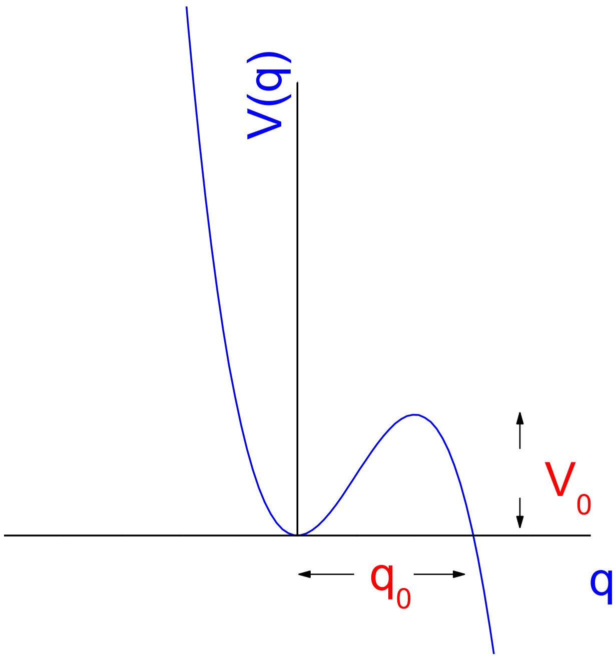
Dissipative quantum tunnelling (finite temperatures)

Metastable potential



$$V(q) = \frac{1}{2} M\omega_0^2 q^2 - \lambda q^3 \qquad (\lambda > 0)$$

$$\Gamma = \frac{2|E_I|}{\hbar}$$

We expect

$$\Gamma = \frac{2\,\mathrm{Im}F}{\hbar} = A(T)\exp - \frac{B(T)}{\hbar}$$

Undamped systems

$$T = (k_B \beta)^{-1} \neq 0 \quad \Longrightarrow \quad E_n^{(0)} \to E_n^{(0)} + i\hbar\Gamma_n^{(0)}/2$$

$$F = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\ln\left[\sum_{n=0}^{\infty}\exp -\beta\left(E_n^{(0)} + i\frac{\hbar\Gamma_n^{(0)}}{2}\right)\right]$$

$$F = -\frac{1}{\beta}\ln Z_R + i\frac{1}{Z_R}\sum_{n=0}^{\infty}\frac{\hbar\Gamma_n^{(0)}}{2}\exp -\beta E_n^{(0)}$$

$$Z_R = \sum_{n=0}^{\infty}\exp -\beta E_n^{(0)} \quad \Longrightarrow \quad \frac{2\mathrm{Im}F}{\hbar} = \langle\Gamma_n^{(0)}\rangle_\beta \equiv \Gamma_\beta^{(0)}$$

Then we need to evaluate

$$Z(\beta) = \int_{-\infty}^{+\infty} dx \, \langle\, x \,|\, \exp -\beta H \,|\, x \,\rangle = \int_{-\infty}^{+\infty} dx \int_{x}^{x} \mathcal{D}q(\tau') \exp - \frac{S_E[q(\tau')]}{\hbar}$$

$$\text{where} \quad S_E[q(\tau')] = \int_{-\hbar\beta/2}^{+\hbar\beta/2} d\tau' \left\{ \frac{1}{2} M \left(\frac{dq}{d\tau'} \right)^2 + V(q) \right\}$$

Two kinds of extrema obeying $q(\hbar\beta/2) = q(-\hbar\beta/2) = x$

Type I : $\dot{q}(\hbar\beta/2) \neq \dot{q}(-\hbar\beta/2)$ which are harmonic oscillator–like paths. We consider only those with negative Euclidean energy

$$E = -|E| = \frac{1}{2} M \dot{q}^2 - V(q)$$

Type II : $\hbar\beta$ periodic solutions which live within the metastable well of the inverted potential

But, close to q_b where $V'(q_b) = 0$ $(V(q_b) = V_0)$, $\omega_b^2 \equiv V''(q_b)/M$

and the period of the motion is $2\pi/\omega_b$ ➡ $\hbar\beta = 2n\pi/\omega_b$

The partition function is then

$$Z(\beta) \approx \int_{-\infty}^{+\infty} dx\, \Delta_I(\beta) \exp - \frac{S_E^{(I)}(x,\beta)}{\hbar} + Z_1(\beta)$$

$$S_E^{(I)}(x,\beta) \longleftrightarrow \Delta_I(\beta) \longleftrightarrow q_c(\tau) = q_c^{(I)}(\tau)$$

⬇

$$N_0(\beta) \left\{\det\left[-M\partial_\tau^2 + M\omega_0^2)\right]\right\}^{-1/2}$$

$$Z_0(\beta) = [2\sinh(\hbar\omega_0\beta/2)]^{-1}$$

$$Z_1(\beta) \quad \longleftrightarrow \quad q_c(\tau) = q_c^{(II)}(\tau)$$

Low temperatures: $\beta^{-1} < \beta_0^{-1} \equiv \hbar\omega_b/2\pi \quad (T_0 \equiv \hbar\omega_b/2\pi k_B)$

$$Z_1(\beta) \approx -\frac{i\hbar\beta}{2}\frac{1}{\sqrt{2\pi\hbar|\tau'(E_\beta)|}}\exp -\left[\frac{2W(E_\beta)}{\hbar} + \beta E_\beta\right]$$

Where $\tau'(E) = d\tau(E)/dE$ and E_β is a solution of

$2dW(E)/dE = -\hbar\beta$ with $2W(E) = \oint \sqrt{2M(V(q) - E)}dq$

Which is another way to write

$$Z_1(\beta) \approx -\frac{i\hbar\beta}{2}\left(\frac{||\dot{q}_c||^2}{2\pi\hbar}\right)^{1/2}\frac{1}{\sqrt{\det'\left[-M\partial_\tau^2 + V''\left(q_c(\tau)\right)\right]}}\times$$
$$\times\exp -\frac{S_E\left[q_c(\tau)\right]}{\hbar}$$

High temperatures: $\beta^{-1} > \beta_0^{-1}$

Lowest positive eigenvalue $\omega_1 - \omega_b > 0 \qquad \omega_1 \equiv 2\pi/\hbar\beta$

$$Z_1(\beta) \approx -\frac{i}{2} N_b(\beta) \frac{1}{\sqrt{|\det[-M\partial_\tau^2 - M\omega_b^2)]|}} \exp -\beta V_0$$
$$= \frac{-i}{4\sin(\beta\hbar\omega_b/2)} \exp -\beta V_0$$

General result ($Z_0 \gg |Z_1|$)

$$F = -\frac{1}{\beta}\ln Z(\beta) \approx -\frac{1}{\beta}\ln Z_0(\beta) + \frac{i}{\beta}\frac{|Z_1(\beta)|}{Z_0(\beta)}$$

$$\frac{2\mathrm{Im}F}{\hbar} = \langle \Gamma_n^{(0)} \rangle_\beta \equiv \Gamma_\beta^{(0)}$$

General result ($Z_0 \gg |Z_1|$) $\frac{2\mathrm{Im}F}{\hbar} = \langle \Gamma_n^{(0)} \rangle_\beta \equiv \Gamma_\beta^{(0)}$

$$\Gamma_\beta^{(0)} = \begin{cases} (2/\hbar)\mathrm{Im}F & \text{if} \quad T \leq T_0 \\ (\omega_b \beta/\pi)\mathrm{Im}F & \text{if} \quad T \geq T_0 \end{cases}$$

$$T < T_0 \longleftrightarrow \Gamma_\beta^{(0)} \approx \frac{2\sinh(\hbar\omega_0\beta/2)}{\sqrt{2\pi\hbar|\tau'(E_\beta)|}} \exp - \left[\frac{2W(E_\beta)}{\hbar} + \beta E_\beta\right]$$

$$T > T_0 \longleftrightarrow \Gamma_\beta^{(0)} \approx \frac{\omega_b \sinh(\beta\hbar\omega_0/2)}{2\pi\sin(\beta\hbar\omega_b/2)} \exp -\beta V_0$$

Classical limit: Arrenhius factor $\Gamma_\beta^{(0)} \approx \frac{\omega_0}{2\pi} \exp -\beta V_0$

Classical activation rate

$$\Gamma_\beta \approx A_{cl}(\beta) \exp -\beta V_0$$

Weak damping $A_{cl}(\beta) \propto \gamma\beta\omega_0/2\pi$

Strong to moderate damping $A_{cl}(\beta) = f(\gamma)\dfrac{\omega_0}{2\pi}$ where

$$f(\gamma) = \sqrt{1 + \left(\frac{\gamma}{\omega_b}\right)^2} - \frac{\gamma}{\omega_b}$$

Very strong damping $A_{cl}(\beta) = \dfrac{\omega_0\omega_b}{4\pi\gamma}$

For weak damping the activation rate is dominated by energy diffusion whereas for strong damping it is dominated by spacial diffusion.

Damped systems

$$S_{eff}[q(\tau')] = \int_{-\hbar\beta/2}^{\hbar\beta/2} \left\{ \frac{1}{2} M \dot{q}^2 + V(q) \right\} d\tau'$$

$$+ \frac{\eta\pi}{4\hbar^2\beta^2} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\tau'' \int_{-\hbar\beta/2}^{\hbar\beta/2} d\tau' \frac{\{q(\tau') - q(\tau'')\}^2}{\sin^2(\pi(\tau' - \tau'')/\hbar\beta)}$$

$$\left.\frac{\delta S_{eff}}{\delta q}\right|_{q_c} = M\ddot{q}_c - \frac{\partial V}{\partial q_c} - \frac{\eta\pi}{\hbar^2\beta^2} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\tau'' \frac{[q_c(\tau') - q_c(\tau'')]}{\sin^2(\pi(\tau' - \tau'')/\hbar\beta)} = 0$$

$$\hat{D}_\beta q(\tau') = -M \frac{d^2 q(\tau')}{d\tau'^2} + V''(q_c) q(\tau') + \hat{O}_\beta q(\tau') = k q(\tau')$$

$$\hat{O}_\beta q(\tau') = \frac{\eta\pi}{\hbar^2\beta^2} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\tau'' \frac{[q(\tau') - q(\tau'')]}{\sin^2(\pi(\tau' - \tau'')/\hbar\beta)}$$

Decay rate $\Gamma_\beta \approx \sqrt{\frac{||\dot{q_c}||^2}{2\pi\hbar}} \left| \frac{\det D_\beta^{(0)}}{\det' D_\beta} \right|^{1/2} \exp - \frac{S_{eff}[q_c(\tau)]}{\hbar}$

Valid only when there is a zero mode or $T < T_R$

Working in Fourier representation

$$q(\tau) = \sum_{n=-\infty}^{\infty} q_n \exp -i\omega_n \tau \qquad \omega_n = 2n\pi/\hbar\beta$$

Equation of motion

$$(M\omega_n^2 + 2M\gamma|\omega_n| + M\omega_0^2)q_n - \frac{3M\omega_0^2}{2q_0} \sum_{m=-\infty}^{\infty} q_m q_{m-n} = 0$$

$$\lambda = 3M\omega_0^2/q_0 \qquad q(\hbar\beta/2) = q(-\hbar\beta/2) = x \longleftrightarrow x = \sum_{n=-\infty}^{\infty} (-1)^n q_n$$

Boundary condition as a Lagrange multiplier

$$(M\omega_n^2 + 2M\gamma|\omega_n| + M\omega_0^2)q_n - \frac{3M\omega_0^2}{2q_0} \sum_{m=-\infty}^{\infty} q_m q_{m-n} = \kappa(-1)^n$$

q as a function of $\kappa = \kappa(x, \omega_n)$ and $q_n = q_n(x, \omega_n)$

$$S_{eff}(z_n) = \hbar\omega_0 \beta B_0 \left[\sum_{n=-\infty}^{\infty} (\nu_n^2 + 2\alpha|\nu_n| + 1) z_n z_{-n} - \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} z_m z_{m-n} z_n \right]$$

$$\nu_n = \omega_n/\omega_0, \; z_n = q_n/q_0 \text{ and } B_0 = M\omega_0 q_0^2/2$$

Dimensionless equation of motion and second variation k in unities of

$$\hbar\omega_0\beta B_0 \qquad (\nu_n^2 + 2\alpha|\nu_n| + 1) z_n - \frac{3}{2} \sum_{m=-\infty}^{\infty} z_m z_{m-n} = 0$$

$$D_\beta f_n = k_n f_n \qquad (\nu_n^2 + 2\alpha|\nu_n| + 1) f_n - 3 \sum_{m=-\infty}^{\infty} z_{n-m}^{(c)} f_m = k_n f_n$$

Low temperature regime

Add $2\int\limits_{\hbar\beta/2}^{\infty} L_E^{(eff)}(q_c(\tau))\,d\tau$ to the zero temperature action. This gives rise to an asymptotic expansion in β^{-1}

$$\Gamma_\beta = A_\beta \exp - B_\beta/\hbar$$

Weak damping regime $B_\beta \approx B - \frac{5B_0}{2\pi}\left(\frac{2\pi}{\hbar\omega_0\beta}\right)^2 = B - 10\pi B_0 \left(\frac{k_B T}{\hbar\omega_0}\right)^2$

Strong damping regime $B_\beta \approx B - \frac{4\pi B}{3}\left(\frac{2\alpha}{\hbar\omega_0\beta}\right)^2$

In both cases $a(\alpha)T^2$

High temperature regime

Now, main contributions to the action come from $q(\tau) = 0$ and $q(\tau) = q_b$

Fluctuations $x(\tau) = \sum_n X_n \exp -i\omega_n \tau$ and $y(\tau) = q_b + \sum_n Y_n \exp -i\omega_n \tau$

Whose actions are respectively
$$\begin{cases} S(X_n) = \frac{M\hbar\beta}{2} \sum_{n=-\infty}^{\infty} \Lambda_n^{(0)} X_n X_{-n} \\ S(Y_n) = \hbar\beta V_0 + \frac{M\hbar\beta}{2} \sum_{n=-\infty}^{\infty} \Lambda_n^{(b)} Y_n Y_{-n} \end{cases}$$

Second variation eigenvalues $\Lambda_n^{(0)} = \omega_n^2 + \omega_0^2 + 2|\omega_n|\gamma$ and $\Lambda_n^{(b)} = \omega_n^2 - \omega_b^2 + 2|\omega_n|\gamma$

$\hbar\beta \to 0$ there is a crossover temperature $T_R \equiv \hbar\omega_R/2\pi k_B$ above which the lowest positive eigenvalue about q_b vanishes

$$\Lambda_R^{(b)} = \omega_R^2 - \omega_b^2 + 2\omega_R\gamma = 0 \begin{cases} T_R = T_0 = \hbar\omega_b/2\pi k_B \ \text{ if } \ \gamma \ll \omega_b \\ T_R = \hbar\omega_b^2/4\pi\gamma k_B \ll T_0 \ \text{ if } \ \gamma \gg \omega_b \end{cases}$$

Evaluating $F = -\frac{1}{\beta}\ln Z(\beta) \approx -\frac{1}{\beta}\ln Z_0(\beta) + \frac{i}{\beta}\frac{|Z_1(\beta)|}{Z_0(\beta)}$

And using the high temperature form of $\Gamma_\beta^{(0)} = \begin{cases} (2/\hbar)\mathrm{Im}F & \text{if} \quad T \leq T_0 \\ (\omega_b\beta/\pi)\mathrm{Im}F & \text{if} \quad T \geq T_0 \end{cases}$

$$\Gamma = \frac{\omega_0}{2\pi}\frac{\omega_R}{\omega_b} f_q \exp -\beta V_0 \qquad \text{with} \qquad f_q = \prod_{n=1}^{\infty} \frac{\omega_n^2 + \omega_0^2 + 2\gamma|\omega_n|}{\omega_n^2 - \omega_b^2 + 2\gamma|\omega_n|}$$

For very weakly damped systems when $\hbar\omega_0\beta \ll 1$

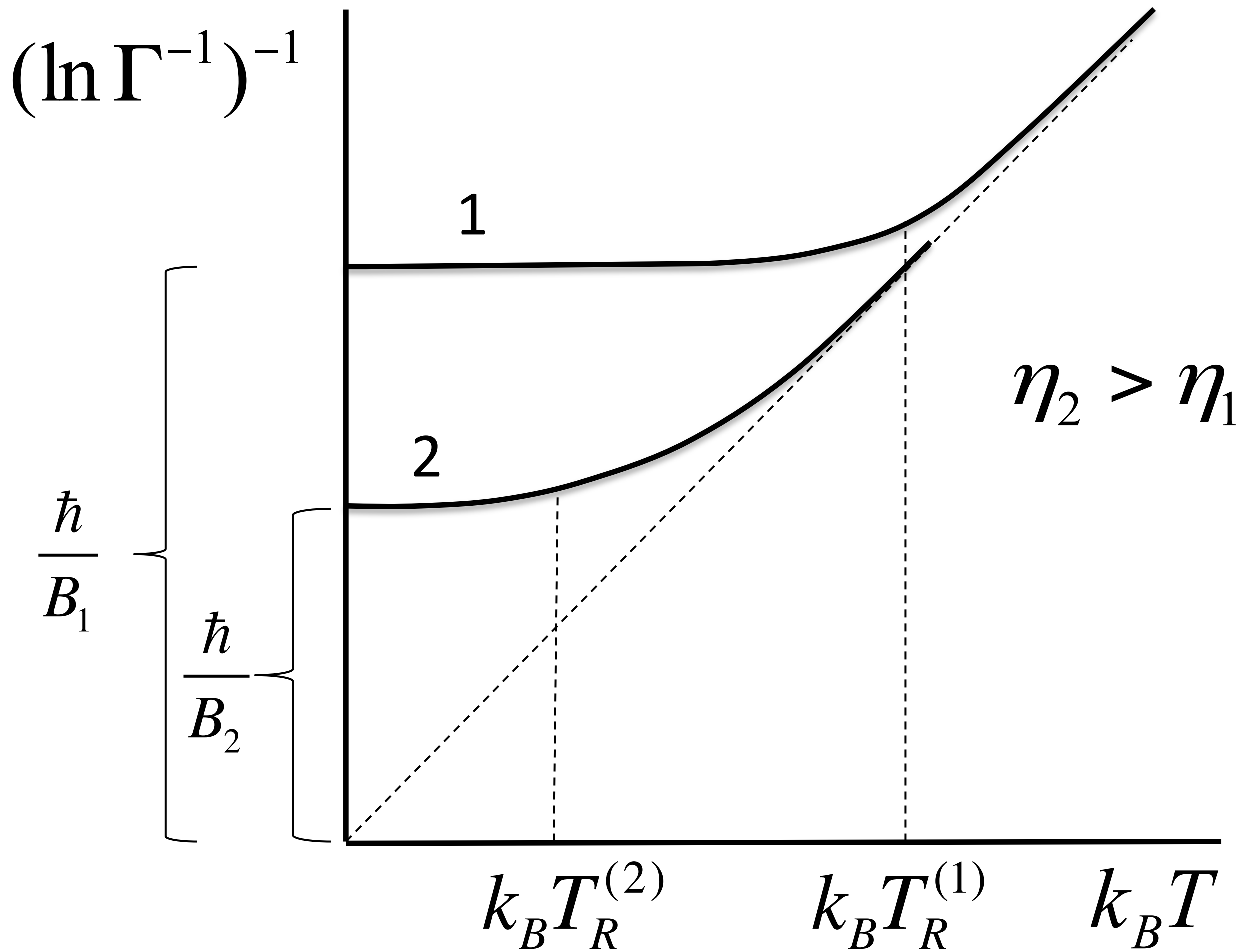
$$f_q \approx \exp\left[\frac{\hbar^2\beta^2}{24}(\omega_0^2 + \omega_b^2)\right] \Longrightarrow \Gamma_\beta = \frac{\omega_0}{2\pi}\exp -\beta\left(V_0 - \frac{\hbar^2\beta}{24}(\omega_0^2 + \omega_b^2)\right)$$

For very strongly overdamped systems when $\hbar\gamma\beta \ll 1$

$$\Gamma_\beta = \frac{\omega_0\omega_b}{4\pi\gamma}\exp -\beta\left(V_0 - \frac{\hbar^2\beta}{24}(\omega_0^2 + \omega_b^2)\right)$$

Finally when $T_R \ll T \ll \dfrac{\hbar\gamma}{k_B}$

$$\Gamma_\beta = \frac{\omega_0\omega_b}{4\pi\gamma}\exp -\beta\left(V_0 - \frac{\hbar(\omega_0^2 + \omega_b^2)}{4\pi\gamma}\ln\frac{\hbar\gamma\beta}{\pi}\right)$$



$(\ln \Gamma^{-1})^{-1}$
1
2
$\eta_2 > \eta_1$
$\frac{\hbar}{B_1}$
$\frac{\hbar}{B_2}$
$k_B T_R^{(2)}$
$k_B T_R^{(1)}$
$k_B T$