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QUANTUM RESONANCES IN PHYSICAL TUNNELING

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ABSTRACT

It has recently been emphasized that the probability of quantum tunneling is a critical function of the shape of the potential. Applying this observation to physical systems, we point out that in principal information on potential surfaces can be obtained by studying tunneling rates. This is especially true in cases where only spectral data is known, since many potentials yield the same spectrum.

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Historically, our intuition on tunneling comes mainly from two places. The first is from alpha decay.¹ There we know that the nucleus eventually decays; it is a resonance coupled to the continuum. The second source of our intuition is from symmetric double-well potentials. There it is well known² that the ground and first excited states are almost degenerate. The ground state has a symmetric wave function (no nodes) and the first excited state has an antisymmetric wave function (one node). The time it takes for a wave packet originally located on one side to get to the other side is given by $\tau = \pi\hbar/(E_1 - E_0)$. The wave packet tunnels back and forth in multiples of this oscillation time.

From the above intuition it might be assumed that given any double-well potential the "particle" will always tunnel to the lower well, given enough time. However, in general this is not true. Whether a state can significantly tunnel to the true vacuum is a very sensitive function of the shape of the potential.

This was recently emphasized in work³ which was motivated by a very different type of study, the early universe. Starting from the dimensionless Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + V(x) \right] \psi = i \frac{d}{dt} \psi, \quad (1)$$

this group studied tunneling from the higher left-hand well in the potentials

$$V = \begin{cases} (x + 2)^2 + U, & x \leq 0 \\ (x - [4 + U]^{1/2})^2, & x \geq 0, \end{cases} \quad (2)$$

$$V = \begin{cases} \frac{5}{(18)^2} (x+3)^2 (x-2)(x-6) , & x \leq \frac{9}{2} \\ -\frac{(25)^2}{(12)(16)} , & \frac{9}{2} \leq x \leq d + \frac{9}{2} \\ \frac{5}{(18)^2} (x-d+3)^2 (x-d-2)(x-d-6) , & d + \frac{9}{2} \leq x \end{cases} , \quad (3)$$

and

$$V = \begin{cases} 6-x, & x \leq -4 \\ 0, & -4 \leq x \leq -1 \\ 2, & -1 \leq x \leq 1 \\ -U, & 1 \leq x \leq 4 \\ 6+x, & 4 \leq x \end{cases} . \quad (4)$$

These potentials are shown in Figs. 1, 2, and 3, respectively.

The true minimum of the potential of Eq. (2) lowers and goes to the right as U is increased. The true minimum of the potential of Eq. (3) expands to the right as d increases, and the true minimum of the potential of Eq. (4) lowers as U increases. In all three potentials a gaussian wave-function, fit to the false minimum, was placed in the left-hand well. Then, in all three cases, the wave-function was numerically integrated in time. In the first case an analytic check was done which agreed with the numerical integration.

Using these results, the maximum probability that the false-vacuum state ever penetrates to the right-hand side, for any time, for arbitrary U (or d) was plotted. This probability is defined as

$$\rho_{\text{RHS}}^{\text{max}}(U) = \max_{\forall t} \int_0^{\infty} dx \psi_0^*(x,t) \psi_0(x,t) \quad (5)$$

In Figs. 4-6 are shown the results for the three potentials.

Figs. 4-6 below

A line plot of the maximum probability which can tunnel from the false vacuum for the potentials in Eq. (2), in Eq. (3), and in Eq. (4). The time evolutions of the wave functions were calculated for times as large as 300. These plots have an accuracy of a few percent. The tunneling times at the maxima are the following: F.4 $\tau = 38, 28$, and 25 for the maxima at $U = 0, 2$, and 4 ; F.5 $\tau \approx 58$ and 69 for the maxima at $d = 0.4$ and 1.975 ; F.6 $\tau = 44, 32$, and 30 for the maxima at $U = 0, 1.98$, and 5.7 . Observe that even at the resonance peaks the maximum probability that tunnels to the true vacuum is not 100%. This is because there always is some fraction of the wavepacket that remains to the left of $x = 0$.

Parabolas

Polynomial

Square Wells

Fig. 4

Fig. 5

Fig. 6

To understand what is going on, look at the first three eigenfunctions of Eq. (2) for $U = 0, 1$, and 2 (Figs. 7, 8, 9).

$U = 0$

$U = 1$

$U = 2$

Figs. 7-9. The first three eigenvectors ϕ_0 , ϕ_1 , and ϕ_2 of Eq. (2) for (7) $U = 0$, (8) $U = 1$, and (9) $U = 2$. The ground state ϕ_0 is represented by the solid line, ϕ_1 by the long-dashed line, and ϕ_2 by the

At $U = 0$, the false-vacuum eigenfunction almost equally overlaps with ϕ_0 and ϕ_1 on the left-hand side. When the tunneling time τ is reached, these two eigenfunctions are out of phase by π , and so the overlap is on the right-hand side. The overlap of ψ_0 with ϕ_2 is almost zero because of the node of ϕ_2 near $x = -2$. For $U = 1$, ψ_0 has an overlap almost exclusively with ϕ_1 which now, however, is almost entirely on the left. Therefore, since ψ_0 has no significant overlap with an eigenfunction with large probability on the right, it can never tunnel to the right. When $U = 2$, we have a situation similar to $U = 0$, except that the two almost degenerate eigenstates are now ϕ_1 and ϕ_2 . They both have nodes near $x = 2.4$. This means that when the wave packet tunnels to the right, it will not be a coherent tunneling, but rather will have two humps.

Clearly this is a resonance condition. It is similar to matching cavities with electromagnetic waves. When the two wells are tuned correctly, the waves can pass back and forth. The tuning is caused by integrating the curvature of the wavefunction properly, this curvature being $[E - V(x)]$. For the present harmonic oscillator-like potential, this means a jump of $U = 2$.

Therefore, as the graphs in Figs. 4-6 show, if one is interested in tunneling, it is important to know how good a fit a particular parametrization of a double-well potential actually is to the "true" potential. As was shown,³ small deviations can have drastic effects on the tunneling rates.

Furthermore, since many potential surfaces are determined by the spectra alone, and not by the scattering data, the picture is more complicated still. For given only a spectrum, there are an uncountable number of potentials which will give the same spectrum. This fact has been beautifully expounded by Abraham

Putting the "one-halves" back in here to conform to the Fig. from Ref. 5, we give an example of AB.⁴ If one adds to the harmonic oscillator potential v_0 the potential v_1 :

$$v = v_0 + v_1 , \quad (6)$$

$$v_0 = \frac{1}{2}z^2 , \quad v_1 = 4\phi(\phi - z) , \quad (7)$$

$$\phi(z) = \frac{e^{-z^2}}{z^{\frac{1}{2}}\text{erfc}(z)} , \quad (8)$$

$$\text{erfc}(z) = \frac{2}{\pi^{\frac{1}{2}}} \int_z^{\infty} e^{-t^2} dt , \quad (9)$$

one has an analytically solvable potential with the same spectrum as the original, but with the ground state removed.⁴⁻⁶ This is shown⁵ in Fig. 10.

Figure 10

The harmonic oscillator potential $v_0(z)$ is a light curve, the contribution $v_1(z)$ is a light dashed curve, and the complete AM potential $v(z)$ is a heavy curve. The number eigenstates are also indicated.

Now by simply adding -1 to the potential, one has the original spectrum. This is the simplest example, but the program works in general, including for potentials with a continuum.

With these points in mind, we became interested in applying these insights to physical systems. We considered the work of Wieser and collaborators.⁸ From spectra, they obtained phenomenological potentials for the methyl-substituted oxetans and thietans of the form

$$V = N_2 x^2 + N_3 x^3 + N_4 x^4 \quad (10)$$

In Table I we give, in the notation of Eq. (i), their values of the N_i for three specific asymmetric compounds.

TABLE I

	2-methyl oxetan	3-methyl oxetan	2-methyl thietan
N_2	-0.6736	-0.5964	-0.862
N_3	-0.0434	-0.05866	-0.0275
N_4	0.07028	0.06856	0.03422
$\rho_{\text{MAX}}^{\text{RHS}}$	0.36	0.51	0.02
τ	3.06	3.10	19.18

Using the above values for the N_i , we found that the oxetans allowed a significant fraction of the wave-packet to tunnel in a short time whereas the thietan allowed almost no tunneling. This is also shown in Table I.

We emphasize that the present calculations apply to no dissipation. Thus, we are talking about a situation where very low temperatures and pressures would be involved. The idea is to try to use the calculated tunneling to test the accuracy of phenomenological potentials in the low energy regime. Hopefully the calculations would be good enough to compare to future experiments.

Cribb and coworkers⁹⁻¹¹ have previously undertaken related tunneling calculations. They used a density matrix formalism in their work. They started⁹ by considering four sets of parameters for a specific potential and showed how the tunneling properties varied with the different sets. They then^{10,11} applied their formalism to chemical systems where pressure and temperature effects are important. These are problems of practical interest in standard chemical reactions.

Our focus is different. We are interested in determining the potential energy surfaces in systems where pressure and temperature effects can be ignored. In that case, tunneling may in principle provide a method to distinguish between slightly different phenomenological potentials in the low energy regime.

Switching quickly to nuclear physics, we mention the observation of Berger at this meeting. In discussing the two-dimensional potential energy surface his group has obtained¹² for the fission of ^{240}Pb , Berger observed¹³ that the small amount of low-energy fission component might be due to resonant tunneling. The tunneling would be from the higher-energy valley to the (approximately parallel) lower-energy valley, both of which are approximately perpendicular to the normal escape direction in the two-dimensional surface. This observation is worthy of further consideration.

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