Path Integral Picture of the Density Matrix

In the past lectures we found that the solution ~~pro~~ of the Langevin Equation with $\vec{f} = -\vec{\nabla}_q E(q)$ was equivalent ~~to~~ to the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \vec{\nabla}_q \cdot \left[\frac{\Gamma}{2} \vec{\nabla}_q P - \frac{1}{2\gamma} \vec{\nabla}_q E \, P \right]$$

for $P = P(\vec{q}, t)$ the probability to find the particle at $\vec{q}$ at time t if it was at $\vec{q} = 0$ at $t = 0$. We also saw that

$$P(\vec{q}, t) = e^{-\frac{1}{2\gamma\Gamma} E(\vec{q})} \langle \vec{q} | U(t,0) | \vec{0} \rangle e^{\frac{1}{2\gamma\Gamma} E(\vec{0})}$$

where $\langle \vec{q} | U(t,0) | 0 \rangle$ satisfies

$$-\frac{\partial}{\partial t} \langle \vec{q} | U(t,0) | 0 \rangle = \tilde{H} \langle \vec{q} | U(t,0) | 0 \rangle$$

where $\tilde{H} = \frac{\Gamma}{2} \hat{\vec{P}}^2 + \frac{\Gamma}{8} (\vec{\partial}_q E)^2 - \frac{\Gamma}{4} \nabla^2 E$

and $\lim_{t \to 0} \langle \vec{q} | U(t,0) | 0 \rangle = 0$

Clearly $U(t,0) = e^{-t \tilde{H}}$ is a density matrix with "$\beta \equiv \frac{1}{t}$"

In equilibrium quantum statistical mechanics we are interested in the density matrix operator $\rho = e^{-\beta H}$ for some H.

We will discuss here a path-integral method that works for both problems (since they are the same!)

Let us consider operators H of the form $H = \frac{\vec{p}^{\,2}}{2m} + V(\vec{q})$

Recall that $[q, p] = i\hbar$

The states $\{|q\rangle\}$ are complete $(\hat{q}|q\rangle = q|q\rangle)$

$$\int_{-\infty}^{+\infty} dq \; |q\rangle\langle q| = \hat{I} \qquad \text{(identity)}$$

$$\Rightarrow \langle q'|\hat{I}|q''\rangle = \delta(q'-q'') = \int_{-\infty}^{+\infty} dq \, \langle q'|q\rangle\langle q|q''\rangle$$

$$= \int dq \; \delta(q'-q)\,\delta(q-q'')$$

$$= \delta(q'-q'') \quad \checkmark$$

But the states $\{|p\rangle\}$ are also complete

$\hat{\vec{p}}\,|\vec{p}\rangle = \vec{p}\,|\vec{p}\rangle$;

Consider now the operator (or rather the matrix element)

$$F(\vec{q},t) = \langle \vec{q} |\, e^{-\frac{t}{\hbar}H} \,| 0 \rangle$$

Let us split the (imaginary!) time interval in N pieces each of length $\Delta\tau$, such that $N\Delta\tau = t$

$$\Rightarrow \quad e^{-\frac{t}{\hbar}H} = \underbrace{e^{-\frac{\Delta\tau}{\hbar}H} \cdots\cdots e^{-\frac{\Delta\tau}{\hbar}H}}_{N \text{ factors}}$$

Let us insert the Identity operator ~~between~~ between each pair of factors $\Rightarrow$ we need a total of $N-1$ expressions of the form

$$I = \int dq \; |q\rangle\langle q|$$

(which is called "the resolution of the identity")

$$\Rightarrow F(\vec{q},t) = \int_{q_j} \langle \vec{q} | e^{-\frac{\Delta t}{\hbar}H} | q_{N-1}\rangle \langle q_{N-1} | e^{-\frac{\Delta t}{\hbar}H} | q_{N-2}\rangle \cdots$$

$$\cdots \langle \vec{q}_1 | e^{-\frac{\Delta t}{\hbar}H} | 0 \rangle$$

$$= \int \prod_{j=1}^{N-1} d\vec{q}_j \; \prod_{j=1}^{N} \langle \vec{q}_j | e^{-\frac{\Delta t}{\hbar}H} | \vec{q}_{j-1}\rangle$$

with $\vec{q}_N \equiv \vec{q}$ and $\vec{q}_0 = 0$

L20 Since $\Delta\tau$ is small we can expand

$$\langle q_j | e^{-\frac{\Delta\tau}{\hbar} H} | q_{j-1}\rangle = \langle q_j | I - \frac{\Delta\tau}{\hbar} H + O(\Delta\tau^2) | q_{j-1}\rangle$$

$$= \langle q_j | I | q_{j-1}\rangle - \frac{\Delta\tau}{\hbar} \langle q_j | H | q_{j-1}\rangle + \cdots$$

Since $H = \frac{\vec{p}^2}{2m} + V(\hat{q})$

$$\langle \quad \rangle = \delta(q_j - q_{j-1}) - \frac{\Delta\tau}{\hbar} \langle q_j | \frac{\vec{p}^2}{2m} | q_{j-1}\rangle - \frac{\Delta\tau}{\hbar} \langle q_j | V(q) | q_{j-1}\rangle + \cdots$$

$$\simeq \delta(q_j - q_{j-1}) - \frac{\Delta\tau}{\hbar} \langle q_j | \frac{\vec{p}^2}{2m} | q_{j-1}\rangle - \frac{\Delta\tau}{\hbar} V\left(\frac{q_j + q_{j-1}}{2}\right) \delta(q_j - q_{j-1}) + \cdots$$

Feynman's midpoint rule.

$$\langle q | \frac{\vec{p}^2}{2m} | q'\rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \langle q | p\rangle \frac{p^2}{2m} \langle p | q'\rangle$$

$$= \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} e^{i\frac{pq}{\hbar}} \frac{p^2}{2m} e^{-i\frac{pq'}{\hbar}}$$

and $\langle q | q'\rangle = \int \frac{dp}{2\pi\hbar} e^{ip(q-q')/\hbar} = \delta(q-q')$

$$\langle \quad \rangle = \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} e^{i\frac{p_j}{\hbar}(q_j - q_{j-1})} \left[1 - \frac{\Delta\tau}{\hbar}\left(\frac{p_j^2}{2m} + V\left(\frac{q_j + q_{j-1}}{2}\right)\right) + \cdots\right.$$

$$= \int \frac{dp_j}{2\pi\hbar} \, e^{i\frac{\Delta\tau}{\hbar} p_j \dot{q}_j - \frac{\Delta\tau}{\hbar}\left(\frac{p_j^{\,2}}{2m} + V\left(\frac{q_j+q_{j+1}}{2}\right)\right) + \cdots}$$

phase space!

$$\Rightarrow F(\vec{q},t) = \int \prod_{j=1}^{N} \frac{dq_j \cdot dp_j}{2\pi\hbar} \, e^{\sum_j \left[i\frac{\Delta\tau}{\hbar} p_j \dot{q}_j - \frac{\Delta\tau}{\hbar}\left(\frac{p_j^{\,2}}{2m} + V(q_j)\right)\right]}$$

In the limit $\Delta\tau \to 0$, $N \to \infty$ we get the formal expression

$$F(\vec{q},t) = \int \mathcal{D}q \, \mathcal{D}p \; e^{\int_0^t \frac{d\tau}{\hbar}\left(i\,\vec{p}\cdot\frac{d\vec{q}}{d\tau} - \frac{\vec{p}^{\,2}}{2m} - V(\vec{q})\right)}$$

$$\int \frac{dp_j}{2\pi\hbar} \, e^{i\frac{\Delta\tau}{\hbar} p_j \dot{q}_j - \frac{\Delta\tau}{\hbar}\cdot\frac{p_j^{\,2}}{2m}} = \# \; e^{-\frac{m\Delta\tau}{2\hbar}\dot{q}_j^{\,2}}$$

$$\Rightarrow \boxed{F(\vec{q},t) = \text{const} \int \mathcal{D}q \; e^{-\frac{1}{\hbar}\int_0^t d\tau\left[\frac{m}{2}\left(\frac{d\vec{q}}{d\tau}\right)^2 + V(\vec{q})\right]}}$$

the constant is independent of V

Feynman Path Integral in imaginary time.

with $\vec{q}(0) = 0$ and $\vec{q}(t) = \vec{q}$.

<u>Note</u>: The Partition Function $Z = \operatorname{tr} e^{-\beta H}$

$$= \int d\vec{q} \, \langle \vec{q} | e^{-\beta H} | \vec{q} \rangle$$

$$\equiv \int d\vec{q} \, \langle \vec{q} | e^{-\frac{(\beta\hbar)H}{\hbar}} | \vec{q} \rangle$$

$$= \int_{\vec{q}(0)=\vec{q}(\beta\hbar)} \mathcal{D}\vec{q} \; e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[\frac{m}{2}\left(\frac{d\vec{q}}{d\tau}\right)^2 + V(\vec{q})\right]}$$

$\vec{q}(0)=\vec{q}(\beta\hbar) \leftrightarrow$ periodic boundary conditions!

Note: For the Langevin Equation, $\hbar = 1$ and

$$m = \frac{1}{\Gamma}$$

$$F(\vec{q},t) = \text{const} \int \mathcal{D}\vec{q}\; e^{-\int_0^t d\tau \left[\frac{1}{2\Gamma}\left(\frac{dq}{dt}\right)^2 + V(q)\right]}$$

$$V(q) = \frac{1}{8\Gamma\gamma^2}\left(\partial_{\vec{q}} E(\vec{q})\right)^2 - \frac{1}{4\gamma}\,\partial_{\vec{q}}^2 E(\vec{q})$$

and $$P(\vec{q},t) = e^{-\frac{1}{2\gamma\Gamma}E(\vec{q})}\; F(\vec{q},t)$$

Since the constant is independent of V, we will fix it for the $V=0$ $(E=0)$ free particle case, i.e. ~~free~~ diffusion. In this case

$\Rightarrow$ $P(q,t) = F(q,t)$ and

$$\frac{\partial P}{\partial \tau} = \frac{\Gamma}{2}\,\partial_q^2 P \quad \Rightarrow D = \frac{\Gamma}{2}$$

$$P = F = (2\pi\Gamma t)^{-d/2}\, e^{-\vec{q}^{\,2}/2\Gamma t}$$

$\Rightarrow$ For free diffusion we ~~must~~ must have

$$\text{const} \times \int \mathcal{D}q\; e^{-\int_0^t d\tau\, \frac{1}{2\Gamma}\left(\frac{d\vec{q}}{dt}\right)} = (2\pi\Gamma t)^{-d/2}\, e^{-\frac{\vec{q}^{\,2}}{2\Gamma t}}$$

We will use this result later on.

How about quantum mechanics at $T=0$?

A quantity of interest is

$$F(t) = \langle \psi(t) | \psi(t') \rangle$$

where $i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$ (Schrödinger Eqn.)

$$-i\hbar \frac{\partial}{\partial t} \langle \psi(t)| = \langle \psi(t)| H \qquad (H^{\dagger} = H)$$

$$\Rightarrow |\psi(t)\rangle = e^{-\frac{i}{\hbar} H(t-t')} |\psi(t')\rangle$$

$$\langle \psi(t)| = \langle \psi(0)| e^{\frac{i}{\hbar} Ht}$$

$$\Rightarrow F(t) = \langle \psi(t')| e^{\frac{i}{\hbar} H(t-t')} |\psi(t')\rangle$$

It is the same object but with $-t \to \frac{it}{\hbar}$ (real time)

The Path Integral now is

$$F(t,t') = \int \mathcal{D}p \, \mathcal{D}q \; e^{\frac{i}{\hbar} \int_{t'}^{t} dt'' \left[p\dot{q} - H(p,q) \right]}$$

If KE $= \frac{p^2}{2m} \Rightarrow$

$$F(t,t') = \int_{\substack{q(t')=q' \\ q(t)=q}} \mathcal{D}q \; e^{\frac{i}{\hbar} \int_{t'}^{t} \left[\frac{m}{2} \dot{q}^2 - V(q) \right] dt''}$$

Note: Action $= S = \int dt'' \left[\frac{m}{2} \dot{q}^2 - V(q) \right] = \int dt \, L$

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How to compute Path Integrals

We will use only imaginary time path-integrals.

Path integrals can be computed exactly only if ~~they are~~ the exponent is a "gaussians", i.e. quadratic form in q and $\dot{q}$

Otherwise ~~~~ some form of perturbation theory must be used, e.g. an expansion in powers of V or a semiclassical expansion. In practice both approaches reduce to the computation of a suitable gaussian path integral and corrections.

Gaussian Path Integrals

The exponent of the integrand of the path integral will be called the (Euclidean) Action

$$\frac{S}{\hbar} = \frac{1}{\hbar}\int_0^t d\tau \left[\frac{1}{2} m \left(\frac{d\vec{q}}{d\tau}\right)^2 + V(\vec{q}(\tau))\right]$$

Semiclassical limit: $\hbar \to 0$ $\Rightarrow$ look for extremal path

$$S = \int_0^t d\tau \; L\,[\partial_\tau q, q]$$

$$\delta S = \int_0^t d\tau \left[\frac{\partial L}{\partial \dot{q}}\,\delta\dot{q} + \frac{\partial L}{\partial q}\,\delta q\right] = \int_0^t d\tau \,\frac{\partial}{\partial \tau}\left[\frac{\partial L}{\partial \dot{q}}\,\delta q\right] +$$

$$+ \int_0^t d\tau \left[-\frac{\partial}{\partial \tau}\left(\frac{\partial L}{\partial \dot{q}}\right) + \frac{\partial L}{\partial q} \right] \delta q(\tau)$$

where $q(0) = 0$ and $q(t) = q$

and $\delta q(0) = \delta q(t) = 0$

$$\Rightarrow \int_0^t d\tau \frac{\partial}{\partial \tau}\left[\frac{\partial L}{\partial \dot{q}} \delta q \right] = 0$$

$$\Rightarrow \delta S = 0 \quad \Longleftrightarrow \quad -\frac{\partial}{\partial \tau}\left(\frac{\partial L}{\partial \frac{dq}{d\tau}} \right) + \frac{\partial L}{\partial q} = 0$$

Euler – Lagrange (or Newton! in real time.)

Here $L = \frac{m}{2} \left(\frac{\partial q}{\partial \tau}\right)^2 + V(q)$

note!

$$\frac{\partial L}{\partial \dot{q}} = m \dot{q} = m \frac{dq}{d\tau}$$

$$\Rightarrow -m \frac{d^2 q}{d\tau^2} + \frac{\partial V}{\partial q} = 0$$

$$\Rightarrow m \frac{d^2 q}{d\tau^2} = + \frac{\partial V}{\partial q}$$

(i.e. Newton's Eqn in an inverted potential.)

We need a solution of this eqn

with $q(0) = 0$ and $q(t) = q$

Expansion: $q(\tau) = q_c(\tau) + \delta q(\tau)$

$\uparrow$ solution of Euler-Lagrange.

$$\Rightarrow \quad S = \int_0^t d\tau \, L(q_c + \delta q, \dot{q}_c + \delta \dot{q})$$

$$= \int_0^t d\tau \Big\{ L(q_c, \dot{q}_c) + \frac{\partial L}{\partial q}\Big|_{q_c} \delta q + \frac{\partial L}{\partial \dot{q}}\Big|_{q_c} \delta \dot{q} + $$

$$+ \frac{1}{2!} \frac{\partial^2 L}{\partial q^2}\Big|_{q_c} (\delta q)^2 + \frac{\partial^2 L}{\partial \dot{q}^2}\Big|_{q_c} (\delta \dot{q})^2 + 2 \frac{\partial^2 L}{\partial q \partial \dot{q}}\Big|_{q_c} \delta q \delta \dot{q}$$

$$+ \ldots \Big\}$$

The terms linear in δq and $\delta \dot{q}$ vanish by construction!

$$\Rightarrow \quad S = S_c + \frac{1}{2!} \int_0^t d\tau \left(\frac{\partial^2 L}{\partial \dot{q}^2} (\delta \dot{q})^2 + \frac{\partial^2 L}{\partial q^2} (\delta q)^2 + 2 \frac{\partial^2 L}{\partial q \partial \dot{q}} \delta q \delta \dot{q} \right.$$

$$+ \ldots$$

$\nearrow$ "classical action"

But $\frac{\partial L}{\partial \dot{q}} = m \dot{q} \Rightarrow \frac{\partial^2 L}{\partial q \partial \dot{q}} = 0$ and $\frac{\partial^2 L}{\partial \dot{q}^2} = m$

and $\frac{\partial L}{\partial q} = \frac{\partial V}{\partial q}$, $\frac{\partial^2 L}{\partial q^2} = \frac{\partial^2 V}{\partial q^2} = V''(q)$

$$\Rightarrow \quad S = S_c + \int_0^t d\tau \left[\frac{1}{2} m (\delta \dot{q})^2 + \frac{1}{2} V''(q)\Big|_{q_c} (\delta q)^2 \right] + \cdots$$

$$\int d\tau \; \delta\dot{q} \; \delta\dot{q} = -\int_0^t d\tau \; \delta q(\tau) \frac{d^2}{d\tau^2} \delta q(\tau)$$

(since $\delta q(0) = \delta q(\tau) = 0$)

$$S = S_c + \int_0^t d\tau \; \delta q(\tau) \; \frac{1}{2} \left[-m \frac{d^2}{d\tau^2} + V''(q_c(\tau)) \right] \delta q(\tau) + \cdots$$

in general it depends on τ

where $S_c = \int_0^t d\tau \left[\frac{1}{2} m \dot{q}_c^2 + V(q_c) \right]$

$$\Rightarrow \quad F(q,t) = e^{-\frac{1}{\hbar} S(\dot{q}_c, q_c)} \int_{\delta q(0) = \delta q(t) = 0} \mathcal{D}q \; e^{-\frac{1}{\hbar} \int_0^t d\tau \; \delta q(\tau) \frac{1}{2} \left[-m \frac{d^2}{d\tau^2} + V''(q_c) \right] \delta q(\tau)} \{ 1 + \cdots$$

correction

The operator $-m \frac{d^2}{d\tau^2} + V''(q_c)$ is Hermitean and it has a spectrum of eigenvalues and eigenvectors :

$$-m \frac{d^2 \varphi_n(\tau)}{d\tau^2} + V''(q_c(\tau)) \varphi_n(\tau) = \varepsilon_n \varphi_n(\tau)$$

where $\varphi_n(0) = \varphi_n(t) = 0$

$\Rightarrow$ We can expand $\delta q(\tau) = \sum_n c_n \varphi_n(\tau)$

$$\Rightarrow \mathcal{D}\delta q \equiv \prod_n dc_n$$

$$\Rightarrow \int \mathcal{D}\delta q \; e^{-\frac{1}{\hbar}\int_0^t d\tau \; \delta q(\tau)\, \frac{1}{2}\left[-m\frac{d^2}{d\tau^2} + V''(q_c)\right]\delta q(\tau)}$$

$$= \int \prod_n dc_n \; e^{-\frac{1}{2\hbar}\sum_{n,n'} c_n c_{n'} \int_0^t d\tau\, \varphi_n(\tau)\left[-m\frac{d^2}{d\tau^2} + V''(q_c)\right]\varphi_{n'}(\tau)}$$

$$= \int \prod_n dc_n \; e^{-\frac{1}{2\hbar}\sum_{n,n'} c_n c_{n'} \int_0^t d\tau\, \varphi_n(\tau)\, \varepsilon_n\, \varphi_{n'}(\tau)}$$

But $\int_0^t d\tau \; \varphi_n(\tau)\varphi_{n'}(\tau) = \delta_{nn'}$ (e.v.'s are orthonormal)

$$= \int \prod_n dc_n \; e^{-\sum_n c_n^2 \frac{\varepsilon_n}{2\hbar}}$$

choose integration measure s.t. $\# = 1$

$$= \# \prod_n \frac{1}{\sqrt{\varepsilon_n}} \qquad (\text{assuming } \varepsilon_n > 0 \;\; \forall n)$$

Note: if $\exists\; \varepsilon_n < 0 \Rightarrow$ unstable expansion! we have the wrong saddle point

$$\Rightarrow \text{Gaussian path integral} = \prod_n \frac{1}{\sqrt{\varepsilon_n}} = \frac{1}{\sqrt{\prod_n \varepsilon_n}}$$

But $\mathrm{Det}\left[-m\frac{d^2}{d\tau^2} + V''\right] = \prod_n \varepsilon_n \Rightarrow$

$$\text{Gaussian Path Integral} = \frac{1}{\left(\mathrm{Det}\left[-m\frac{d^2}{d\tau^2} + V''\right]\right)^{1/2}}$$

$$\Rightarrow F(q,t) = e^{-\frac{S_c}{\hbar}} \left[\mathrm{Det}\left(-m\frac{d^2}{d\tau^2} + V''(q_c)\right)\right]^{-1/2} \{1 + O(\hbar)\}$$

Note: This expression is exact for quadratic actions i.e. harmonic oscillators and free particles.

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How to compute determinants: (Coleman's method

The function $V''(q_c(\tau)) = W(\tau)$

where $0 \leq \tau \leq t$

Let us construct the function $\psi_\lambda(\tau)$

$$-m\frac{d^2\psi_\lambda}{d\tau^2} + W(\tau)\psi_\lambda = \lambda\psi_\lambda$$

We will require $\psi_\lambda(\tau)$ to obey "initial conditions"

$\psi(0) = 0$ and $\frac{\partial\psi_\lambda}{\partial\tau}(0) = 1$

Consider now $\psi_\lambda(t) \Rightarrow \psi_\lambda(t) = 0 \Leftrightarrow \lambda \in \{E_n\}$

$\Rightarrow$ the zeros of $\psi_\lambda(t)$ are the eigenvalues $\{E_n\}$

We will assume that $W(\tau)$ is such that the spectrum has only non-degenerate eigenvalues and that the spectrum is discrete. Consider now two such potentials W_1 and W_2 and the ratio

$$\frac{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_1(\tau)-\lambda\right)}{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2(\tau)-\lambda\right)} \qquad \text{where } \lambda\in\mathbb{C}$$

$\Rightarrow$ the ratio has simple zeros on the spectrum of $-m\frac{d^2}{d\tau^2}+W_1$ and simple poles on the spectrum of $-m\frac{d^2}{d\tau^2}+W_2$

Let $\psi_1(t,\lambda)$ and $\psi_2(t,\lambda)$ be their associated functions $\Rightarrow$ $\frac{\psi_1(t,\lambda)}{\psi_2(t,\lambda)}$ also has simple zeros on the spectrum of $-m\frac{d^2}{d\tau^2}+W_1$ and simple poles on the spectrum of $-m\frac{d^2}{d\tau^2}+W_2$

$$\Rightarrow \frac{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_1-\lambda\right)}{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2-\lambda\right)} \Big/ \frac{\psi_1(t,\lambda)}{\psi_2(t,\lambda)} = \Phi(\lambda)$$

which is a meromorphic function with ~~which has~~ no zeros and no poles on the entire complex plane $\Rightarrow$ $\Phi(\lambda)$ is constant

Furthermore, away from the Real axis $\Phi(\lambda)\xrightarrow[|\lambda|\to\infty]{} 1$

$\Rightarrow$ $\Phi(\lambda)=1$ $\Rightarrow$

$$\frac{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_1-\lambda\right)}{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2-\lambda\right)} = \frac{\psi_1(t,\lambda)}{\psi_2(t,\lambda)}$$

Since we want

$$\frac{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_1\right)}{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2\right)} = \frac{\psi_1(t,0)}{\psi_2(t,0)}$$

i.e. we only need $\psi_i(t,0)$ (i.e. the "zero mode"

$\Rightarrow$ we will write

$$\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_1\right) = \mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2\right)\frac{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_1\right)}{\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2\right)}$$

$$= \mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W_2\right)\frac{\psi_1(t,0)}{\psi_2(t,0)}$$

In practice we will chose $W_2=0$ (free particle) and $W_1=W$

$$\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}+W\right) = \mathrm{Det}\left(-m\frac{d^2}{d\tau^2}\right)\frac{\psi(t,0)}{\psi_0(t,0)}$$

free particle

$$\Rightarrow -m\frac{d^2}{d\tau^2}\psi_0(\lambda,\tau) = \lambda\,\psi_0(\lambda,\tau)$$

$$\lambda=0 \Rightarrow \frac{d^2\psi}{d\tau^2}=0 \Rightarrow \psi = a + b\,\tau \Rightarrow \begin{cases}\psi(0)=0 \Rightarrow a=0\\ \psi'(0)=1 \Rightarrow b=1\end{cases}$$

$$\Rightarrow \quad F(q,t) = e^{-\frac{S_c}{\hbar}(q,\dot{q})} \left[\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}\right)\right]^{-1/2} \left[\frac{\psi(t;0)}{\psi_0(t,0)}\right]^{-1/2}$$

$$\mathrm{Det}\left(-m\frac{d^2}{d\tau^2}\right) = \frac{2\pi\hbar t}{m} \qquad (\text{free particle})$$

$$\psi_0(t) = t \qquad (d=1)$$

$$F(q,t) = e^{-\frac{S_c}{\hbar}(q,\dot{q})} \sqrt{\frac{m}{2\pi\hbar}} \left(\psi(t,0)\right)^{-1/2}$$

For the linear harmonic oscillator we have:

$$V = \frac{1}{2} k q^2 \Rightarrow V'' = k$$

$$\Rightarrow \quad W = -m\frac{d^2}{d\tau^2} + k$$

and

$$-m\frac{d^2\psi}{d\tau^2} + k\psi = 0 \qquad (\lambda = 0)$$

$$\psi = A\, e^{\sqrt{\frac{k}{m}}\tau} + B\, e^{-\sqrt{\frac{k}{m}}\tau}$$

$$\psi(0) = 0 \Rightarrow A = -B$$

$$\psi'(0) = 1 \Rightarrow A = \frac{1}{2}\sqrt{\frac{m}{k}} = \frac{1}{2\omega}$$

$$\psi(t,0) = \frac{\sinh(\omega t)}{\omega}$$

$$F(q,t) = e^{-\frac{S_c}{\hbar}(q,t)} \sqrt{\frac{m}{2\pi\hbar t}} \sqrt{\frac{\omega t}{\sinh\omega t}}$$

If we are interested in $q(t) = q$ with $q(0) = 0$

$$\Rightarrow \quad m \frac{d^2 q}{d\tau^2} = k\, q$$

$$q(\tau) = a\, e^{\omega\tau} + b\, e^{-\omega\tau}$$

$$\Rightarrow q(0) = 0 \Rightarrow a = -b$$

$$q(t) = q = a\left(e^{\omega t} - e^{-\omega t}\right)$$

$$q = 2a \sinh(\omega t)$$

$$\cancel{\sinh \omega t = q} \qquad a = \frac{q}{2 \sinh \omega t}$$

$$\frac{S_c}{\hbar} = \frac{1}{\hbar}\int_0^t d\tau \left[\frac{m}{2}\left(\frac{dq_c}{d\tau}\right)^2 + \frac{k}{2} q_c^2\right]$$

$$= \frac{1}{\hbar}\int_0^t d\tau \left[\frac{m}{\cancel{2}} \cancel{4}^{2} a^2 \omega^2 \cosh^2 \omega\tau + \frac{k}{\cancel{2}} \cancel{4}^{2} a^2 \sinh^2 \omega\tau\right]$$

$$= \frac{2k}{\hbar} a^2 \int_0^t d\tau \left(\cosh^2 \omega\tau + \sinh^2 \omega\tau\right)$$

$$= \frac{2k a^2}{\hbar} \int_0^t d\tau \quad \cosh(2\omega\tau)$$

$$\frac{S_c}{\hbar} = \frac{\cancel{2} k a^2}{\hbar} \frac{1}{\cancel{2}\omega} \sinh(2\omega\tau)$$

$$\Rightarrow \frac{S_c}{\hbar} = \frac{\cancel{2} m \omega^{\cancel{2}} q^2}{\hbar\, \cancel{4}\, \sinh^2(\omega t)} \quad \frac{\sinh 2\omega t}{2\cancel{\omega}} = \frac{m\omega q^2}{2\hbar} \coth(\omega t)$$

$$F(q,t) = e^{-\frac{m\omega q^2 \coth(\omega t)}{\cancel{2}\hbar}} \left(\frac{m\omega}{2\pi\hbar \sinh \omega t}\right)^{1/2}$$

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Application 1

Diffusion in $d=1$ in a Harmonic Potential:

$E = \frac{1}{2} k q^2$. Set $\hbar = 1$ and

$$L = \frac{1}{2\Gamma}\left(\frac{dq}{d\tau}\right)^2 + V(q)$$

$$V(q) = \frac{k^2 q^2}{8\Gamma\gamma^2} - \frac{k}{4\gamma}$$

$\Rightarrow$

$$P(q,t) = e^{-\frac{1}{4}\frac{k}{\gamma\Gamma}q^2} e^{-\frac{kq^2}{\cancel{4}\Gamma\gamma}\coth\left(\frac{kt}{2\gamma}\right)} e^{\frac{kt}{4\gamma}}$$

$$\times \left[\frac{k}{4\pi\Gamma\gamma \sinh\left(\frac{kt}{2\gamma}\right)}\right]^{1/2}$$

Note:

$$\lim_{t\to\infty} P(q,t) = e^{-\frac{k}{4\gamma\Gamma}q^2} e^{-\frac{kq^2}{\cancel{4}\gamma\Gamma}} \left(\frac{k}{2\pi\Gamma\gamma}\right)^{1/2}$$

$$\times \lim_{t\to\infty} \cancel{e^{\frac{kt}{4\gamma}}} \cancel{\left(e^{-\frac{kt}{2\gamma}}\right)^{1/2}}$$

$$= e^{-\frac{\frac{1}{2}kq^2}{\gamma\Gamma}}$$

$\Rightarrow \gamma\Gamma \equiv k_B T$ ✓

How fast is the approach to equilibrium?

$$P(q,t) = e^{-\frac{kq^2}{2\gamma\Gamma}\frac{1}{1-e^{-kt/\gamma}}} \left[\frac{k}{2\pi\Gamma\gamma(1-e^{-kt/\gamma})}\right]^{1/2}$$

e.g.

$$P(0,t) = \left[\frac{k}{2\pi\Gamma\gamma(1-e^{-kt/\gamma})}\right]^{1/2} \underset{\frac{kt}{\gamma}\gg 1}{\approx} \left(\frac{k}{2\pi\Gamma\gamma}\right)^{1/2}\left[1+\frac{1}{2}e^{-\frac{kt}{\gamma}}+\cdots\right]$$

exponentially fast

Also as $\frac{kt}{\gamma} \ll 1$

$$\Rightarrow \quad 1-e^{-kt/\gamma} \approx \frac{kt}{\gamma}$$

$$P(q,t) \longrightarrow \frac{e^{-\frac{q^2}{2\Gamma t}}}{(2\pi\Gamma t)^{1/2}}$$

✓ free diffusion at short times.

Application 2

Quantum Linear Harmonic Oscillator at finite temperature:

Since $\rho = e^{-\beta H}$ $\qquad \beta = \frac{1}{k_B T}$

Boltzmann!

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}kq^2$$

$$S = \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{dq}{d\tau}\right)^2 + \frac{1}{2}kq^2\right]$$

$$F(q,T) = \langle q | e^{-\beta H} | 0 \rangle$$
$$= e^{-\frac{m\omega q^2}{2\hbar}\coth\left(\frac{\hbar\omega}{kT}\right)} \left[\frac{m\omega}{2\pi\hbar\sinh\left(\frac{\hbar\omega}{kT}\right)}\right]^{1/2}$$

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Partition Function: We will discuss two approaches

(1) Look for periodic solutions of the eqn. of motion

e.g. for the LHO we have

$$m\frac{d^2\bar{q}}{d\tau^2} = k\,\bar{q}$$

$$\bar{q}(\tau) = A\,e^{\omega\tau} + B\,e^{-\omega\tau}$$

$$\Rightarrow \quad \bar{q}(0) = \bar{q}(\beta\hbar) = q =$$

$$q = A + B \mp A\,e^{\beta\hbar\omega} + B\,e^{-\beta\hbar\omega}$$

$$A[1 - e^{\beta\hbar\omega}] = B[e^{-\beta\hbar\omega} - 1]$$

$$A = B\,e^{-\beta\hbar\omega}$$

$$q = A + B = B(1 + e^{-\beta\hbar\omega})$$

$$B = \frac{q}{1 + e^{-\beta\hbar\omega}}$$

$$\bar{q}(\tau) = q\,\frac{e^{-\beta\hbar\omega}e^{\omega\tau} + e^{-\omega\tau}}{1 + e^{-\beta\hbar\omega}} = q\,\frac{\cosh\left(\omega\tau - \frac{\beta\hbar\omega}{2}\right)}{\cosh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\frac{1}{\hbar} S(\bar{q}, \dot{\bar{q}}) = \int_0^{\beta\hbar} d\tau \left[\frac{m}{2\hbar}\left(\frac{d\bar{q}}{d\tau}\right)^2 + \frac{k}{2\hbar}\, \bar{q}^{\,2} \right]$$

$$= \frac{m\omega^2 q^2}{2\hbar} \int_0^{\beta\hbar} d\tau \; \frac{\sinh^2(\omega\tau - \frac{\beta\hbar\omega}{2}) + \cosh^2(\omega\tau - \frac{\beta\hbar\omega}{2})}{\cosh^2 \frac{\beta\hbar\omega}{2}}$$

$$= \frac{m\omega^2 q^2}{2\hbar} \int_0^{\beta\hbar} d\tau \; \frac{\cosh(2\omega\tau - \beta\hbar\omega)}{\cosh^2(\frac{\beta\hbar\omega}{2})}$$

$$= \frac{m\omega^2 q^2}{2\hbar} \; \frac{1}{\cancel{2}\omega} \; \frac{\cancel{2}\, \sinh(\beta\hbar\omega)}{\cosh^2(\frac{\beta\hbar\omega}{2})}$$

$$\frac{S}{\hbar} = \frac{m\omega q^2}{\hbar} \tanh\left(\frac{\beta\hbar\omega}{2}\right)$$

$$\Rightarrow Z = \int_{-\infty}^{+\infty} dq \; \langle q | e^{-\beta H} | q \rangle$$

$$= \int_{-\infty}^{+\infty} dq \; e^{-\frac{m\omega q^2}{\hbar} \tanh\left(\frac{\beta\hbar\omega}{2}\right)} \left[\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)} \right]^{1/2}$$

$$= \frac{\sqrt{2\pi}}{\left[\frac{2\cancel{m\omega}}{\cancel{\hbar}} \tanh\left(\frac{\beta\hbar\omega}{2}\right)\right]^{1/2}} \left[\frac{\cancel{m\omega}}{2\cancel{\pi\hbar} \sinh(\beta\hbar\omega)} \right]^{1/2}$$

$$= \left(2\tanh\left(\frac{\beta\hbar\omega}{2}\right) 2\sinh\frac{\beta\hbar\omega}{2}\cosh\frac{\beta\hbar\omega}{2}\right)^{-1/2} = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\Rightarrow Z = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

check:

$$Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} = e^{-\frac{\hbar\beta\omega}{2}} \frac{1}{1-e^{-\beta\hbar\omega}}$$

$$= \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} \checkmark$$

Second Approach: Fourier Expansion.

Since $q(\tau) = q(\tau + \beta\hbar) \Rightarrow$

$$q(\tau) = \sum_{n=-\infty}^{+\infty} q_n e^{i\omega_n\tau} \qquad \text{with } q_n^* = -q_n$$

and $e^{i\omega_n\beta\hbar} = 1 \Rightarrow \beta\hbar\omega_n = 2\pi n$

$$\omega_n = \frac{2\pi}{\beta\hbar} n = \frac{2\pi}{\hbar} k_B T n \qquad \text{"Matsubara Frequencies"}$$

$$\frac{1}{\hbar} S[q,\dot{q}] = \frac{m}{2\cancel{\hbar}} \beta\cancel{\hbar} \sum_{n=-\infty}^{+\infty} |q_n|^2 \omega_n^2 + \frac{k}{2\cancel{\hbar}} \beta\cancel{\hbar} \sum_{n=-\infty}^{+\infty} |q_n|^2$$

$$= \frac{\beta}{2} \sum_{n=-\infty}^{+\infty} |q_n|^2 (m\omega_n^2 + k)$$

$$= \frac{\beta}{2}\left[q_0^2 k + 2\sum_{n=1}^{\infty} |q_n|^2 (m\omega_n^2 + k)\right]$$

$$Z = \mathcal{N} \int_{-\infty}^{+\infty} dq_0 \prod_{n=1}^{\infty} \int_{-\infty}^{+\infty} d\,\mathrm{Re}\,q_n \int_{-\infty}^{+\infty} d\,\mathrm{Im}\,q_n \; e^{-\frac{\beta k}{2\hbar} q_0^2} \prod_{n=1}^{\infty} e^{-\frac{\beta m}{2\hbar}(\omega_n^2+\omega^2)|q_n|^2}$$

$\uparrow$ normalization constant

$$= \mathcal{N}\left[\int_{-\infty}^{+\infty} dq_0 \; e^{-\frac{\beta k}{2\hbar} q_0^2}\right]\left(\prod_{n=1}^{\infty} \int_{-\infty}^{+\infty} d\,\mathrm{Re}\,q_n \; e^{-\frac{\beta m}{2\hbar}(\omega_n^2+\omega^2)(\mathrm{Re}\,q_n)^2}\right)$$

$$\left(\prod_{n=1}^{\infty} \int_{-\infty}^{+\infty} d\,\mathrm{Im}\,q_n \; e^{-\frac{\beta m}{2\hbar}(\omega_n^2+\omega^2)(\mathrm{Im}\,q_n)^2}\right)$$

$$\Rightarrow \quad Z = \mathcal{N} \sqrt{2\pi} \sqrt{\frac{\hbar}{\beta k}} \prod_{n=1}^{\infty} \frac{2\pi\hbar}{\beta m(\omega_n^2+\omega^2)}$$

Identity: $$\prod_{n=1}^{\infty} \frac{1}{1+\frac{z^2}{n^2}} = \frac{\pi z}{\sinh \pi z}$$

$$\omega_n = \frac{2\pi n}{\beta\hbar} \qquad\qquad \frac{\omega}{\omega_n} = \frac{\beta\hbar\omega}{2\pi}\,\frac{1}{n} \equiv \frac{z}{n}$$

$$Z = \mathcal{N} \sqrt{\frac{2\pi\hbar}{\beta k}} \left[\prod_{n=1}^{\infty} \frac{2\pi\hbar}{\beta m\omega_n^2}\right] \prod_{n=1}^{\infty} \frac{1}{1+\frac{\omega^2}{\omega_n^2}}$$

$$Z = \mathcal{N} \sqrt{\frac{2\pi\hbar}{\beta k}} \left[\prod_{n=1}^{\infty} \frac{2\pi\hbar}{\beta m\omega_n^2}\right] \frac{\cancel{\pi}\,\frac{\beta\hbar\omega}{2\cancel{\pi}}}{\sinh \cancel{\pi}\frac{\beta\hbar\omega}{2\cancel{\pi}}}$$

$$Z = \left[\mathcal{N} \sqrt{\frac{2\pi\hbar}{\beta m}} \left(\prod_{n=1}^{\infty} \frac{2\pi\hbar}{\beta m\omega_n^2}\right) \beta\hbar\right] \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

Thus we must choose $\mathcal{N}$ to cancel the bracket or, in other words, choose the Jacobian properly.

$$Z = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\Rightarrow \quad dq_0 \equiv \sqrt{\frac{m}{2\pi\hbar^2\beta}}\, dq_0 \quad ; \quad \frac{d\,\mathrm{Re}\,q_n \, d\,\mathrm{Im}\,q_n}{2\pi/(\beta m \omega_n^2)} \equiv d\,\mathrm{Re}\,q_n \, d\,\mathrm{Im}\,q_n$$

Correct for a classical system!

Perturbation Expansions:

Let us now consider a case in which we want to perturb a density matrix. Thus, let us take $H = H_0 + V$. Say let $H_0 = \frac{p^2}{2m}$ and $V \equiv g\,V$, i.e. a scattering problem $\Rightarrow$ How do we compute

$$\langle \vec{q} |\, \rho^{*} | 0 \rangle \equiv \rho(\vec{q}, 0; T) \; ?$$

$$\rho(\vec{q}, 0; T) = \int_{\substack{q(0)=0 \\ \vec{q}(\beta\hbar)=\vec{q}}} \mathcal{D}q \; e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{d\vec{q}}{d\tau}\right)^2 + gV[\vec{q}(\tau)]\right]}$$

Let us expand in powers of g:

$$\rho(\vec{q};0;T) = \sum_{n=0}^{\infty} \frac{\left(-\frac{g}{\hbar}\right)^n}{n!} \int_0^{\beta\hbar} d\tau_1 \cdots \int_0^{\beta\hbar} d\tau_n \int \mathcal{D}q \, e^{-S_0[q]}$$

$V[q(\tau_1)] \cdots V[q(\tau_n)]$

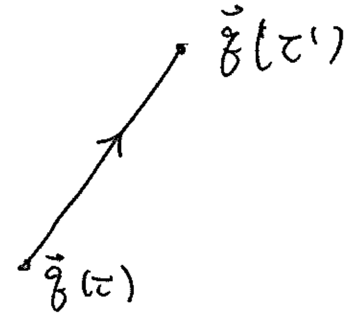
Let us look at the first order, $O(g)$, term:

$$\frac{1}{1!}\left(\frac{-g}{\hbar}\right) \int_0^{\beta\hbar} d\tau_1 \int_{\substack{q(0)=0 \\ q(\beta\hbar)=q}} \mathcal{D}q \; e^{-S_0[q]} \; V[q(\tau_1)]$$

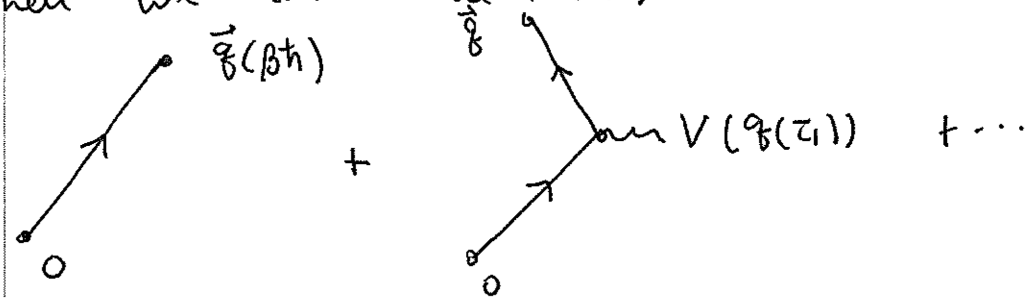
$$= \frac{1}{1!}\left(\frac{-g}{\hbar}\right) \int_0^{\beta\hbar} d\tau_1 \int d\vec{q}[\tau_1] \, \langle \vec{q} | e^{-\beta H_0} | \vec{q}(\tau_1) \rangle \, V(\vec{q}(\tau_1)) \, \langle \vec{q}(\tau_1) | e^{-\beta H_0} | \vec{q}(0) \rangle$$

If we represent

$$\langle \vec{q} | \, e^{-\beta H_0} \, | \vec{q}\,' \rangle \quad \longleftrightarrow$$



Then we have the series



In other words this is the Born series of multiple scattering processes. Thus, if we know the unperturbed density matrix, we can construct the series.

Finally, we will derive the following useful expression for the generating function:

$$Z[J] = \cancel{\mathcal{N}} \int_{PBC's} \mathcal{D}q \; e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{dq}{d\tau}\right)^2 + \frac{k}{2}q^2 + Jq\right]}$$

(i.e. $Z = \operatorname{tr} e^{-\beta H}$) ($\mathcal{N}$: same as before)

where $J \equiv J(\tau) \equiv J(\tau+\beta\hbar)$

Since $q(\tau) = q(\tau+\beta\hbar)$ we can compute this path integral by a simple method. Let us shift the variable $q(\tau)$,

$q \Rightarrow \bar{q} + \xi$ (both periodic)

$$\text{Action} = \int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{d\bar{q}}{d\tau}\right)^2 + \frac{k\bar{q}^2}{2} + J\bar{q} + \frac{m}{2}\left(\frac{d\xi}{d\tau}\right)^2 + \frac{k\xi^2}{2} + m\frac{d\bar{q}}{d\tau}\frac{d\xi}{d\tau} + k\bar{q}\xi + J\xi\right]$$

$$\int_0^{\beta\hbar} d\tau \, \frac{d\bar{q}}{d\tau} \frac{d\xi}{d\tau} = \underbrace{\int_0^{\beta\hbar} d\tau \, \frac{d}{d\tau}\left[\xi \frac{d\bar{q}}{d\tau}\right]}_{=0 \quad (\text{PBC's})} - \int_0^{\beta\hbar} d\tau \, \xi \frac{d^2\bar{q}}{d\tau^2}$$

$\Rightarrow$ Choose $\bar{q}$ /
$$-m \frac{d^2\bar{q}}{d\tau^2} + k\bar{q} + J = 0$$

Let $G(\tau,\tau')$ / $\left(-m\frac{d^2}{d\tau^2} + k\right) G(\tau,\tau') = \delta(\tau-\tau')$ (periodic!)

$$\Rightarrow \quad \bar{q}(\tau) = -\int_0^{\beta\hbar} d\tau' \, G(\tau-\tau') \, J(\tau')$$

$$\Rightarrow Z[J] = Z[0] \, e^{+\frac{1}{2\hbar}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau' \, J(\tau) G(\tau-\tau') J(\tau')}$$

L25 Computation of G:

$$\left(-m\frac{d^2}{d\tau^2} + k\right) G(\tau-\tau') = \delta(\tau-\tau')$$

$$G(\tau+\beta\hbar-\tau') = G(\tau-\tau')$$

$$G(\tau-\tau') = \sum_{n=-\infty}^{+\infty} G_n \, e^{i\omega_n(\tau-\tau')}$$

periodic!

$$\sum_{n=-\infty}^{+\infty} (m\omega_n^2 + k) \, G_n \, e^{i\omega_n(\tau-\tau')} = \delta(\tau-\tau')$$

$$G_n = \frac{1}{k+m\omega_n^2}\frac{1}{\beta\hbar} = \frac{1}{m\beta\hbar}\frac{1}{\omega^2+\omega_n^2}$$

$$\Rightarrow G(\tau-\tau') = \frac{1}{m\beta\hbar}\sum_{m=-\infty}^{+\infty} \frac{e^{i\omega_n(\tau-\tau')}}{\omega_n^2+\omega^2}$$

$$\omega_n = \frac{2\pi}{\beta\hbar}\, n$$

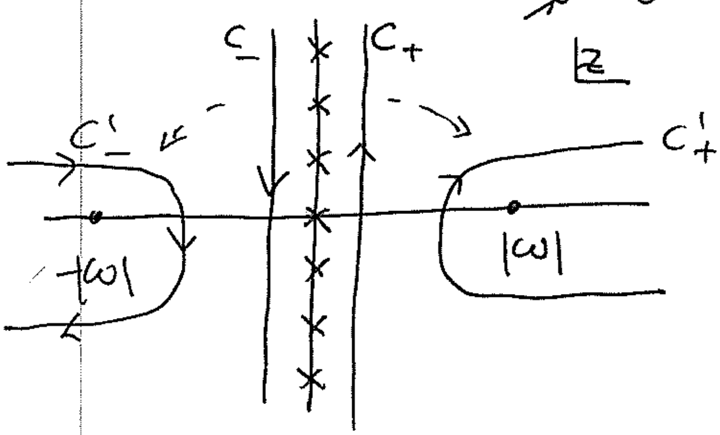
Let us consider the function $f(z)$

$$f(z) = \frac{\beta\hbar}{e^{\beta\hbar z}-1} \qquad \text{where } z \in \mathbb{C}$$

$f(z)$ has simple poles at $\beta\hbar z_n = 2\pi n i$

$$z_n = \frac{2\pi n}{\beta\hbar}\, i \equiv i\omega_n$$

$$\mathrm{Res}\left[f(z), i\omega_n\right] = \frac{\cancel{\beta\hbar}}{\cancel{\beta\hbar}\, e^{\beta\hbar z_n}} = \frac{1}{e^{i\beta\hbar\omega_n}} = 1$$



$$\Rightarrow \oint_C \frac{dz}{2\pi i}\, f(z)\, F(z) = \sum_{n=-\infty}^{\infty} \frac{\cancel{2\pi i}}{\cancel{2\pi i}}\, F(z_n)\cdot 1$$

Residue Thm.

let $$F(z) = \frac{e^{(\tau-\tau')z}}{\omega^2 - z^2}$$

$$\Rightarrow \sum_{n=-\infty}^{+\infty} F(z_n) = \sum_{n=-\infty}^{+\infty} \frac{e^{i\omega_n(\tau-\tau')}}{\omega^2 + \omega_n^2} \quad \checkmark$$

$$\Rightarrow \cancel{\sum_n} G(\tau-\tau') = \oint_C \frac{dz}{2\pi i}\left(\frac{\beta\hbar}{e^{\beta\hbar z}-1}\right)\frac{e^{(\tau-\tau')z}}{\omega^2-z^2}\frac{1}{\beta\hbar m}$$

(neg. oriented!)

$$= -\oint_{C'_+} \frac{dz}{2\pi i}\frac{\beta\hbar}{e^{\beta\hbar z}-1}\frac{e^{(\tau-\tau')z}}{\omega^2-z^2}\frac{1}{\beta\hbar m}$$

$$- \oint_{C'_-} \frac{dz}{2\pi i}\left(\frac{\beta\hbar}{e^{\beta\hbar z}-1}\right)\frac{e^{(\tau-\tau')z}}{\omega^2-z^2}\frac{1}{\beta\hbar m}$$

$$= \frac{1}{\beta\hbar m}\left[\frac{\beta\hbar}{e^{\beta\hbar\omega}-1}\frac{e^{\omega(\tau-\tau')}}{+2\omega} - \frac{\beta\hbar}{e^{-\beta\hbar\omega}-1}\frac{e^{-\omega(\tau-\tau')}}{+2\omega}\right]$$

$$= \frac{\cancel{\beta\hbar}}{2\omega}\frac{1}{\cancel{\beta\hbar} m}\frac{\cosh\left[\omega(\tau-\tau') - \frac{\beta\hbar\omega}{2}\right]}{\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$G(\tau-\tau') = \frac{1}{m\omega} \frac{\cosh\left(\omega|\tau-\tau'| - \frac{\beta\hbar\omega}{2}\right)}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\Rightarrow Z[J] = Z[0]\, e^{\frac{1}{2\hbar}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, J(\tau)\, G(\tau-\tau')\, J(\tau')}$$

Suppose that $g V(q) = g q^4$

First Order Correction:

$$\frac{1}{1!}\left(-\frac{g}{\hbar}\right)\int_0^{\beta\hbar} d\tau_1 \int \mathcal{D}q\, e^{-S_0(q)}\, V(q(\tau_1))$$

$$= -\frac{g}{\hbar}\int_0^{\beta\hbar} d\tau_1 \int \mathcal{D}q\, e^{-S_0(q)}\, [q(\tau_1)]^4$$

$$[q(\tau_1)]^4 = \left[-\hbar\frac{\delta}{\delta J(\tau_1)}\right]^4 e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, J(\tau)\, q(\tau)}\Bigg|_{J=0} Z[0]$$

$$\Rightarrow = -\frac{g}{\hbar}\int_0^{\beta\hbar} d\tau_1 \left[-\hbar\frac{\delta}{\delta J(\tau_1)}\right]^4 Z[J]\Bigg|_{J=0}$$

$$= -\frac{g}{\hbar}\,\frac{1}{2!}\left(\frac{1}{2\hbar}\right)^2 \#\, \hbar^4 \int_0^{\beta\hbar} d\tau_1 \left[G(\tau_1-\tau_1)\right]^2 Z[0]$$

where $\# =$ combinatorial factor $= 4!$

$$G(0) = \frac{1}{2m\omega}\coth\left(\frac{\beta\hbar\omega}{2}\right)$$

$$= -\frac{3}{4}\frac{g\hbar^2\beta}{(m\omega)^2}\coth^2\left(\frac{\beta\hbar\omega}{2}\right)\frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$Z = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}\left[1 - \frac{3g\hbar^2\beta}{4(m\omega)^2}\coth^2\left(\frac{\beta\hbar\omega}{2}\right) + O(g^2)\right]$$

$$Z = e^{-\beta F}$$

$$F = F_0 + gF_1 + O(g^2)$$

$$F = -k_BT\log Z$$

$$F = -k_BT\log Z_0 - k_BT\log\left[1 - \frac{3g\hbar^2\beta}{4(m\omega)^2}\coth^2\left(\frac{\beta\hbar\omega}{2}\right) + O(g^2)\right]$$

$$F = \frac{\hbar\omega}{2} + k_BT\log\left(1 - e^{-\beta\hbar\omega}\right)$$

$$+\frac{3g\hbar^2}{4(m\omega)^2}\coth^2\left(\frac{\beta\hbar\omega}{2}\right) + O(g^2)$$

gnd. state level shift

$$\lim_{T\to 0} F(T) = E_0 = \frac{\hbar\omega}{2} + \frac{3g\hbar^2}{4(m\omega)^2} + O(g^2) \equiv E_0(g)$$

$$F(T) = E_0(g) + k_BT\log\left(1 - e^{-\beta\hbar\omega}\right) + \frac{3g\hbar^2}{(m\omega)^2}\frac{e^{-\beta\hbar\omega}}{\left(1 - e^{-\beta\hbar\omega}\right)^2} + O(g^2)$$

Note: $g\left(\frac{\hbar}{m\omega}\right)^2 \ll \hbar\omega$ but not w.r.t. kT !

Is this consistent?

Check:

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① At low T
$$Z = e^{-\frac{E_0(g)}{kT}} + e^{-\frac{E_1(g)}{kT}} + \cdots$$

$$Z = e^{-\frac{E_0(g)}{kT}}\left[1 + e^{-\frac{E_1(g)-E_0(g)}{kT}} + \cdots\right]$$

$$F = -kT\log Z$$
$$= E_0(g) - kT\, e^{-\frac{(E_1(g)-E_0(g))}{kT}} + \cdots$$

$$\Rightarrow -kT\, e^{-\beta\hbar\omega} + \frac{3g\hbar^2}{m^2\omega^2}\, e^{-\beta\hbar\omega} + \cdots$$

$$\equiv -kT\, e^{-\beta\hbar\omega}\left(1 - \frac{3g\hbar^2}{m^2\omega^2}\frac{1}{kT} + \cdots\right)$$

$$\equiv -kT\, e^{-\beta\hbar\omega}\, e^{-\frac{3g\hbar^2}{m^2\omega^2}\frac{1}{kT}} + \mathcal{O}(g^2)$$

(this checks out at higher orders!)

$$\Rightarrow \quad E_1(g) - E_0(g) = \hbar\omega + 3g\xi^4 + O(g^2)$$

$$\xi^2 = \frac{\hbar}{m\omega}$$

first order shift of the first excited state!

We have actually calculated the shifts of <u>all</u> the levels!

What about high Temperatures? This should be the classical limit. Here we use $\beta \hbar \omega \to 0$

$$F(T) = E_0(g) + kT \log\left(\frac{\hbar\omega}{kT}\right) + 3 g \xi^4 \left(\frac{kT}{\hbar\omega}\right)^2 + \cdots$$

$$= E_0(g) + kT \log\left(\frac{\hbar\omega}{kT}\right) + 3 \frac{g \cancel{\hbar^2}}{m^2\omega^2} \left(\frac{kT}{\cancel{\hbar}\omega}\right)^2 + \cdots$$

note: $\hbar$ drops out!

Is this correct?

Classical Calculation:

$$Z = \int \frac{dp\, dq}{2\pi\hbar}\, e^{-\frac{\beta p^2}{2m} - \frac{\beta m \omega^2 q^2}{2} - \beta g q^4}$$

$$= \sqrt{2\pi} \sqrt{\frac{m}{\beta}} \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dq\, e^{-\frac{\beta m\omega^2 q^2}{2} - g\beta q^4}$$

scale β out $\quad x = \sqrt{\beta m \omega^2}\, q$

$$= \sqrt{\frac{2\pi \cancel{m}}{\beta}} \frac{1}{2\pi\hbar} \frac{1}{\sqrt{\beta \cancel{m} \omega^2}} \int_{-\infty}^{+\infty} dx\, e^{-\frac{x^2}{2} - \frac{g \cancel{\beta} x^4}{(\cancel{\beta} m\omega^2)^2}}$$

$$Z = \frac{kT}{\hbar\omega} \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-\frac{x^2}{2} - \frac{g\, kT}{m^2\omega^4} x^4}$$

$$\approx \frac{kT}{\hbar\omega} \left\{ 1 - \frac{3 g kT}{m^2 \omega^4} + \cdots \right\}$$

This behavior is correct only if $\frac{g\,kT}{m^2\omega^4} \ll 1$

For kT large, the q^4 term dominates and

$$\sqrt{kT} \int \frac{dq}{\sqrt{2\pi}} \; e^{-\beta \frac{m\omega^2}{2} q^2 - \beta g q^4} \approx \# \, (kT)^{3/4} + \cdots$$

Thus, in the classical limit, as a function of g there is a cross over from $Z \sim kT$ to

$$Z \sim \frac{(kT)^{3/4}}{g^{1/4}} + \cdots$$

which is non-analytic in g! This is not accessible in perturbation theory.