

Model tunneling problems in a high magnetic field

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We have studied simple tunneling problems in two dimensions in the presence of a high transverse magnetic field both by numerical integration of the Schrödinger equation and by semiclassical evaluation of the path integral. We have chosen three model potentials: (i) asymmetric single well, (ii) symmetric double well, and (iii) quadruple well. We find that the semiclassical approach is analytically tractable and gives a very accurate description of the exponential and oscillatory behaviors of the tunneling matrix elements. A precise definition of the Aharonov-Bohm phase for the tunneling paths is given. In addition to the Aharonov-Bohm phase, there is also a geometrical phase coming from the fluctuation determinant, and we find that for every closed loop it is exactly $\pm\pi$.

I. INTRODUCTION

Since the advent of high-quality molecular beam epitaxy, it has become possible to study the properties of electrons in a nearly perfect two-dimensional system. The discovery of the fractional quantum Hall effect has led to an especially intensive study of the nature of the electronic states in the presence of a high transverse magnetic field. In particular, a recent theory¹ of the two-dimensional electron gas in a large magnetic field focuses on the effect on the ground state of exchange processes involving the cooperative tunneling of rings of electrons. However, the study of tunneling processes in a high magnetic field is in its infancy.

In the absence of magnetic field there has been ample study of tunneling processes using semiclassical methods,² of which the Wentzel-Kramers-Brillouin (WKB) approximation is one specific example. Let us consider a symmetric double-well potential for example. Solving the Schrödinger equation separately in each well produces a doubly degenerate ground state. The actual ground state, however, consists of two nondegenerate levels whose eigenfunctions are approximately given by the even and odd combinations of the individual ground-state wave functions of the two wells; the degeneracy being lifted because of the overlap of the two individual ground states. In the path-integral approach one obtains the partition function (and hence the energy levels) by considering all the paths that begin and end at the same point. The paths responsible for the splitting of the ground state are the ones that tunnel from one quantum well into the other. These paths are called "instantons" (because they are localized in time), and the splitting they produce is called the tunnel splitting. There exist powerful instanton techniques for computing the tunnel splitting. We refer the reader to Ref. 3 where it is shown for the example of a one-dimensional symmetric double-well potential that the tunnel splitting calculated using the dilute in-

stanton gas approximation agrees (in the regime of its validity) with the correct tunnel splitting obtained from solving the Schrödinger equation. Our work is in essence a generalization of these techniques to two-dimensional potentials in the presence of a high transverse magnetic field. A brief report of parts of this work has been published.⁴

A high magnetic field fundamentally alters the nature of the quantum states—it leads to quantization of the (rapid) cyclotron motion, producing Landau levels separated by energy $\hbar\omega_c = \hbar(eB/mc)$. If $\hbar\omega_c$ is large compared with all other energies in the problem (formally, if we take the effective mass $m \rightarrow 0$), then the cyclotron degrees of freedom are confined to the lowest Landau level. The remaining degrees of freedom are the electron guiding-center coordinates. These have no kinetic energy; a free electron in the lowest Landau level will remain localized about a given guiding center indefinitely. In this sense, the kinetic energy is quenched by the magnetic field. The resulting Hamiltonian involving the particle guiding-center coordinate \mathbf{R} alone is not, however, purely classical since the coordinates now specify the center of a Gaussian-localized probability amplitude of width l determined by the condition that the cyclotron orbit encloses one flux quantum: $2\pi l^2 = \phi_0/B = hc/eB$. We shall see that the dynamics of the guiding centers in the presence of an external potential $V(\mathbf{r})$ is equivalent to the quantum dynamics of a particle in a two-dimensional phase space such that R_x plays the role of the spatial coordinate, R_y that of the momentum of the particle, and l^2 plays the role of \hbar .

By virtue of this analogy, it is possible to use a phase-space or coherent-state path-integral expression^{1,2,5} for the partition function to compute the energy spectrum of a particle in a high magnetic field. The advantage of this is that we can study the effect of exponentially small tunneling processes on the spectrum by using semiclassical methods to evaluate the path integral. We know of no

other method, short of numerically integrating the Schrödinger equation, to compute tunneling effects in this limit. However, there are two problems with the approach. The first is that the coherent-state path integral is not in and of itself a mathematically well-defined object in the sense that there exists no measure for it which is analogous to the Wiener measure for the diffusion integral. It can indeed be defined (for analytic potentials) as a limit of other well-defined objects,⁶ such as the vanishing time-step limit of a discrete-time path integral or as the vanishing-mass limit of a normal path integral. The problem with this is that any manipulations of the path integral, such as a regrouping of the paths, or an approximation to the action, must be performed using the more complicated objects before the limit is taken, rather than the relatively simple path integral itself. In particular, the analytic continuation of the paths to complex space, which we encounter as soon as we begin to search for classical paths, involves untested implicit assumptions concerning the nature of the contours which pass through the various saddle points. Thus it is not *a priori* clear that the semiclassical expression for the partition function is reliable. The second problem is that no useful method has been developed for evaluating the fluctuation determinant or, in other words, for computing the prefactors in the expressions for the tunneling matrix elements. It has not even been proven possible to derive index theorems, such as those that are known for the regular path integral, to determine the phase of the prefactor.

In this paper we study three model potentials: the anisotropic single well, the double well, and the quadruple well. These potentials are simple enough that the exact spectrum can be computed numerically. We can also compute the splitting of the lowest energy levels (tunnel splitting) using the semiclassical approximation. Based on the comparison between the semiclassical expressions and the exact results, we have drawn the following conclusions. (1) The semiclassical expressions for the exponential dependences of tunneling matrix elements are analytically simple (hence useful) and extremely accurate. The magnitude of the resulting tunnel splitting can be very different from what one would expect based on the overlap of two Gaussian wave functions. (2) The prefactors are in general unspectacular in their dependences on the parameters in the problem. For instance, in the double-well problem, over a range of parameters in which the tunnel splitting varies by 16 orders of magnitude, the prefactor varies only by a factor of 2. (3) There are non-trivial phase factors associated with the fluctuation prefactor whenever there are multiple tunneling paths between wells. We have empirically determined that there is a phase $\pm\pi$ (i.e., a phase factor -1) associated with any classical path which forms a closed loop. We want to emphasize right here that this phase is *not* the usual Aharonov-Bohm phase that originates from the flux enclosed by the classical path; rather, this phase comes from the fluctuations around the classical path. We find that this phase depends only on the geometry of the system (and not on the shape) and hence we call it the geometrical phase. (4) Whenever there is more than one tunneling path, there is interference between them. In

the usual case when the electron moves in a magnetic-field-free region of space, the relevant phase for a closed path is the Aharonov-Bohm phase given by $2\pi\phi/\phi_0$, where ϕ is the flux enclosed by the closed path and $\phi_0 = hc/e$. In the present case, however, the magnetic field is everywhere and the electron moves (as we will show later) along complex classical trajectories, thus complicating the meaning of "enclosed" flux. We shall give a precise definition of the Aharonov-Bohm phase for these situations. The interference leads to an oscillatory behavior of the tunnel splitting. In particular, when the total phase difference between the two paths is $(2n+1)\pi$, they interfere destructively and the tunnel splitting they produce vanishes. This may seem surprising at first because intuitively one thinks that the odd parity state is always of higher energy than the even parity state, and hence the tunnel splitting can never vanish, but this is true only in the absence of a magnetic field. Which state has higher energy in the presence of magnetic field is not obvious, and we find that the path-integral techniques again provide a simple answer.

The plan of the paper is as follows. In Sec. II we review how the Schrödinger equation reduces to a difference equation in the high-field limit which can then be solved by numerical methods. (The numerical results are "exact" in the sense that in principle one can calculate the energy levels to any accuracy one desires. In practice, however, we determine the energy levels with such an accuracy as to get the tunnel splitting correct to four or five significant figures. In this whole paper, the word "exact" is to be understood as "accurate to at least four or five significant figures.") In Sec. III we set up the path integral and obtain equations for the classical paths. Sec. IV contains the canonical example of a harmonic oscillator, and Sec. V deals with a symmetric double-well potential in detail. We study the energy levels both using semiclassical and numerical methods, and compare the results. In Sec. VI we discuss the phase associated with a tunneling matrix element; a precise definition of the Aharonov-Bohm phase is given here. In Sec. VII the quadruple well potential is studied in order to test our conjecture about the geometrical phase. Sec. VIII contains a discussion of the prefactor, and especially of why it is so difficult to compute explicitly. The paper is finally concluded in Sec. IX.

II. EXACT SOLUTION

In order to get the exact solution we first project the potential onto the lowest Landau level (LLL). The eigenstates of an electron in the LLL in symmetric gauge are given by

$$(2^{n+1}\pi n!)^{-1/2} z^n \exp(-\frac{1}{4}|z|^2), \quad (1)$$

where $z = x + iy$, $n = 0, 1, 2, \dots$, and (x, y) are position coordinates measured in units of Landau length $l = \sqrt{\hbar c / eB}$. (In the rest of the paper, we shall take $l = 1$.) By the phrase "projection onto the LLL" we mean that we want to express the potential $V(z, z^*)$ in terms of z and its derivatives alone in such a way that its matrix elements in the LLL remain unchanged. The pro-

cedure is well known,⁵ but we outline it here briefly for completeness. If V is of polynomial form, then a specific term in V is of the form $z^{r_1}(z^*)^{r_2}$ and its matrix element between two LLL states of quantum numbers m and n is

$$\int dz \int dz^* e^{-|z|^2/2}(z^*)^m [z^{r_1}(z^*)^{r_2}] z^n,$$

which can be rewritten as

$$\int dz \int dz^* \left[\left[-2 \frac{\partial}{\partial z} \right]^{r_2} e^{-|z|^2/2}(z^*)^m \right] (z^{r_1} z^n),$$

and then as

$$\int dz \int dz^* e^{-|z|^2/2}(z^*)^m \left[\left[2 \frac{\partial}{\partial z} \right]^{r_2} z^{r_1} \right] z^n.$$

Now the way to project V onto the LLL is clear: Expand V as a power series in z and z^* . Normal order each term so that all the z^* 's are to the left of the z 's. Now replace z^* by $2(\partial/\partial z)$. Notice that this operator only operates on the polynomial part of the wave function; it does not act on the exponential. Thus the projected form of the time independent Schrödinger equation for $V(z^*, z)$ can be expressed as

$$V_p \left[2 \frac{\partial}{\partial z}, z \right] f(z) = E f(z), \quad (2a)$$

where V_p is the projected potential, and $f(z)$ is the polynomial part of the wave function, $\psi(z) = f(z) \exp(-\frac{1}{4}|z|^2)$. The most general form for f is

$$f(z) = \sum_{n=0}^{\infty} A_n z^n / (\pi 2^{n+1} n!)^{1/2} \equiv \sum_{n=0}^{\infty} a_n z^n. \quad (2b)$$

For an analytic potential the eigenvalue equation thus reduces to a difference equation which relates the values of successive coefficients a_n and can thus be solved numerically. Solutions can be found for any E and the coefficients depend on the value of E . The values of E which correspond to eigenvalues are those for which the eigenfunction $\psi_E(z)$ is normalizable. It can be easily seen that this normalizability condition is equivalent to the requirement that the series

$$\sum_n |A_n|^2 = \sum_n |a_n|^2 n! 2^{n+1} \pi \quad (3)$$

be convergent. For studying the convergence of the sum in (3) one needs to know a_n for large n , which can be obtained by looking at the asymptotic form of the (Schrödinger) difference equation. We do this in detail for the symmetric double-well potential (Sec. V) and show that the convergence of (3) is guaranteed if $|a_n| \rightarrow 0$ for $n \rightarrow \infty$. This criterion is obviously necessary (but not sufficient, as one must show in each case that a_n goes to zero fast enough) and we assume it for other potentials as well without proving it rigorously.

Thus the numerical method to obtain the eigenvalues is as follows. For each value of E we compute a_n as a function of E for very large n . (We vary E by small steps of size ΔE .) The eigenvalue is determined within an interval ΔE to be that value of E for which $a_n(E) = 0$, i.e., where

a_n changes sign. Now, in this interval the eigenvalue can be more precisely located by choosing yet smaller steps ΔE , and by continuing this process until the desired accuracy is attained. We are interested in the tunnel splitting which is the difference between the symmetric and antisymmetric eigenvalues. This difference is at times (e.g., when the wells are very far apart) extremely small compared to the individual eigenvalues, so that a reasonable accuracy in the tunnel splitting requires a determination of the eigenvalues to an extremely high precision. We are able to determine the splittings of up to 20 orders of magnitude smaller than the eigenvalues themselves, and it is remarkable that this uses typically only a few seconds of cpu time on a UNIVAC.

III. PATH INTEGRAL

A matrix element of the temperature Green's function

$$G(\mathbf{r}_i, \mathbf{r}_f; \beta) = \langle \mathbf{r}_f | e^{-\beta H} | \mathbf{r}_i \rangle$$

can be written as a weighted sum over all paths from point i to point f , and this is termed its path-integral representation. For an electron in a potential $V(x, y)$ with a perpendicular magnetic field $\mathbf{B} = B \hat{\mathbf{z}}$, the Hamiltonian is given by

$$H = \frac{1}{2m} \left[\mathbf{p} - \frac{e \mathbf{A}}{c} \right]^2 + V(\mathbf{r}), \quad (4)$$

where $\mathbf{A} = \frac{1}{2} B \mathbf{r} \times \hat{\mathbf{z}}$. We want to obtain the path-integral representation for magnetic fields that are so high that the electron always stays in the LLL.

One approach is to start with the standard² (real time) path-integral representation,

$$\langle x_f y_f | \exp(-i \hbar^{-1} H t) | x_i y_i \rangle = \int \mathcal{D}(\mathbf{r}) \exp(i \hbar^{-1} S),$$

where the action functional is given by

$$S = \int_0^t \left[\frac{1}{2} m \left(\frac{d\mathbf{r}}{d\tau} \right)^2 + \frac{e}{c} \frac{d\mathbf{r}}{d\tau} \cdot \mathbf{A} - V(\mathbf{r}) \right] d\tau.$$

With the substitution $t \rightarrow -i \hbar \beta$ we get the desired imaginary time (Euclidean) form

$$\langle \mathbf{r}_f | e^{-\beta H} | \mathbf{r}_i \rangle = \int \mathcal{D}(\mathbf{r}) \exp(-S), \quad (5)$$

$$S = \int_0^\beta \left[\frac{1}{2} \frac{\dot{x}^2 + \dot{y}^2}{\hbar \omega_c} - i \dot{x} y + V(x, y) \right] d\tau,$$

where we have rescaled all lengths by the magnetic length l , and $\omega_c = eB/mc$ is the cyclotron frequency. In Eq. (5) the $B \rightarrow \infty$ limit is taken by letting $\hbar \omega_c \rightarrow \infty$, which finally yields

$$S = \int_0^\beta [-i \dot{x} y + V_{\text{eff}}(x, y)] d\tau. \quad (6)$$

Even though this procedure implies that $V_{\text{eff}}(x, y) = V(x, y)$, we have introduced a new symbol, V_{eff} , for reasons that will be made clear below. The limit $B \rightarrow \infty$ described above is more properly the limit $m \rightarrow 0$, since we have explicitly kept the magnetic length fixed. In this limit the kinetic degrees of freedom of the electron are

frozen, since the spacing between Landau levels, $\hbar\omega_c$, is large compared with all other energies in the problem.

Another approach is to proceed to a path integral from the projected problem directly, as in Ref. 1. In symmetric gauge the wave function for an electron in the LLL with guiding-center position \mathbf{R} can be written as

$$\langle \mathbf{r} | \mathbf{R} \rangle = \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{1}{4}(\mathbf{r}-\mathbf{R})^2 + \frac{i}{2}(\mathbf{r} \times \mathbf{R}) \cdot \hat{\mathbf{z}} \right], \quad (7)$$

which has the same form as a coherent state in a two-dimensional phase space.² The states $|\mathbf{R}\rangle$ form a nonorthogonal, overcomplete basis;

$$\langle \mathbf{R}_1 | \mathbf{R}_2 \rangle = \exp \left[-\frac{1}{4} |\mathbf{R}_1 - \mathbf{R}_2|^2 + \frac{i}{2} (\mathbf{R}_1 \times \mathbf{R}_2) \cdot \hat{\mathbf{z}} \right]. \quad (8)$$

The LLL projection operator is given by

$$P_0 \equiv \frac{1}{2\pi} \int d^2\mathbf{R} |\mathbf{R}\rangle \langle \mathbf{R}|, \quad (9)$$

which is unity within the LLL since

$$\langle \mathbf{R}_1 | P_0 | \mathbf{R}_2 \rangle = \langle \mathbf{R}_1 | \mathbf{R}_2 \rangle.$$

Now the path-integral representation of $G(\mathbf{r}_f, \mathbf{r}_i; \beta)$ can be obtained in the usual way.² First the inverse temperature β is broken into a large number of equal intervals ϵ , i.e., $e^{-\beta H}$ is written as $[\exp(-\epsilon H)]^N$, and then the projection operator P_0 is inserted at each infinitesimally small interval (ensuring that the electron is in the LLL throughout its motion in imaginary time). Then

$$G(\mathbf{R}_i, \mathbf{R}_f; \beta) = \frac{1}{(2\pi)^N} \int \prod_{k=1}^N d^2\mathbf{R}_k \prod_{j=0}^N \langle \mathbf{R}_{j+1} | e^{-\epsilon H} | \mathbf{R}_j \rangle,$$

where $\mathbf{R}_0 \equiv \mathbf{R}_i$, $\mathbf{R}_{N+1} \equiv \mathbf{R}_f$, and $\epsilon N = \beta$. For $\epsilon \rightarrow 0$ the matrix element can be written as

$$\begin{aligned} \langle \mathbf{R}_{j+1} | e^{-\epsilon H} | \mathbf{R}_j \rangle &= \langle \mathbf{R}_{j+1} | \mathbf{R}_j \rangle \exp \left[-\epsilon \frac{\langle \mathbf{R}_{j+1} | H | \mathbf{R}_j \rangle}{\langle \mathbf{R}_{j+1} | \mathbf{R}_j \rangle} \right] \\ &= \exp \left[-\epsilon \left[-\frac{i}{2} \dot{\mathbf{R}}_j \times \mathbf{R}_j \cdot \hat{\mathbf{z}} + V_{\text{eff}}(\mathbf{R}_j) \right] \right], \end{aligned}$$

with the help of which we obtain

$$G(\mathbf{R}_i, \mathbf{R}_f; \beta) = \int \mathcal{D}(\mathbf{R}) \exp(-S), \quad (10a)$$

where the Euclidean action S is given by

$$S = \int_0^\beta [-i\dot{X}Y + V_{\text{eff}}(X, Y)] d\tau \quad (10b)$$

with

$$V_{\text{eff}}(X, Y) = \langle \mathbf{R} | V(x, y) | \mathbf{R} \rangle. \quad (11)$$

The trace of $G(\mathbf{R}, \mathbf{R}; \beta)$ over all \mathbf{R} is the partition function. The path integral defined in Eq. (10) is not a mathematically well-defined object, due to the fact that discontinuous paths have finite action, and hence dominate the path integral, which reflects the overcomplete-

ness of the basis we are using.

Notice that nowhere do we have to assume that \mathbf{R} is real. In fact, Eq. (7) with complex \mathbf{R} also satisfies the Schrödinger equation (although it is unnormalizable) and the subsequent equations follow as well.

Now we come to the definitions of V_{eff} in Eqs. (11) and (6). For nonzero l , these definitions are inequivalent, whereas they coincide for $l \rightarrow 0$. A few examples are

$$\begin{aligned} \langle \mathbf{R} | x | \mathbf{R} \rangle &= X, \\ \langle \mathbf{R} | x^2 | \mathbf{R} \rangle &= X^2 + 1, \\ \langle \mathbf{R} | x^3 | \mathbf{R} \rangle &= X^3 + 3X, \\ \langle \mathbf{R} | x^4 | \mathbf{R} \rangle &= X^4 + 6X^2 + 3, \end{aligned} \quad (12)$$

where we recall that x and X are measured in units of l . This shows that the choice of $V_{\text{eff}}(x, y)$ in the definition of the path integral is uniquely defined only to zeroth order in l . A unique choice of V_{eff} is determined only when the path integral is defined as the limit of well-defined quantities, and the proper choice depends on how the limit is taken.

It is interesting that a path-integral representation (PIR) with $V_{\text{eff}}(X, Y) = V(X, Y)$ can also be obtained within the coherent state scheme. This is done as follows:⁷ We know that in the LLL

$$1 = \int \frac{d^2\mathbf{R}}{2\pi} |\mathbf{R}\rangle \langle \mathbf{R}|,$$

using which we define

$$e^{-\epsilon V} \equiv \int \frac{d^2\mathbf{R}}{2\pi} e^{-\epsilon V(\mathbf{R})} |\mathbf{R}\rangle \langle \mathbf{R}|, \quad (13)$$

where $\epsilon = \beta/N$ is very small. It is easy to see that to order ϵ , $V'(\mathbf{R}) = V(\mathbf{R})$ because

$$\langle \mathbf{R} | V | \mathbf{R} \rangle \equiv \int d^2r V(x, y) |\langle \mathbf{r} | \mathbf{R} \rangle|^2$$

implies

$$\langle \mathbf{R} | V | \mathbf{R} \rangle = \int \frac{d^2\mathbf{R}'}{2\pi} V(\mathbf{R}') |\langle \mathbf{R}' | \mathbf{R} \rangle|^2.$$

By multiplying Eq. (13) N times we obtain $e^{-\beta V}$ and the path integral thus derived is given by Eq. (10) with

$$V_{\text{eff}}(X, Y) = V(X, Y). \quad (14)$$

Thus we see that even within the coherent-state PIR there is no unique choice for $V_{\text{eff}}(X, Y)$ although the $\lim_{l \rightarrow 0} V_{\text{eff}}(X, Y)$ is unambiguously defined.

As several authors have observed^{4,6,7} this ambiguity in the definition of V_{eff} has to do with the ordering of operators which quantum mechanically do not commute. This ambiguity results since \mathbf{R} only specifies the location of the particle to within a magnetic length, and there is no reason *a priori* to favor any of the class of functions V_{eff} of the form $V_{\text{eff}}(R_y, R_x) = V(\mathbf{R}')$, where $|\mathbf{R}' - \mathbf{R}| \lesssim l$. Only a careful study of which function V_{eff} produces the propagator corresponding to the desired operator ordering can resolve this ambiguity. We have not yet derived a prescription for determining the correct choice in gen-

eral, but have found in all the examples we have considered to date that the "correct" results are obtained if we average the above prescriptions:

$$V_{\text{eff}}(X, Y) = \frac{1}{2} [V(\mathbf{R}) + \langle \mathbf{R} | V | \mathbf{R} \rangle] . \quad (15)$$

This ambiguity in the definition of V_{eff} is clearly one of the difficulties in the determination of the prefactor. (There are other complications that we shall come to in Sec. VIII.) We also find, surprisingly, that different choices of V_{eff} yield phases of the path integral that are different even in the limit $\hbar \rightarrow 0$.

Now we come to the classical paths $\mathbf{R}_{\text{cl}}(t)$ (also called stationary paths, or extremal paths) which are saddle points of the action functional, given by $\delta S / \delta \mathbf{R}(t)_{\mathbf{R}=\mathbf{R}_{\text{cl}}} = 0$. According to Eq. (10) these paths satisfy the equations of motion

$$\begin{aligned} i\dot{X}_{\text{cl}} &= \left. \frac{\partial V_{\text{eff}}}{\partial Y} \right|_{\text{cl}} , \\ i\dot{Y}_{\text{cl}} &= - \left. \frac{\partial V_{\text{eff}}}{\partial X} \right|_{\text{cl}} . \end{aligned} \quad (16)$$

These are nothing but the familiar (from classical electrodynamics) equations of motion (in imaginary time) of a massless particle in the presence of a magnetic field. It is immediately obvious from these equations that in general one must allow an analytic continuation of X_{cl} and Y_{cl} to complex space (unlike in analogous problems without magnetic field^{1,2}). This is not too disturbing because, as we mentioned earlier, Eq. (9) holds even for complex \mathbf{R} . A more serious drawback, however, is that there are four boundary conditions and only two first-order differential equations, which means that Eq. (16) does not in general have solutions connecting two arbitrary points in the two-dimensional space. This can be remedied by keeping $\hbar\omega_c$ finite in Eq. (5), so that there are two *second-order* differential equations, and taking the limit $\hbar\omega_c \rightarrow \infty$ only in the end. Fortunately, we shall not need to do that because we shall be interested only in paths joining two equipotential points for which Eqs. (16) do allow solutions. That the classical paths lie along equipotential contours is physically obvious as the kinetic energy is frozen, and can also be easily seen from Eqs. (16), which lead to

$$\dot{V}_{\text{eff}}(X_{\text{cl}}, Y_{\text{cl}}) = 0 . \quad (17)$$

If we define $V_{\text{eff}}(X_i, Y_i) = V_{\text{eff}}(X_f, Y_f) = 0$, then according to Eq. (17)

$$V_{\text{eff}}(X_{\text{cl}}, Y_{\text{cl}}) = 0 . \quad (18)$$

This equation greatly simplifies the calculations. From Eq. (10), the contribution of a classical path to the action is then

$$S_{\text{cl}} = -i \int_i^f Y_{\text{cl}} dX_{\text{cl}} , \quad (19)$$

which can be trivially evaluated by solving Eq. (18) for Y_{cl} . Thus one does not need to actually solve Eqs. (16) to get the classical action.

S_{cl} is in general complex. The imaginary part of S_{cl} is the Aharonov-Bohm phase for the tunneling path. Note that there may also be a phase coming from the prefactor, or, in other words, from the fluctuations around the classical path. When there is more than one path, the total amplitude is obtained by summing the contributions of all different paths. Different phases from the paths produce interference effects, as we shall see later.

IV. ASYMMETRIC SINGLE WELL

The harmonic oscillator is the mandatory first example in any path-integral study. In this section we consider an electron in the asymmetric harmonic well potential:

$$V = V_0(x^2 + Ky^2) . \quad (20)$$

A. Numerical solution

Expressing V in terms of z and z^* ,

$$V = \frac{V_0}{4} [(z^2 + z^{2*})(1-K) + 2zz^*(1+K)] ,$$

and then projecting it onto the LLL, we get

$$V_p = \frac{V_0}{4} \left[\left(z^2 + 4 \frac{\partial^2}{\partial z^2} \right) (1-K) + 4 \frac{\partial}{\partial z} z (1+K) \right] . \quad (21)$$

Equation (2) yields the following difference equation for the coefficients a_n of Eq. (2b):

$$\begin{aligned} (1-K)a_{n-2} + 4(1-K)(n+2)(n+1)a_{n+2} \\ + [4(1+K)(n+1) - 4E/V_0]a_n = 0 . \end{aligned} \quad (22)$$

Even and odd n 's are decoupled. Starting from the boundary conditions $a_0=1$, $a_{-2}=0$ or from $a_1=1$, $a_{-1}=0$ one can calculate a_n for even and odd wave functions, respectively for a given E . It is then straightforward to calculate numerically the energy eigenvalues following the procedure sketched in Sec. II. We typically determine the eigenvalues to four or five significant figures.

B. Semiclassical treatment

The path integral is given by

$$\int \mathcal{D}X \int \mathcal{D}Y \exp \left[- \int_0^\beta d\tau [-i\dot{X}Y + V_{\text{eff}}(X, Y)] \right] , \quad (23)$$

where V_{eff} is calculated according to Eq. (15) and is given by

$$V_{\text{eff}}(X, Y) = V_0(X^2 + KY^2) + \frac{V_0}{2}(1+K) .$$

The only classical path is the trivial one, $X(\tau) = Y(\tau) = 0$, this leaves us with the fluctuation determinant, which is also given by Eq. (23) [but, of course, with different boundary conditions: $X(0) = X(\beta) = Y(0) = Y(\beta) = 0$]. We evaluate it in the following manner. First, write Eq. (23) as

$$\exp\left[-\beta\frac{V_0}{2}(1+K)\right] \int \cdots \left[\prod_i \mathcal{D}X_i \mathcal{D}Y_i\right] \\ \times \exp\left[-\epsilon \sum_i [-iX_i Y_i + V_0(X_i^2 + KY_i^2)]\right]$$

and do the Y_i integral to obtain

$$\exp\left[-\beta\frac{V_0}{2}(1+K)\right] \int \mathcal{D}X \\ \times \exp\left[-\int_0^\beta \left(\frac{\dot{X}^2}{4V_0K} + V_0X^2\right)\right].$$

Now the integral corresponds to the fluctuation determinant of a one-dimensional harmonic oscillator of mass $1/(2V_0K)$ and frequency $2V_0\sqrt{K}$. So the integral in the above equation is equal to the partition function $\sum_m \exp[-\beta(m + \frac{1}{2})2V_0\sqrt{K}]$ of a one-dimensional harmonic oscillator. Thus the total energy spectrum is

$$E_m = \frac{V_0}{2}(1 + \sqrt{K})^2 + m2V_0\sqrt{K}, \\ m=0,1,2,\dots \quad (24)$$

This is in exact agreement with our numerical calculations. We speculate that it is, in fact, exact.

This gives the first indication of why we made the specific choice of $V_{\text{eff}}(X, Y)$ given by Eq. (15); any other choice would give a wrong value for the ground-state energy E_0 , even though the spacing between levels would be correctly predicted by any reasonable choice of V_{eff} .

It is worth pointing out that for a symmetric well ($K=1$) the eigenenergies are given by

$$E_m^{\text{symm}} = (m+1)2V_0,$$

which can also be seen from the fact that they satisfy the eigenvalue equation

$$V_p^{\text{symm}} z^m = E_m^{\text{symm}} z^m,$$

with

$$V_p^{\text{symm}} = 2V_0 \frac{\partial}{\partial z} z.$$

V. SYMMETRIC DOUBLE WELL

We choose the model potential

$$V = V_0(x^2 + y^2 - r_0^2)^2 + \frac{1}{2}Ky^2. \quad (25)$$

Without the term $\frac{1}{2}Ky^2$ this potential would be circularly symmetric, but for nonzero K it has two minima at $(\pm r_0, 0)$. For $K=0$ there is a hill at the origin and the electron has two paths along the circle $x^2 + y^2 = r_0^2$ (one clockwise, one counterclockwise) that it takes from one minimum to the other. As K is increased, the hill at the origin becomes less and less prominent, and finally for $K > 4V_0r_0^2$ there is not a hill but a saddle point at the origin. Thus for small values of K , we expect to have two

classical paths going around the hill, whereas for large values of K we expect only a single path going through the origin. (This statement will be made precise later.) The potential near either well is that of an asymmetric single well studied in the previous section.

A. Numerical solution

For $K=0$ the potential is circularly symmetric, and the eigenvalue problem

$$V_0 \left[4 \frac{\partial^2}{\partial z^2} z^2 - 4r_0^2 \frac{\partial}{\partial z} z + r_0^4 \right] f_m = E_m f_m$$

can be easily solved with the result

$$f_m = z^m, \\ E_m = V_0[4(m+2)(m+1) - 4r_0^2(m+1) + r_0^4]. \quad (26)$$

For $K \neq 0$, however, an analytic solution is not possible and one must get the eigenvalues numerically. The projected potential is now

$$V_0 \left[4 \frac{\partial^2}{\partial z^2} z^2 - 4r_0^2 \frac{\partial}{\partial z} z + r_0^4 \right] - \frac{K}{8} \left[z^2 + 4 \frac{\partial^2}{\partial z^2} - 4 \frac{\partial}{\partial z} z \right],$$

which leads to the eigenvalue equation

$$a_n \left\{ V_0[4(n+2)(n+1) - 4(n+1)r_0^2 + r_0^4] - E \right. \\ \left. + \frac{K}{2}(n+1) \right\} - \frac{K}{8}[a_{n-2} + a_{n+2}4(n+2)(n+1)] = 0. \quad (27)$$

Even and odd n 's are decoupled; starting with boundary conditions $a_0=1, a_{-2}=0$ one gets the even wave functions, and with $a_1=1, a_{-1}=0$ one gets the odd eigenfunctions.

As promised earlier, we now discuss in detail how we extract the energy eigenvalues from the difference equation (27). Let us first consider the asymptotic behavior of (27) and obtain the condition for which the wave function is normalizable. For very large n the difference equation (27) reduces to

$$4(n+2)(n+1)a_n = \frac{K}{8V_0}[4(n+2)(n+1)a_{n+2} + a_{n-2}]. \quad (28)$$

On the right-hand side either a_{n+2} or a_{n-2} may dominate. To be specific we shall consider even n .

Case 1. If a_{n+2} dominates then

$$a_n = \frac{K}{8V_0} a_{n+2},$$

whose solution is (for $n=2m$)

$$a_{2m}^{\text{g}} = \left[\frac{8V_0}{K} \right]^m a_0. \quad (29)$$

For these coefficients the series in Eq. (3) is clearly divergent and the wave function is not normalizable.

Case 2. If a_{n-2} dominates then we have

$$(n+2)(n+1)a_n = \frac{K}{32V_0} a_{n-2},$$

with the solution

$$a_{2m}^2 = 2a_0 \left[\frac{K}{32V_0} \right]^m \frac{1}{(2m+2)!}, \quad (30)$$

for which the wave function is normalizable. Thus the energy eigenvalues are those values of E for which the asymptotic form of the coefficients is given by Eq. (30).

A general asymptotic solution can be written as a combination of the growing and shrinking solutions of (29) and (30):

$$a_{2m} = A(E) \left[\frac{K}{32V_0} \right]^m \frac{1}{(2m+2)!} + B(E) \left[\frac{8V_0}{K} \right]^m \quad (31)$$

and the eigenvalue is obtained when $B(E)=0$. For large m , the first term on the right-hand side is very small, so that the eigenvalue condition becomes $\lim_{m \rightarrow \infty} a_{2m} = 0$. Thus the recipe to obtain the eigenvalues is simple: change E gradually in Eq. (27) and calculate numerically a_n with sufficiently large n . An eigenvalue is obtained whenever a_n changes sign.

We shall mainly be interested in the splitting of the lowest energy levels due to tunneling. This is given by the difference of the lowest eigenvalues of the even and odd wave functions which are even and odd combinations of the wave functions in the individual potential well. For large r_0^2 , the tunnel splitting is very small and to get reasonably accurate information about it we often need to calculate the eigenvalues correct up to twenty or more significant figures. Also, in order to make sure that we are in the tunneling regime, we consider only ground-state energies that lie below the smallest potential barrier along the y axis, i.e., below $V_0 r_0^4$ (when there is a saddle point at the origin) or $\frac{1}{2}K(r_0^2 - K/8V_0)$ (when there is a hill at the origin).

B. Classical action

The tunnel splitting can be obtained from the partition function, which is the trace of

$$G(\mathbf{R}, \mathbf{R}; \beta) = \langle \mathbf{R} | e^{-\beta H} | \mathbf{R} \rangle$$

over all \mathbf{R} . The classical paths are (i) the trivial path, in which the electron stays at the bottom of one well, and (ii) the instanton paths, in which it goes to the bottom of the other well and comes back an arbitrary number of times. It is clear that one must consider the paths in (ii) in order to get the splitting of the energy levels; keeping only the trivial path would reproduce the results of the previous section. We refer the reader to literature where the contributions from an arbitrary number of instantons^{2,3} at arbitrary times have been summed up in the dilute instanton gas approximation to derive the splitting of the ground-state energy. We only want to mention here that this has to be done in a careful manner because of the appearance of zero mode due to time translation in-

variance. The final result states that the tunnel splitting Δ is proportional to the one instanton contribution, which is also called the "barrier penetration factor":

$$\Delta \approx V_0 \sum M e^{i\gamma} \exp(-S_{cl}), \quad (32)$$

with

$$S_{cl} = -i \int_{\text{one well}}^{\text{other well}} Y_{cl} dX_{cl}. \quad (33)$$

The sum in (32) represents the sum over all the classical paths. $M e^{i\gamma}$ is the prefactor associated with the classical path and is proportional to $D'[\mathbf{R}_{cl}]/D^0$ where D' refers to the fluctuation determinant of $\langle \text{other well} | e^{-\beta H} | \text{one well} \rangle$ without the contribution of the zero mode, and D^0 is the fluctuation determinant of the trivial path. We have defined M to be real and positive and γ is the phase associated with the prefactor. Validity of the semiclassical approach would demand that the rapid variations be described by $\exp(-S_{cl})$ and the prefactor M be a slowly varying function of the different parameters.

The V_{eff} corresponding to the potential in (25) that appears in the definition of the path integral is given by (ignoring the constant terms)

$$V_{\text{eff}} = V_1 [(X^2 + Y^2 - 1)^2 + 4\lambda Y^2], \quad (34)$$

where

$$\begin{aligned} (r'_0)^2 &= r_0^2 - 2, \\ V_1 &= V_0 (r'_0)^4, \\ \lambda &= K/8V_0 (r'_0)^2, \end{aligned} \quad (35)$$

and X, Y are expressed in units of r'_0 . Notice that $(r'_0)^2 = r_0^2 - 2$ arises due to the prescription in Eq. (15); Eq. (14) or (11) would have given $(r'_0)^2 = r_0^2$ or $(r'_0)^2 = r_0^2 - 4$, respectively, leaving the rest of the V_{eff} unchanged except for the constant terms.

The classical action is given by

$$S_{cl} = -i(r'_0)^2 \int_{-1}^1 Y_{cl} dX_{cl}, \quad (36)$$

$$Y_{cl} = i[\sqrt{\lambda} - (X_{cl}^2 + \lambda - 1)^{1/2}]. \quad (37)$$

One can learn something about the nature of the classical paths without solving Eqs. (16). From Eqs. (37) and (16) it is clear that if $(X_{cl}(\tau), Y_{cl}(\tau))$ is a classical path, so is $(X_{cl}^*(\tau), -Y_{cl}^*(\tau))$. For $\lambda > 1$, $(X_{cl}^2 + \lambda - 1)^{1/2}$ is always real for real X_{cl} and therefore the classical path is such that X_{cl} is purely real and Y_{cl} is purely imaginary throughout the path. Therefore there is only one path. On the other hand, for $\lambda < 1$, both $X_{cl}(\tau)$ and $Y_{cl}(\tau)$ are in general complex giving rise to two distinct paths in the complex space related by $(X_{cl}^{(1)}, Y_{cl}^{(1)}) \rightleftharpoons (X_{cl}^{(2)*}, -Y_{cl}^{(2)*})$. Also, from Eq. (36) it can be seen that the classical actions for these paths are complex conjugates of each other.

For $\lambda > 1$ the integral in Eq. (36) can be easily performed with the result

$$S_{cl} = (r'_0)^2 \left[\sqrt{\lambda} - (\lambda - 1) \ln \left[\frac{1 + \sqrt{\lambda}}{\sqrt{\lambda - 1}} \right] \right],$$

which can be analytically continued to $\lambda < 1$ to give

$$S_{cl} = (r'_0)^2 \left[\sqrt{\lambda} - (\lambda - 1) \ln \left[\frac{1 + \sqrt{\lambda}}{\sqrt{|\lambda - 1|}} \right] \right. \\ \left. \pm \Theta(1 - \lambda) i \frac{\pi}{2} (1 - \lambda) \right]. \quad (38)$$

Here one can explicitly see that the actions of the two classical paths for $\lambda < 1$ are complex conjugate of each other. For $\lambda < 1$, we have also done the integral (36) numerically by numerically solving the equations of motion for the classical paths, and confirmed the validity of the analytic continuation to values of λ below 1.

Thus we obtain an analytical expression for the classical action. Fluctuations about this path determine the value of the prefactor M in Eq. (32). Although we do not calculate M , we are able to say something about it using physical arguments. At $\lambda = 1$ all the three paths are classically available to the electron and the fluctuations will be large. For λ close to unity, the electron is, in a manner of speaking, not absolutely sure which path to choose, making fluctuations important. But for λ sufficiently far from unity the fluctuations about the classical path(s) should not be important and M ought to be a slowly varying function of $(r'_0)^2$, which here plays the role analogous to $1/\hbar$ of usual path integrals. Also, the method of steepest descent is valid only for large values of $(r'_0)^2$.

For $\lambda > 1$, the tunnel splitting is given by

$$\Delta = M_1 e^{-S_{cl}}, \quad (39a)$$

where the phase of the prefactor must be $n\pi$ because S_{cl} is real. For $\lambda < 1$ we must sum the contributions from the two different paths:

$$\Delta = M_2 e^{i\gamma} e^{-S_{cl}} + M_2 e^{-i\gamma} e^{-S_{cl}^*} \\ = 2M_2 \cos(\gamma - \text{Im}S_{cl}) \exp(-\text{Re}S_{cl}) \\ = 2M_2 \cos \left[\gamma - (r'_0)^2 \frac{\pi}{2} (1 - \lambda) \right] \exp(-\text{Re}S_{cl}). \quad (39b)$$

Here we have used the fact that the prefactors from the two classical paths must be complex conjugates of each other so as to produce a real Δ . As argued earlier, M_1 and M_2 are expected to be slowly varying functions of $(r'_0)^2$ and λ for λ sufficiently far from unity.

Thus, for fixed λ , the exponential behavior of Δ is given by $\exp(-r_0^2 \times \text{constant})$. The oscillatory behavior is predicted to have the property that if Δ is zero for some particular value of r_0^2 , then the next zero will occur at $r_0^2 + 2/(1 - \lambda)$. We have not obtained a general analytic expression for the prefactors (see Sec. VII) and we must extract the information about γ from a comparison between Eq. (39) and the numerical results. The value of γ (modulus 2π) can be determined by determining the zeros of Δ from the exact numerical calculations. In

Table I we tabulate for some values of λ (less than unity) and r_0^2 for which $\Delta = 0$. These have an uncertainty of ± 1 in their last digit. Clearly, the spacing between successive values of r_0^2 is *exactly* $2/(1 - \lambda)$ as predicted by the semiclassical theory. Moreover, the phase γ coming from the prefactor is independent of λ and is $\pi/2$. Thus, the total phase factor of a loop (in which the electron goes from one well to another by one path and comes back by the other) is -1 . This result apparently depends only on the geometry but not on the specific parameters (r_0 , λ , etc.) of the system. We conjecture that to any general closed path is associated a geometrical phase $\pm\pi$. In the next section we shall test this for a quadrupole well.

The value of γ is independent of whether we use Eq. (11), (14), or (15) to define V_{eff} , which can be verified from numerical calculations.

Given that γ is a geometrical factor, a heuristic calculation of its value can be performed by considering the problem with $\lambda = 0$ (when there is no tunneling). The exact eigenenergies can be obtained analytically from Eq. (27) with $K = 0$:

$$E_n = [4(n + 2)(n + 1) - 4(n + 1)r_0^2 + r_0^4] V_0,$$

and degeneracies occur ($\Delta = 0$) when $E_n = E_{n+1}$. This occurs whenever $r_0^2 = 2m$, $m = 2, 3, \dots$, which is consistent with the semiclassical expression in Eq. (39b) with $\lambda = 0$ ($K = 0$) provided $\gamma = \pi/2$. Thus, to the extent that γ is truly independent of parameters, it can be computed by comparison with an exactly soluble case.

Finally we consider the exponential behavior of the amplitude. For certain values of λ greater than unity we plot the prefactor $\Delta e^{+S_{cl}}$ in Fig. 1 as a function of r_0^2 , where Δ is the numerical value of the tunnel splitting. We find that it is a very slowly varying function of r_0^2 . In Fig. 1 we also plot $\Delta e^{\text{Re}S_{cl}} / \sin(\text{Im}S_{cl})$ for certain values of λ less than unity and again come to the same conclusion. We also see that, as expected, the variation in these quantities is less when λ is farther away from 1. In Figs. 2 and 3 we plot the same quantities as a function of λ for some large values of r_0^2 . Again, there is a rapid variation at λ close to unity. The \times 's in Figs. 1 and 2 show the values of r_0^2 or λ for which Δ vanishes; these oscillations are exactly described by the term $\sin(\text{Im}S_{cl})$ in Eq. (39b). Also, in Fig. 1 the tunnel splitting changes typically by 16 orders of magnitude over the range of r_0^2 shown, while the prefactor changes by merely a factor of 2. Thus we see that the semiclassical path-integral method accu-

TABLE I. The values of r_0^2 are given for the double-well potential for which the tunnel splitting is found to be zero by numerical methods. The difference between two successive values of r_0^2 agrees with the semiclassical prediction of $2/(1 - \lambda)$. The geometrical phase γ is found to be $\pi/2$ for all λ using Eq. (39b).

λ	r_0^2 for which $\Delta = 0$	$\frac{2}{1 - \lambda}$	γ
0.01	6.040, 8.060, 10.808, ...	2.020	$\pi/2$
0.1	6.444, 8.666, 10.888, ...	2.222	$\pi/2$
0.2	7.000, 9.5000, 12.000, ...	2.500	$\pi/2$
0.4	8.666, 11.999, 15.332, ...	3.333	$\pi/2$

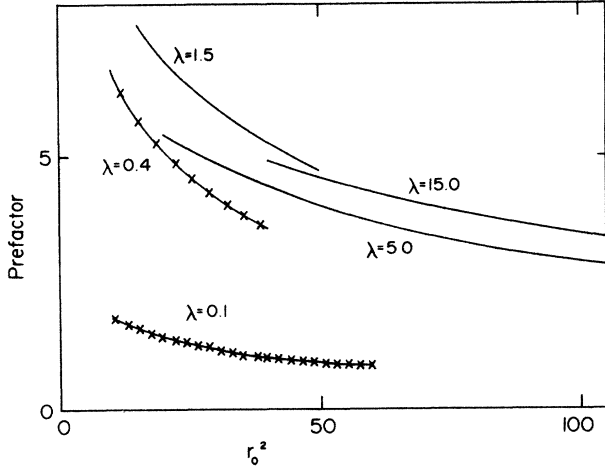


FIG. 1. The prefactor [defined as $\Delta \exp(S_{cl})$ for $\lambda > 1$ and $\Delta \exp(\text{Re}S_{cl})/\sin(\text{Im}S_{cl})$ for $\lambda < 1$] plotted as a function of r_0^2 . For $\lambda < 1$, the \times 's show the values of r_0^2 for which the tunnel splitting Δ [or $\sin(\text{Im}S_{cl})$] is zero.

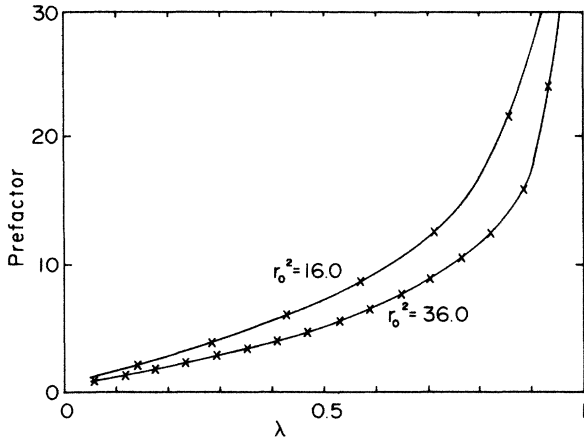


FIG. 2. The prefactor $\Delta \exp(\text{Re}S_{cl})/\sin(\text{Im}S_{cl})$ plotted as a function of λ for two different values of r_0^2 . The \times 's show the values of λ for which the tunnel splitting Δ is zero.

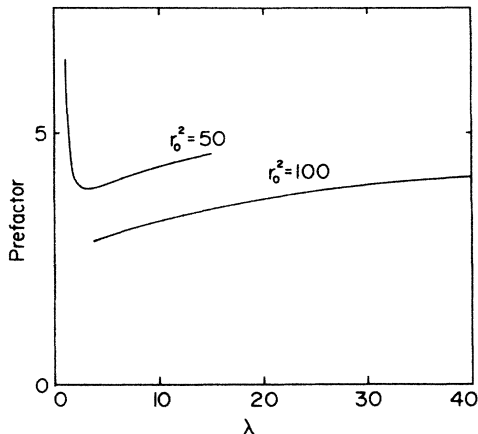


FIG. 3. The prefactor, $\Delta \exp(S_{cl})$, plotted as a function of λ . We cannot go to very small values of λ because the tunnel splitting Δ becomes smaller than the numerical accuracy we can obtain.

rately predicts the exponential and the oscillatory behaviors of the tunnel splitting for the symmetric double-well problem under consideration.

The tunnel splitting decreases as r_0^2 is increased, and increases as λ is increased. Thus in Fig. 1 there is only a limited range of r_0^2 at fixed λ that we can study, because for very small r_0^2 the ground-state energy goes above the potential barrier and is not in the tunneling regime, while for very large r_0^2 the tunnel splitting is too small ($\Delta \lesssim 10^{-18} V_1$) to allow an accurate numerical determination. An analogous situation is true for Figs. 2 and 3.

VI. THE PHASE

Now that we believe the oscillatory behavior predicted by the semiclassical approach, we are in a position to define the Aharonov-Bohm phase of a tunneling path. From Eq. (32), the imaginary part of the classical action is

$$\text{Im}S_{cl} = - \int (Y_1 dX_1 - Y_2 dX_2),$$

where (X_1, Y_1) and (X_2, Y_2) are the real and imaginary parts of \mathbf{R}_{cl} . This implies that for a closed loop the Aharonov-Bohm phase is given by

$$\phi_{AB} = 2\pi \frac{A_{eff} B}{\phi_0}, \quad (40)$$

where the effective area (A_{eff}) is the projected area of the complex loop on the real plane minus its projected area on the imaginary plane. For a path lying completely in the real space this coincides with the usual definition. Thus in order to compute the Aharonov-Bohm phase associated with a closed tunneling path one needs to determine the classical paths of the particle in complex space.

Notice that $\text{Im}S_{cl}$ is nothing but the Berry's⁸ "phase" of a particle in the coherent state (7) taken adiabatically around the classical path. It is not real because of the overcompleteness of the basis. As a matter of fact, for tunneling problems in high magnetic fields it necessarily has an imaginary part because the classical path must foray into complex space in order to find equipotential contours.

As we have mentioned before, besides the Aharonov-Bohm phase, which arises from the classical path, there is another phase contribution which comes from fluctuations around the classical path. The Aharonov-Bohm phase is dependent on the parameters that control the shape of the potential, but the phase of the fluctuation prefactor is independent of these parameters, and hence we call it the geometrical phase. Moreover, in the double-well problem we find that it contributes a phase factor -1 for a closed loop. We postulate this to be generally true for any closed tunneling path, and test it for the quadrupole-well potential in the following section. Incidentally, we point out that the knowledge of phase also settles the problem of which of the even and odd parity states has the lower energy. The tunnel splitting in Eqs. (39) is defined as $\Delta = E_{odd} - E_{even}$, and it is clear that Δ is positive for $\lambda > 1$, whereas for $\lambda < 1$ the sign of Δ is

the same as the sign of $\sin(\text{Im}S_{\text{cl}})$. Thus as long as there is only one classical path connecting the two wells, the usual rule ($E_{\text{odd}} > E_{\text{even}}$) holds. On the other hand, with multiple classical paths, the interference between different paths complicates the issue, but the correct answer can still be found using semiclassical methods.

VII. QUADRUPLE WELL

In the last section we found in the two-well problem that when there are two classical paths going from the bottom of one well to the other, the electron suffers in addition to the Aharonov-Bohm phase another phase change of $\pm\pi$ in going around the loop. This led us to speculate that to every closed tunneling path is associated a universal phase factor -1 in addition to the phase factor arising from the Aharonov-Bohm effect. To test the validity of this conjecture, we now consider a quadruple-well potential with four minima around a ring. This potential allows closed paths in which the electron goes around the ring. The potential we choose is

$$V = V_0(x^2 + y^2 - r_0^2) + \frac{K_1}{4}(x^2 - y^2)^2. \quad (41)$$

This has four minima at

$$(x, y) = (\pm r_0/\sqrt{2}, \pm r_0/\sqrt{2})$$

and maxima at

$$(0, 0), \quad \left[0, \pm r_0 \left[\frac{4V_0}{K_1 + 4V_0} \right]^{1/2} \right],$$

and

$$\left[\pm r_0 \left[\frac{4V_0}{K_1 + 4V_0} \right]^{1/2}, 0 \right].$$

At the minima this potential is zero, at the origin $V_0 r_0^4$, and at other maxima $V_0 K_1 r_0^4 / (4V_0 + K_1)$. In order to make sure that one is in the tunneling regime one must only consider energy levels below $V_0 K_1 r_0^4 / (4V_0 + K_1)$.

The eigenvalue equation is given by the following difference equations:

$$a_n \{ V_0 [4(n+2)(n+1) - 4r_0^2(n+1) + r_0^4] + \frac{1}{2} K_1 (n+2)(n+1) - E \} \\ + \frac{K_1}{16} [16a_{n+4}(n+4)(n+3)(n+2)(n+1) + a_{n-4}] = 0. \quad (42)$$

This equation couples every fourth coefficient leading to four wave functions with different symmetry under rotation, given by

$$\sum_{n=0}^{\infty} a_{4n+p} z^{4n+p} e^{-|z|^2/4}, \quad p = 1, 2, 3, 4, \quad (43)$$

which can be obtained starting from four different boundary conditions. The energy eigenvalues are obtained as in the double well, i.e., when $a_{n \rightarrow \infty}$ changes sign as a function of E . The four lowest eigenenergies correspond to four nonequivalent combinations of the wave functions in the separate wells. In particular, the wave function with $p=0$ in Eq. (43) corresponds to a symmetric combination, because z^4 is invariant under a rotation of the axes by 90° , i.e., under the transformation $x, y \rightarrow y, -x$.

Now we come to the semiclassical treatment. We evaluate $V_{\text{eff}}(X, Y)$ according to Eq. (15):

$$V_{\text{eff}}(X, Y) = V_1 \left[(X^2 + Y^2 - 1)^2 + \frac{K}{4}(X^2 - Y^2)^2 \right], \quad (44)$$

where

$$V_1 = V_0(r'_0)^4, \quad K = K_1/V_0, \quad (r'_0)^2 = r_0^2 - 2 - \frac{K}{4}, \quad (45)$$

and X and Y are measured in units of r'_0 . The minima are now at $(X, Y) = (\pm 1/\sqrt{2}, \pm 1/\sqrt{2})$, and the energy levels below $K_1(r'_0)^4/(K+4)$ are in the tunneling regime.

The tunneling can occur along the sides [e.g., from

$(-1/\sqrt{2}, 1/\sqrt{2})$ to $(1/\sqrt{2}, 1/\sqrt{2})$] or along the diagonal [e.g., from $(-1/\sqrt{2}, 1/\sqrt{2})$ to $(+1/\sqrt{2}, -1/\sqrt{2})$]. If r_0 is very large then only the tunneling along the sides will be important because the tunneling matrix elements decay exponentially with the square of the distance. For the sake of simplicity, we shall only consider large r_0 (which is anyway a requirement for the validity of the semiclassical approach) and neglect completely the exponentially small contribution of the tunneling through the origin.

The classical action for tunneling along the sides is given by

$$S_{\text{cl}} = -i(r'_0)^2 \int_{-1/\sqrt{2}}^{1/\sqrt{2}} Y_{\text{cl}} dX_{\text{cl}}, \quad (46)$$

where

$$Y_{\text{cl}} = \left[\frac{1 - [1 - (i/2)\sqrt{K}] X_{\text{cl}}^2}{1 + (i/2)\sqrt{K}} \right]^{1/2}. \quad (47)$$

The integral can be performed without difficulty (although one must be careful about the branch cut) and yields

$$S_{\text{cl}} = \frac{(r'_0)^2}{\sqrt{K+4}} \ln \left[\frac{i\sqrt{K+4} - 2 + i\sqrt{K}}{i\sqrt{K+4} + 2 - i\sqrt{K}} \right] \\ = \frac{(r'_0)^2}{\sqrt{K+4}} \ln \left[\frac{4\sqrt{K+4}}{4 + (\sqrt{K+4} - \sqrt{K})^2} \right] + i\frac{\pi}{2} \frac{(r'_0)^2}{\sqrt{K+4}}. \quad (48)$$

Thus we see that the semiclassical path-integral method again provides an analytical solution for the classical action.

Again we sum over instantons in the dilute gas approximation. The result is a spectrum for the tunnel splitting which can be obtained from a tight binding model with the Hamiltonian

$$H = \sum_n (TC_n^\dagger C_{n+1} + T^* C_{n+1}^\dagger C_n), \quad (49)$$

where the site index $n = 1, 2, 3, 4$ ($n = 5$ is identified with $n = 1$). C^\dagger and C are the creation and destruction operators, respectively, and T is the tunneling matrix element. We have defined the zero of energy such that in the absence of tunneling the ground-state energy is zero. The Hamiltonian can be diagonalized by Fourier transform:

$$H = \sum_k \frac{1}{4} (Te^{ik} + T^* e^{-ik}) C_k^\dagger C_k, \quad (50)$$

where

$$C_n = \frac{1}{2} \sum_k e^{ikn} C_k; \quad k = 0, \pm \frac{\pi}{2}, \pi.$$

The energy eigenvalues are

$$E_k = \frac{1}{2} \text{Re}(Te^{ik}). \quad (51)$$

The tunneling matrix element is written as

$$T = 2T_0 e^{i\gamma} e^{-S_{cl}}, \quad (52)$$

where γ is the phase coming from the fluctuation prefactor and T_0 is real and positive. Then

$$E_k = T_0 e^{-\text{Re}S_{cl}} \cos(\gamma + k - \text{Im}S_{cl}).$$

From Eq. (50) it is clear that $k = 0$ corresponds to a completely symmetric combination of the wave functions of the individual wells, with energy eigenvalue

$$E_{\text{symm}} = T_0 e^{-\text{Re}S_{cl}} \cos(\gamma - \text{Im}S_{cl}). \quad (53)$$

The other eigenvalues are

$$\begin{aligned} & -T_0 e^{-\text{Re}S_{cl}} \cos(\gamma - \text{Im}S_{cl}), \\ & \pm T_0 e^{-\text{Re}S_{cl}} \sin(\gamma - \text{Im}S_{cl}). \end{aligned} \quad (54)$$

These imply the following properties for the energy eigenvalues for large r_0 . (i) The eigenvalues occur in doublets; i.e., if they are measured from their average, then they occur in pairs with energies equal in magnitude but opposite in sign. (ii) Since

$$\text{Im}S_{cl} = \frac{\pi}{2} \frac{(r'_0)^2}{\sqrt{K+4}},$$

if one specific wave function (say, the symmetric one) has zero eigenvalue at some r_0^2 then the next zero will be at $r_0^2 + 2\sqrt{K+4}$. Thus the separation between two successive zeros is $2\sqrt{K+4}$. (iii) The magnitude of the energy splitting is governed by the factor $\exp(-\text{Re}S_{cl})$.

We checked these predictions by numerical determination of the eigenvalues. In Table II we give the four ground-state energies for three different values of r_0^2 for $K = 2.25$. It is clear that for each r_0^2 , there are two pairs of energies with opposite sign. The two energies of a doublet are not exactly equal in magnitude, which is due to the fact that the prediction of their equality involves the assumption of the neglect of any diagonal tunneling. This approximation becomes more and more accurate as r_0^2 increases and, indeed, in Table II, we find that for larger r_0^2 , the energies of the doublets are much closer in magnitude. (This serves as a measure of how good the approximation of ignoring the diagonal tunneling is for a given r_0^2 .) Let us now look for r_0^2 for which $E_{\text{symm}} = 0$. These are: 10.984, 16.459, 21.256, 26.330, 31.307, 36.314, 41.312, 46.313, 51.312, 56.313, These values of r_0^2 are accurate with an uncertainty of ± 1 in the last digit. Clearly for large r_0^2 , the difference between two successive values is 5.0, which is exactly equal to $2\sqrt{K+4}$ with $K = 2.25$. The same is true for any other K , as we show in Table III for a few values of K , where some of the values of r_0^2 for which $E_{\text{symm}} = 0$ are shown.

As before, we determine the value of the phase contributed by the prefactor by comparing those values of r_0^2 for which $E_{\text{symm}} = 0$ given in Table III with the semiclassical expression

$$\cos \left[\frac{\pi}{2} \frac{r_0^2}{\sqrt{K+4}} - \frac{\pi}{2} \frac{2+K/4}{\sqrt{K+4}} - \gamma \right] = 0. \quad (55)$$

This allows us to determine γ , which we also tabulate in the table. We find that it is independent of the parameters (i.e., K , r_0^2 , V_0) and is equal to $\frac{5}{4}\pi$. Thus the phase of

TABLE II. For the quadruple-well potential the four ground-state eigenvalues are given for three different values of r_0^2 .

r_0^2	E_1	E_2	E_3	E_{symm}
30	-3.10153×10^{-4}	-3.35177×10^{-4}	3.09818×10^{-4}	3.35511×10^{-4}
40	-1.75850×10^{-5}	-1.90217×10^{-5}	1.75834×10^{-5}	1.90233×10^{-5}
50	-1.00748×10^{-6}	-1.08988×10^{-6}	1.00748×10^{-6}	1.08989×10^{-6}

TABLE III. For the quadruple-well potential the values of r_0^2 are given for which E_{symm} is found to be zero by numerical methods. The difference between two successive values of r_0^2 agrees with the semiclassical prediction of $2\sqrt{K+4}$. The geometrical phase γ is found to be $5\pi/4$ for all K using Eq. (55).

K	r_0^2 , where $E_{\text{symm}}=0$	$2\sqrt{K+4}$	γ
0.2	..., 103.495, 107.593, ...	4.099	$\frac{5}{4}\pi$
1.0	..., 36.902, 41.384, 45.852, 50.326, 54.797 ...	4.472	$\frac{5}{4}\pi$
2.0	..., 40.466, 45.366, 50.265, ...	4.899	$\frac{5}{4}\pi$
2.25	..., 36.314, 41.312, 46.313, 51.312, ...	5.000	$\frac{5}{4}\pi$
5.0	..., 37.750, 43.750, 49.750, ...	6.000	$\frac{5}{4}\pi$

an electron going around the loop is 5π , which contributes a phase factor $e^{i5\pi} = -1$. (This is in addition to the Aharonov-Bohm phase.) This is in agreement with our conjecture.

We must mention that there is a certain amount of ambiguity in the phase γ , having to do with the choice of the specific form of V_{eff} given in Eq. (15). If we chose either Eq. (11) or Eq. (14) to define V_{eff} , we would get a different value of γ which would be shape (K) dependent and would not agree with our conjectured value. However, *only* the choice of V_{eff} in Eq. (15) gives a parameter-independent value of γ , which we consider an appealing additional reason to believe that Eq. (15) is the correct choice for V_{eff} .

Now we come to the exponential behavior of the tunnel splitting. We choose $K=2.25$ so that changing r_0^2 by 10.0 does not change the cosine in Eq. (53). Then we plot in Fig. 4 the prefactor $E_{\text{symm}}\exp(+S_{\text{cl}})$ as a function of r_0^2 for $r_0^2=10n$, where n is an integer. Clearly this is a very slowly varying function of r_0^2 , even though E_{symm} changes (in units of V_1) from 0.1 at $r_0^2=10$ to 10^{-17} at $r_0^2=140$.

From Eqs. (53) and (54), if we know the E_{symm} for some r_0^2 , then we can calculate the other energies. For $r_0^2=50$ this short exercise yields the values $\pm 1.007485 \times 10^{-6}$ and -1.08989×10^{-6} for the other three energies, which are again in excellent agreement with the other eigenvalues given in the table.

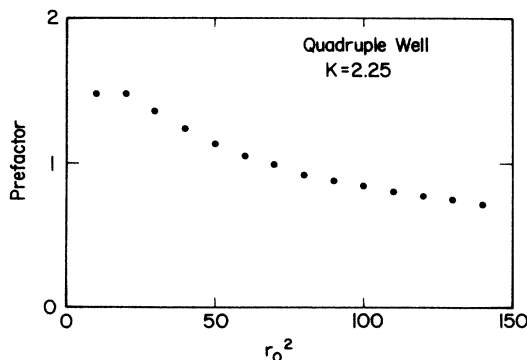


FIG. 4. The prefactor, $E_{\text{symm}}\exp(S_{\text{cl}})$, plotted as a function of r_0^2 for the quadruple-well problem.

VIII. THE PREFACTOR

Prefactor calculations are always different and in the present case they involve all the subtleties of a sum over discontinuous paths.^{2,4-6} (Recall that most paths are discontinuous due to the overcompleteness of the basis set; even the classical paths are typically discontinuous due to the overspecification of the boundary conditions for the semiclassical equations of motion.) Fortunately, the prefactor rarely has interesting dependences on the parameters (and whenever it does, they can often be deduced without actually evaluating it). Indeed, as we have discussed, this has been the case in the present model problems where the prefactors have typically varied by a factor of 2 while the tunnel splitting has varied by 17 orders of magnitude. Thus for practical applications, the magnitude of the prefactor is rarely important. However, for completeness, in this section we discuss the results of some preliminary investigations of the prefactor. To be specific we shall talk about the prefactor in the context of the double-well problem; the prefactor for the asymmetric single well has already been evaluated in Sec. IV.

The first source of difficulty in the determination of the prefactor is the ambiguity in the definition of V_{eff} . Different possible choices of V_{eff} produce different constant terms (which we did not write explicitly), which do not affect the classical paths whatsoever, but appear in the prefactor. In the double-well problem the constant terms implicit in Eq. (34) would contribute a term

$$\exp \left[-\frac{2}{(r'_0)^2} \left(1 + \lambda + \frac{2}{(r'_0)^2} \right) \right],$$

which multiplies the factor coming from the fluctuations around the classical path. Fortunately, this contribution tends to unity for very large $(r'_0)^2$. The same is true for other choices of V_{eff} . Thus for $(r'_0)^2 \rightarrow \infty$ (which is the regime in which the semiclassical approximation holds) there is no ambiguity in the prefactor arising from the ambiguity in defining V_{eff} , and it is given by

$$\int D\eta \int D\xi \exp \left\{ \int d\tau \left[-i(r'_0)^2 \dot{\eta} \xi + \frac{1}{2} \eta^2 V_{\text{eff}}^{xx} + \frac{1}{2} \xi^2 V_{\text{eff}}^{yy} + \eta \xi V_{\text{eff}}^{xy} \right] \right\}, \quad (56)$$

where η and ξ are fluctuations in X and Y from the classical path (X_{cl}, Y_{cl}) ;

$$V_{\text{eff}}^{xx} = \frac{\partial^2}{\partial x^2} V_{\text{eff}} \Big|_{(X_{cl}, Y_{cl})},$$

etc.; and we have retained only up to quadratic terms in the fluctuations.

We first consider the case of $\lambda > 1$ where Y_{cl} is purely imaginary and X_{cl} is purely real. We can then make the substitution $Y \rightarrow iY$ so that the new path integral

$$\int \mathcal{D}X \int \mathcal{D}Y \exp \left[- \int d\tau \left(\frac{1}{2} (r'_0)^2 (\dot{X}Y - \dot{Y}X) + V_{\text{eff}}(X, Y) \right) \right] \quad (57)$$

with

$$V_{\text{eff}}(X, Y) = V_1 [(X^2 - Y^2 - 1)^2 - 4\lambda Y^2]$$

gives rise to the prefactor

$$\int \mathcal{D}\eta \int \mathcal{D}\xi \exp \left[- \frac{1}{2} \int d\tau \left((r'_0)^2 (\dot{\eta}\xi - \dot{\xi}\eta) + \eta^2 V_{\text{eff}}^{xx} + \xi^2 V_{\text{eff}}^{yy} + 2\eta\xi V_{\text{eff}}^{xy} \right) \right] \quad (58)$$

with

$$\begin{aligned} V_{\text{eff}}^{xy} &= -8V_0 X_{cl} Y_{cl}, \\ V_{\text{eff}}^{xx} &= 4V_0 (3X_{cl}^2 - Y_{cl}^2 - 1), \\ V_{\text{eff}}^{yy} &= -4V_0 (X_{cl}^2 - 3Y_{cl}^2 - 1 + 2\lambda). \end{aligned} \quad (59)$$

Notice that all terms in (59) are real. The expression in the large parentheses of Eq. (58) can be written as

$$(\eta \ \xi) R \begin{pmatrix} \eta \\ \xi \end{pmatrix} \quad (60a)$$

with

$$R = \begin{pmatrix} V_{\text{eff}}^{xx} & i(r'_0)^2 \left[i \frac{d}{d\tau} \right] + V_{\text{eff}}^{xy} \\ -i(r'_0)^2 \left[i \frac{d}{d\tau} \right] + V_{\text{eff}}^{xy} & V_{\text{eff}}^{yy} \end{pmatrix}. \quad (60b)$$

Here R is a Hermitian operator. Thus, as usual,^{2,3} evaluation of the prefactor boils down to calculating the fluctuation determinant which is the product of the eigenvalues of the operator R . There is no conceptual difficulty, but we have not been able to do this analytically except in the limit $\lambda \rightarrow \infty$ which we shall come to later. However, one can explicitly show with the help of Eq. (16) that there exists a zero eigenvalue which corresponds to the eigenvector

$$\begin{pmatrix} \eta_0 \\ \xi_0 \end{pmatrix} \propto \begin{pmatrix} \dot{X}_{cl} \\ \dot{Y}_{cl} \end{pmatrix} \propto \begin{pmatrix} [\sqrt{\lambda} - (X_{cl}^2 + \lambda - 1)^{1/2}] (X_{cl}^2 + \lambda - 1)^{1/2} \\ -[\sqrt{\lambda} - (X_{cl}^2 + \lambda - 1)^{1/2}] X_{cl} \end{pmatrix}. \quad (61)$$

As usual, this is a result of the time translational invariance of the problem. So long as this is the only zero mode, it does not lead to a divergence of the prefactor (as one would naively think) because it has already been accounted for while summing up over an arbitrary number of instantons at arbitrary times, and the final formula for the tunnel splitting involves a product of all eigenvalues of R *excluding* the zero eigenvalue. Let us now consider in detail the wave function associated with the zero mode as a function of X_{cl} shown in Fig. 5. The forms are intuitively understandable: Y_{cl} starts from zero at $\tau = -\infty$ (or $X_{cl} = -1$) and ends at zero at $\tau = \infty$ ($X_{cl} = 1$), which means that the "velocity" \dot{Y}_{cl} must change sign at least once during this interval; \dot{X}_{cl} on the other hand does not need to change sign at all. As λ goes toward unity from above, the velocity \dot{X}_{cl} at the origin becomes smaller and smaller and at $\lambda = 1$ it vanishes. This happens due to the incipient appearance of a hill at the origin rather than a saddle point for $\lambda < 1$. For $\lambda = 1$ there is a second zero mode $(\eta_1, \xi_1) = (\xi_0 \text{sgn}(x_{cl}), \eta_0)$. Thus, we expect that the prefactor will diverge as $\lambda \rightarrow 1$ from above. This can be seen in Fig. 3.

When λ is less than one, X_{cl} and Y_{cl} are both in general complex and it is not straightforward to write the action in a form analogous to Eq. (60) with a Hermitian R . However, Eq. (61) still gives the zero modes for the two classical paths that go around the hill at the origin. It is physically transparent that near $\lambda = 1$, when the classical path bifurcates, large fluctuations are possible because there exist nearby paths that are almost classical. When λ is just below unity, there is a very small hill at the origin and although the paths with the least action go around it, the paths going through the hill will not have a large action either. Thus, we also expect the prefactor to diverge as $\lambda \rightarrow 1$ from below, as seen in Fig. 2.

Let us now consider the limit $\lambda \rightarrow \infty$ where an analytic solution for the prefactor can be obtained. This is made possible because in the potential V_{eff} , the X and Y dependent terms decouple for large λ :

$$V_{\text{eff}} = V_1 [(X^2 - 1)^2 + 4\lambda Y^2], \quad (62)$$

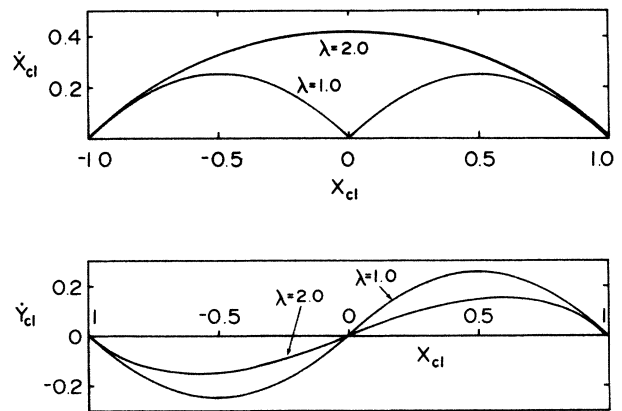


FIG. 5. The zero mode $(\dot{X}_{cl}, \dot{Y}_{cl})$ for the double-well problem for two different values of λ .

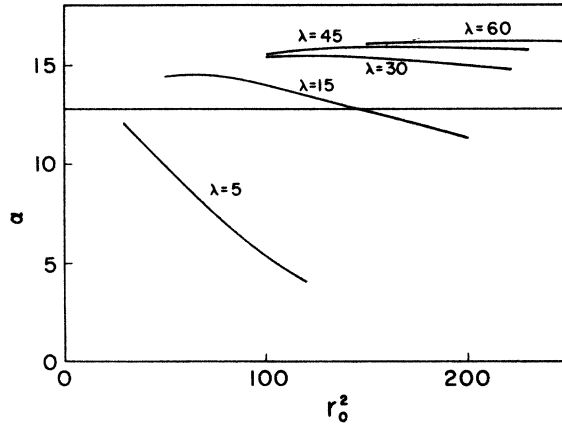


FIG. 6. Numerical curves for α [defined in Eq. (65)] plotted as a function of r_0^2 for various values of λ . The horizontal straight line is at $\alpha = 16\sqrt{2}/\pi = 12.77$, which is the theoretical value of α in the limit $\lambda, r_0^2 \rightarrow \infty$.

where X, Y are expressed, as in Eq. (34), in units of r'_0 . With this simplified potential the classical Euclidean action is given by

$$S = \int_0^\beta d\tau \left[4\lambda V_1 \left[Y - \frac{i\dot{X}(r'_0)^2}{8\lambda V_1} \right]^2 + \frac{1}{16\lambda V_1} (r'_0)^4 \dot{X}^2 + V_1 (X^2 - 1)^2 \right]. \quad (63)$$

Now as in Sec. IV, we integrate out the Y degrees of freedom to get

$$S_x = \int_0^\beta d\tau \left[\frac{1}{16\lambda V_1} (r'_0)^4 \dot{X}^2 + V_1 (X^2 - 1)^2 \right]$$

which after some rescaling becomes

$$S_x = \frac{1}{g} \int_0^{\beta g} d\tau \left[\frac{1}{2} \dot{X}^2 + \frac{1}{8} \omega^2 (X^2 - 1)^2 \right], \quad (64)$$

with

$$g = \frac{\sqrt{8\lambda V_1}}{(r'_0)^2},$$

$$\omega^2 = 8V_1.$$

Thus the problem of an electron in a two-dimensional double-well potential in the presence of extremely high magnetic field reduces to the simple problem of an electron in a one-dimensional double-well potential $V(X) = \frac{1}{8}\omega^2(X^2 - 1)^2$, whose solution is well known.^{2,3,9} The result for the tunnel splitting for Eq. (64) is

$$\Delta = 16 \left[\frac{2}{\pi} \right]^{1/2} \frac{V_1}{r'_0} \lambda^{1/4} \exp \left[- \frac{2(r'_0)^2}{3\sqrt{\lambda}} \right]. \quad (65)$$

The classical action [Eq. (38)] in the $\lambda \rightarrow \infty$ limit is $2(r'_0)^2/3\sqrt{\lambda}$, which explains the exponential term. To check the prefactor, we plot in Fig. 6 the empirical value of α , defined as

$$\alpha = \frac{\Delta r'_0}{V_1 \lambda^{1/4}} \exp \left[\frac{2}{3} \frac{(r'_0)^2}{\sqrt{\lambda}} \right], \quad (66)$$

where we obtain Δ numerically. It is clear that for large λ , α is only very weakly dependent on λ and r_0 . Moreover, its value is approximately 16 in the range of r_0 shown in the figure, which is in reasonable agreement with $16\sqrt{2}/\pi \approx 12.77$ as predicted by Eq. (65) in the limit $\lambda \rightarrow \infty$ and $r_0 \rightarrow \infty$. Unfortunately, we cannot go to larger r_0 due to numerical restrictions (i.e., very small Δ) where we expect an improved agreement as α is slowly decreasing with increasing r_0 (Fig. 6).

IX. CONCLUSION

We have studied the tunneling of an electron through a smooth potential in two dimensions in the presence of an extremely high transverse magnetic field. We have taken three different kinds of model potentials for which exact numerical solutions for the energy eigenvalues are possible. The semiclassical expression for the tunnel splitting contains a slowly varying factor (the prefactor), a rapidly varying function (the exponential), and sometimes an oscillatory factor. We do not obtain a general analytic form for the prefactor but calculate it by comparing the semiclassical expression with the numerical solution. It is in general unspectacular in its dependence on different parameters. We find that the semiclassical approach exactly describes the rapid (exponential and oscillatory) variations of the tunneling matrix elements, which establishes the validity of this approach in similar problems¹ beyond any reasonable doubt. There are two different types of phase associated with a classical path. One is analogous to the Aharonov-Bohm phase, and must be calculated by tracing out the classical path in the complex space. The second is a geometrical phase coming from the fluctuation prefactor. We empirically find that the geometrical phase factor of a closed loop is independent of the shape of the potential and is $e^{\pm i\pi} = -1$. Although we have shown this only for symmetric double and quadruple wells, we propose that it is true in general. In Ref. 1 it was necessary to assume the existence of such a phase factor in order that cooperative ring exchanges lower the ground-state energy of a collection of fermions. Our results thus lend support to this assumption.

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