# Quantum Tunneling, Dissipation, and Fluctuations

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A theory of quantum tunneling with dissipation is constructed. The frequency-dependent transmission coefficient is calculated at zero and finite temperatures. A fluctuation-dissipation theorem for tunneling particles is derived.

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The understanding of the properties of tunneling particles coupled to the degrees of freedom representing the environment is of crucial importance to a large number of interesting problems in physics. The tunneling of a test particle from a metastable state has been studied by Caldeira and Leggett[1] and a number of other workers[2] using instanton methods, and applied to tunneling of flux quanta in Josephson junctions.[3] In a second case, depicted in Fig. 1, a particle of given energy $E$ hits a barrier and suffers multiple inelastic collisions with collective modes in the barrier, and the transmitted particle emerges with a distribution of energies $E'$. This is essentially a *scattering* problem with many applications such as tunneling of Cooper pairs through Josephson junctions,[4] tunneling of electrons out of a metal through vacuum (scanning tunneling microscopy[5]), and resonance tunneling of electrons in a dirty conductor[6] in the presence of phonons (finite-temperature conductivity).

In this Letter a theory of tunneling for this very general case will be presented. The theory is essentially a WKB theory with weak coupling to the heat bath for tunneling with dissipation. For a given problem which can be solved in the absence of dissipation within WKB we calculate the complete frequency-dependent transmission coefficient, or spectral function, at zero and finite temperatures. The transmission coefficient can be thought of as the scattering cross section of the barrier. We derive a fluctuation-dissipation theorem, relating the spectral function of the particle to the response function of the external degrees of freedom (the "heat bath"). From the spectral function the average energy loss or gain and the integrated tunneling rate $T_E$ can be readily calculated and we present explicit expressions for the case of coupling to a longitudinal phonon branch. At zero temperature the tunneling rate may either increase or decrease because of dissipation; at finite temperatures the tunneling rate increases exponentially with temperature to the second power which was also found for tunneling from metastable wells.[2] All the steps of the derivation have a well-defined physical meaning; we do not invoke imaginary time and instanton constructions which limit the possibility of intuitively understanding the results and the approximations. The theory has two limitations: The energy of the particle and the coupling energy should both be well below the barrier height.

The starting point is the Feynman path-integral expression[7] for the combined probability amplitude of particle and bath:

$$K(Q_f,X_f,T|Q_i,X_i)=\int_{Q(0)=Q_i}^{Q(T)=Q_f} D[Q]\int_{X(0)=X_i}^{X(T)=X_f} D[X]\exp\left[\frac{i}{\hbar}\int_0^T\left(\tfrac{1}{2}M\dot{Q}^2-V(Q)-V_1(Q)\sum_\alpha x_\alpha(t)+\tfrac{1}{2}\sum_\alpha m(\dot{x}_\alpha^2-\omega_\alpha^2x_\alpha^2)\right)dt\right]. \quad (1)$$

The potential $V(Q)$ represents a barrier through which the particle with coordinate $Q$ and mass $M$ has to tunnel while coupled with coupling strength $V_1$ to a set of oscillator degrees of freedom $x_\alpha$, collectively denoted by $X$. These modes (phonons, etc.) represent the "heat bath" with which the particle interacts.

Our strategy[8] is to deal with the functional integral over the $Q$ coordinate first by means of a time-dependent WKB approximation, and perform the functional integral over the $X$ coordinates rigorously with use of a formalism developed by Feynman and Vernon[7] for linear coupling to the external coordinates. The wave function of the particle by itself for a given $x_\alpha(t)$ is

$$\psi(Q,T)=\int dQ_i\,\psi^E(Q_i)\int_{Q(0)=Q_i}^{Q(T)=Q} D[Q]\exp\left[\frac{i}{\hbar}\int_0^T\left(\tfrac{1}{2}M\dot{Q}^2-V(Q)-V_1(Q)\sum_\alpha x_\alpha(t)\right)dt\right], \quad (2)$$

where $\psi^E(Q_i)$ is a wave packet of energy $E$ hitting the "left-hand" side of the barrier (near $Q=0$) at time $T=0$. The wave function in the barrier can be found by use of WKB if we assume for the moment that $\sum_\alpha x_\alpha(t)$ is just a time-dependent potential (and not a set of quantum mechanical coordinates). In WKB, $\psi(Q,T)=A \times \exp[iS(Q,T)/\hbar]$ where, with $f(t)\equiv\sum_\alpha x_\alpha(t)$,

$$\frac{\partial S}{\partial T}=-\frac{1}{2M}\left(\frac{\partial S}{\partial Q}\right)^2-V(Q)-V_1(Q)f(T)+\cdots. \tag{3}$$

We set $S=S_0+S_1$ where $S_0$ is the usual WKB result in the absence of the coupling $V_1$:

$$S_0=-Et+i\hbar\int_0^Q \kappa(Q')dQ',\quad \kappa(Q)=\{2M[V(Q)-E]\}^{1/2}/\hbar \tag{4}$$

and $S_1$ is the correction due to $V_1 f$. To lowest order in $V_1 f$

$$S_1=i\int_{-\infty}^{\infty}d\omega\, f(\omega)e^{i\omega T}g(\omega),\quad g(\omega)=\int_0^Q\frac{dQ'}{2\pi}\frac{MV_1(Q')}{\hbar\kappa(Q')}\exp\left(-\int_{Q'}^{Q}dQ''\frac{M\omega}{\hbar\kappa(Q'')}\right). \tag{5}$$

Equations (5) were investigated in detail by Büttiker and Landauer[9] for $f(t)$ periodic with frequency $\omega$. There is a characteristic traversal time $\tau=\int_0^L(M/\{2[V(Q)-E]\})^{1/2}dQ$ for a barrier of length $L$ such that for frequencies $\omega<1/\tau$ the particle tunnels through an effectively static barrier while for $\omega>1/\tau$ it tunnels through a time-averaged barrier picking up inelastic sidebands at $E\pm\hbar\omega$, $E\pm 2\hbar\omega$, etc. We shall see that $\tau$ is also the characteristic time scale in the presence of a thermal bath.

To compute the probability amplitude $A(E,E')$ for the particle to have energy $E'$ after tunneling, we set $Q=L$ in Eq. (5) and assume that the coupling is switched off after tunneling:

$$A(E,E')=A_0\int\frac{dT}{2\pi}\exp\left(i(E'-E)T/\hbar-\frac{1}{\hbar}\int_{-\infty}^{\infty}d\omega\, f(\omega)g(\omega)e^{i\omega T}\right), \tag{6}$$

where $A_0$ is the tunnel amplitude in the absence of dissipation. To compute the transmission probability per unit interval of energy $E'$ per second, $P_{E,E'}=\langle|A(E,E')|^2\rangle/T_m$, with $T_m$ the measuring time, we need to average $|A(E,E')|^2$ over the bath, taking into account the quantum mechanical nature of the coordinates $x_\alpha$.

Note that the coupling term $S_1$ can be written as

$$S_1=\int_{-\infty}^{+\infty}f(t)\tilde{Q}_T(t)dt,\quad \tilde{Q}_T(t)=i\int_{-\infty}^{+\infty}\exp[-i\omega(t-T)]g(\omega)d\omega.$$

This shows that $\tilde{Q}_T(t)$ acts as a complex driving force on $x_\alpha$, leading to an *effective* Lagrangean for the bath

$$\tilde{L}_T(t)=\sum_\alpha \tfrac{1}{2}m[\dot{x}_\alpha(t)^2-\omega_\alpha^2x_\alpha^2(t)]+\tilde{Q}_T\sum_\alpha x_\alpha(t). \tag{7}$$

The resulting functional integrals over the $x_\alpha$ coordinates become

$$P_{E,E'}=(T_mN)^{-1}\int dT_1\,dT_2\exp[(i/\hbar)(E'-E)(T_1-T_2)]\int dX_f\,dX_f'\,dX_i\,dX_i'\,D[X]\,D[X']\,\delta(X_f-X_f')$$
$$\times\exp\left(\frac{i}{\hbar}\int_{-\infty}^{\infty}dt[\tilde{L}_{T_1}(t)-\tilde{L}^*_{T_2}(t)]\right)\sum_n e^{-\beta E_n}\phi_n(X_i)\phi_n^*(X_i'), \tag{8}$$

where $\phi_n$ are the energy eigenfunctions of the oscillators, $\beta=1/kT$, and $N$ is a normalization factor. In Eq. (8) we summed over all the final states of the bath leading to the $\delta$ function for $X_f$. The integral over the forced harmonic oscillators can be performed by the methods of Feynman and Vernon,[7] since the coupling to the oscillators is linear. We find, assuming a frequency cutoff $\omega_m$,

$$P_{E,E'}=|A_0|^2\exp\left(-\frac{4\pi}{\hbar}\int_0^{\omega_m}d\omega\, g(\omega)g(-\omega)\chi''(\omega)\coth(\beta\hbar\omega/2)\right)$$
$$\times\left[\int_{-\infty}^{\infty}\frac{dt}{2\pi}\exp\left(i(E'-E)t/\hbar-(4\pi/\hbar)\int_{-\omega_m}^{\omega_m}d\omega\, g^2(\omega)\chi''(\omega)[1-e^{-\beta\hbar\omega}]^{-1}e^{i\omega t}\right)\right]. \tag{9}$$

Here $\chi''$ is the imaginary part of the frequency-dependent susceptibility of the bath, $\chi(\omega)=f(\omega)/F(\omega)$, where $f(\omega)$ is the response of a force $F(\omega)$ on the oscillators. Equation (9) is our fundamental result. It gives the complete energy distribution of the outgoing particles. The formula can be thought of as a fluctuation-dissipation

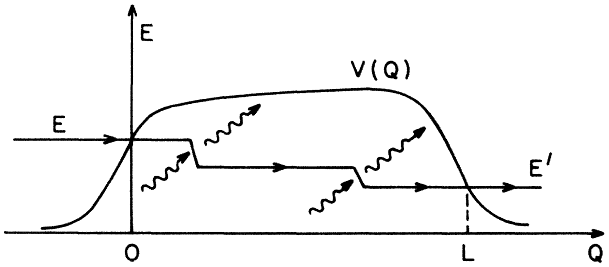


FIG. 1. Particle with initial energy $E$ tunneling through a barrier $V(Q)$ emerging with a distribution of energies $E'$ after collisions with collective modes.

theorem for tunneling particles since it relates the spectral function of the particle to the dissipative part of the frequency-dependent response function of the bath.

The effect of the collective modes is thus completely characterized by the frequency-dependent susceptibility $\chi''(\omega)$ which may be related to the density of states $D(\omega)$ through[7]

$$\chi''(\omega) = -\tfrac{1}{2}\pi D(\omega)/m\omega, \quad \omega < \omega_m. \tag{10}$$

In order to mimic Ohmic dissipation, which extrapolates to a classical damping term and is believed to be relevant for the Josephson junction, we consider phonons with velocity $v$ and $D(\omega) = \omega^2/2\pi^2 v^3$ per unit volume, so that

$$\chi''(\omega) = -\omega R, \tag{11}$$

with $R = 1/4\pi m v^3$ playing the role of a resistance. From Eq. (5) we find that approximately

$$g(\omega) \approx (\bar{V}_1/2\pi\omega)[1-\exp(-\omega\tau)], \tag{12}$$

where $\bar{V}_1$ is the average coupling constant.

The line shape given by Eq. (9) with Eqs. (10)–(12) is highly asymmetric. If we define

$$S(\omega) = -(\hbar/\pi)[1-\exp(-\beta h\omega)]^{-1}\chi''(\omega) \tag{13}$$

and expand the exponent to lowest order we find, for $|E'-E| = |\Delta E| < \hbar\omega_m$,

$$P_{E,E'} = T_E\left[\delta\left(\frac{-\Delta E}{\hbar}\right) + \frac{4\pi^2}{\hbar^2}g^2\left(\frac{\Delta E}{\hbar}\right)S\left(\frac{\Delta E}{\hbar}\right) + \dots\right], \tag{14}$$

where

$$T_E = A_0^2 \exp\left(\frac{4\pi^2}{\hbar^2}\int_{-\omega_m}^{\omega_m} d\omega\, g(\omega)g(-\omega)S(\omega)\right). \tag{15}$$

The function $S(\omega)$ can be identified as the *dynamic structure factor* of the bath:

$$S(\omega) = \int_{-\infty}^{+\infty}(dt/2\pi)\langle f(t)f(0)\rangle \exp(-i\omega t).$$

This follows directly from the fluctuation-dissipation theorem. The first term in Eq. (14) represents elastic tunneling reduced by a factor which has a similar form to the Debye-Waller factor which reduces the intensity of Bragg spots in elastic x-ray scattering. The second term represents absorption or emission of a single quantum of energy at $\omega = (E'-E)/\hbar$. The relation between the scattering cross section and the dynamic structure factor is a standard result of the linear-response theory of scattering. The factor $g(\omega)$ is the effective frequency-dependent coupling. Note that for zero temperature, $S(\omega) = 0$ for $\omega < 0$: No energy can be absorbed from the bath in its ground state. If we use the approximation of Eq. (12) in Eq. (14) then the energy distribution of the inelastically scattered particles has a maximum at $E'-E \simeq \hbar\tau^{-1}$ and a halfwidth $\Delta E_{1/2} \simeq \hbar\tau^{-1}$ at $\beta = \infty$.

If we raise the temperature then $P_{E,E'}$ acquires a larger tail for $E > E'$. For $\beta^{-1} > \beta_{co}^{-1} = 2\hbar/\tau$ the contribution of frequencies near the cutoff $\omega_m$ will dominate and for $\beta^{-1} \gg \beta_{co}^{-1}$ the tunneling is dominated by particles which absorb enough energy to emerge at the top of the barrier. This happens especially for long barriers for which $\tau$ is also long. Our theory cannot describe this crossover between quantum tunneling and thermal activation.

The linear-response result could have been found more easily with the use of Fermi's "golden rule" with $g(\omega)$ as matrix element. However, as the dimensionless parameter $R\bar{V}_1^2\tau^2\omega_m^2/\hbar$ grows, linear-response theory fails but we can still use Eq. (9) to go beyond linear-response theory. The first moment of the distribution of $P_{E,E'}$, $\langle\Delta E\rangle = \langle E - E'\rangle$, is

$$\langle\Delta E\rangle = [4\pi^2/\hbar]\int_{-\omega_m}^{\omega_m} d\omega\,\omega g^2(\omega)S(\omega), \tag{16}$$

which in the case of Ohmic dissipation with $\omega_m\tau \gg 1$ and $\beta_{co} > \beta$ becomes

$$\langle\Delta E\rangle = \frac{\bar{V}_1^2 R}{\pi}\left[\omega_m - \frac{\pi}{\beta\hbar}\left(\frac{3}{2}\cot\frac{\pi\tau}{\beta\hbar} + \frac{1}{2}\tan\frac{\pi\tau}{\beta\hbar}\right)\right]. \tag{17}$$

Hence, for $\beta = \infty$ the particle is losing energy, whereas for finite temperature the tunneling particles may actually on average gain energy, notwithstanding dissipation! As $1/\beta$ approaches $1/\beta_{co}$, $\langle E'-E\rangle$ increases rapidly with $1/\beta$ and we expect crossover to thermal activation. For $\omega_m\tau \ll 1$ and $\hbar\omega_m \gg 1/\beta$, we have

$$\langle\Delta E\rangle = \bar{V}_1^2 R\tau^2\omega_m^3\left(\frac{1}{3\pi} - \frac{2}{15}\pi^3\frac{1}{(\beta\hbar\omega_m)^4}\right). \tag{18}$$

The first case corresponds to the sideband limit of Büttiker and Landauer, the second case to the static limit.

We can also integrate Eq. (9) with respect to $E'$ to find the *total* tunneling probability

$$T_E=|A_0|^2\exp\left[-\frac{2\pi}{\hbar}\int_0^{\omega_m}d\omega\left\{[g^2(\omega)-g^2(-\omega)]\chi''(\omega)+[g(\omega)+g(-\omega)]^2\chi''(\omega)\coth\frac{\beta\hbar\omega}{2}\right\}\right]. \qquad (19)$$

The first term in the exponent represents the effect of dissipation; it suppresses tunneling. The second term represents the effect of a Gaussian random force acting on the tunneling particle; it is the fluctuation term and it enhances tunneling. In the limit $\beta\to\infty$ we can compute the temperature dependence for the Ohmic case $\chi''(\omega)=-R\omega$:

$$T_E(\beta)=T_E(\beta=\infty)\exp(\pi\bar{V}_1^2\tau^2R/3\hbar^3\beta^2), \qquad (20a)$$

where, for $\omega_m\tau \ll 1$,

$$T_E(\beta=\infty)=|A_0|^2\exp(\bar{V}_1^2\tau^2R\omega_m^2/\pi\hbar). \qquad (20b)$$

The tunneling rate at $\beta=\infty$ is enhanced because the electron can tunnel rapidly when the fluctuating barrier is low. The dissipative term which reduces tunneling is of higher order. The tunneling rate at finite temperature increases like $\ln T\sim 1/\beta^2$ due to thermal fluctuations.

The approximations we have made can be expressed in terms of the dimensionless parameters $\epsilon_1=\kappa^2L'^2$ and $\epsilon_2=R\bar{V}_1^2\tau^2\omega_m^2/\hbar$, where $L'$ is a characteristic length $\sim L$ over which the potential $V$ does not vary significantly. For WKB to apply we assume $\epsilon_1 \gg 1$, and for weak coupling $(S_1/S_0 \ll 1)$ to hold, $\epsilon_2 \gg \epsilon_1$. Note that $\epsilon_2 \ll 1$ is the linear-response regime. These simple approximations do not impose noticeable restrictions on the applicability to the experiments discussed in the introduction. In the realistic case where the dissipation is due to coupling to acoustic phonons, the electron-phonon coupling is proportional to $\omega$, implying $g(\omega)\sim\omega$ for small $\omega$. Equation (19) then leads to a tunneling rate $\ln T\sim 1/\beta^4$, in agreement with the result of Grabert, Weiss, and Hanggi.[2] The tunneling rate at zero temperature is always suppressed in this case.

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