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QUANTUM TUNNELING AND NEGATIVE EIGENVALUES

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In the path-integral approach to the decay of a metastable state by quantum tunneling, the tunneling process is dominated by a solution to the imaginary-time equations of motion, called the bounce. In all known cases, the second variational derivative of the euclidean action at the bounce has one and only one negative eigenvalue. This note explains this phenomenon by showing it is an inevitable feature of the bounce for a wide class of systems. This class includes a set of particles interacting through potentials obeying some mild technical restrictions, and also theories of interacting scalar and gauge fields. There may exist solutions in other ways like bounces and which have more than one negative eigenvalue, but, even if they do exist, they have nothing to do with tunneling.

In the semiclassical approximation to quantum dynamics, we frequently study false ground states, time-independent states that are classically stable but decay through quantum tunneling. The decay probability per unit time of such a state is of the form

$$\Gamma = A\,\mathrm{e}^{-B/\hbar}(1+\mathrm{O}(\hbar)). \tag{1}$$

For field-theory applications, it's useful to have a manifestly Lorentz-invariant method of computing A and B. The usual one is based on the euclidean (imaginary-time) version of Feynman's sum over histories [1]. One begins by finding a bounce, a time-reversal invariant solution of the imaginary-time equations of motion that approaches the false ground state at infinity. (The trivial constant solution is excluded.) The coefficient B is the euclidean action evaluated at the bounce. The coefficient A is the product of certain collective-coordinate factors and the square root of the absolute value of the determinant of the second variation of the action evaluated at the bounce (with zero eigenvalues from collective coordinates omitted).

In all known cases the second variation at the bounce has one and only one negative eigenvalue. There is a hand-waving argument for this. The bounce shifts the energy of the false ground state in the same way an instanton shifts the energy

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of a true ground state. The formula for the instanton energy shift *is* the formula described in the preceding paragraph, without the phrase "absolute value". Thus the negative eigenvalue is necessary to insure that the energy shift is imaginary, that is to say, that the state becomes unstable.

Even if we're gullible enough to swallow this argument, we're still left with an unanswered question. What are we to do if we find a solution for which the second variation has more than one negative eigenvalue? Is any number of negative eigenvalues satisfactory? Or must the number of negative eigenvalues be odd? Or perhaps equal to one modulo four?

There exist somewhat more plausible and considerably more elaborate arguments connecting the bounce to tunneling, but they are no more helpful on this point. The purpose of this note is to answer the question by showing that, for a wide class of dynamical systems, the bounce has one and only one negative eigenvalue. If we find a solution with more than one negative eigenvalue, we should throw it away; it's the wrong solution and has nothing to do with the tunneling process.

Let q^a be the generalized coordinates of our system, where a runs over a finite or infinite set. I shall establish the stated result when the euclidean lagrangian is of the form

$$L = \tfrac{1}{2} m_{ab}(q)\dot{q}^a \dot{q}^b + V(q)\,. \tag{2}$$

Here the sum over repeated indices is implied, m_{ab} is some positive-definite symmetric matrix function of the q's, V is some function of the q's, and the overdot denotes differentiation with respect to imaginary time.

I will choose coordinates such that the false ground state is at the origin, $q^a = 0$, and add a constant to V such that $V(0) = 0$. Because the false ground state is classically stable, the origin must be a local minimum of V. Because tunneling occurs, V must be negative somewhere. Thus we have a situation like that sketched in fig. 1: The origin is surrounded by a region of positive V, separated by a surface, Σ, on which V vanishes, from an exterior region of negative V. I shall have to make one technical assumption* about V, that ∇V vanishes nowhere on Σ. This ensures that Σ has everywhere a well-defined normal.

Some comments:

(i) As advertised, this is a wide class of systems. It includes both the theory of an arbitrary number of particles interacting through arbitrary velocity-independent potentials, and the theory of a set of scalar fields interacting through nonderivative interactions, coupled to abelian or nonabelian gauge fields (in temporal gauge). Unfortunately, it does not include one very interesting problem, quantum tunneling from de Sitter space in the theory of scalar fields coupled to einsteinian gravity. (At least, I have not been able to put this problem into appropriate form, or into any tractable generalization of it.)

* This assumption can be weakened considerably; see the appendix.

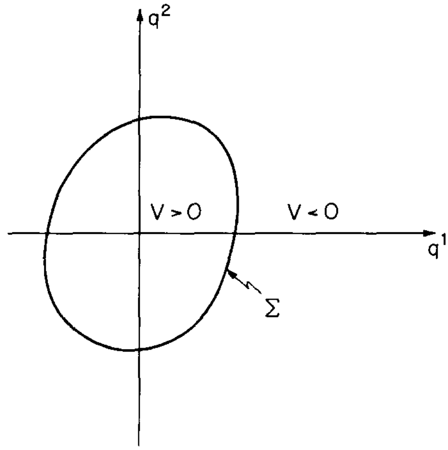

Fig. 1. The shape of the potential, V, for a tunneling problem. The system tunnels from the origin, where $V=0$, through a region of positive V, to the surface Σ, where V vanishes, and from which it can escape to the region of negative V.

(ii) Fig. 1 is drawn for the simplest case. However, it would not affect the argument if things were more complicated. For example, there could be additional regions of positive V, disconnected from the origin. Likewise, the region of positive V connected to the origin could extend to infinity in some directions, which would make Σ noncompact or even disconnected.

(iii) Although I'll deal with infinite numbers of degrees of freedom, I'll make no attempt at rigorous functional analysis; I'll blithely assume that all sums are as convergent and all functionals as smooth as I need.

Now for the argument:

For the systems under study, there is a well-developed WKB theory of barrier penetration [2], which can be summarized by the statement that the system tunnels through the barrier along the path of least resistance. In more detail: We define a metric in configuration space by

$$\mathrm{d}l^2 = m_{ab}\,\mathrm{d}q^a\,\mathrm{d}q^b , \tag{3}$$

and define a functional of paths that begin at the origin and terminate somewhere on Σ,

$$S_\mathrm{B}[q(l)] = \int \mathrm{d}l \sqrt{2V(q(l))} \, . \tag{4}$$

To avoid worrying about paths that penetrate the region of negative V, by convention we terminate all paths on their first intersection with Σ. (The suffix B denotes barrier penetration. This is the first of three closely related functionals we shall encounter.) A minimal barrier penetration path, $q_0(l)$, is one that minimizes S_{B}. The coefficient B in eq. (1) is given by

$$B = 2S_{\mathrm{B}}[q_0(l)]\,. \tag{5}$$

For many problems, only the absolute minimum of S_{B} is important, but in other cases, even local minima are of interest. For example, penetration of Σ at different points might lead to escape into different valleys in V, and we might be interested in the probability of tunneling into each of these valleys, even if the probabilities for some valleys are exponentially small compared to those for others. In any case, local saddle points or maxima are of no interest. Thus, the second variation at the stationary point must be positive semidefinite operator,

$$\delta^2 S_{\mathrm{B}}\Big|_{q_0(l)} \geqslant 0\,. \tag{6}$$

This equation will eventually be connected to the paucity of negative eigenvalues.

Eq. (6) must be interpreted with a small amount of care. The reason is that the domain of S_{B}, the set of paths on which S_{B} is defined, is not an open set (in any of the usual topologies for path space). In particular, there exist smooth curves in path space, passing through $q_0(l)$, such that every path on one side of $q_0(l)$ is in the domain of S_{B}, while every path on the other side penetrates the region of negative V. I can say nothing, and need to say nothing, about the derivatives of S_{B} along such a curve. I only assert that, for twice-differentiable curves which pass through $q_0(l)$ and which lie completely in the domain of S_{B}, at $q_0(l)$ the derivative of S_{B} along the curve vanishes and the second derivative is positive.

Let us define a functional

$$S'[q(t)] = \int \mathrm{d}t\, L(\dot{q}(t), q(t))\,, \tag{7}$$

for motions that begin at the origin and end on Σ. Just as for S_{B}, by convention all motions are terminated at their first intersection with Σ; thus V is never negative in the region of integration. Note that although the integral is like that in Hamilton's principle, the boundary conditions are non-hamiltonian; the final endpoint is not completely fixed, nor is the time interval. However, a stationary point of S' is *a fortiori* stationary under variations that do leave the final endpoint and the time fixed, and thus is a solution of the Euler-Lagrange equations,

$$\frac{\mathrm{d}}{\mathrm{d}t} m_{ab} \frac{\mathrm{d}q^b}{\mathrm{d}t} = \frac{\partial L}{\partial q^a}\,. \tag{8}$$

This implies that the euclidean energy,

$$E = \frac{1}{2}\left(\frac{\mathrm{d}l}{\mathrm{d}t}\right)^2 - V, \tag{9}$$

is a constant of the motion.

Every motion $q(t)$ defines a unique path $q(l)$. (Of course, the mapping is not invertible; there are many motions that traverse the same path at different speeds.) S' may be written in terms of $q(l)$ and $\mathrm{d}l/\mathrm{d}t$:

$$S' = \int \mathrm{d}l \left[\frac{1}{2}\frac{\mathrm{d}l}{\mathrm{d}t} + V\frac{\mathrm{d}t}{\mathrm{d}l}\right]. \tag{10}$$

Because the time interval is not fixed, to stationarize this for fixed $q(l)$ requires just ordinary calculus, not calculus of variations. We see that the stationary point is a minimum (because V is positive) and obeys

$$\frac{\mathrm{d}l}{\mathrm{d}t} = \sqrt{2V}\,. \tag{11}$$

If we insert this in eq. (10), S' becomes S_{B}. In equations,

$$S'[q(t)] \geqslant S_{\mathrm{B}}[q(l)]\,, \tag{12}$$

with equality obtained for that $q(t)$ which obeys eq. (11).

Thus there is a one-to-one correspondence between the stationary points of S' and those of S_{B}.* In particular, for $q_0(t)$, the motion that corresponds to $q_0(l)$,

$$S'[q_0(t)] = S_{\mathrm{B}}[q_0(l)] = \tfrac{1}{2}B\,, \tag{13}$$

and, from eqs. (6) and (12),

$$\delta^2 S'\Big|_{q_0(t)} \geqslant 0\,. \tag{14}$$

Of course, this equation must be interpreted with the same care as eq. (6).

By eq. (11), $q_0(t)$ is a zero-energy solution of the equations of motion. Thus it approaches the origin in infinite time. Because ∇V nowhere vanishes on Σ, $q_0(t)$ reaches Σ in finite time. Thus, with no loss of generality we can take t to occupy the range $[-\infty, 0]$. At $t=0$, again by eq. (11), $\dot{q}_0^a = 0$. Thus we can extend $q_0(t)$ to a

* This correspondence is very close to that which connects Hamilton's principle to Jacobi's principle of least action [3]. I have used this correspondence before in discussing the connection between the path-integral and WKB formulations of tunneling [4]. However, I have chosen to give the argument from first principles here, rather than referring to the literature, both because my boundary conditions are not quite the usual ones and because I need somewhat more information about the correspondence than I can find in the literature.

solution of the equations of motion for all time, by reflection:

$$q_0(-t) = q_0(t)\,. \tag{15}$$

The extended $q_0(t)$ is the bounce. It stationarizes the usual euclidean action,

$$S = \int_{-\infty}^{\infty} L(\dot{q}(t), q(t))\,\mathrm{d}t\,, \tag{16}$$

restricted to functions that approach the origin at plus and minus infinity.

We now turn to a study of the eigenvalues and eigenfunctions of $\delta^2 S$ evaluated at $q_0(t)$.

(i) Because q_0 is an even function of t, we can always choose the eigenfunctions to be either even or odd functions of t.

(ii) Because of the time-translation invariance of the equations of motion, $\dot{q}_0$ is an eigenfunction with eigenvalue zero. It is an odd function of t.

(iii) The eigenfunction(s) with lowest eigenvalue must be even.

Proof: Let $\psi(t) = -\psi(-t)$ be an eigenfunction with lowest eigenvalue. Define

$$\tilde{\psi} = \begin{cases} \psi\,, & t > 0 \\ -\psi\,, & t < 0\,. \end{cases} \tag{17}$$

Because $\psi(0) = 0$, this is continuous and piecewise continuously differentiable. If ψ is normalized, so is $\tilde{\psi}$, and the expectation value of $\delta^2 S$ for $\tilde{\psi}$ is the same as that for ψ. Since this is the minimum expectation value, the lowest eigenvalue, $\tilde{\psi}$ must also be an eigenfunction with lowest eigenvalue. So therefore is $\psi + \tilde{\psi}$. But this is preposterous, since this function vanishes on the entire negative axis, and can hardly be a solution of the eigenvalue equation, an ordinary differential equation.

Thus there must be at least one even eigenfunction with a negative eigenvalue, which I will call ψ_1. If there is a second eigenfunction with a negative eigenvalue, ψ_2, it may be either even or odd. I shall show that in either case there is a contradiction.

If ψ_2 is even, we can find coefficients a and b such that

$$\left(a\psi_1(0) + b\psi_2(0)\right) \cdot \nabla V(q_0(0)) = 0\,. \tag{18}$$

Thus we can construct a one-parameter family of motions,

$$q_\lambda(t) = q_0(t) + \lambda\left(a\psi_1(t) + b\psi_2(t)\right) + \mathrm{O}(\lambda^2)\,, \tag{19}$$

such that for sufficiently small λ, $q_\lambda(0)$ is in Σ,

$$V(q_\lambda(0)) = 0\,. \tag{20}$$

I wish to evaluate S' for $q_\lambda(t)$, restricted to $t \leqslant 0$. However, before I can do this, I must check that this function is among those for which S' is defined, that is to say, that q_λ lies in the region of positive V for all negative t. I'll do this by computing the time derivatives of $V(q_\lambda(t))$ at $t=0$. Because $q_\lambda(t)$ is an even function of t,

$$\left.\frac{\mathrm{d}V(q_\lambda(t))}{\mathrm{d}t}\right|_{t=0} = 0, \tag{21}$$

while

$$\left.\frac{\mathrm{d}^2V(q_\lambda(t))}{\mathrm{d}t^2}\right|_{t=0} = \left.\frac{\mathrm{d}^2V(q_0(t))}{\mathrm{d}t^2}\right|_{t=0} + \mathrm{O}(\lambda) = \nabla V\cdot m^{-1}\nabla V + \mathrm{O}(\lambda), \tag{22}$$

by the Euler-Lagrange equations. Thus V is positive for sufficiently small λ and for t in some neighborhood of zero. But for t outside this neighborhood, $q_0(t)$ is strictly in the interior of the region of positive V, and thus so is $q_\lambda(t)$ for sufficiently small λ. Hence, for sufficiently small λ, it is legitimate to compute $S'[q_\lambda(t)]$.

Because q_λ is an even function of t,

$$S[q_\lambda(t)] = 2S'[q_\lambda(t)]. \tag{23}$$

Thus,

$$\left.\frac{\mathrm{d}^2S[q_\lambda(t)]}{\mathrm{d}\lambda^2}\right|_{\lambda=0} = 2\left.\frac{\mathrm{d}^2S'[q_\lambda(t)]}{\mathrm{d}\lambda^2}\right|_{\lambda=0}. \tag{24}$$

The left side of this equation is negative, because ψ_1 and ψ_2 are eigenfunctions with negative eigenvalues. But the right side is non-negative by eq. (14).

If ψ_2 is odd, we can find coefficients a and b such that

$$\left(a\dot\psi_2(0) + b\ddot q_0(0)\right)\cdot\nabla V(q_0(0)) = 0. \tag{25}$$

If we construct the one-parameter family of motions,

$$q_\lambda(t) = q_0(t) + \lambda\left(a\psi_2(t) + b\dot q_0(t)\right), \tag{26}$$

$q_\lambda(0) = q_0(0)$ is in Σ for all λ. Furthermore, for sufficiently small λ, $q_\lambda(t)$, for $t \leqslant 0$, is in that class of functions for which S' is defined. The reasoning here is the same as before; note that eq. (25) is necessary to establish (21). Because the coefficient of λ in eq. (26) is an odd function of t,

$$S[q_\lambda(t)] = S'[q_\lambda(t)] + S'[q_{-\lambda}(t)]. \tag{27}$$

Differentiating this twice, we again obtain eq. (24). The left side of this equation is negative, because ψ_2 is an eigenfunction with negative eigenvalue and $\dot q_0$ is an eigenfunction with eigenvalue zero. But the right side is positive, by eq. (14).

This completes the argument. It has been long and niggling; perhaps a short sloppy summary will be useful. The WKB formulation of tunneling tells us to search for a minimal barrier penetration path; the path-integral formulation tells us to search for a bounce. These two prescriptions are equivalent, in much the same way that Hamilton's principle and Jacobi's principle are equivalent. But there is an apparent paradox. The minimal barrier penetration path is a true minimum; all small deviations from it increase the action. However, the problem of small vibrations about the bounce has an eigenfunction with negative eigenvalue; small deviations in this direction decrease the action. The resolution of the paradox is the observation that not all small deviations from the bounce map into possible barrier penetration paths; they may over- or undershoot the escape surface, Σ. However, if there are two eigenfunctions with negative eigenvalues, we can always build a deviation that lands dead on Σ, and we have a true contradiction.

This work was completed while I was a visitor to the Theory Division of CERN. I would like to thank CERN for its hospitality.

Appendix

WHAT HAPPENS IF ∇V VANISHES?

In the body of this paper, I made a technical assumption, that ∇V vanishes nowhere on Σ. This can be replaced by a considerably weaker assumption, that at every point on Σ for which ∇V vanishes, the matrix of second derivatives of V is invertible. This can in turn be replaced by an even weaker (though somewhat less natural) assumption, that the matrix has at least one negative eigenvalue. (This follows from invertibility because Σ is the boundary of a region of negative V.)

I shall show that, under the stated assumption, the minimal barrier penetration path can not intersect Σ at a point where ∇V vanishes. Thus, in the neighborhood of the minimal path, we have nonvanishing ∇V, and the rest of the proof follows as before.

The argument proceeds by contradiction. I shall assume that $q_0(t)$, the minimum of S', intersects Σ at a point where ∇V vanishes. I shall then construct a path arbitrarily close to $q_0(l)$ with a smaller value of S'.

Because ∇V vanishes at the assumed intersection point, it takes an infinite time for $q_0(t)$ to reach Σ. Thus t occupies the range $[-\infty, \infty]$. By our assumption, there exists a vector of unit length, e, such that at the intersection point,

$$e^a \frac{\partial^2 V}{\partial q^a \partial q^b} e^b \equiv V' < 0 . \tag{28}$$

(Note that this equation is true even if there are only continuous negative eigenvalues, as could be the case for an infinite number of variables.)

I shall define a new motion, $q_1(t)$, by

$$q_1(t) = q_0(t), \qquad t \leqslant T,$$
$$= q_0(t) + Ae\sin[\omega(t-T)], \qquad t \geqslant T, \tag{29}$$

where A, T, and ω are real parameters which I shall choose shortly.

The parameter A is fixed by demanding that q_1 intersect Σ at $T' = T + \pi/(2\omega)$. Let us expand $V(T')$ in a series in powers of A, neglecting terms of higher than second order. (I shall justify this neglect shortly.)

$$V(T') = V_0 + AV_1 + A^2V_2. \tag{30}$$

For sufficiently large T, $V_0 = V(q_0(T'))$ is arbitrarily small. So is V_1, which is proportional to $\nabla V(q_0(T'))$. V_2 is the first coefficient that does not go to zero for large T; it is arbitrarily close to the negative constant, V''. Because V_0 is positive, the quadratic equation for A, $V(T') = 0$, has two real roots, one positive and one negative. For both roots, A is arbitrarily small for sufficiently large T. This justifies neglecting the higher terms in the series. Because A can be made arbitrarily small, $q_1(l)$ can be made arbitrarily close to $q_0(l)$.

Now let us expand $S'[q_1(t)]$ in a series in powers of A,

$$S'[q_1(t)] = S_0' + AS_1' + A^2S_2' + \cdots. \tag{31}$$

I shall analyze the terms in this expression one by one: (i) S_0' is an integral over the same positive integrand as that which defines $S'[q(t)]$, but the range of integration is smaller, $[-\infty, T']$ rather than the whole line. Thus S_0' is strictly less than $S'[q_0(t)]$. (ii) AS_1' can always be made less than or equal to zero by choosing the sign of A appropriately. (iii) For T sufficiently large,

$$A^2S_2' = \tfrac{1}{2}A^2\int_T^{T'} \mathrm{d}t\left[\omega^2\cos^2\omega(t-T) + V''\sin^2\omega(t-T)\right]$$
$$= \tfrac{1}{8}\pi A^2(\omega^2 + V''). \tag{32}$$

If we choose ω^2 to be less than $-V''$, this is strictly negative. (iv) Thus the first three terms in the series all make $S'[q_1(t)]$ less than $S'[q_0(t)]$. But since the term proportional to A^2 has a nonzero coefficient, the higher terms can not change this inequality, for sufficiently small A. This completes the proof.

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