Euclidean Methods

How to estimate ground state energies via path integrals

$$\rho_N(x,y,\beta) = \langle x|e^{-\beta\mathcal{H}}|y\rangle = \int_y^x \mathcal{D}q(\tau)\, e^{-S_E[q(\tau)]/\hbar}$$

$$S_E[q(\tau)] = \int_0^{\hbar\beta} d\tau\, L_E(q,\dot{q}) \qquad \text{and} \qquad L_E(q,\dot{q}) = \frac{1}{2}M\dot{q}^2 + V(q)$$

$$\rho(x,y,\beta) = \langle x|e^{-\beta\mathcal{H}}|y\rangle = \sum_{n=0}^{\infty} \psi_n(x)\,\psi_n^*(y)\,e^{-\beta E_n}$$

$$\lim_{\beta\to\infty} \int_y^x \mathcal{D}q(\tau)\, e^{-S_E[q(\tau)]/\hbar} \approx \psi_0(x)\,\psi_0^*(y)\,e^{-\beta E_0}$$

$$\lim_{\beta\to\infty}\int_y^x \mathcal{D}q(\tau)\, e^{-S_E[q(\tau)]/\hbar} \approx \psi_0(x)\,\psi_0^*(y)\, e^{-\beta E_0}$$

Saddle point approximation $\left.\dfrac{\delta S_E}{\delta q}\right|_{q_c} = -M\ddot{q}_c + V'(q_c) = 0$

$$q_c(0) = y \text{ and } q_c(\hbar\beta) = x \text{ when } \hbar\beta \to \infty$$

$$S_E[q(\tau)] \simeq S_E[q_c(\tau)] + \frac{1}{2}\int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau'\, d\tau''\, \delta q(\tau')\, \delta q(\tau'') \left.\frac{\delta^2 S_E}{\delta q(\tau')\,\delta q(\tau'')}\right|_{q_c}$$

$$\left.\frac{\delta^2 S_E}{\delta q(\tau')\,\delta q(\tau'')}\right|_{q_c} = -M\frac{d^2}{d\tau'^2}\delta(\tau' - \tau'') + V''(q_c)\delta(\tau' - \tau'')$$

$$\delta q(\tau') = q(\tau') - q_c(\tau') \qquad\qquad \delta q(\hbar\beta) = \delta q(0) = 0$$

$$S_E[q(\tau)] \simeq S_E[q_c(\tau)] + \frac{1}{2} \int_0^{\hbar\beta} \int_0^{\hbar\beta} d\tau'\, d\tau''\, \delta q(\tau')\, \delta q(\tau'') \frac{\delta^2 S_E}{\delta q(\tau')\, \delta q(\tau'')} \bigg|_{q_c}$$

Expansion in orthogonal functions $\quad \delta q(\tau') = \sum_{n=0}^{\infty} c_n q_n(\tau')$ with $q_n(\hbar\beta) = q_n(0) = 0$

and $\displaystyle \int_0^{\hbar\beta} d\tau'\, q_n(\tau')\, q_m(\tau') = \delta_{mn}$

$$S_E[q(\tau')] \to S_E(c_0, ..., c_n, ...) = S_E[q_c] + \frac{1}{2} \sum_{n=0}^{\infty} \lambda_n c_n^2$$

$$\int_y^x \mathcal{D}q(\tau)\, e^{-S_E[q(\tau)]/\hbar} \approx e^{-S_E[q_c]/\hbar}\, \frac{\mathcal{J}}{\mathcal{N}} \int \dots \int dc_0\, dc_1 \dots dc_n \dots \exp - \sum_n \frac{\lambda_n c_n^2}{2\hbar}$$

$$\int_y^x \mathcal{D}q(\tau)\, e^{-S_E[q(\tau)]/\hbar} \approx e^{-S_E[q_c]/\hbar}\, \frac{\mathcal{J}}{\mathcal{N}} \prod_n \left(\frac{2\pi\hbar}{\lambda_n}\right)^{1/2}$$

$$\equiv \frac{1}{\mathcal{N}_R} \left(\frac{1}{\det[-M\partial_\tau^2 + V''(q_c)]}\right)^{1/2} e^{-S_E[q_c]/\hbar}$$

$$\mathcal{N}_R \equiv \mathcal{N}/(\mathcal{J} \prod_n \sqrt{2\pi\hbar})$$

Harmonic oscillator

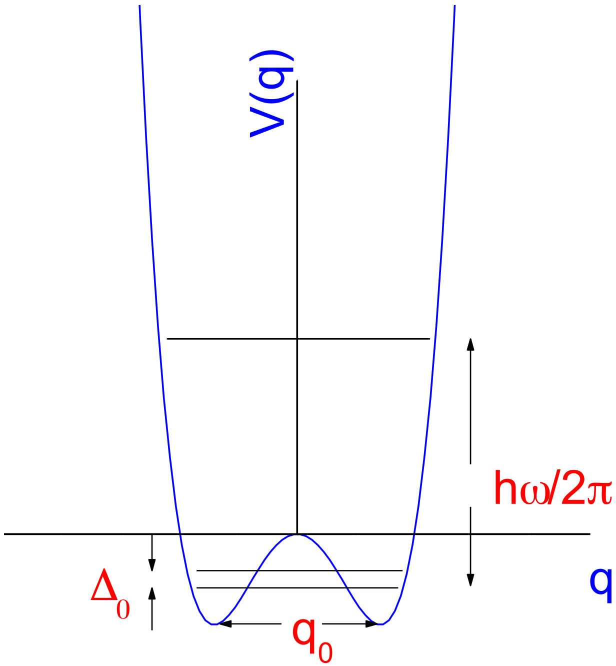
The classical solution $q_c(\tau) = 0$ ➡ $S_E[q_c] = 0$

Then we need $\rho(0, 0, \beta)$ which is given by

$$\frac{1}{\mathcal{N}_R}\left(\frac{1}{\det[-M\partial_\tau^2 + M\omega^2]}\right)^{1/2} \approx \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \exp -\frac{\hbar\omega\beta}{2}$$

From which we get $|\psi_n(0)|^2 = (M\omega/\pi\hbar)^{1/2}$ and $E_0 = \hbar\omega/2$

Bistable potential



$$V(q) = -\frac{1}{2}M\omega_0^2 q^2 + \frac{1}{4}\lambda q^4 \qquad (\lambda > 0).$$

Euclidean energy

$$\frac{1}{2}M\dot{q}_c^2 - V(q_c) = 0$$

$q_c(-\hbar\beta/2) = -a$ and $q_c(\hbar\beta/2) = a$ → instantons

$q_c(-\hbar\beta/2) = a$ and $q_c(\hbar\beta/2) = -a$ → anti-instantons

$q_c(-\hbar\beta/2) = a$ and $q_c(\hbar\beta/2) = a$

$q_c(-\hbar\beta/2) = -a$ and $q_c(\hbar\beta/2) = -a$

3 main steps

a) Action of N excursions = NB where

$$S_E[q_c] = \int_{-\infty}^{\infty} d\tau' \left\{ \frac{1}{2} M \dot{q}_c^2 + V(q_c) \right\} = \int_{-\infty}^{\infty} d\tau' \, M \dot{q}_c^2 \equiv B$$

b) Determinant of N excursions

$$\frac{1}{\mathcal{N}_R} \left(\frac{1}{\det[-M\partial_\tau^2 + V''(q_c)]} \right)^{1/2} = \frac{K^N}{\mathcal{N}_R} \left(\frac{1}{\det[-M\partial_\tau^2 + M\omega^2]} \right)^{1/2}$$

$$= K^N \left(\frac{M\omega}{\pi\hbar} \right)^{1/2} \exp - \frac{\hbar\omega\beta}{2}$$

c) Integrating over the centers of the excursions

$$\lim_{\beta\to\infty} \int_{-\hbar\beta/2}^{\hbar\beta/2} d\bar{\tau}_1 \int_{-\hbar\beta/2}^{\bar{\tau}_1} d\bar{\tau}_2 \ldots \int_{-\hbar\beta/2}^{\bar{\tau}_{N-1}} d\bar{\tau}_N = \lim_{\beta\to\infty} \frac{(\hbar\beta)^N}{N!}$$

Therefore

$$\rho(-a,-a,\beta) = \rho(a,a,\beta) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \exp -\frac{\hbar\omega\beta}{2} \sum_{\text{even } N} \frac{(Ke^{-B/\hbar}\hbar\beta)^N}{N!}$$

$$\rho(a,-a,\beta) = \rho(-a,a,\beta) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \exp -\frac{\hbar\omega\beta}{2} \sum_{\text{odd } N} \frac{(Ke^{-B/\hbar}\hbar\beta)^N}{N!}$$

which give us $\rho(\pm a,-a,\beta) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \exp -\frac{\hbar\omega\beta}{2}$

$$\times \frac{1}{2}\left[\exp(Ke^{-B/\hbar}\hbar\beta) \mp \exp(-Ke^{-B/\hbar}\hbar\beta)\right]$$

But we know that $\quad |\psi_E\rangle \equiv |+\rangle \;\text{ and }\; |\psi_O\rangle \equiv |-\rangle$

And then $\quad E_\pm = \dfrac{\hbar\omega}{2} \mp \hbar K e^{-B/\hbar}$

with

$$|\langle+|\pm a\rangle|^2 = |\langle-|\pm a\rangle|^2 = \langle+|-a\rangle\langle a|+\rangle = -\langle-|-a\rangle\langle a|-\rangle = \frac{1}{2}\left(\frac{M\omega}{\pi\hbar}\right)^{1/2}$$

But we still need to compute K !

The zero eigenvalue problem

$$-M\partial_\tau \ddot{q}_c + V''(q_c)\dot{q}_c = -M\partial_\tau^2 \dot{q}_c + V''(q_c)\dot{q}_c = 0$$

Then $q_0(\tau) = \dfrac{\dot{q}_c(\tau)}{||\dot{q}_c||} = \left(\dfrac{B}{M}\right)^{1/2} \dot{q}_c(\tau)$ is a normalized eigenfunction with zero eigenvalue

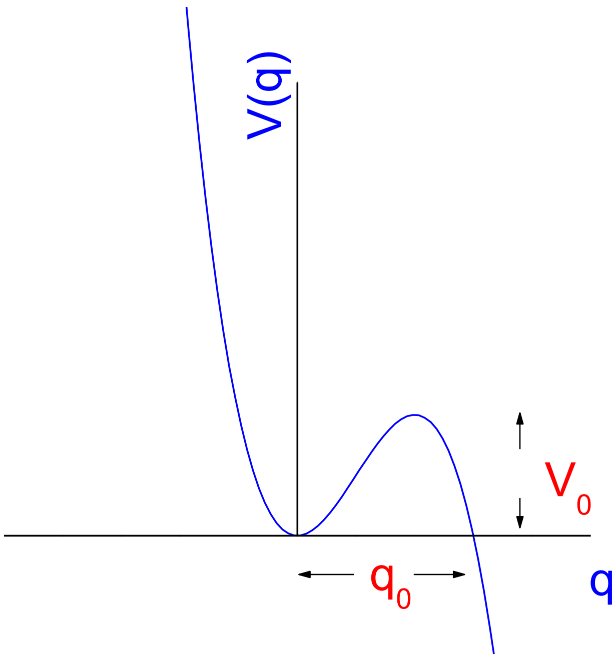
Variation along this direction $\delta q(\tau') = dc_0\, q_0(\tau') = \dfrac{dq_c(\tau')}{d\tau'}\, d\bar{\tau}$

Integral already performed $\dfrac{dc_0}{\sqrt{2\pi\hbar}} = \left(\dfrac{B}{2\pi\hbar M}\right)^{1/2} d\bar{\tau}$

And finally,

$$K = \left(\frac{B}{2\pi M\hbar}\right)^{1/2} \left(\frac{\det(-M\partial_\tau^2 + M\omega^2)}{\det'(-M\partial_\tau^2 + V''(q_c))}\right)^{1/2}$$

Metastable potential



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

$$\psi(q,t) \propto e^{-i(E_R + iE_I)t/\hbar}$$

$$\psi^*(q,t)\psi(q,t) \propto e^{-2|E_I|t/\hbar} \Rightarrow \Gamma = \frac{2|E_I|}{\hbar}$$

Appropriate solution for the Euclidean action : the bounce

Then $\rho(0,0,\beta) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \exp -\frac{\hbar\omega\beta}{2} \sum_N \frac{(Ke^{-B/\hbar}\hbar\beta)^N}{N!}$

$$= \left(\frac{M\omega}{\pi\hbar}\right)^{1/2} \exp -\frac{\hbar\omega\beta}{2} \exp(Ke^{-B/\hbar}\hbar\beta)$$

From which $E_0 = \frac{\hbar\omega}{2} - \hbar K e^{-B/\hbar}$

Analysis of the zero mode shows us that there must be a negative eigenvalue in the second variation problem.

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Analytic extension in function space

Eigenfunctions of zero and negative eigenvalues: $q_1(\tau)$ and $q_0(\tau)$

Path in function space parametrized by $f_z(\tau)$

$$f_0(\tau) = 0, \;\; f_1(\tau) = q_c(\tau), \;\text{ and } \partial f_z / \partial z|_{z=1} = q_0(\tau)$$

Integral to be evaluated $I \equiv \int \frac{dz}{\sqrt{2\pi\hbar}} \exp - \frac{S_E(z)}{\hbar}$

$$z > z_0 \qquad (S_E(z_0) = 0) \quad \Longrightarrow \quad S_E(z) < 0$$

$$S_E(1) = B \quad \text{is a saddle point} \quad \Longrightarrow \quad d^2 S_E(1)/dz^2 < 0$$

Along an appropriate contour z

Integral acquires an imaginary part

$$\mathrm{Im} I = \int_{1}^{1+i\infty} \frac{dz}{\sqrt{2\pi\hbar}} \exp -\frac{S_E(1)}{\hbar} \ \exp -\frac{S_E^{''}(1)}{2\hbar}(z-1)^2$$

$$= \frac{|S_E^{''}(1)|^{-1/2}}{2} \exp -\frac{S_E(1)}{\hbar}$$

which can be rewritten as $\mathrm{Im} \int \mathcal{D}q(\tau) \ \exp -\frac{S_E[q(\tau)]}{\hbar} =$

$$= \frac{1}{2\mathcal{N}_R}\left(\frac{B}{2\pi M\hbar}\right)^{1/2} \hbar\beta \left|\frac{1}{\det'[-M\partial_\tau^2 + V''(q_c)]}\right|^{1/2} \exp -\frac{B}{\hbar}$$

But as $\mathrm{Im} \int \mathcal{D}q(\tau) \ \exp -\frac{S_E[q(\tau)]}{\hbar} = \frac{\hbar\beta}{\mathcal{N}_R} \mathrm{Im} K \left|\frac{1}{\det[-M\partial_\tau^2 + M\omega^2)]}\right|^{1/2} \exp -\frac{B}{\hbar}$

$$\mathrm{Im}K = \frac{1}{2}\left(\frac{B}{2\pi M\hbar}\right)^{1/2}\left|\frac{\det[-M\partial_\tau^2 + M\omega^2]}{\det'[-M\partial_\tau^2 + V''(q_c)]}\right|^{1/2}$$

$$\Gamma = \left(\frac{B}{2\pi M\hbar}\right)^{1/2}\left|\frac{\det[-M\partial_\tau^2 + M\omega^2]}{\det'[-M\partial_\tau^2 + V''(q_c)]}\right|^{1/2} \exp -\frac{B}{\hbar}$$