Lecture 17: Path integral description of many-body physics

In the last lecture, we have seen that the formalism of "second-quantization" in which various terms in the Hamiltonian of many-body systems are described in terms of creation and annihilation operators, provides a economical language in which simple leading order perturbation theory calculations can be formulated. Later in this course, we will also see that this formalism also suggests simple mean-field theory type approximations that yield an amazingly good description of interesting phenomena like superconductivity and superfluidity.

In other contexts, for instance the study of phase transitions at which superfluidity is lost, an alternative description in terms of path integrals is also very useful. In this lecture, we will therefore develop such a description, focusing on the bosonic case for simplicity, since the fermionic path integral, although simple to set up, involves somewhat unfamiliar mathematics.

As a preliminary, consider a single pair of bosonic creation and annihilation operators satisfying the commutation relation

$$[a, a^\dagger] = 1 \ , \tag{1}$$

and let us construct eigenstates $|\phi\rangle$ of the annihilation operator a.

To do this, we assume

$$|\phi\rangle = \sum_{n=0}^{\infty} C_n(\phi)|n\rangle \tag{2}$$

and fix $C_n(\phi)$ by requiring

$$a|\phi\rangle = \phi|\phi\rangle \tag{3}$$

[allowed eigenvalues are of course those values of ϕ for which we can find $C_n(\phi)$ that satisfy this requirement]. Since

$$a|\phi\rangle = \sum_{n=1}^{\infty} C_n(\phi)\sqrt{n}|n-1\rangle \tag{4}$$

this involves comparing with $\phi C_n(\phi)$ the coefficient of $|n\rangle$ in the above, *i.e.* $C_{n+1}\sqrt{n+1}$, and demanding that the two be equal for each n. This gives the recursion relation

$$\sqrt{n+1}C_{n+1} = \phi C_n \tag{5}$$

which has solution

$$C_n = \frac{\phi^n}{\sqrt{n!}} C_0(\phi) \tag{6}$$

where $C_0(\phi)$ controls the overall normalization of the state, and may be chosen equal to 1. With this choice, we write the un-normalized eigenstate as

$$|\phi\rangle = \sum_{n=0}^{\infty} \frac{\phi^n}{\sqrt{n!}} |n\rangle \tag{7}$$

Since $|n\rangle$ itself is given as

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle. \tag{8}$$

we may also write this as

$$\begin{aligned} |\phi\rangle &= \sum_{n=0}^{\infty} \phi^n \frac{(a^\dagger)^n}{n!} |0\rangle \\ &= e^{\phi a^\dagger} |0\rangle \end{aligned} \tag{9}$$

Clearly, there is no restriction placed on ϕ by any of the above, so there is an eigenstate $|\phi\rangle$ for every complex number ϕ. If we consider the overlap $\langle\phi'|\phi\rangle$ of two such states, it is easy to see that this has a simple closed form expression:

$$\begin{aligned} \langle\phi'|\phi\rangle &= \sum_{n,m} \frac{(\phi'^\star)^n \phi^m}{\sqrt{n!}\sqrt{m!}} \langle n|m\rangle \\ &= \sum_n \frac{(\phi'^\star \phi)^n}{n!} = e^{\phi'^\star \phi}. \end{aligned} \tag{10}$$

In addition, it is easy to see one can write the identity operator using this basis of coherent states via the following completeness relation

$$\begin{aligned} \mathbf{1} &= \int [d\phi d\phi^\star] e^{-\phi^\star \phi} |\phi\rangle\langle\phi| \\ [d\phi d\phi^\star] &= \frac{dRe\phi dIm\phi}{\pi}. \end{aligned}$$

To verify this, one simply notes that

$$
\begin{aligned}
& \int \frac{dxdy}{\pi} e^{-(x^2+y^2)} \sum_n \frac{(x+iy)^n}{\sqrt{n!}} \frac{(x-iy)^n}{\sqrt{m!}} |n\rangle\langle m| \\
= & \int \frac{rdrd\theta}{\pi} e^{-r^2} \sum_{nm} \frac{1}{\sqrt{n!m!}} e^{(n-m)i\theta} r^{n+m} |n\rangle\langle m| \\
= & \sum_n \int 2rdr \frac{1}{n!} e^{-r^2} r^{2n} |n\rangle\langle n| \qquad (11)
\end{aligned}
$$

And finally, setting $r^2 = p$, we obtain

$$
\begin{aligned}
\int [d\phi d\phi^\star] e^{-\phi^\star\phi} |\phi\rangle\langle\phi| &= \sum_n \left(\int dp \frac{e^{-p} p^n}{n!} \right) |n\rangle\langle n| \\
&= \sum_n |n\rangle\langle n| \\
&= \mathbf{1} \qquad (12)
\end{aligned}
$$

as claimed.

In some contexts, it is also useful to understand the action of $a^\dagger$ on $|\phi\rangle$. This may be done by noting

$$
\begin{aligned}
a^\dagger e^{\phi a^\dagger} |0\rangle &= \sum_{n=0}^{\infty} \frac{\phi^n}{n!} (a^\dagger)^{n+1} |0\rangle \\
&= \frac{\partial}{\partial\phi} e^{\phi a^\dagger} |0\rangle \\
&= \frac{\partial}{\partial\phi} |\phi\rangle \qquad (13)
\end{aligned}
$$

Thus, when acting on $|\phi\rangle$, $a^\dagger$ acts in the same way as $\frac{\partial}{\partial\phi}$. Likewise:

$$
\langle\phi| a = \frac{\partial}{\partial\phi^\star} \langle\phi|. \qquad (14)
$$

Now, any state can be written, using the resolution of identity developed earlier, as an expansion

$$
|\psi\rangle = \int [d\phi d\phi^\star] e^{-\phi^\star\phi} \psi(\phi^\star) |\phi\rangle \qquad (15)
$$

Here

$$\psi(\phi^\star) = \langle\phi|\psi\rangle \tag{16}$$

is the "wavefunction" corresponding to the state $|\psi\rangle$. Since

$$\langle\phi|a|\psi\rangle = \frac{\partial}{\partial\phi^\star}\langle\phi|\psi\rangle = \frac{\partial}{\partial\phi^\star}\psi(\phi^\star) \tag{17}$$

and

$$\langle\phi|a^\dagger|\psi\rangle = \phi^\star\psi(\phi^\star). \tag{18}$$

we see that

$$\begin{aligned} a &= \frac{\partial}{\partial\phi^\star} \\ a^\dagger &= \phi^\star \end{aligned} \tag{19}$$

in the same sense in which

$$\begin{aligned} \hat{x} &= x \\ \hat{p} &= -i\frac{\partial}{\partial x} \end{aligned}$$

when working with coordinate-space wavefunctions of ordinary single particle quantum mechanics.

It is conventional in many situations to work with so-called "normal-ordered" expressions $A(a^\dagger, a)$ in which all the creation operators are to the "*left* of the annihilation operators. Such normal operators have the following simple matrix elements between two coherent states:

$$\langle\phi|A(a^\dagger, a)|\phi'\rangle = A(\phi^\star, \phi')e^{\phi^\star\phi'} \tag{20}$$

where $A(\phi^\star, \phi')$ is obtained from $A(a^\dagger, a)$ by replacing $a^\dagger$ by $\phi^\star$ and a by ϕ'. Also, the trace of such a normal ordered operator can be written as

$$\begin{aligned} \mathrm{Tr}A &= \sum_n \langle n|A|n\rangle \\ &= \int [d\phi d\phi^\star] \sum_n \langle n|\phi\rangle\langle\phi|A|n\rangle e^{-\phi^\star\phi} \\ &= \int [d\phi d\phi^\star] \langle\phi|A| \sum_n |n\rangle\langle n|\phi\rangle e^{-\phi^\star\phi} \end{aligned}$$

$$\begin{aligned} &= \int [d\phi d\phi^\star] e^{-\phi^\star \phi} \langle \phi | A | \phi \rangle \\ &= \int [d\phi d\phi^\star] A(\phi^\star, \phi) \end{aligned} \tag{21}$$

Clearly, all of this generalizes readily to a set of creation and annihilation operators $\{a_k^\dagger, a_k\}$ that create We have a set of a_{α_k} where $\{|\alpha_k\rangle\}$ form a complete orthonormal basis of single particle staqtes. Simultaneous eigenstates of all the a_{α_k} are now labeled not by one complex number ϕ, but by a complex-valued function $\phi(k)$ of the index k.

$$\begin{aligned} |\phi(k)\rangle &= \sum_{n_1, n_2 \cdots} \frac{\left[\phi(1)^{n_1} (a_{\alpha_1}^\dagger)^{n_1} \phi(2)^{n_2} (a_{\alpha_2}^\dagger)^{n_2} \cdots\right]}{n_1! n_2! \cdots} |0\rangle \\ &= e^{\sum_k \phi(k) a_{\alpha_k}^\dagger} |0\rangle \end{aligned}$$

For instance, if we use the position states $\{|x\rangle\}$ as the single-particle basis, then the corresponding simultaneous eigenstates of a_x are labeled by a complex valued function $\phi(x)$ and given as

$$|\phi(x)\rangle = e^{\int d^3x \phi(x) a^\dagger(x)} |0\rangle \tag{22}$$

This concludes our discussion of the coherent state basis. Before we use this basis to develop a path integral representation of the partition function, it is useful to see how properties of these basis states play a role in actual computations involving these states. To this end, we consider two examples: First and most basic, let us ask what is the expected number of particles in a coherent state. For concreteness, consider a system of bosons that lives on a lattice with sites labeled by j. We have $\hat{N} = \sum_j n_j$, where $n_j = a_j^\dagger a_j$ denotes the particle number at a site j. Now, one can transform to any other orthonormal basis of single particle states, say $\{|\alpha_k\rangle\}$, and as we have seen earlier, $\sum_j n_j$ transforms to $\sum_k n_k$, where $n_k = a_{\alpha_k}^\dagger a_{\alpha_k}$. Working in the basis of coherent states $\{|\phi(k)\rangle\}$ and suppressing the argument k of the function $\phi(k)$ to avoid confusion, we have

$$\begin{aligned} \langle \hat{N} \rangle &= \frac{\langle \phi | \sum_j n_j | \phi \rangle}{\langle \phi | \phi \rangle} \\ &= \sum_k \langle \phi | a_{\alpha_k}^\dagger a_{\alpha_k} | \phi \rangle \langle \phi | \phi \rangle \\ &= \sum_k \phi^\star(k) \phi(k) \end{aligned} \tag{23}$$

Next, we compute the expectation value of $\hat{N}^2$. To do this, we first express $\hat{N}^2$ in terms of the a_{α_k} by writing

$$\begin{aligned}
\hat{N}^2 &= \sum_{k,k'} a^\dagger_{\alpha_k} a_{\alpha_k} a^\dagger_{\alpha_{k'}} a_{\alpha_{k'}} \\
&= \sum_{k,k'} (a^\dagger_{\alpha_k} a^\dagger_{\alpha_{k'}} a_{\alpha_{k'}} a_{\alpha_k} + a^\dagger_{\alpha_k} a_{\alpha_{k'}} \delta_{k,k'}) \\
&= \hat{N} + \sum_{k,k'} a^\dagger_{\alpha_k} a^\dagger_{\alpha_{k'}} a_{\alpha_{k'}} a_{\alpha_k} \qquad (24)
\end{aligned}$$

Then, we have

$$\begin{aligned}
\langle \hat{N}^2 \rangle &= \frac{\langle \phi | \hat{N}^2 | \phi \rangle}{\langle \phi | \phi \rangle} \\
&= \sum_k \phi^\star(k)\phi(k) + \sum_{k,k'} \phi^\star(k)\phi^\star(k')\phi(k')\phi(k) \\
&= \langle \hat{N} \rangle + \langle \hat{N} \rangle^2 \qquad (25)
\end{aligned}$$

In the thermodynamic limit of a large number of particles at finite density, this result tells us that although coherent states are eigenstates of a "phase variable" $\phi(k)$, they nevertheless have quite sharply defined particle-number. In a certain well-defined sense that we will explore later, this phase variable is canonically conjugate to the particle number, and from this perspective, our coherent states are like the minimum-uncertainty wavepackets in which one may have reasonably well-defined values for *both* position and momentum.

With this background, we now develop a path integral representation of the partition function in the basis of these coherent states. To do this, it is convenient to assume that the Hamiltonian $H[a^\dagger, a]$ is a "normal-ordered" function of creation and annihilation operators, *i.e.*, it is written in such a way that all the creation operators are to the left of all the annihilation operators in every term of the Hamiltonian. If the original expression for the Hamiltonian is not of this form, it can always be put in this form using the commutation relations, so this is not a real restriction. Also, for notational convenience, we suppress the fact the ϕ is a function of the single-particle basis label k and denote the function $\phi(k)$ simply as ψ. This is useful since $\phi(k)$ also acquires the usual additional "imaginary-time" dependence in our derivation of the path integral, and keeping the k dependence explicit would simply clutter our notation—thus, arguments or subscripts of ψ refer to this imaginary time dependence, and $\psi_n^\star\psi_n \equiv \sum_k \phi_n^\star(k)\phi_n(k)$ in our short-hand notation.

With these two things in mind, we have

$$Z \;=\; \mathrm{Tr}\; e^{-\beta H[a^\dagger,a]} = \int [d\psi_0^\star\psi_0]\langle\psi_0|e^{-\beta H[a^\dagger,a]}|\psi_0\rangle e^{-\psi_0^\star\psi_0}$$

We now break up the exponential as

$$e^{-\beta H[a^\dagger,a]} = e^{-\frac{\beta}{M}H[a^\dagger,a]}\cdots e^{-\frac{\beta}{M}H[a^\dagger,a]} \tag{26}$$

where there are M identical factors on the right hand side. Next we introduce a resolution of identity between two consecutive factors on the right hand side of the above expression. This gives

$$Z \;=\; \int [d\psi_0 d\psi_0^\star][d\psi_1 d\psi_1^\star]\cdots[d\psi_{M-1}d\psi_{M-1}^\star]e^{-\sum_{k=0}^{M-1}\psi_k^\star\psi_k}\prod_{k=0}^{M-1}\langle\psi_{k+1}|e^{-\epsilon H}|\psi_k\rangle \tag{27}$$

with the understanding that $\psi_M \equiv \psi_0$. Thinking of $\epsilon \equiv \beta/M$ as a time-step along an imaginary time direction τ, this is equivalent to saying that $\psi(\tau)$ is periodic with fixed period $\beta \equiv M\epsilon$. Next, we note that if H is normal-ordered, the smallness to ϵ guarantees that $\exp(-\epsilon H)$ is also normal ordered to leading order in ϵ. This allows us to write:

$$\begin{aligned}
&= \int [d\psi_0 d\psi_0^\star][d\psi_1 d\psi_1^\star]\cdots[d\psi_{M-1}d\psi_{M-1}^\star]e^{+\sum_{k=0}^{M-1}[\psi_{k+1}^\star\psi_k-\psi_k^\star\psi_k-\epsilon H(\psi_{k+1}^\star,\psi_k)]}\\
&= \int [d\psi_0 d\psi_0^\star][d\psi_1 d\psi_1^\star]\cdots[d\psi_{M-1}d\psi_{M-1}^\star]e^{+\epsilon\sum_{k=0}^{M-1}[\frac{1}{\epsilon}(\psi_{k+1}^\star-\psi_k^\star)\psi_k-H(\psi_{k+1}^\star,\psi_k)]}\\
&= \int [d\psi_0 d\psi_0^\star][d\psi_1 d\psi_1^\star]\cdots[d\psi_{M-1}d\psi_{M-1}^\star]e^{-\epsilon\sum_{k=1}^{M}[\frac{1}{\epsilon}\psi_k^\star(\psi_k-\psi_{k-1})+H(\psi_k^\star,\psi_{k-1})]}
\end{aligned} \tag{28}$$

valid to leading order in ϵ. In the last line above, we have used the discrete version of integration by parts and the periodic boundary conditions on ψ to transfer the finite difference on to ψ instead of $\psi^\star$, and it is understood throughout that we are taking the limit $M \to \infty$, $\epsilon \to 0$, such that $M\epsilon = \beta$ remains fixed.

Formally, in this limit, the sum in the exponential can be thought of as a Riemann sum whose limit gives an integral expression. In other words, we may identify

$$\epsilon \sum_{k=1}^{M} [\frac{1}{\epsilon}\psi_k^\star(\psi_k - \psi_{k-1}) + H(\psi_k^\star, \psi_{k-1})] \;=\; \int_0^\beta d\tau [\psi^\star(\tau)\partial_\tau\psi(\tau) + H(\psi^\star(\tau), \psi(\tau))] \tag{29}$$

In the same limit, the multiple integral can be thought of as *defining an integral over paths in the space of coherent states*:

$$\int [d\psi_0 d\psi_0^\star][d\psi_1 d\psi_1^\star] \cdots [d\psi_{M-1} d\psi_{M-1}^\star] \;=\; \int \mathcal{D}\psi(\tau)\mathcal{D}\psi^\star(\tau) \tag{30}$$

This path integral representation is somewhat analogous to the coherent state path integrals for spins, which we developed in earlier lectures. Indeed, the time derivative term in the exponential is clearly a pure imaginary quantity, and therefore represents the analog of the Berry phase that we encountered in the spin path integral.

This concludes our derivation of the coherent state path integral for bosonic systems. In the next few lectures, we will explore the physics of such systems using this and other tools.