or, equivalently, the internal energy $U$ and the specific heat $c$ at $\Gamma=2$. Their excess parts per particle are found to be

$$U_{\text{exc}}/N = -\tfrac{1}{4}e^2 \ln(\pi\rho L^2) - \tfrac{1}{4}e^2 C, \qquad (18)$$

and

$$c_{\text{exc}}/N = k_B(\ln 2 - \pi^2/24). \qquad (19)$$

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# Quantum-Statistical Metastability

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Consider a system rendered unstable by both quantum tunneling and thermodynamic fluctuation. The tunneling rate $\Gamma$, at temperature $\beta^{-1}$, is related to the free energy $F$ by $\Gamma=(2/\hbar)\,\mathrm{Im}F$. However, the classical escape rate is $\Gamma=(\omega\beta/\pi)\,\mathrm{Im}F$, $-\omega^2$ being the negative eigenvalue at the saddle point. A general theory of metastability is constructed in which these formulas are true for temperatures, respectively, below and above $\omega\hbar/2\pi$ with a narrow transition region of $O(\hbar^{3/2})$.

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Consider a system with a localized metastable ground state and a saddle point through which the system can escape to the true ground state. A simple example is a particle in the one-dimensional (1D) potential of Fig. 1. I shall at first concentrate on this example and then generalize to an arbitrary system (which may be a field theory). One may safely assume that both the ground-state energy, $\frac{1}{2}\hbar\omega_0\ [V''(x_0)=\omega_0{}^2]$, and the temperature are small compared to the barrier height, $V_0$; otherwise, the system would not be metastable.

At temperatures small compared to $\hbar\omega_0$ the particle is mainly in the low-lying metastable states. These have wave functions that vanish at $-\infty$, are standing waves normalized to 1 in the well, and give an exponentially small probability current, $J$, at positive $x$, which is identified with the decay rate, $\Gamma(E)$. The nonconservation of $J$ requires that $E$ have an (exponentially small) imaginary part[1] which obeys $\Gamma=(2/\hbar)\,\mathrm{Im}E$. Taking a Boltzmann average of $\Gamma(E)$, we find $\Gamma=(2/\hbar)\,\mathrm{Im}F$, to lowest order in exponentially small quantities.

At temperatures large compared to $\hbar\omega_0$ (but still small compared to $V_0$) we would expect classical thermodynamic fluctuations to dominate. The classical rate[2] is calculated by setting up a

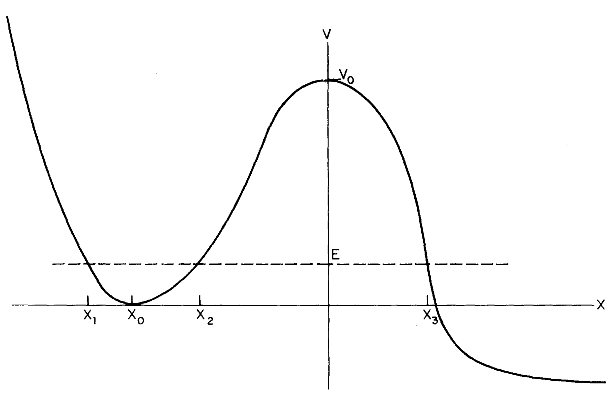


FIG. 1. The potential for a 1D metastable system.

 

Boltzmann distribution of particles to the left of the barrier and identifying $\Gamma$ with the probability current across the barrier:

$$\Gamma = \frac{\int dp\,dx\,(2\pi\hbar)^{-1}\exp\{-\beta[\frac{1}{2}p^2+V(x)]\}\,\delta(x)p\theta(p)}{\int dp\,dx\,(2\pi\hbar)^{-1}\exp\{-\beta[\frac{1}{2}p^2+V(x)]\}}$$
$$\approx \frac{\omega_0}{2\pi}\exp(-\beta V_0)\,. \qquad (1)$$

The step function $\theta(p)$ is inserted because there are no particles entering the well from the right. The partition function integral is dominated by the minimum of $V$. The free energy picks up a small imaginary part from the contribution of the "saddle point" ($x=0$) to the partition function.[1] Continuing the $x$ integral into the complex plane at $x=0$, one finds

$$\mathrm{Im}F = (\omega_0/2\omega\beta)\exp(-\beta V_0),$$
$$\Gamma = (\omega\beta/\pi)\,\mathrm{Im}F. \qquad (2)$$

The low- and high-temperature formulas for $\Gamma$ agree at $\beta_0^{-1} \equiv \hbar\omega/2\pi$. The best one could hope is that each is true everywhere, respectively, below and above $\beta_0^{-1}$. Amusingly, this turns out to be almost true; there is a narrow crossover region of $O(\hbar^{3/2})$, where $\Gamma$ is given by a more complicated expression which is derived below. (The exponential suppression factor in $\Gamma$, obtained here, is fairly well known.[3] However, a consistent semiclassical procedure for calculating $\Gamma$ at all temperatures has not been given before and hence the value of the prefactor has not been clear.)

To proceed I must define $\Gamma$ more carefully. It is the Boltzmann average of the probability current over a set of quantum states. For $E<V_0$, these states were defined above. At $E \gtrsim V_0$, they consist of waves, incident from the left, reflected and transmitted at the barrier. The incident flux per unit energy is set equal to the classical value, $1/2\pi\hbar$. This generalizes the classical notion of a Boltzmann distribution of particles to the left of the barrier. Furthermore, for $E<V_0$ the reflection coefficient goes to 1 and these states merge with the ones defined previously whose density, $\rho$ (as given by the WKB condition[4]), leads to the same incident flux per unit energy, $1/2\pi\hbar$. For $E<V_0$, the WKB linear turning-point formula gives[4]

$$\rho(E)\Gamma(E) = (2\pi\hbar)^{-1}\exp[-W(E)/\hbar], \qquad (3)$$
$$W(E) = 2\int_{x_2}^{x_3} dx[2(V-E)]^{1/2} \qquad (4)$$

(see Fig. 1). For $E \gtrsim V_0$ the linear turning-point formula is invalid but the transmission occurs very close to the top of the well so that one may use the transmission coefficient for a parabolic barrier,[4]

$$\rho(E)\Gamma(E) = (2\pi\hbar)^{-1}\{1+\exp[-2\pi(E-V_0)/\hbar\omega]\}^{-1}. \qquad (5)$$

This formula gives the correct classical limit above barrier, $\rho(E)\Gamma(E)\to(2\pi\hbar)^{-1}$ and agrees with the WKB result below barrier,

$$\rho(E)\Gamma(E)\to(2\pi\hbar)^{-1}\exp[-2\pi(V_0-E)/\hbar\omega]$$
$$\approx(2\pi\hbar)^{-1}\exp[-W(E)/\hbar]. \qquad (6)$$

One may now compute the equilibrium decay rate,

$$\Gamma = Z_0^{-1}\int_0^\infty dE\,\rho(E)\Gamma(E)\exp(-\beta E), \qquad (7)$$

$$Z_0 = \sum_{n=0}^{\infty}\exp[-(n+\tfrac{1}{2})\hbar\omega_0\beta] \qquad (8)$$
$$= [2\sinh(\tfrac{1}{2}\beta\hbar\omega_0)]^{-1}.$$

[Actually at $E=O(\hbar)$ the formula for $\Gamma(E)$ is not correct and the integral should be replaced by a sum; however, as we shall see, this has a negligible effect on $\Gamma$.] At low temperatures the integral is dominated by a stationary point, $\beta\hbar = 2\int_{x_2}^{x_3}dx[2(V-E)]^{-1/2}\equiv T(E)$, the period of the classical orbit in the potential $-V$ with energy $-E$. One can assume that $T(E)$ is monotone decreasing; generalizations are straightforward. Thus $2\pi/\omega \le T(E)\le\infty$ and a maximum exists for $\beta^{-1}<\beta_0^{-1}\equiv 2\pi/\hbar\omega$, with

$$\Gamma = Z_0^{-1}|2\pi\hbar T'|^{-1/2}\exp(-S/\hbar), \qquad (9)$$

where $S$ is the action of the classical path. For $\beta^{-1}>\beta_0^{-1}$ the integral cannot be done by steepest descents; however, it is dominated by $E\gtrsim V_0$ where Eq. (5) for $\Gamma(E)\rho(E)$ is valid:

$$\Gamma = Z_0^{-1}\int_{-\infty}^{\infty}dE\,(2\pi\hbar)^{-1}\{1+\exp[-2\pi(E-V_0)/\hbar\omega]\}^{-1}\exp(-\beta E)$$
$$= Z_0^{-1}\omega[4\pi\sin(\tfrac{1}{2}\beta\hbar\omega)]^{-1}\exp(-\beta V_0). \qquad (10)$$

For $\beta^{-1} \approx \beta_0^{-1}$ the integral is dominated by energies strictly less than but close to $V$. With use of

$$W(E) = (2\pi/\omega)(V_0 - E) + \tfrac{1}{2}|T'(V_0)|(V_0 - E)^2, \tag{11}$$

$$\Gamma = Z_0^{-1}\int_{-\infty}^{V_0} dE\,(2\pi\hbar)^{-1}\exp[-W(E)/\hbar]$$
$$= Z_0^{-1}|2\pi\hbar T'|^{-1/2}\operatorname{erf}[(\beta - \beta_0)|\hbar/T'|^{1/2}]\exp[-\beta V_0 + (\beta - \beta_0)^2\hbar/|2T'|], \tag{12}$$

where erf($x$) is the error function, $\operatorname{erf}(x) \equiv (2\pi)^{-1/2}\int_{-\infty}^{x} dy\,\exp(-\tfrac{1}{2}y^2)$. Asymptotically this formula gives

$$\Gamma = Z_0^{-1}|2\pi\hbar T'|^{-1/2}\exp[-\beta V_0 + (\beta - \beta_0)^2\hbar/|2T'|]$$

at temperatures below $\beta_0^{-1}$ and $\Gamma = Z_0^{-1}(2\pi\hbar)^{-1}(\beta_0 - \beta)^{-1}\exp(-\beta V_0)$, above $\beta_0^{-1}$, thus matching smoothly onto Eqs. (9) and (10) near $\beta_0^{-1}$. The more complicated Eq. (12) is only required for $(\beta^{-1} - \beta_0^{-1})$ of $O(\hbar^{3/2}(\omega/2\pi)^2|T'|^{1/2})$.

One now must calculate Im$F$. This is done by writing $Z$ as a functional integral and evaluating it by steepest descents. Saddle points are periodic solutions of the equations of motion with potential $-V$. The trivial saddle point, $x(T) = x_0$, gives

$$Z_0 = N[\operatorname{Det}(-d^2/d\tau^2 + \omega_0^2)]^{-1/2} = [2\sinh(\tfrac{1}{2}\hbar\omega_0\beta)]^{-1}. \tag{13}$$

[The determinant is calculated for eigenfunctions obeying periodic boundary conditions and the constant, $N$, has been chosen to make $Z_0$ agree with Eq. (8).] There is another saddle point, the periodic orbit discussed previously, $\bar{x}(\tau)$. [For $\beta^{-1} > \beta_0^{-1}$ this reduces to a constant, $\bar{x}(\tau) = 0$.] The second variation operator, $-d^2/d\tau^2 + V''(\bar{x})$, has (for $\beta^{-1} < \beta_0^{-1}$) a periodic zero mode, $\dot{\bar{x}}$, and since $\dot{\bar{x}}$ has one node, there must be one negative eigenvalue. Introducing a time-translation collective coordinate[5] to eliminate the zero mode and deforming the integration contour with respect to the negative mode,[1] I find

$$\operatorname{Im}F = (\hbar/2)Z_0^{-1}(W/2\pi\hbar)^{1/2}N|\operatorname{Det}'[-d^2/d\tau^2 + V''(\bar{x})]|^{-1/2}\exp(-S/\hbar). \tag{14}$$

(Det′ has the zero eigenvalue omitted.) Finally Det′ can be related to the classical motion,[6] $N^{-2}\operatorname{Det}'[-d^2/d\tau^2 + V''(\bar{x})] = T'W$, verifying the relation $\Gamma = 2\hbar^{-1}\operatorname{Im}F$. For $\beta^{-1} > \beta_0^{-1}$, there is no zero mode but there is still a (constant) negative mode:

$$\operatorname{Im}F = Z_0^{-1}(2\beta)^{-1}N|\operatorname{Det}(-d^2/d\tau^2 - \omega^2)|^{-1/2}\exp(-\beta V_0),$$
$$= Z_0^{-1}[4\beta\sin(\tfrac{1}{2}\beta\hbar\omega)]^{-1}\exp(-\beta V_0), \tag{15}$$

verifying $\Gamma = (\omega\beta/\pi)\operatorname{Im}F$.

The classical limit occurs for $\beta^{-1} \gg \beta_0^{-1}$:

$$\Gamma = (\omega/2\pi)[\sinh(\tfrac{1}{2}\beta\hbar\omega_0)/\sin(\tfrac{1}{2}\beta\hbar\omega)]\exp(-\beta V_0) \to (\omega_0/2\pi)\exp(-\beta V_0). \tag{16}$$

It is also clear that the correct zero-temperature limit is achieved since $\operatorname{Im}F \to \operatorname{Im}E_0$, where $E_0$ is the ground-state energy.

All that remains is to generalize to multidimensional systems. Thus consider a particle in an $n$-dimensional potential with a relative minimum at $\vec{x}_0$, $V = \tfrac{1}{2}\omega_0^2 x_1'^2 + \tfrac{1}{2}\sum_{i=2}^{n}(\omega_0^{i})^2 x_i'^2$ for some set of coordinates $x_i'$, and a saddle point at $\vec{0}$, $V = -\tfrac{1}{2}\omega^2 x_1^2 + \tfrac{1}{2}\sum_{i=2}^{n}(\omega^{i})^2 x_i^2$. The contribution to $\Gamma$ from states of energy $E < V_0$ is again suppressed by $\exp[-W(E)/\hbar]$, where now $W(E) = \int ds[2V - E)]^{1/2}$, with $s$ labeling distance along the orbit of energy $-E$. The prefactor in $\rho(E)\Gamma(E)$ is now rather complicated. Fortunately, life simplifies for $V_0 - E \ll V_0$. At these energies the classical solution becomes 1D, $x_1 \propto \sin(\omega\tau)$, $x_i = 0$, $i > 1$. Furthermore, the tunneling region becomes very narrow and so the quadratic approximation to $V$ may be used. Thus the wave-function factors, $\psi(\vec{x}) = \prod_{i=1}^{n}\psi_i(x_i)$. For $i > 1$, $\psi_i$ must be a harmonic oscillator wave function with frequency $\omega_i$. $\psi_1$ is simply the 1D solution used above. Writing $E = \sum_{i=1}^{n}E_i$, the transmission coefficient depends on $E_1$ only and takes the 1D form. The Boltzmann integral takes the 1D form multiplied by a discrete sum over harmonic-oscillator energies for the transverse degrees of freedom,

$$\Gamma = Z_0^{-1}\int_0^{\infty} dE_1\exp(-\beta E_1)\rho(E_1)\Gamma(E_1)\prod_{i=2}^{n}\sum_{n_i=0}^{\infty}\exp[-\beta\hbar\omega_i(n_i + \tfrac{1}{2})]. \tag{17}$$

Similar factorization occurs in $Z_0$, giving

$$\Gamma_n = \Gamma_1 \prod_{i=2}^{n} \sinh(\tfrac{1}{2}\omega_0{}^i\hbar\beta)/\sin(\tfrac{1}{2}\omega^i\hbar\beta), \qquad (18)$$

where $\Gamma_1$ is given by Eqs. (9), (12), and (10) as the temperature increases from somewhat below $\hbar\omega/2\pi$ right up to the classical range.

Now consider Im$F$. As the temperature approaches $\beta_0{}^{-1}$ from below, the Gaussian fluctuations in transverse directions approximately factor, giving $\prod_{i=2}^{n}\{\mathrm{Det}[-d^2/d\tau^2+(\omega^i)^2]\}^{-1/2}$; above $\beta_0{}^{-1}$ this factorization becomes exact since the classical solution is then time independent. These extra factors are just the ones occurring in $\Gamma_n$ verifying the two formulas relating $\Gamma$ to Im$F$ at all temperatures above $\beta_0{}^{-1}$ and also at temperatures somewhat below $\beta_0{}^{-1}$. As the temperature is lowered further, I expect $\Gamma = (2/\hbar)\,\mathrm{Im}F$ to remain true by the general argument in the second paragraph. These results are directly applicable to quantum field theory.[7]

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