Advanced Quantum Mechanics

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Lecture #24

Path Integrals and QM

Recap of Last Class

- Replica Trick and Linked Cluster Theorem

- Two point correlators in Gaussian Theory : Matsubara Frequencies

- Evaluating Matsubara sums: 1st order corrections to Z

- Rotation to real frequencies ⟶ poles of time-ordered functions

- Perturbation Expansion for 2-point function

Path Integrals for Many-Particle Systems

Let us recap how we obtained path integral formalism for single particle QM

- Start with matrix element of time evolution operator $U = e^{-iHt}$ between position eigenstates

- Break it up into products of matrix elements of infinitesimal evolution operator between intermediate position eigenkets. Obtain a large number of integrals over intermediate co-ord.

$$\hat{U}(x_f, t_f; x_i, t_i) = \int dx_1 dx_2 .. dx_{N-1} \, [$$

$$\langle x_f | \hat{U}(t_f, t_i + (N-1)\epsilon) | x_{N-1} \rangle \langle x_{N-1} | \hat{U}(t_i + (N-1)\epsilon, t_i + (N-2)\epsilon) | x_{N-2} \rangle \langle x_{N-2} | ...$$

$$| x_2 \rangle \langle x_2 | \hat{U}(t_i + 2\epsilon, t_i + \epsilon) | x_1 \rangle \langle x_1 | \hat{U}(t_i + \epsilon, t_i) | x_i \rangle]$$

- For infinitesimal matrix elements, introduce momentum states [Note H=H(x,p)] and use normal ordering to convert this to exponential of the infinitesimal Lagrangian.

- Work out momentum integrals, take continuum limit, to get

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

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

Path Integrals for Many-Particle Systems

For many particle systems, the natural operators to write the Hamiltonian are creation/annihilation operators, i.e. $H = H(a^\dagger, a)$. These are the conjugate operators with (anti) commutation relations.

We can simply follow the derivation for one particle QM, if we can find the eigenstates of the creation/annihilation operators and introduce resolution of identity with these states.

The many-body basis that we have seen till now is the occupation no. basis $\longrightarrow$ not eigenstates of $a^\dagger$, a. Search for new basis $\longrightarrow$ Many Body Coherent States

The equivalent of Path Integrals, written in these bases, are called functional integrals

Coherent States

Recap of Harmonic Osc.: $H = \left[\frac{-\nabla^2}{2m} + \frac{1}{2}m\omega_0^2 x^2\right] = \omega_0\left[b^\dagger b + \frac{1}{2}\right]$

Coherent states are defined as the right eigenstates of the annihilation operator $b|\xi\rangle = \xi|\xi\rangle$

Corresponding to $|\xi>$, $\langle\xi|b^\dagger = \langle\xi|\xi^*$

- Linear Comb. of diff. number states: $|\xi\rangle = e^{-|\xi|^2/2}\sum_n \frac{\xi^n}{\sqrt{n!}}|n\rangle = e^{\xi a^\dagger - \xi^* a}|0\rangle$
- Orthogonality: $\langle\xi|\eta\rangle = e^{-\frac{1}{2}(|\xi|^2+|\eta|^2)+\xi^*\eta}$
- (Over)completeness: $\frac{1}{\pi}\int d^2\xi|\xi\rangle\langle\xi| = 1$
- Linear Dependence: $\int d^2\xi e^{-\frac{1}{2}|\xi|^2}\xi^n|\xi\rangle = 0$

The coherent states can still be used as basis set to obtain unique expansion of an arbitrary state, as long as we restrict the expansion co-efficients to be of the form

$|\psi\rangle = \frac{1}{\pi}\int d^2\xi|\xi\rangle e^{-\frac{1}{2}|\xi|^2} f(\xi^*)$ f is a fn. of only ξ^* and not of ξ

Many-Body Coherent States

Let us generalize the defn. of a coherent state as the right eigenstate of all the annihilation operators, one for each single-particle basis state.

$$a_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle \qquad \forall\ \alpha$$

We will immediately see that coherent states for Bosons and Fermions have very different description.

Bosons: $[a_\alpha, a_\beta]|\phi\rangle = 0 \Rightarrow [\phi_\alpha, \phi_\beta] = 0$ $\qquad$ ϕ_α is a complex number

Fermions: $\{a_\alpha, a_\beta\}|\phi\rangle = 0 \Rightarrow \{\phi_\alpha, \phi_\beta\} = 0$ $\qquad$ ϕ_α and ϕ_β anticommute

Grassmann Numbers

Will not work with Grassmann Numbers in this course

Bosonic Coherent States

A Bosonic coherent state is the right eigenstate of all the annihilation operators, one for each single-particle basis state.

$$a_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle \qquad \forall \ \alpha$$

where ϕ_α is a complex number

Similarly the left eigenstate of all the creation operators, one for each single-particle basis state.

$$\langle\phi|a_\alpha^\dagger = \langle\phi|\phi_\alpha^*$$

Expansion in occupation no. basis:

$$|\phi\rangle = \sum_{\{n_\alpha\}} \frac{\phi_{\alpha_1}^{n_{\alpha_1}}\phi_{\alpha_2}^{n_{\alpha_2}}}{\sqrt{n_{\alpha_1}!n_{\alpha_2}!..}}|n_{\alpha_1}, n_{\alpha_1}..\rangle$$

$$= \sum_{\{n_\alpha\}} \prod_\alpha \frac{(\phi_\alpha a_\alpha^\dagger)^{n_\alpha}}{n_\alpha!}|0\rangle = e^{\sum_\alpha \phi_\alpha a_\alpha^\dagger}|0\rangle$$

Clearly

$$a_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle \qquad \forall \ \alpha$$

This is an un-normalized state. However with these states, one has the relations

$$a_\alpha^\dagger|\phi\rangle = \frac{\partial}{\partial\phi_\alpha}|\phi\rangle \qquad \langle\phi|a_\alpha = \frac{\partial}{\partial\phi_\alpha^*}\langle\phi|$$

Bosonic Coherent States

(Non) Orthogonality of Bosonic Coherent States:

$$\langle\phi^{'}|\phi\rangle = \langle 0| e^{\sum_\alpha \phi^{'*}_\alpha a_\alpha} e^{\sum_\beta \phi_\beta a^\dagger_\beta}|0\rangle$$

$$= \langle 0| \sum_{\{n_\alpha\}} \prod_\alpha \frac{(\phi^{'*}_\alpha a_\alpha)^{n_\alpha}}{n_\alpha!} \sum_{\{n_\beta\}} \prod_\beta \frac{(\phi_\beta a^\dagger_\beta)^{n_\beta}}{n_\beta!}|0\rangle$$

Note: In each term, each $n_\alpha = n_\beta$ for the expectation to be non zero. For $n_\alpha = n_\beta$, one factor of $n_\alpha!$ is cancelled by the matrix elements of $(aa^\dagger)^{n\alpha}$

$$= \sum_{\{n_\alpha\}} \prod_\alpha \frac{(\phi^{'*}_\alpha \phi_\alpha)^{n_\alpha}}{n_\alpha!}$$

$$= e^{\sum_\alpha \phi^{'*}_\alpha \phi_\alpha}$$

Extension of SHO coherent states
with different normalization.

Bosonic Coherent States

Resolution of identity: $$\int \prod_\alpha \frac{d\phi^*_\alpha d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} |\phi\rangle\langle\phi| = 1$$ in Fock Space

where $$\frac{d\phi^*_\alpha d\phi_\alpha}{2\pi i} = \frac{d(Re\phi_\alpha)d(Im\phi_\alpha)}{\pi}$$

For a state $|\phi>$ in Fock space

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

wavefunction

Trace of an operator A

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

$$= \int \prod_\alpha \frac{d\phi^*_\alpha d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \langle\phi|\hat{A} \left(\sum_n |n\rangle\langle n|\right) |\phi\rangle$$

$$= \int \prod_\alpha \frac{d\phi^*_\alpha d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \langle\phi|\hat{A}|\phi\rangle$$

Bosonic Coherent States

Matrix Elements:

$$\langle\phi|a_\alpha^\dagger|f\rangle = \phi_\alpha^* f(\phi^*) \qquad \langle\phi|a_\alpha^\dagger|f\rangle = \phi_\alpha^* f(\phi^*)$$

$$a_\alpha \to \frac{\partial}{\partial\phi_\alpha^*} \qquad a_\alpha^\dagger \to \phi_\alpha^*$$

Schrodinger Equation: $$H(a_\alpha^\dagger, a_\alpha)|\phi\rangle = E|\phi\rangle \to H\left(\phi_\alpha^*, \frac{\partial}{\partial\phi_\alpha^*}\right)\psi(\phi^*) = E\psi(\phi^*)$$

Normal Ordered Operators: An operator where all creation operators occur to the left of all annihilation operators

$$: a_x^\dagger a_x a_y^\dagger a_y := a_x^\dagger a_y^\dagger a_x a_y$$

For normal ordered operators, $$\langle\phi|\hat{A}(a_\alpha^\dagger, a_\alpha)|\phi^{'}\rangle = A(\phi_\alpha^*, \phi_\alpha^{'})$$

Functional Integrals for many Bosons

Since any state in Fock space can be expanded in coherent state basis.

Start with the matrix element of the time evolution operator between two coherent states.

$$U(\phi_f, t_f; \phi_i, t_i) = \langle \phi_f | e^{-i\hat{H}(a^\dagger, a)t} | \phi_i \rangle$$

Break up into products of large no. of infinitesimal evolution operators

$$= \langle \phi_f | \prod_{n=0}^{N-1} e^{-i\hat{H}(a^\dagger, a)(t_{n+1}-t_n)} | \phi_i \rangle$$

$t_0 = t_i$, $t_N = t_f$, $t_n = t_i + n\,\varepsilon$

Introduce resolution of identity with many-body coherent states. $\int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} |\phi\rangle\langle\phi| = 1$

between each infinitesimal operator

Remember that for each time index, we have a product over single particle basis α

Introduce $\phi_\alpha(t)$ where t takes discrete values on the lattice $t_0 = t_i$, $t_N = t_f$, $t_n = t_i + n\,\varepsilon$

E.g. if α is the position basis x, we can use $\phi(x,t)$

Functional Integrals for many Bosons

$$U(\phi_f, t_f; \phi_i, t_i) = \int \prod_\alpha \frac{d\phi^*_\alpha(t_1) d\phi_\alpha(t_1)}{2\pi i} e^{-\sum_\alpha \phi^*_\alpha(t_1)\phi_\alpha(t_1)} \int \prod_\beta \frac{d\phi^*_\beta(t_2) d\phi_\beta(t_2)}{2\pi i} e^{-\sum_\beta \phi^*_\beta(t_2)\phi_\beta(t_2)}$$

$$.. \int \prod_\gamma \frac{d\phi^*_\gamma(t_{N-1}) d\phi_\gamma(t_{N-1})}{2\pi i} e^{-\sum_\gamma \phi^*_\gamma(t_{N-1})\phi_\gamma(t_{N_1})}$$

$$\langle \phi_f | e^{-i\hat{H}(a^\dagger, a)\epsilon} | \phi_{N-1} \rangle \langle \phi_{N-1} | e^{-i\hat{H}(a^\dagger, a)\epsilon} | \phi_{N-2} \rangle \langle \phi_{N-2} | \ldots\ldots$$

$$\ldots. | \phi_2 \rangle \langle \phi_2 | e^{-i\hat{H}(a^\dagger, a)\epsilon} | \phi_1 \rangle \langle \phi_1 | e^{-i\hat{H}(a^\dagger, a)\epsilon} | \phi_i \rangle$$

Focus on the matrix element of the infinitesimal time-evolution operator

$$\langle \phi_{n+1} | e^{-i\hat{H}(a^\dagger, a)\epsilon} | \phi_n \rangle$$

Evidently, if all $a^\dagger$ occur to the left of all a in the infinitesimal exponential, (normal ordering)

$\langle \phi | a^\dagger_\alpha = \langle \phi | \phi^*_\alpha$ and $a_\alpha | \phi \rangle = \phi_\alpha | \phi \rangle$, we can simply replace $a^\dagger_\alpha$ by ϕ^*_α and a_α by ϕ_α

The exponential operator is however not normal ordered in general.

The Infinitesimal Evolution operator

Unlike the case of single particle Hamiltonian $H = \frac{\hat{p}^2}{2m} + V(\hat{x})$

where H is already normal ordered, and Trotter errors in $e^{-iH\varepsilon}$ arise in 2nd order in ε

the many body H is not necessarily normal ordered

E.g. : $$H = \sum_x a_x^\dagger \frac{-\nabla^2}{2m} a_x + \sum_{xx'} V(x-x') a_x^\dagger a_x a_{x'}^\dagger a_{x'}$$

So, it is important to start with a normal ordered form of the many-body H

$$H = \sum_x a_x^\dagger \left[\frac{-\nabla^2}{2m} + V(x-x'=0) \right] a_x + \sum_{xx'} V(x-x') a_x^\dagger a_{x'}^\dagger a_{x'} a_x$$

From now on, we will assume that many-particle Hamiltonians are written in their normal ordered forms.

With this assumption, the Trotter errors can be neglected as they are $\mathcal{O}(N\epsilon^2) \to 0$

in the continuum limit

Functional Integral for Bosons

Taking all these together, we have

$$\langle \phi_{n+1} | e^{-i\hat{H}(a^\dagger_\alpha, a_\alpha)\epsilon} | \phi_n \rangle = e^{-iH(\phi^*_\alpha(n+1), \phi_\alpha(n))\epsilon} \langle \phi_{n+1} || \phi_n \rangle + \mathcal{O}\epsilon^2$$

$$= e^{-iH(\phi^*_\alpha(t_{n+1}), \phi_\alpha(t_n))\epsilon} e^{\sum_\alpha \phi^*_\alpha(t_{n+1})\phi_\alpha(t_n)} + \mathcal{O}\epsilon^2$$

Note: ϕ^* always appears at a time point ε shifted from the time pt. at which ϕ appears

Remember that the resolution of identity at t_{n+1} gives an additional factor

$$e^{-\sum_\alpha \phi^*_\alpha(t_{n+1})\phi_\alpha(t_{n+1})}$$

Let us now collect them together to get

$$e^{-\sum_\alpha \phi^*_\alpha(t_{n+1})[\phi_\alpha(t_{n+1}) - \phi_\alpha(t_n)] - i\epsilon H[\phi^*_\alpha(t_{n+1}), \phi_\alpha(t_n)]}$$

$$= e^{i\epsilon \left\{ \sum_\alpha \phi^*_\alpha(t_{n+1}) \left[i \frac{\phi_\alpha(t_{n+1}) - \phi_\alpha(t_n)}{\epsilon} \right] - H[\phi^*_\alpha(t_{n+1}), \phi_\alpha(t_n)] \right\}}$$

Note that there are N matrix elements, but N-1 insertion of identity resolutions. So all the terms cannot be paired up in this way.

Choice: Keep the $e^{\sum_\alpha \phi^*_\alpha(t_N)\phi_\alpha(t_{N-1})}$ coming from the final matrix element hanging around

Functional Integral for Bosons

$$U(\phi_f, t_f; \phi_i, t_i) = \left(\prod_{m=1}^{N-1} \prod_\alpha \int \frac{d\phi_\alpha^*(t_m)\phi_\alpha(t_m)}{2\pi i} \right) e^{\sum_\alpha \phi_\alpha^*(t_f)\phi_\alpha(t_{N-1})}$$

$$e^{i\epsilon \sum_{m=1}^{N-1} \left\{ \sum_\alpha \phi_\alpha^*(t_{m+1}) \left[i \frac{\phi_\alpha(t_{m+1}) - \phi_\alpha(t_m)}{\epsilon} \right] - H[\phi_\alpha^*(t_{m+1}), \phi_\alpha(t_m)] \right\}}$$

dt

$i\, \partial_t \phi_\alpha$

Continuum Limit : Remember, by convention $\phi^*(t) = \phi^*(t)$, and $\phi(t) = \phi(t-\varepsilon)$

Short hand notation: $\left(\prod_{m=1}^{N-1} \prod_\alpha \int \frac{d\phi_\alpha^*(t_m)\phi_\alpha(t_m)}{2\pi i} \right) = \int \mathcal{D}[\phi_\alpha^*(t), \phi_\alpha(t)]$

$$U(\phi_f, t_f; \phi_i, t_i) = \int \mathcal{D}[\phi_\alpha^*(t), \phi_\alpha(t)] e^{\sum_\alpha \phi_\alpha^*(t_f)\phi_\alpha(t_f)} e^{iS}$$

where the action $S = \sum_\alpha \int_{t_i}^{t_f} dt \left\{ \phi_\alpha^*(t) i\partial_t \phi_\alpha(t) - H[\phi_\alpha^*(t), \phi_\alpha(t)] \right\}$

Functional Integral for Bosons

For specificity, let us choose the single particle basis α to be the position basis

$$U(\phi_f, t_f; \phi_i, t_i) = \int \mathcal{D}[\phi^*(x,t), \phi(x,t)] \; e^{\int d^3x \phi^*(x,t_f)\phi(x,t_f)} \; e^{iS}$$

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

Lagrangian density

$\phi^*(x,t)$ and $\phi(x,t)$ are "operator valued" functions of space and time. These are the quantum fields.

The action is now a space time integrated object (no notion of "paths"). The integrand is the Lagrangian density of the system.

The matrix element of the time evolution operator is a functional integral over all possible field configurations, with each configuration contributing e^{iS} (times the boundary term), where S is the action written in terms of the fields and their derivatives wrt space and time.

In this way of approaching many-particle QM, the external input is the nature of the fields (bosonic or fermionic, spin –> multiple fields, bosonic+fermionic etc.) and the action written in terms of these fields. The output is the propagator and related quantities.

Weakly Repulsive Spin 0 Bose Gas

The Hamiltonian for a repulsive Bose gas interacting with local (delta fn) interaction potential. (normal ordered form)

$$H = \int d^3x a_x^\dagger \left(\frac{-\nabla^2}{2m} - \mu \right) a_x + g a_x^\dagger a_x^\dagger a_x a_x$$

The chemical potential absorbs quadratic terms coming from normal ordering

$$= \int d^3k a_k^\dagger \left(\frac{k^2}{2m} - \mu \right) a_k + \frac{g}{V} \int d^3k \int d^3k' \int d^3q \;\; a_k^\dagger a_{k'}^\dagger a_{k'-q} a_{k+q}$$

Introduce Bosonic fields: $\phi^*(x,t)$ and $\phi(x,t)$ or $\phi^*(k,t)$ and $\phi(k,t)$

The action for this system is given by

$$S = \int_{t_i}^{t_f} dt \int d^3x \left\{ \phi^*(x,t) \left(i\partial_t + \frac{\nabla^2}{2m} + \mu \right) \phi(x,t) \; - g \; \phi^*(x,t)\phi^*(x,t)\phi(x,t)\phi(x,t) \right\}$$

$$U(\phi_f, t_f; \phi_i, t_i) = \int \mathcal{D}[\phi^*(x,t), \phi(x,t)] \;\; e^{\int d^3x \phi^*(x,t_f)\phi(x,t_f)} \;\; e^{iS}$$

A quadratic/gaussian theory is obtained in the non-interacting limit.