\text{arbitrary}$$

$$I_2=\left(n_2+\frac{1}{4}\gamma_2\right)\hbar, \quad \theta_2=\text{arbitrary} \tag{4.3}$$

[and for the potential (1.6), the Maslov constants are $\gamma_1=\gamma_2=2$]. Appropriate trajectories are determined by a shooting method: the final action n_2 is a function of the initial action n_1 and of the angle θ_1, and the initial condition θ_1 is adjusted so as to make n_2 integer valued. If the outward part of the trajectory continues in the same direction as the inward part, it contributes to the element $T_{n_2n_1}$ of the transmission matrix; otherwise it contributes to the reflection matrix element $R_{n_2n_1}$.

Miller and George showed [12] that this method can also be applied to classically forbidden processes for which there is no real classical trajectory such that n_2 is integer valued; instead, this condition is satisfied by taking complex valued trajectories. Any observed variables must take real values, but unobserved variables are free to take any value, including complex values. The initial and final conditions of the trajectory are as follows

$$\begin{array}{cc} & \text{initial} \\ x_1 & \text{real, arbitrary} \\ p_1 & \text{real, } \sqrt{2\mu(E-E_{n_1})} \\ \theta_1 & \text{complex, variable} \\ I_1 & \text{real, specified} \end{array} \quad \rightarrow \quad \begin{array}{cc} & \text{final} \\ x_2 & \text{real, arbitrary} \\ p_2 & \text{real, } \sqrt{2\mu(E-E_{n_2})} \\ \theta_2 & \text{complex, free} \\ I_2 & \text{real, specified} \end{array} . \tag{4.4}$$

(x_1 and x_2 should be located in either left or right asymptotic regions, but otherwise they are arbitrary.) The trajectory can be integrated along any path in the complex t plane. Integration of Hamilton's equations in complex phase space along a specified path in the complex t plane gives a final transverse action I_f which depends on the initial transverse action I_1 and angle θ_1:

$$I_f(\theta_1,I_1)=I_2. \tag{4.5}$$

The complex value of θ_1 is adjusted (using a Newton-Raphson iteration or similar procedure) until a zero of the complex function I_f-I_2 is located.

The choice of path in the complex t plane is an important issue. For most continuous deformations of a path, the values of any physical observable will not change. There are, however, singular points in the complex t plane, such that a physical quantity will change discontinuously when the contour passes these points. We will discuss these singular points in more detail when we describe our numerical results.

Having found a suitable complex time path for the classically forbidden process, we assume (following Miller) that there exists a contribution to the sum (4.1) from this path, provided the imaginary part of the action is positive, so that the contribution to the matrix element has magnitude less than unity. Except when there are symmetries in the problem, all of these trajectories will have different values of ImW, and usually only that trajectory with the smallest positive value of ImW need be retained, as the others will be exponentially small by comparison. The matrix elements corresponding to classically forbidden transmissions will therefore be written

$$t_{n_2n_1}=\left[\frac{i\hbar}{2\pi}\frac{\partial^2 W^{(t)}_{n_2n_1}}{\partial I_{n_1}\partial I_{n_2}}\right]^{1/2}\exp[iW^{(t)}_{n_2n_1}/\hbar] \tag{4.6}$$

and similarly for classically forbidden reflections, with $W^{(r)}_{n_2n_1}$, the action for the reflection path, replacing $W^{(t)}_{n_2n_1}$.

We can now give a simple formula for the splitting in terms of canonically invariant quantities. First note that the phases Φ_n appearing in (3.11) and (3.13) are related to the action variable J for the longitudinal motion: $2\pi J=\hbar\Phi_n(E)$. It follows that

$$\hbar\frac{d\Phi_n}{dE}=2\pi\left(\frac{\partial H}{\partial J}\right)^{-1}. \tag{4.7}$$

Combining (4.6) and (4.7) with (3.11), we find

$$\Delta E=\frac{\hbar^{3/2}}{2\pi^2}\left[2\pi i\frac{\partial^2 W}{\partial I_1\partial I_2}\frac{\partial H}{\partial J_1}\frac{\partial H}{\partial J_2}\right]^{1/2}\exp(iW/\hbar) \tag{4.8}$$

where (I_1,J_1) and (I_2,J_2) are the transverse and longitudinal actions for the two states.

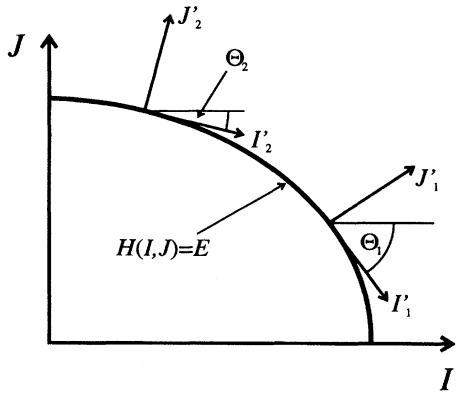

FIG. 1. Illustrating the definition of the two sets of action variables (I,J) and (I',J') discussed in Sec. IV; the latter are, respectively, tangential and perpendicular to contours of $H(I,J)$.

Equation (4.8) is equivalent to an expression previously obtained by one of us [6] using an entirely different method: the earlier expression was of the form

$$\Delta E=\frac{\hbar^{3/2}}{2\pi^2}\left[2\pi i\,\frac{\partial^2 W}{\partial I_1'\partial I_2'}\frac{\partial H}{\partial J_1'}\frac{\partial H}{\partial J_2'}\right]^{1/2}\exp(iW/\hbar), \quad (4.9)$$

where I' and J' are action variables measured, respectively, tangential and perpendicular to a contour of the Hamiltonian $H(I,J)$ (see Fig. 1). [We remark that in writing (4.9) we have corrected an error in (3.18) of Ref. [6], in which a term proportional to $d\mathbf{r}^2$ was dropped in Eq. (3.13) of that paper.] In (4.8) of this paper, W is differentiated at constant energy E, implying that

$$\frac{\partial^2 W}{\partial I_1'\partial I_2'}=\frac{\partial^2 W}{\partial I_1\partial I_2}\frac{\partial I_1}{\partial I_1'}\frac{\partial I_2}{\partial I_2'}=\frac{\partial^2 W}{\partial I_1\partial I_2}\cos\Theta_1\cos\Theta_2, \quad (4.10)$$

where the angles Θ_1 and Θ_2 are defined in Fig. 1. Also, in (4.8) the factors $\partial H/\partial J$ are evaluated at fixed I, implying that

$$\frac{\partial H}{\partial J_1'}=\frac{\partial H}{\partial J_1}\frac{\partial J_1}{\partial J_1'}=\frac{\partial H}{\partial J_1}\frac{1}{\cos\Theta_1}. \quad (4.11)$$

The factors involving $\cos\Theta_1$ and $\cos\Theta_2$ cancel, implying that (4.8) is equivalent to (4.9).

The earlier paper considered a double well potential, and manipulated the expression for the tunneling splitting to this canonically invariant form. It was hypothesized that the tunneling splitting should be an invariant quantity, and that this formula should apply to the dynamical tunneling problem, as well as double well problems. The new derivation avoids making assumptions about canonical invariance, but it is only applicable in its present form when the KAM tori correspond to asymptotic channels of a scattering problem.

V. NUMERICAL RESULTS

We wrote computer programs to calculate the energy splittings ΔE and the elements of the S matrix directly from the Schrödinger equation, and also to calculate elements of the S matrix semiclassically. The programs for the quantum mechanical computations require little discussion. To determine the energy splittings we computed the energy levels numerically by a matrix diagonalization method. We calculated the elements of the S matrix numerically by using an R-matrix propagation method described in [15]. We had to use a large number (up to 2000) of steps in the x direction because we required very small amplitudes corresponding to tunneling: S matrix elements of magnitude 10^{-12} could be calculated accurate to three significant figures.

Our semiclassical calculation of the S matrix elements follows Miller's approach, using a shooting method to determine an appropriate complex classical trajectory, as discussed in Sec. IV. Our earlier discussion did not specify how to determine the path in the complex t plane along which the trajectory is computed. This depends on the form of the scattering potential used; in general this issue must be addressed by locating the singularities in the complex t plane numerically, and testing all the different topologies with which the path can wind around the singularities in order to find a tunneling trajectory with the smallest action. In the numerical investigations which we report below, the coefficients ϵ and ϵ' are small, implying that the potential is close to separable. The singular points are easily determined in the separable case, and can be used as a guide in the slightly perturbed nonseparable cases of interest. In the separable case the motion of the x coordinate is independent, and can be obtained by solving the implicit equation

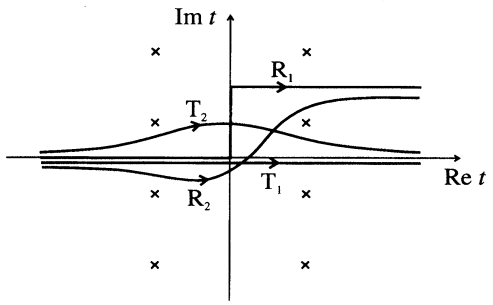

FIG. 2. Singularities in the complex t plane and paths that produce transmitting trajectories (T_1 and T_2) and reflecting trajectories (R_1 and R_2).

$$t=\left(\frac{1}{2}\mu\right)^{1/2}\int_0^x dx'[E-V(x')]^{-1/2} \quad (5.1)$$

for $x(t)$. The singularities in the complex t plane occur when the potential $V(x)$ is singular. For the potential $V(x)=\alpha\,\mathrm{sech}^2(x)$, $V(x)$ diverges at $x=\pi/2i+n\pi i$, which correspond to the singular times

$$t=\pm t_s\pm n\pi i\sqrt{\frac{\mu}{2E}},\quad t_s=\sqrt{\frac{\mu}{2E}}\sinh^{-1}\left(i\sqrt{\frac{E}{E-\alpha}}\right), \quad (5.2)$$

where we choose $t=0$ as the time at which the particle is at $x=0$. The arrangement of these singularities in the complex t plane is shown in Fig. 2, which also shows two paths which generate trajectories corresponding to transmission over the top of the barrier (T_1 and T_2), and two paths which lead to reflecting trajectories (R_1 and R_2). For the potential $V(x)=\alpha\exp(-x^2/2)$, although the potential $V(x)$ is finite for any finite x in the complex x plane, it is possible for the trajectory $x(t)$ to escape to infinity in a finite complex time.

TABLE I. Splittings determined by the matrix element $t_{n_1n_2}$, for the sech^2 potential (1.7). The parameters were $\hbar=0.2$, $\alpha=0.01$. The avoided crossing between $n_1=0^+$ and $n_2=1^+$ states occur close to $E\approx0.36056$ and $K\approx-0.1744$; for the $n_1=0^+$, $n_2=2^+$ crossings, $E\approx0.55406$ and $K\approx-0.2723$.

ϵ	ϵ'	n_1,n_2	ΔE_{QM}	ΔE_{mix}	ΔE_{SC}
0.001	0.0	0,1	3.9×10^{-5}	3.9×10^{-5}	3.9×10^{-5}
0.001	0.0005	0,1	3.9×10^{-5}	3.9×10^{-5}	4.5×10^{-5}
0.0	0.001	0,1	0.0	0.0	0.0
0.001	0.0005	0,2	1.6×10^{-6}	1.9×10^{-6}	1.7×10^{-6}
0.0	0.001	0,2	3.8×10^{-6}	3.8×10^{-6}	3.6×10^{-6}

TABLE II. Splittings determined by the matrix element $t_{n_1 n_2}$, for the Gaussian potential (1.8). The parameters were $\hbar=0.2$, $\alpha=0.05$. The avoided crossings between $n_1=0^+$ and $n_2=1^+$ states occur close to $E\approx 0.534\,022$, $K\approx 0.211\,64$; for the $n_1=0^+$, $n_2=2^+$ crossings, $E\approx 0.657\,858$ and $K\approx 0.212\,82$.

ϵ	ϵ'	n_1,n_2	$\Delta E_{\rm QM}$	$\Delta E_{\rm mix}$	$\Delta E_{\rm SC}$
0.001	0.0	0,1	7.7×10^{-5}	7.7×10^{-5}	8.1×10^{-5}
0.001	0.001	0,1	7.7×10^{-5}	7.7×10^{-5}	7.7×10^{-5}
0.0	0.001	0,1	0.0	0.0	0.0
0.001	0.001	0,2	9.3×10^{-6}	9.4×10^{-6}	9.0×10^{-6}
0.0	0.001	0,2	9.4×10^{-6}	9.4×10^{-6}	9.0×10^{-6}

The transmitting and reflecting trajectories are divided by such a singular point in this case.

We have to be careful not to come close to such a singularity in the numerical integration in order to keep sufficient accuracy. In our numerical calculations, transmission amplitudes were calculated along a real t path for both potentials from $x=-L/2$ to $\mathrm{Re}x=L/2$. For reflection in the sech^2 model, we first move t along real axis until $\mathrm{Re}x$ reaches 0, then along a purely imaginary time increment $i\tau=\pi i\sqrt{\mu/2E}$, and finally we move t in a purely real direction until $\mathrm{Re}x$ returns to $-L/2$. The same procedure was used for reflection of the Gaussian model, except that $i\tau$ is replaced by the value for which the velocity changes sign in the separable case.

We tabulate results for three different estimates of the splitting of the degeneracy: $\Delta E_{\rm QM}$ is the splitting determined from a diagonalization of the quantum Hamiltonian, $\Delta E_{\rm SC}$ is determined using the semiclassical formula (4.8), and $\Delta E_{\rm mix}$ uses the quantum mechanically calculated S-matrix elements with the formula (3.11) or (3.13) for the splitting. The latter quantity is tabulated for two reasons: first it specifies the magnitude of the quantum S-matrix elements, and secondly, in cases where the agreement between the quantum and semiclassical results is not perfect, it indicates whether the discrepancy lies in the semiclassical approximation or in the reduction to a 2×2 matrix.

We studied three different types of splittings, and we will refer to them by means of the S-matrix elements which occur in the formula for the splitting. Symmetry related doublets at $K=0$, which correspond to direct reflection of the mode n^+ into the mode n^-, are determined by the element r_{nn}. We also studied the splittings of two types of avoided crossings produced by varying K, in which the degenerate quasi-modes correspond to propagation in the same direction, or in different directions: we refer to these as $t_{n_1 n_2}$ and $r_{n_1 n_2}$ splittings, respectively.

TABLE III. Matrix elements r_{nn} of the S matrix for the Gaussian potential (1.8). The parameters were $\alpha=0.05$, $\epsilon=0.01$. The energy is $E\approx 0.7459$.

$\hbar$	n_y	$\lvert S_{\rm QM}\rvert$	$\lvert S_{\rm SC}\rvert$
0.7	0	3.40×10^{-2}	5.69×10^{-2}
0.7/3	1	1.24×10^{-4}	1.23×10^{-4}
0.7/5	2	3.76×10^{-7}	3.56×10^{-7}
0.7/7	3	1.18×10^{-9}	1.23×10^{-9}
0.7/9	4	3.53×10^{-12}	3.71×10^{-12}

TABLE IV. Splittings determined by the matrix element r_{nn}, for the Gaussian potential (1.8). The parameters and the energy are the same as Table III.

$\hbar$	(n_x,n_y)	$\Delta E_{\rm QM}$	$\Delta E_{\rm mix}$	$\Delta E_{\rm SC}$
0.7	(2,0)	4.19×10^{-3}	4.19×10^{-3}	7.0×10^{-3}
0.7/3	(6,1)	4.86×10^{-6}	5.09×10^{-6}	5.0×10^{-6}
0.7/5	(10,2)	2.73×10^{-7}	9.26×10^{-9}	8.8×10^{-9}
0.7/7	(14,3)	1.31×10^{-10}	2.07×10^{-11}	2.2×10^{-11}
0.7/9	(18,4)	5.38×10^{-12}	4.82×10^{-14}	5.1×10^{-14}

In Tables I and II we give examples of splittings involving the $t_{n_1 n_2}$ scattering matrix element; Tables I and II contain data for the potentials (1.7) and (1.8), respectively. For both of these examples we used $\mu=\lambda=1$ and $L=10$; the other parameter values are listed in the captions of the tables. In these tables semiclassical estimates $\Delta E_{\rm SC}$ obtained from (4.8) agree well with quantum results $\Delta E_{\rm QM}$, as well as with $\Delta E_{\rm mix}$. We remark that if both the coupling constants ϵ and ϵ' are zero, the splitting vanishes, implying that this splitting is an inherently two-dimensional tunneling process. In the case where $\epsilon=0$, for both potentials we found two solutions with the same imaginary part of the action. This degeneracy comes from the symmetry of the potential: these two solutions have the same phase for splitting between $n=0$ and $n=2$, whereas they have the opposite signs for splitting $n=0$ and $n=1$ states, so that the splitting is zero.

Next we consider splittings determined by direct reflection by the matrix element r_{nn}. The direct reflection occurs even when ϵ and ϵ' are zero. Thus, this type of splitting can be essentially either one dimensional or two dimensional. We examined this point carefully, by changing values of $\hbar$, so that we calculate splittings of states for which the quantized tori are the same. Tables III and IV show the elements of the S-matrix element r_{nn} and the energy splittings, respectively, for the potential (1.8), where the same values of μ, λ, and L

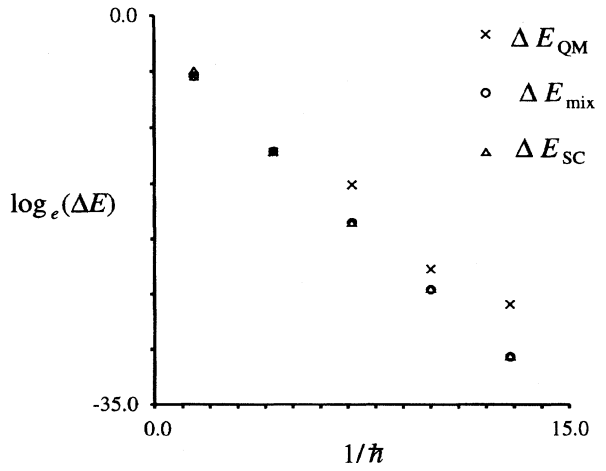

FIG. 3. Energy splitting as a function of $1/\hbar$ for the Gaussian potential (1.8). The data are taken from Table IV.

are used as above. From Table III we see that for fixed classical parameters, Miller's theory is valid in the limit of $\hbar \to 0$: the semiclassical results agree with quantum ones for $\hbar \leq 0.7/3$. Next consider the energy splittings given in Table IV and plotted in Fig. 3: we find that for $\hbar \leq 0.7/5$, S_{SC} agrees well with S_{QM}, but ΔE_{SC} does not agree with ΔE_{QM}. This implies that the reduction to a 2×2 matrix breaks down in the limit of $\hbar \to 0$. Note that the formula (4.8) gave an underestimate of the splitting. These observations imply that, in these cases, the splitting of the degeneracy is dominated by multiple scattering. The deviation from simple exponential dependence of splitting on $1/\hbar$ given is similar to that seen in the results of [8].

We verified the multiple-scattering interpretation in several cases by calculating the splitting using a succession of approximations of the exact determinant quantization condition; in these cases we only obtained accurate estimates of the splitting when matrix elements allowing transitions via intermediate states were included.

Finally, we remark that all the examples of $r_{n_1 n_2}$ splittings that we examined appear to be determined by the multiple scattering mechanism.

VI. DISCUSSION

In this paper we have given the first example of quantitative agreement with a two-dimensional semiclassical theory for splittings between KAM quantized quasimodes. Our discussion was specific to problems which can be represented in terms of a scattering region connecting incoming and outgoing channels, but the approach can be extended to potentials with bound states. Our analysis gives a formula which is equivalent to one suggested in Ref. [6], based on consideration of a double well potential.

Our analysis also indicates a mechanism by which the simple formulas for the splitting, (3.11) and (3.13) can fail. Our derivation depends on the neglect of a remainder term in the determinant quantization condition. If this remainder cannot be neglected, our formulas, based on the assumption that the splitting is due to a single-scattering event, are not valid. Individually, the elements of the S matrix describe a process (one traversal of the scatterer) occurring in a finite time, whereas the fine structure of the spectrum contained in the splittings between energy levels carries information about the dynamics on very long time scales. It should not, therefore, be too surprising that the predictions of (3.11) or (3.13), which contain information about only one S matrix element, can break down. By taking account of multiple-scattering processes, we can describe the propagation over longer periods and obtain more accurate information about the splittings.

To see how this can lead to a quantitative theory, note that multiple traversals of the scatterer can produce a larger probability for transitions between two states, and the effects of transitions involving scattering via intermediate states must be included. For example, if the matrix element $t_{n_1 n_2}$ is very small, the product $t_{n_1 n_i} t_{n_i n_2}$, describing scattering via an intermediate mode with transverse quantum number n_i, may make a dominant contribution to the corresponding matrix element of $\tilde{M}'^2$. The reduction of the quantization condition (3.7) to a 2×2 matrix depends on the matrix element coupling the states with transverse quantum numbers n_1 and n_2 being sufficiently large to guarantee that the remainder term in (3.8) can be neglected. Even if this condition is not satisfied by the matrix $\tilde{M}'$, it may be satisfied by the matrix $\tilde{M}'^2$, which includes the effects of transitions via one intermediate state. Similarly, the matrix $\tilde{M}'^N$, which describes N traversals of the scatterer, may satisfy the condition for reduction to a 2×2 form, implying that the splitting is dominated by scattering via $N-1$ intermediate modes.

Finally we remark that it may be possible to extend (4.8) to the multiple-scattering case, by regarding the potential as having a periodicity of NL rather than L. The longitudinal action J is increased by a factor of N, and the complex tunneling trajectory extending over N periods may have a smaller tunneling action $\mathrm{Im}W$ than for a path which is constrained to lie within one period. The value of N would be increased until the smallest tunneling action was found at $N=N^*$; because N^* may depend upon $\hbar$, the splitting need not decrease exponentially with $\hbar$ in the multiple-scattering case.

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[1] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York, 1990).
[2] R. T. Lawton and M. S. Child, Mol. Phys. **44**, 709 (1981).
[3] M. J. Davies and E. J. Heller, J. Chem. Phys. **75**, 246 (1981).
[4] J. von Neumann and E. P. Wigner, Phys. Z. **30**, 467 (1929).
[5] M. Wilkinson, J. Phys. A **20**, 635 (1987).
[6] M. Wilkinson, Physica D **21**, 341 (1986).
[7] T. Uzer, D. W. Noid, and R. A. Marcus, J. Chem. Phys. **79**, 4412 (1983).
[8] O. Bohigas, D. Boosé, R. Egydio de Carvalho, and V. Marvulle, Nucl. Phys. A **560**, 197 (1993).
[9] R. Roncaglia, L. Bonci, F. M. Izrailev, B. J. West, and P. Grigolini, Phys. Rev. Lett. **73**, 802 (1994).
[10] R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation* (Academic, New York, 1974).
[11] W. H. Miller, Adv. Chem. Phys. **25**, 69 (1974).
[12] W. H. Miller and T. F. George, J. Chem. Phys. **56**, 5668 (1972).
[13] E. Doron and S. D. Frischat (unpublished).
[14] A. Lenard, Ann. Phys. (NY) **6**, 261 (1959).
[15] J. C. Light and R. B. Walker, J. Chem. Phys. **65**, 4272 (1976).