Advanced Quantum Mechanics

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Lecture #25

Path Integrals and QM

Recap of Last Class

- Functional Integrals for many body systems

- Many Body Coherent States for Bosons

- Deriving the functional Integral

- Repulsive Spin 0 Bose gas

Imaginary time and Z

Partiton Function $$Z = Tr\ e^{-\beta \hat{H}}$$

Trace of an operator A $$Tr\ \hat{A} = \sum_n \langle n|\hat{A}|n\rangle \ = \int \prod_\alpha \frac{d\phi^*_\alpha d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \langle \phi|\hat{A}|\phi\rangle$$

So $$Z = \int \prod_\alpha \frac{d\phi^*_\alpha(\tau_f) d\phi_\alpha(\tau_f)}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha(\tau_f)\phi_\alpha(\tau_f)} \langle \phi(\tau_f)|e^{-\beta \hat{H}}|\phi(\tau_f)\rangle$$

We can once again follow the steps we took in writing the path integral for a particle in imaginary time. The matrix element of e-βH can itself be written as a functional integral over field configurations at intermediate (imaginary) time points.

$$\langle \phi(\tau_f)|e^{-\beta \hat{H}}|\phi(\tau_f)\rangle = \int_{\phi(0)=\phi(\tau_f)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{\sum_\alpha \phi^*(\tau_f)\phi_\alpha(\tau_f)} e^{-S_E[\phi^*,\phi]}$$

where $$S = \int_{t_i}^{t_f} dt \int d^3x \, \{\phi^*(x,t)(i\partial_t)\phi(x,t) - H[\phi^*(x,t), \phi(x,t)]\}$$

$$\Downarrow$$

$$S_E = \int_0^\beta d\tau \int d^3x \, \{\phi^*(x,\tau)\partial_\tau \phi(x,\tau) + H[\phi^*(x,\tau), \phi(x,\tau)]\}$$

Imaginary time and Z

$$Z = \int \prod_{\alpha} \frac{d\phi^*_\alpha(\tau_f) d\phi_\alpha(\tau_f)}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha(\tau_f)\phi_\alpha(\tau_f)} \langle \phi(\tau_f)| e^{-\beta \hat{H}} |\phi(\tau_f)\rangle$$

$$\langle \phi(\tau_f)| e^{-\beta \hat{H}} |\phi(\tau_f)\rangle = \int_{\phi(0)=\phi(\tau_f)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{\sum_\alpha \phi^*(\tau_f)\phi_\alpha(\tau_f)} e^{-S_E[\phi^*,\phi]}$$

$$S_E = \int_0^\beta d\tau \int d^3x \, \{\phi^*(x,\tau)\partial_\tau \phi(x,\tau) + H[\phi^*(x,\tau), \phi(x,\tau)]\}$$

The exponential term from the definition of Z cancels the exponential term coming from the functional integral involving the fields at the final time.

$$Z = \int_{\phi(0)=\phi(\beta)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{-S_E[\phi^*,\phi]}$$

The partition fn is a functional integral over periodic field config. with each field config contributing a factor of e^{-S}

If you are interested in ground state properties, you can set $\beta \rightarrow \infty$ at the end of the calc.

Stationary Phase Approximation

Asymptotic expansion of $I(l) = \int_{-\infty}^{\infty} dt e^{-\ell f(t)}$ in powers of 1/ l (useful for large l)

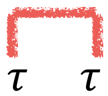
$f_0=f(t_0)$, where df/dt=0

$f^{(n)}_0=d^n/dt^n\, f(t_0)$

$$= e^{-\ell f_0}\sqrt{\frac{2\pi}{\ell f_0''}}\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{2\pi}} e^{-\frac{\tau^2}{2}-\sum_{n=3}^{\infty}\frac{\tau^n}{n!}\frac{f_0^{(n)}}{\ell^{n/2-1}(f_0'')^{n/2}}}$$

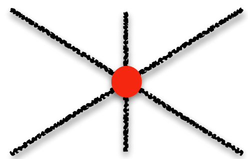
$$= e^{-\ell f_0}\sqrt{\frac{2\pi}{\ell f_0''}}\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{2\pi}} e^{-\frac{\tau^2}{2}}\left[1-\sum_{n=3}^{\infty}\frac{\tau^n}{n!}\frac{f_0^{(n)}}{\ell^{n/2-1}(f_0'')^{n/2}}+\frac{1}{2}\left(\sum_{n=3}^{\infty}\frac{\tau^n}{n!}\frac{f_0^{(n)}}{\ell^{n/2-1}(f_0'')^{n/2}}\right)^2+\ldots\right]$$

These are integrals of powers of τ over a Gaussian measure. Use Feynman Diagrams

Define contraction 

$$= \int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{2\pi}}\tau^2 e^{-\frac{\tau^2}{2}} = 1$$

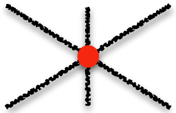
Co-eff of τ^n is denoted by a vertex with n lines coming out of it.
Note there will be vertices with different no. of lines.



$$V_n = \frac{1}{n!}\frac{f_0^{(n)}}{\ell^{n/2-1}(f_0'')^{n/2}}$$

Stationary Phase Approximation

Diagrams: draw any no. of vertices (of any degree n) and connect all the lines. In addition, a diagram with N vertices have $(-1)^N/N!$, coming from expansion of the exponential.



$$V_n = \frac{1}{n!}\frac{f_0^{(n)}}{\ell^{n/2-1}(f_0'')^{n/2}}$$

1

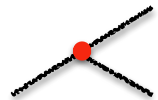
$$I(\ell) = e^{-\ell f_0}\sqrt{\frac{2\pi}{\ell f_0''}}\,e^{(\text{ sum of all connected diagrams })}$$

Stationary phase approx.:

Group all diagrams having same power of (1/l) .

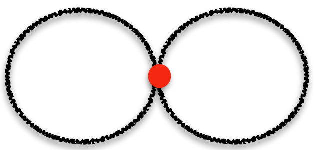
Mixes order in perturbation theory (i.e. diagrams at a specific order has diff. no. of vertices)

It is clear that odd powers of τ do not contribute — no way to close the lines

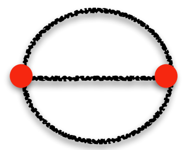


To lowest order in 1/l

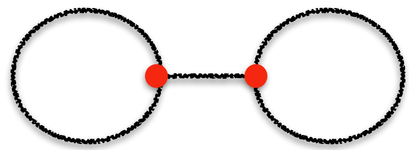
$1/l^{(4/2-1)}$



$[1/l^{(3/2-1)}]^2$



$[1/l^{(3/2-1)}]^2$



$$\frac{(-1)}{1!}\times 3\times\frac{f_0^{(4)}}{4!(f_0'')^2} = \frac{-3}{4!}\frac{f_0^{(4)}}{(f_0'')^2}$$

$$\frac{(-1)^2}{2!}\times 3\times 2\times\left(\frac{f_0^{(3)}}{3!(f_0'')^{3/2}}\right)^2 = \frac{1}{12}\frac{(f_0^{(3)})^2}{(f_0'')^3}$$

$$\frac{(-1)^2}{2!}\times 3\times 3\times\left(\frac{f_0^{(3)}}{3!(f_0'')^{3/2}}\right)^2 = \frac{1}{8}\frac{(f_0^{(3)})^2}{(f_0'')^3}$$

$$I(\ell) = e^{-\ell f_0 + \frac{1}{2}\ln\frac{2\pi}{\ell f_0''} + \frac{1}{\ell}\left(\frac{5}{24}\frac{(f_0^{(3)})^2}{(f_0'')^3} - \frac{1}{8}\frac{f_0^{(4)}}{(f_0'')^2}\right) + \mathcal{O}(1/\ell^2)}$$

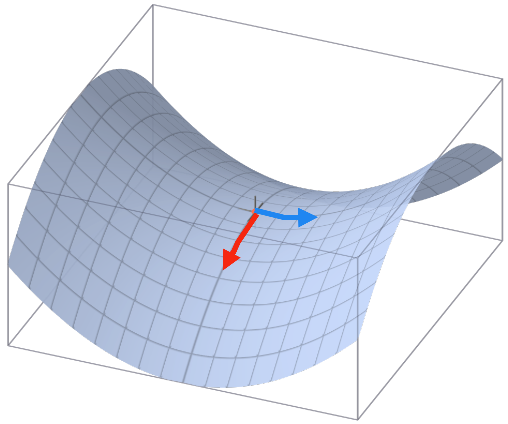
Stationary Phase Approximation

f(z) is an analytic fn and

For $z=z_0$, $f'(z_0) = 0$

Integrals of Complex variables: $$I(\ell) = \int dz^* dz e^{-\ell f(z)}$$

Cauchy's Integral formula —> z_0 can only be a saddle point of Re f[z]



Choose the contour passing through z_0, which keeps Im f[z] constant.
Otherwise large oscillations wash out the integral

$$I(\ell) = e^{-\ell Im f[z_0]} \int_C ds e^{-\ell Re f[s]}$$

Use $f^{''}(z_0) = \rho_0 e^{i\phi_0}$ Near z_0 $$f(z_0 + \rho e^{i\phi}) = f(z_0) + \frac{1}{2}\rho_0 \rho^2 e^{i(\phi_0 + 2\phi)}$$

The directions $\phi = -\phi_0/2$ and $\phi = -\phi_0/2 + \pi/2$ keep Im f constant. This also correspond to maximum +ve and -ve curvature for Re f . Contour C is chosen along the path of steepest descent.

The real integral along this contour is evaluated as the asymptotic expansion shown before.

Stationary Phase Approx.: Path Integrals

A path integral is nothing but multiple integrals

$$U(x_f,t_f;x_i,t_i) = \left(\frac{mN}{2\pi i(t_f-t_i)}\right)^{1/2}\int \mathcal{D}[x(t)]e^{iS[x(t)]}$$

$$S[x(t)] = \int_{t_i}^{t_f} dt\left[\frac{1}{2}m\dot{x}^2(t) - V(x(t))\right] = \int_{t_i}^{t_f} dt\mathcal{L}[x(t),\dot{x}(t)]$$

Imaginary time Path Integral

$$U(x_f,\tau_f;x_i,\tau_i) = \left(\frac{m}{2\pi\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)]e^{-S_E[x(\tau)]}$$

$$S_E[x(\tau)] = \int_{\tau_i}^{\tau_f} d\tau\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V[x(\tau)]$$

Remember that $\int \mathcal{D}[x(\tau)] \sim \prod_{i=1}^{N-1}\int_{-\infty}^{\infty} dx_i$ i.e. we have multiple integrals over exp functions

But where is the large l in this ?

Bring back hbar !!

The argument of the exponential is dimensionless and S has dim. of hbar

$$U(x_f,\tau_f;x_i,\tau_i) = \left(\frac{m}{2\pi\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)]e^{-\frac{S_E[x(\tau)]}{\hbar}}$$

Large l as hbar --> 0 —— Classical Limit !!

Stationary Phase Approx.: Path Integrals

Large l as hbar –> 0 —— Classical Limit !!

Remember that the path integral is actually a multiple integral and S is a fn of many x variables (one for each time point t). So we have to find the minimum wrt each of the x variables.

Differentiation wrt all the x variables —–> functional derivative wrt. paths.

The saddle point is nothing but the classical path

$$\frac{\delta S}{\delta x(t)} = 0 \qquad \left[\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x}\right]\Bigg|_{x_{cl}(t)} = 0$$

Euler Lagrange Equation

For H = $p^2/2m+V(x)$, $\quad m\ddot{x} = -\nabla V(x)$

and the corresponding path integral is just the exponential of the saddle point action.

Stationary Phase Approx.: Path Integrals

Expanding around the saddle point $x(t) = x_c(t) + \sqrt{\hbar} y(t)$

$$U(x_f, t_f; x_i, t_i) = e^{i\frac{S_c}{\hbar}} \int_{(0,t_i)}^{(0,t_f)} \mathcal{D}[y(t)] e^{i\int_{t_i}^{t_f} dt \frac{1}{2} y(t)\left[-m\frac{d^2}{dt^2} - V''[x_c(t)]\right] y(t) + \sum_{n=3}^{\infty} \frac{\hbar^{n/2-1}}{n!} V^{(n)}[x_c(t)] y^n(t)}$$

From this it is evident why quadratic Lagrangians have special properties.

In this sense they are often called "classical" — terms with +ve powers of hbar are absent in the stationary phase expansion.

The leading order correction to the classical contribution is a Harmonic oscillator with the frequency of the oscillator set by the small oscillation frequencies around the classical path.

Stationary Phase Approx.: Functional Integrals

The partition function function for many bosons is a functional integral over field config of Exp($-S_E$). This is nothing but many more complex integrals, one for each space-time point. (or one for each k and each τ).

The basic idea of stationary phase approximation works in this case provided a large number multiplying the action can be found.

For the time being, introduce fictitious l

$$Z(\ell) = \int_{\phi(0)=\phi(\beta)} \mathcal{D}[\phi_\alpha^*(\tau), \phi_\alpha(\tau)] e^{-\ell S_E[\phi^*,\phi]}$$

$$S_E = \int_0^\beta d\tau \int d^3x \, \{\phi^*(x,\tau)\partial_\tau \phi(x,\tau) + H[\phi^*(x,\tau), \phi(x,\tau)]\}$$

Classical Field Config. is given by saddle point equations $\frac{\delta S_E}{\delta \phi^*(x,\tau)} = 0$ $\frac{\delta S_E}{\delta \phi(x,\tau)} = 0$

$$\phi(x,\tau) = \phi_c(x,\tau) + \sqrt{\frac{1}{\ell}}\delta\phi(x,\tau)$$

and we will drop the δ for notational convenience

$$Z(\ell) = e^{-\ell S_E[\phi_c]} \int_{\phi(x,0)=\phi(x,\beta)=0} \mathcal{D}[\phi(x,\tau)] e^{-\frac{1}{2}\int_0^\beta d\tau \int_0^\beta d\tau' \int d^3x \int d^3x' \left.\frac{\partial^2 \mathcal{L}_E}{\partial\phi^*(x,\tau)\partial\phi(x',\tau')}\right|_{\phi_c} \phi^*(x,\tau)\phi(x',\tau') + \mathcal{O}(1/\ell)}$$

Stationary Phase Approximation for Bosons

Put in a fictitious (for now) factor of l in front of the action

$$Z(\ell) = \int_{\phi(0)=\phi(\beta)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{-\ell S_E[\phi^*, \phi]}$$

$$S_E = \int_0^\beta d\tau \int d^3x \, \{\phi^*(x,\tau)\partial_\tau \phi(x,\tau) + H[\phi^*(x,\tau), \phi(x,\tau)]\}$$

$$= \int_0^\beta d\tau \int d^3x \left\{\phi^*(x,\tau)\left[\partial_\tau - \frac{\nabla^2}{2m} - \mu\right]\phi(x,\tau) + g\phi^*(x,\tau)\phi^*(x,\tau)\phi(x,\tau)\phi(x,\tau)\right\}$$

$$= \int_0^\beta d\tau \int d^3x \left\{\phi(x,\tau)\left[-\partial_\tau - \frac{\nabla^2}{2m} - \mu\right]\phi^*(x,\tau) + g\phi^*(x,\tau)\phi^*(x,\tau)\phi(x,\tau)\phi(x,\tau)\right\}$$

The Saddle Point is obtained for a field configuration which satisfies

$$\frac{\delta S_E}{\delta \phi^*(x,\tau)} = 0 \quad \longrightarrow \quad \left[\partial_\tau - \frac{\nabla^2}{2m} - \mu\right]\phi(x,\tau) + 2g|\phi(x,\tau)|^2\phi(x,\tau) = 0$$

$$\frac{\delta S_E}{\delta \phi(x,\tau)} = 0 \quad \longrightarrow \quad \left[-\partial_\tau - \frac{\nabla^2}{2m} - \mu\right]\phi^*(x,\tau) + 2g|\phi(x,\tau)|^2\phi^*(x,\tau) = 0$$

The Saddle Point Solution

Working in real time

$$\left[-i\partial_t - \frac{\nabla^2}{2m} - \mu\right]\phi(x,t) + 2g|\phi(x,t)|^2\phi(x,t) = 0 \qquad i\partial_t\phi(x,t) = \left[-\frac{\nabla^2}{2m} - \mu\right]\phi(x,t) + 2g|\phi(x,t)|^2\phi(x,t)$$

For g = 0, this is simply the single particle Schrodinger Equation

For g ≠ 0, this eqn. is called the non-linear Schrodinger Equation or Gross-Pitaevski equation for Bosons.

Possible Solutions :

- ϕ(x,t) = 0 is always a solution. This is the trivial or vacuum solution.
- ϕ(x,t) = ϕ_0, a space-time independent solution (static saddle point)

$$-\mu\phi_0 + 2g|\phi_0|^2\phi_0 = 0 \Rightarrow |\phi_0| = \sqrt{\frac{\mu}{2g}}$$

We will work with this

- More non-trivial space-time dependent solutions depending on boundary conditions.

Gaussian Fluctuations around Saddle point

$$S_E = \int_0^\beta d\tau \int d^3x \, \{\phi^*(x,\tau)\partial_\tau\phi(x,\tau) + H[\phi^*(x,\tau), \phi(x,\tau)]\}$$

Expanding around the saddle point $\phi(x,\tau) = \phi_0 + \sqrt{\frac{1}{\ell}}\delta\phi(x,\tau)$

$$\ell S_E = \ell S_c + S^{(2)} + \frac{1}{\sqrt{\ell}}S^{(3)} + \frac{1}{\ell}S^4$$

$$\ell S_c = -\frac{\ell\beta}{2}\frac{\mu^2}{2g}$$

$$S^{(2)} = \frac{1}{2}\int_0^\beta d\tau \int d^3x [\phi^*(x,\tau), \phi(x,\tau)]\mathcal{D}^{-1}(x,\tau)\left[\begin{array}{c} \phi(x,\tau) \\ \phi^*(x,\tau) \end{array}\right]$$

$$\mathcal{D}^{-1}(x,\tau) = \left[\begin{array}{cc} \partial_\tau - \frac{\nabla^2}{2m} + g\phi_0^2 & g\phi_0^2 \\ g\phi_0^2 & -\partial_\tau - \frac{\nabla^2}{2m} + g\phi_0^2 \end{array}\right]$$

Note that for BEC, the condensate $\Phi_0 = N\phi_0$

provides a large parameter N in real situations

Quadratic action and Bogoliubov Theory

The Bogoliubov theory is obtained by retaining terms upto $S^{(2)}$

$$S^{(2)} = \frac{1}{2}\int_0^\beta d\tau \int d^3x [\phi^*(x,\tau), \phi(x,\tau)] \mathcal{D}^{-1}(x,\tau) \left[\begin{array}{c} \phi(x,\tau) \\ \phi^*(x,\tau) \end{array} \right]$$

$$\mathcal{D}^{-1}(x,\tau) = \left[\begin{array}{cc} \partial_\tau - \frac{\nabla^2}{2m} + g\phi_0^2 & g\phi_0^2 \\ g\phi_0^2 & -\partial_\tau - \frac{\nabla^2}{2m} + g\phi_0^2 \end{array} \right]$$

Work in momentum and Matsubara frequency space

$$S^{(2)} = \frac{1}{2}\sum_m \int d^3k [\phi^*(k,i\omega_m), \phi(-k,-i\omega_m)] \mathcal{D}^{-1}(k,i\omega_m) \left[\begin{array}{c} \phi(k,i\omega_m) \\ \phi^*(-k,-i\omega_m) \end{array} \right]$$

$$\mathcal{D}^{-1}(k,i\omega_m) = -\left[\begin{array}{cc} i\omega_m - \frac{k^2}{2m} - g\phi_0^2 & -g\phi_0^2 \\ -g\phi_0^2 & -i\omega_m - \frac{k^2}{2m} - g\phi_0^2 \end{array} \right]$$

Quadratic action and Bogoliubov Theory

$$S^{(2)} = \frac{1}{2}\sum_m \int d^3k[\phi^*(k, i\omega_m), \phi(-k, -i\omega_m)]\mathcal{D}^{-1}(k, i\omega_m)\left[\begin{array}{c}\phi(k, i\omega_m)\\ \phi^*(-k, -i\omega_m)\end{array}\right]$$

$$\mathcal{D}^{-1}(k, i\omega_m) = -\left[\begin{array}{cc} i\omega_m - \frac{k^2}{2m} - g\phi_0^2 & -g\phi_0^2 \\ -g\phi_0^2 & -i\omega_m - \frac{k^2}{2m} - g\phi_0^2\end{array}\right]$$

Diagonalizing D^{-1} gives the quasiparticle co-ordinates of the Bogoliubov Theory

Note that D^{-1} has the form $(i\ \omega_m\ \sigma^3 - H)$, where H is the quadratic Bogoliubov Hamiltonian

$$\hat{H} = -\frac{1}{2}\sum_k \frac{k^2}{2m} + g\rho + \frac{1}{2}\sum_k \left(\begin{array}{cc} a_k^\dagger & a_{-k}\end{array}\right)\left(\begin{array}{cc}\frac{k^2}{2m} + g\rho & g\rho \\ g\rho & \frac{k^2}{2m} + g\rho\end{array}\right)\left(\begin{array}{c} a_k \\ a_{-k}^\dagger\end{array}\right)$$

This is why simple diagonalization of the Hamiltonian does not yield correct answer for the Bosons.

Quadratic action and Bogoliubov Theory

$$\mathcal{D}^{-1}(k, i\omega_m) = -\begin{bmatrix} i\omega_m - \frac{k^2}{2m} - g\phi_0^2 & -g\phi_0^2 \\ -g\phi_0^2 & -i\omega_m - \frac{k^2}{2m} - g\phi_0^2 \end{bmatrix}$$

To find the eigen values look at the Determinant

$$Det\mathcal{D}^{-1} = [(i\omega_m)^2 - (\epsilon_k + g\phi_0^2)^2 + g^2\phi_0^4] = [(i\omega_m)^2 - E_k^2]$$

$$E_k = \sqrt{(\epsilon_k + g\phi_0^2)^2 - g^2\phi_0^4} = \sqrt{2g\phi_0^2 k^2/m + \left(\frac{k^2}{2m}\right)^2}$$ is the Bogoliubov Spectrum

Going to real frequencies, Det D^{-1} has zeroes at $\omega = \pm E_k$

This means the matrix D has poles at $\omega = \pm E_k$

Similarly, one can show that D is diagonalized by $\begin{bmatrix} u_k & v_k \\ v_k & u_k \end{bmatrix}$

where $u_k^2 = 1 + v_k^2 = \frac{1}{2}\left[1 + \frac{\frac{k^2}{2m} + g\rho}{E_k}\right]$ $\qquad u_k v_k = \frac{g\rho}{2E_k}$