Tunneling of Bound Systems at Finite Energies: Complex Paths Through Potential Barriers.

G.F. Bonini\textsuperscript{a}, A.G. Cohen\textsuperscript{b}, C. Rebbi\textsuperscript{b} and V.A. Rubakov\textsuperscript{c}

\textsuperscript{a}Institut für theoretische Physik, University of Heidelberg, D-69120 Heidelberg, Germany
\textsuperscript{b}Department of Physics, Boston University, Boston, MA 02215, USA
\textsuperscript{c}Institute for Nuclear Research of the Russian Academy of Sciences, Moscow 117312, Russia

(January 19, 1999)

We adapt the semiclassical technique, as used in the context of instanton transitions in quantum field theory, to the description of tunneling transmissions at finite energies through potential barriers by complex quantum mechanical systems. Even for systems initially in their ground state, not generally describable in semiclassical terms, the transmission probability has a semiclassical (exponential) form. The calculation of the tunneling exponent uses analytic continuation of degrees of freedom into a complex phase space as well as analytic continuation of the classical equations of motion into the complex time plane. We test this semiclassical technique by comparing its results with those of a computational investigation of the full quantum mechanical system, finding excellent agreement.

PACS: 03.65.Sq, 02.70.-c

1. Tunneling phenomena are inherent in numerous quantum systems, from atoms to condensed matter to quantum field theory. Even in systems with a small parameter—coupling constant—a quantitative description of tunneling is possible only in a limited number of cases. Perhaps the best known example is the WKB approximation familiar from one-dimensional wave mechanics; similar techniques, such as the “most probable escape path” and instanton methods, are used to study tunneling from the bottom of potential wells. In the latter cases the calculation of the tunneling probability may be reduced to the solution of classical equations of motion for real generalized coordinates in imaginary (“Euclidean”) time, supplemented by the analysis of small fluctuations about this classical Euclidean trajectory. However, these methods often fail in describing tunneling of systems with more than one degrees of freedom at finite energies.

It has been suggested recently, in the context of instanton transitions in quantum field theory, that semiclassical techniques may be used for calculating the exponential suppression factors in a class of processes where multi-dimensional systems tunnel at finite energies. The proposal involves a double analytic continuation: the degrees of freedom are continued into a complex phase space as well as analytic continuation of the classical equations of motion into the complex time plane. The tunneling exponent is determined by an appropriate solution of the classical, albeit complexified, equations of motion. Computation by numerical methods is then feasible even for systems with a large number of degrees of freedom, as has already been demonstrated in a field theoretic model. A problem with the formalism of Refs. is that its derivation from first principles is still lacking, although its plausibility has been supported by perturbative calculations about an instanton.

The purpose of this paper is two fold. First, we adapt the technique of Refs. to tunneling of quantum mechanical bound systems through high and wide potential barriers. As an example, we consider a system of two degrees of freedom with linear binding force. We find that if the bound system is initially in a highly excited state, the tunneling exponent is indeed calculable in a semiclassical way. This result is hardly surprising, as the initial state itself can be described in semiclassical terms.

We formulate the complexified classical boundary value problem relevant to the calculation of the exponent in this case.

Second, the real strength of this formalism is that it also enables one to treat barrier penetration when the bound system is initially in a low lying state, e.g. the ground state. This is far from obvious, as this initial state cannot be described semiclassically. Nevertheless, we argue that in this case the tunneling exponent can be obtained by an appropriate limiting procedure. The resulting technique is less-well justified, so we have chosen to test it by direct computation of the transmission probability in the full quantum theory. We briefly describe the numerical methods involved, and present the results of both the full quantum mechanical and semiclassical analyses. We find good agreement between the two, confirming the validity of the semiclassical approach.

2. To be specific, let us consider a quantum mechanical system of two particles of equal mass $m = 1/2$ moving in one dimension. Let these particles be bound by the harmonic potential $(\omega^2/8)(x_1 - x_2)^2$, and one of these particles be repelled from the origin by a positive semidefinite potential $V(x_1)$ that vanishes as $x_1 \to \pm\infty$ (we could of course allow $V$ to depend on $x_2$ as well, provided it couples to the internal degree of freedom). We take this...
potential to have the form $V(x_1) = g^{-2}U(gx_1)$, where $g$ is a small constant. We set $\hbar = 1$, so the classical limit corresponds to $g \to 0$. In what follows we present the results of numerical calculations for $\omega = 1/2$ and gaussian potential, $U(x) = \exp(-x^2/2)$, although the treatment of other potentials would be similar. In terms of the center-of-mass and relative coordinates, $X = (x_1 + x_2)/2$ and $y = (x_1 - x_2)/2$, the Lagrangian reads

$$L = \frac{1}{2} X^2 + \frac{1}{2} y^2 - \frac{1}{2} \omega^2 g^2 - \frac{1}{g^2} U[g(X + y)]$$

Far from the origin ($|X| \to \infty$), the center-of-mass and internal degrees of freedom decouple and the system can be characterized by its center-of-mass momentum $P$ and oscillator excitation number $n$, or, equivalently, by $n$ and the total energy $E = P^2/2 + \omega(n+1/2)$. We wish to calculate the probability $T_n(E)$ for transmission of the system through the barrier $V$. Of particular interest is $T_0(E)$, the transmission probability of this system initially in its oscillator ground state.

It is convenient to introduce rescaled total energy and occupation number $\epsilon = g^2 E$ and $\nu = g^2 n$. With our choice of $U$, the top of the barrier corresponds to a potential energy $\epsilon = 1$. For $\epsilon < 1$ transmission is possible only via tunneling. For $\epsilon$ just above 1 classical over-barrier transitions are possible for very special initial states. Indeed, there exists an unstable, static classical solution with both particles stationary at the top of the barrier, $x_1 = x_2 = 0$, so that $\epsilon = 1$. If one perturbs this solution by giving an arbitrarily small, common positive velocity to both particles, they will move toward $X = \infty$. The reversed evolution takes the system to $X = -\infty$, with the classical oscillator characterized by a certain excitation energy $\epsilon_0^{osc} \equiv \omega \nu_0$ (and a certain phase of the classical oscillator). The combined evolution is the classical transition over the barrier from this particular asymptotic state. By solving the (real time) classical equations of motion numerically, we found that $\nu_0 \approx 0.9$ for $\omega = 1/2$.

The classical evolution of the system initially in the classical oscillator ground state ($x_1 = x_2$) leads to the excitation of the oscillator as it approaches the barrier. Classical transition over the barrier occurs in this case only if the total energy exceeds some critical value. In our example we found numerically $\epsilon_{crit} = 1.8$.

If $\epsilon$ and $\nu$ are such that classical transitions over the barrier are not possible, the system has to tunnel. We will shortly see that at $\epsilon$ and $\nu$ fixed, and $g \to 0$ (i.e., at large total energy and initial occupation number, $E, n \propto g^{-2}$) the transmission probability has the semiclassical form

$$T_0(E) = C_0(\epsilon) e^{-\frac{1}{\pi} F_0(\epsilon)}$$

and that the exponent is obtained by taking the limit

$$F_0(\epsilon) = \lim_{\nu \to 0} F(\epsilon, \nu)$$

One of the main purposes of this paper is to check this limiting procedure by comparison with a fully quantum mechanical calculation.

3. To see that Eq. (3) is indeed valid, and to obtain the procedure for calculating the exponent $F(\epsilon, \nu)$, let us consider the transmission amplitude $A(X_f, y_f; P, n) = \langle X_f, y_f | \exp[-iH(t_f - t_i)] | P, n \rangle$, where $X_f$ ($>0$) and $y_f$ are the coordinates at time $t_f$, and we eventually take the limit $(t_f - t_i) \to \infty$. This amplitude may be written as a convolution of the evolution operator in the coordinate basis and the wave function of the initial state. The former is given by the path integral $\langle X_f, y_f | \exp[-iH(t_f - t_i)] | X_i, y_i \rangle = \int [dX][dy] \exp iS$ where the integration runs over paths satisfying $(X, y)(t_i) = (X_i, y_i)$, $(X, y)(t_f) = (X_f, y_f)$. For an initial state with $P \propto g^{-1}$, $n \propto g^{-2}$, the initial wave function is semiclassical and has the exponential form. In the case of a harmonic binding potential, this follows from the integral representation in the coherent state formalism:

$$\langle X_i, y_i | P, n \rangle = \frac{e^{iPX_i}}{\sqrt{2\pi}} \frac{i}{2\pi} e^{-\frac{1}{2} \int i \sqrt{\nu} y_i} e^{-\frac{i}{2} \frac{1}{\sqrt{\nu} \omega^2} \sqrt{\nu} \omega^2 y_i}$$

(One may replace $\sqrt{n}/\sqrt{n}$ by $\exp(n \log \bar z /\sqrt{n} + n/2)$ at large $n$.) By introducing the rescaled integration variables $X \to gX$, $y \to gy$, etc., we observe that $A(X_f, y_f; P, n)$ is given by an integral of an exponential of the form $\exp(-g^{-2} \Gamma)$ where $\Gamma$ depends only on the rescaled integration variables, $\nu$ and $\epsilon$, and does depend explicitly on $g^2$. This allows for a semiclassical analysis: we find stationary points of $\Gamma$ and evaluate the integrals using a stationary phase approximation. We outline the main steps in the derivation of the stationary point equations.

Variation of $\Gamma$ with respect to $X(t)$ and $y(t)$ for $t_i < t < t_f$ leads to the conventional classical equations of motion. When classical transitions are forbidden, there will be no real solutions satisfying the boundary conditions. Nevertheless there will be solutions with complex values of the integration variables. When performing the analytic continuation we will, in general, encounter singularities. To deal with this problem, we note that the time contour, originally the real axis, can be distorted into the complex plane, keeping the end points $t_i$, $t_f$ fixed. This deformation of the time contour allows us to avoid these singularities. Thus, our strategy is to search for complex solutions of the classical equations of motion along a contour ABCDE in the complex time plane, as shown in Fig. 1.
There are further stationary point equations coming from variation of $\Gamma$ with respect to the integration variables at the end point $t_f$. It is convenient to formulate these equations along part B of the contour, where $t = iT/2 + t'$, $t' = \text{real} \rightarrow -\infty$ (this is possible because the equations of motion decouple in the asymptotic past). Instead of $\epsilon$ and $\nu$ we introduce new real parameters $T$ and $\theta$; $T$ enters the problem through the shape of the contour. The general complex solution at large negative $t'$ is $X(t') = X_0 + pt'$, $y(t') = ue^{-i\omega t'} + ve^{i\omega t'}$ where $X_0$, $p$, $u$ and $v$ are complex parameters. The stationary point equations at the initial time lead to the following boundary conditions: (i) $X(t')$ is real (i.e. $p$ is real and $T$ may be chosen so that $X_0$ is also real), (ii) the positive and negative frequency parts of $y(t')$ are related to each other by $v = u^*e^{i\theta}$.

More boundary conditions appear when one evaluates the total transmission probability, i.e. integrates $|A(X_f, y_f; P, n)|^2$ over $X_f$ and $y_f$, again in a gaussian approximation. These conditions involve the final time and simply require that (iii) $X(t)$ and $y(t)$ are real on the DE part of the contour.

\[ F(\epsilon, \nu) = 2\text{Im}S_0 - \epsilon T - \nu \theta \]

where

\[ S_0 = -\int_{\text{BCDE}} dt \left[ \frac{1}{2}X\partial_x^2X + \frac{1}{2}y\partial_y^2y + \frac{\omega^2}{2}y^2 + U(X + y) \right] \]

is the (rescaled) classical action for the complex solution of the above boundary value problem. The total energy and excitation number are related to $T$ and $\theta$ by

\[ \frac{\partial(2\text{Im}S_0)}{\partial T} = \epsilon, \quad \frac{\partial(2\text{Im}S_0)}{\partial \theta} = \nu \]

i.e. the pairs $(\epsilon, \nu)$ and $(T, \theta)$ are Legendre-conjugate.

We have solved the equations of motion numerically along the contour BCDE subject to the boundary conditions (i)–(iii). In particular, we have evaluated the limit $\nu \rightarrow 0$. The result of this semiclassical calculation is shown in Fig. 3.

4. To check this semiclassical procedure, we have performed a numerical analysis of the full quantum system defined by (4). This is conveniently done in a basis of center-of-mass coordinate $X$ eigenstates and oscillator excitation number $n$. In this basis the state is represented by a multi-component wave function $\psi_n(X) \equiv \langle X, n | \Psi \rangle$, and the time-independent Schrödinger equation reads

\[ -\frac{\partial^2 \psi_n(X)}{\partial X^2} + \left( n + \frac{1}{2} \right) \omega \psi_n(X) + \sum_{n'} V_{nn'}(X) \psi_{n'}(X) = E \psi_n(X) \tag{5} \]

where $V_{nn'}(X) = \langle n | V(X + y) | n' \rangle$. Our choice of a gaussian potential $V$ enables us to calculate $V_{nn'}(X)$ by a numerical iteration procedure. Equation (5) is supplemented with the standard boundary conditions: (a) the incoming wave $(X \rightarrow -\infty)$ is in a state of given center-of-mass momentum $P$ and excitation number $n$; (b) only outgoing waves exist at $X \rightarrow +\infty$.

To solve the system (5) numerically, we introduce a lattice with equal spacing, $X_k = ka$, and discretize eq. (5) using the Numerov–Cowling algorithm (which reduces the discretization error to $O(a^6)$). We also truncate the system to a finite number of oscillator modes $n \leq N_0$. In order to insure good accuracy of the solution, we have chosen the number of lattice sites $2N_X$ and the cutoff $N_0$ as large as $2N_X = 2\cdot4096$, $N_0 = 400$. This corresponds to over 3 million coupled complex equations. To deal with them, we take advantage of the special form of Eq. (5).

Indeed, by inverting a set of $(N_0 + 1) \times (N_0 + 1)$ matrices, which is computationally feasible, Eq. (5) can be recast in the form $\psi_n(X_k) = \sum_{n'} [L_k \psi_{n'}(X_{k-1}) + R_k \psi_{n'}(X_{k+1})]$. The elimination of $\psi_n$ at definite $X_k$ leads to a system of similar form for the remaining variables (with suitably redefined $L$ and $R$), again after $(N_0 + 1) \times (N_0 + 1)$ matrix algebra and matrix inversion. In this way we progressively eliminate variables at intermediate values of $X_k$ and ultimately obtain a system that linearly relates $\psi_n$ at the end points $X = -N_X a$ and $X = +N_X a$. With a discretized version of the boundary conditions (a) and (b), this final system is straightforward to solve. The transmission probability is then determined by $|\psi_n|^2$ at the end point $X = N_X a$.

We performed a series of checks of this numerical procedure to insure that our calculations are sufficiently precise and that the results are close to the continuum limit.
We present in Figs. 2 and 3 the results of the full quantum mechanical computation of the transmission probability for the system initially in its oscillator ground state. The potential $V$ is gaussian, and $\omega = 1/2$. Figure 2 shows that the transmission probability $T_0(E)$ indeed has the functional form (8): at fixed $\epsilon \equiv g^2 E$, the logarithm of $T_0$ is very well fit by a linear function of $g^{-2}$. We use this fit to obtain the exponent $F_0(\epsilon)$. Both the full quantum mechanical results for $F_0(\epsilon)$ and the semiclassical results (the latter obtained by implementing the limiting procedure (4)) are shown in Fig. 3. Clearly, there is good agreement between the two. (The slight discontinuities in the quantum mechanical results are an artifact of the energy dependence of the $g^2$ range from which we can extract $F_0$. They provide an indication of the errors due to higher order effects.) We conclude that the validity of the semiclassical approach is confirmed by the direct quantum mechanical computation.

5. Full quantum mechanical computations (analytic or numerical) of barrier penetration probabilities are rarely possible. Even for our simplified system, values of $g$ smaller than 0.1 are difficult to study, as one has to deal with very small transmission coefficients. On the other hand, limitations of the semiclassical computations are far less severe. The generalization of the semiclassical approach to quantum-mechanical systems with harmonic binding of more than two particles in more than one space dimension is straightforward, and we also expect that other binding potentials may be treated in a similar way provided their semiclassical wave functions are known. Indeed, in all such cases the transmission amplitudes with highly excited initial states will be given by (path) integrals of exponential functions, and the tunneling exponents will be determined by appropriate stationary points. The latter will be complex solutions to classical field equations on contours in complex time, with boundary conditions depending on the binding potential. A limit analogous to Eq. (4) will then determine the tunneling exponent for incoming systems in low lying bound states.

The semiclassical calculability of pre-exponential factors is less clear. While it is plausible that these factors are given by functional determinants about complex classical solutions for highly excited incoming states (finite $\nu$ in our model), we do not expect that a limiting property similar to Eq. (4) will continue to hold for the pre-exponents. The calculation of such pre-exponential factors for low lying states remains an interesting open problem.

Acknowledgements. We are indebted to P. Tinyakov for helpful discussions. This research was supported in part under DOE grant DE-FG02-91ER40676, Russian Foundation for Basic Research grant 96-02-17449a and by the U.S. Civilian Research and Development Foundation for Independent States of FSU (CRDF) award RP1-187. Two of the authors (C.R. and V.R.) would like to thank Professor Miguel Virasoro for hospitality at the Abdus Salam International Center for Theoretical Physics, where part of this work was carried out.

[1] T. Banks, M. Bender and T.T. Wu, Phys. Rev. D8 (1973) 3346; T. Banks and M. Bender, Phys. Rev. D8 (1973) 3366.
[2] S. Coleman, The uses of instantons, In: The whys of subnuclear physics. Proc. 1977 Int. School on Subnuclear Physics, ed. A. Zichichi, Plenum, N.Y., 1979.
[3] V.A. Rubakov and P.G. Tinyakov, Phys. Lett. B279 (1992) 165.
[4] V.A. Rubakov, D.T. Son, and P.G. Tinyakov, Phys. Lett. B287 (1992) 342.
[5] A.N. Kuznetsov and P.G. Tinyakov, Mod. Phys. Lett. A11 (1996) 479; Phys. Rev. D56 (1997) 1156.
[6] P.G. Tinyakov, Phys. Lett. B284 (1992) 410.
[7] A.H. Mueller, Nucl. Phys. B401 (1993) 93.