Tunneling and Instantons

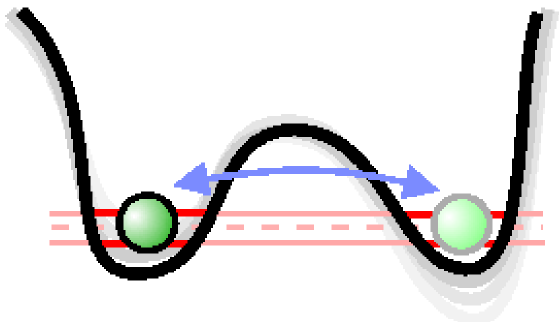
Remarkably, the same mathematical equations describe both the 1D Ising model, and quantum mechanical tunneling in a double-well potential. Here, the domain wall solution describe the barrier penetration event, sometimes called the "instanton". This is our first example illustrating how certain quantum mechanical problems can be rigorously mapped onto models of classical statistical mechanics, allowing direct solutions using standard theoretical tools.

Quantum statistical mechanics of a tunneling two-state system

Now consider a (single) quantum-mechanical particle moving in a double well potential of the form

$$V(x) = \frac{1}{2}rx^2 + \frac{1}{4}ux^4,$$

with $r < 0$. Classically, a low energy particle will be confined to one of the two wells, with a doubly degenrate ground state at $x = \pm x_o = \pm(|r|/u)^{1/2}$. Quantum mechanically, there is a finite (even if small) probability for tunneling through the barrier. The corresponding tunneling rate will depend on the form and the size of the barrier, and it will determine the "tunnel splitting" Δ between the "bonding" (ground) and the "antibonding" (first excited) quantum energy state.



While the tranditional calculation of the barrier penetration rate has been first performed by the so-called WKB (semiclassical) approximation, an equivalent result can also be obtained by examining the quantum statistical mechanics of the same problem, which is easiest to do in the so-called imaginary time (Matsubara) formulation.

Matsubara formalism for a single particle

The partition function for the system can be written as

$$Z = Tr[e^{-\beta \mathbf{H}}] = \sum_n e^{-\beta E_n},$$

where $\mathbf{H}$ is the Hamiltonian of this system with eigenvalues $E_0, E_1, ...$, and the density matrix (statistical operator)

$$\rho = \frac{1}{Z} e^{-\beta \mathbf{H}}.$$

The (modified) Heisenberg representation for the position operator $\mathbf{x}$ is defined by

$$\mathbf{x}(\tau) = e^{\tau \mathbf{H}/\hbar} \mathbf{x} e^{-\tau \mathbf{H}/\hbar}.$$

The imaginary time auto-correlation function can be written using a time-ordered product operator $\mathbf{T}_\tau$ as

$$\chi(\tau) = Tr[\rho \mathbf{T}_\tau \{\mathbf{x}(\tau)\mathbf{x}(0)\}].$$

Finally, it is easy to see (homework problem HW#6.2) that at low temperature ($\beta \longrightarrow \infty$), this reduces to

$$\chi(\tau) \sim e^{-\tau \Delta/\hbar}.$$

Thus, the imaginary time decay rate of $\chi(\tau)$ measures the tunnel splitting Δ between the ground state and the first excited state.

Path integral represenation

A convenient representation for evaluating the partition function of the system is provided by the Feynmann path-integral representation in imaginary time

$$Z = \int Dx(\tau) e^{-S[x]},$$

where the action is [we measure the time in units such that the particle mass $m = 1$]

$$S[x(t)] = \int_0^{\beta\hbar} dt \left[\frac{1}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x) \right].$$

Furthermore, the imaginary-time auto correlation function $\chi(\tau)$ can also be evaluated usign this path integral represenatation as

$$\chi(\tau) = \frac{1}{Z} \int Dx(\tau) x(\tau) x(0) e^{-S[x]}$$

As we can see, this action looks exactly identical to the Landau-Ginzburg action for the ϕ^4 theory (continuum limit of the Ising model)! The problem, therfore, is formally reduced to an equivalent classical statistical mechanical problem. Here, the (imaginary) time of the quantum particle corresponds to the saptial coordinate of the classical problem. Solving the tunneling problem is, thefore, equivalent to solvinf the $d = 1$ classical Ising model!

Instanton solution

In evaluating this path integral, one has to sum over all possible paths in imaginary time, which contribute to the partition function according to their respective Boltzmann weights determined by the action $S[x(t)]$. For "thick" enough barriers, the leading contributions can be obtained by a *semi-classical* approximation, which corresponds to trajectories with minimal action. These are calculated from the saddle-point condition

$$\frac{\delta S}{\delta x(t)} = 0,$$

giving

$$-\frac{d^2x}{d\tau^2} + rx + ux^3 = 0.$$

This equation is identical to our Landau-Ginzburg equation we used for the domain wall calculation. It again describes the classical trajectory of a particle moving in the **inverted potential** $-V(x)$! Here, the domain wall corresponds to a trajectory describing the tunneling of a particle from one to the other potential well. It essentially takes place in a rather short time interval

$$\tau^* = |r|^{-1/2},$$

so that

$$x(\tau) = x_0 \tanh\left[(\tau - \tau_o)/\tau^*\right],$$

and is thus called the **"instanton"** solution. Note that, just as any domain wall, it can be "centered" about an arbitrary time τ_o. It is called "instanton", since tits "thickness" in time τ^* becomes very small for thick barriers ($|r|$ large), so in a way tunneling is (almost) instantenious.

Dilute instanton gas

To compute the partition function, we need to sum over all possible tunneling events, just as we summed over all the possible configurations of the domain walls in the 1D Ising model. The rest of the calculation is done in complete analogy as before, and we find that the "correlation time" takes the form

$$\tau_\xi \sim \exp\{S_o\},$$

where the "barrier height" is given by

$$S_o \sim \frac{|r|^{3/2}}{u}.$$

Physically, this correlation time corresponds to the **average time** between consecutive tunneling events across the barrier. For "thick barriers", where S_o is large, the the correlation time $\tau_\xi \gg \tau^*$, so a particle typically spends a long time in each well, before almost instantaneously tunneling to the other well. In this regime, the instantons can be considered as a noninteracting "gas", as we have assumed in the above calculation of the correlation time. Following the procdure we developed for the classical domain wall gas, we can now calculate also the autocorrelation function (see homework problem HW#6.1), and find

$$\chi(\tau) \sim e^{-\tau/\tau_\xi}.$$

By comparing with the result from the Matsubara calculation (homework problem HW#6.2), we find that the tunnel splitting between the "bonding" and "antibonding" levels in the double well problem

$$\Delta = \frac{\hbar}{\tau_\xi} \sim \exp\{-S_o\}.$$

We conclude that it is exponentially large in terms of the barrier height, in agreement with the WKB formula.

The formal analogy of the two problems is our first encounter of the formal mapping of quantum mechanical (QM) problems in d dimensions to equivalent problems in classical statistical mechanics in $d+1$ dimensions (d spatial and one time). In this case, the QM problem was a local tunneling center, thus a "zero-dimensional" problem (e.g. has only one degree of freedom). It was mapped onto the one dimensional Ising model, and this analogy provides a deeper understanding of the WKB behavior on one side, and the thermodynamic behavior at the lower critical dimension on the other side.