Lecture 18: Calculating with the Bosonic path integral.

In the last lecture, we have developed the coherent state path integral representation for a system of many bosonic particles. As was clear from the derivation, the path integral is defined as a formal limit of an infinitely fine mesh in the imaginary time direction, and is usually written in continuous time τ.

This formal representation suffices for most purposes, since the main role of the path integral representation is to suggest new and physically well-motivated approximation schemes and provide physical insight. For instance, our derivation of the quantum rotor Hamiltonian as the low-energy effective theory for an antiferromagnetic insulator with short-range Néel order relied crucially on the physical intuition provided by the spin coherent state path integral. The physical picture that emerged from our manipulations of the formally defined path integral told us that the low temperature physics is dominated by near-collinear configurations characterized by a Néel vector that varies slowly in space and time, and that the Berry phase associated with the time-evolution of the system within this class of configurations can be thought of as the kinetic energy of a quantum rotor which points in the direction of the Néel vector. In arriving at these conclusions, we never actually needed to use the details of the time-discretization to calculate anything.

However, sometimes it is necessary to be able to go back to the more precise time-discretized version to resolve ambiguities and be sure that we know what we are doing. So in this lecture, we will try and do some very simple calculations with the bosonic path integral, keeping the discretization in the time direction explicit, as a way of gaining familiarity with path integral methods.

The first calculation we will do is that of the partition function Z_0 of a many-body system of non-interacting bosonic particles with single-particle energy levels ϵ_α. Absorbing the chemical potential into the single-particle energies to define $E_\alpha = (\epsilon_\alpha - \mu)$, we may write the non-interacting Hamiltonian in second-quantized form as

$$H_0 = \sum_\alpha E_\alpha a_\alpha^\dagger a_\alpha \tag{1}$$

From the previous lecture, we have the following expression for the partition function written as a path integral:

$$Z = \prod_\alpha \left(\int [d\psi_\alpha(\tau_0) d\psi_\alpha^\star(\tau_0)] \cdots [d\psi_\alpha(\tau_{M-1}) d\psi_\alpha^\star(\tau_{M-1})] e^{-\psi_\alpha^\star(\tau_i) S_{ij}^\alpha \psi_\alpha(\tau_j)} \right) \tag{2}$$

where the S_{ij}^α is an $M \times M$ matrix which we may construct based on our derivation in the previous lecture (remember, $M\epsilon = \beta$ is held fixed and the imaginary time spacing ϵ is sent to zero to formally define the "path integral"):

$$S^\alpha = \begin{bmatrix} 1 & 0 & 0 & \cdots & -a_\alpha \\ -a_\alpha & 1 & 0 \cdots & 0 & 0 \\ 0 & -a_\alpha & 1 \cdots & 0 & 0 \\ 0 & 0 & -a_\alpha \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -a_\alpha & 1 \end{bmatrix} \tag{3}$$

with $a_\alpha = -\epsilon E_\alpha + 1$

Thus evaluating the path integral reduces to doing a Gaussian integral over many complex variables. While this is rather standard material in a mathematical methods course, it is nevertheless useful to remind oneself of the basic results before proceeding further in our discussion. To this end, we first note that the Gaussian integral over one variable, namely

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}} \, , \tag{4}$$

generalizes readily to the following n-fold Gaussian integral

$$\int \frac{dx_1 \cdots dx_n}{(2\pi)^{n/2}} e^{-\frac{1}{2}\sum_{ij} x_i A_{ij} x_j + \sum_i x_i J_i} = \frac{1}{\sqrt{\det A}} e^{\frac{1}{2}\sum_{ij} J_i A_{ij}^{-1} J_j} \tag{5}$$

which is valid for any positive definite matrix A.

The argument is straightforward at least for those A that can be diagonalized by an orthogonal transformation and proceeds by two changes of variables. First, we shift the $\{x_i\}$ to eliminate the linear terms in the exponent:

$$y_i = x_i - \sum_j A_{ij}^{-1} J_j \tag{6}$$

The Jacobian for this transformation is clearly unity since it only involves a shift by a constant vector. Next, one transforms from the $\{y_i\}$ to the eigenmodes of the A matrix:

$$z_k = \sum_i O^{-1}_{ki} y_i \tag{7}$$

where O is the matrix whose columns are the orthonormal eigenvectors of A so that

$$O^T A O = \begin{bmatrix} a_1 & 0 & 0 & \cdots & 0 \\ 0 & a_2 & 0 & \cdots & 0 \\ 0 & 0 & a_3 & 0\cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_n \end{bmatrix}. \tag{8}$$

where the a_i are the eigenvalues of A. As a result of the orthonormality of these eigenvectors, the matrix O is orthogonal, and therefore the Jacobian of the second transformation is also unity. Therefore,

$$\int \frac{dx_1 \cdots dx_n}{(2\pi)^{n/2}} e^{-\frac{1}{2}\sum_{ij} x_i A_{ij} x_j + \sum_i x_i J_i} = \int \frac{dy_1 \cdots dy_n}{(2\pi)^{n/2}} e^{-\frac{1}{2}\sum_i a_i z_i^2} \tag{9}$$

and the required result follows from the answer for a Gaussian integral over a single variable. Indeed, the final result is actually true for Gaussian integrals involving a larger class of complex matrices with a positive definite hermitean part:

$$\int \prod_i \frac{d\mathrm{Re}x_i d\mathrm{Im}x_i}{\pi} e^{-\sum_{ij} x_i^\star K_{ij} x_j + \sum_i J_i^\star x_i + \sum_i J_i x_j^\star} \tag{10}$$

for any K with +ve hermitian part.

This is the result we need to use to evaluate the discrete form of the path integral. Using this result, we have

$$Z = \prod_\alpha \frac{1}{\mathrm{det} S^\alpha} \tag{11}$$

We calculate $\mathrm{det}S^\alpha$ by expanding along the first row of S^α:

$$\mathrm{det}S^\alpha = \begin{vmatrix} 1 & 0\cdots & 0 & 0 \\ -a_\alpha & 1\cdots & 0 & 0 \\ 0 & -a_\alpha\cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & -a_\alpha & 1 \end{vmatrix} + (-1)^{M-1}(-a) \begin{vmatrix} -a_\alpha & 1 & 0\cdots & 0 \\ 0 & -a_\alpha & 1\cdots & 0 \\ 0 & 0 & -a_\alpha\cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -a_\alpha \end{vmatrix}$$

$$= \quad 1 + (-1)^{M-1}(-a)^M = (1 - a^M)$$

Now, it is straightforward to take the $M \to \infty$ limit

$$\lim_{M\to\infty} \left(1 - \left(1 - \frac{\beta}{M} E_\alpha\right)^M\right) \quad = \quad (1 - e^{-\beta E_\alpha}) \tag{12}$$

to obtain the final result for the partition function

$$Z \quad = \quad \prod_\alpha \frac{1}{1 - e^{-\beta E_\alpha}} \tag{13}$$

Not surprisingly, this tallies exactly with the result for a non-interacting bosonic system obtained by elementary means.

In many applications, it is useful to represent various response functions (studied in our earlier lectures on linear response theory) in path integral language. The basic building block of such a path integral representation of these response functions is the so-called imaginary time ordered Green function:

$$\mathcal{G}(\alpha_1\tau_1|\alpha_2\tau_2) = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}\mathcal{T}[a^H_{\alpha_1}(\tau_1)(a^\dagger_{\alpha_2})^H(\tau_2)]\right] \tag{14}$$

where the superscript H on the creation and annihilation operators indicates that they are Heisenberg operators:

$$\begin{aligned} a^H(\tau) \quad &= \quad e^{H\tau} a e^{-H\tau} \\ (a^\dagger)^H(\tau) \quad &= \quad e^{H\tau} a^\dagger e^{-H\tau} \end{aligned} \tag{15}$$

and the imaginary time ordering symbol $\mathcal{T}$ places Heisenberg operators at a later time τ to the left of those at an earlier time τ'. This is augmented by the convention that we place $a^\dagger$ to left of a for $\tau_1 = \tau_2$.

What is the path integral representation of this object? To work this out, it is simplest to work through the two cases separately, one with $\tau_1 > \tau_2$ and the other with $\tau_2 > \tau_1$. In the former case, the time-ordering produces the expression

$$\frac{1}{Z}\mathrm{Tr}e^{-\beta H}e^{H\tau_1}a_{\alpha_1}e^{-H\tau_1}e^{H\tau_2}a^\dagger_{\alpha_2}e^{-H\tau_2} \quad = \quad \frac{1}{Z}\mathrm{Tr}e^{-(\beta-\tau_1)H}a_{\alpha_1}e^{-H(\tau_1-\tau_2)}a^\dagger_{\alpha_2}e^{-H\tau_2} \tag{16}$$

while in the latter case one has

$$\frac{1}{Z}\mathrm{Tr}e^{-(\beta-\tau_2)H}a^\dagger_{\alpha_2}e^{-H(\tau_2-\tau_1)}a_{\alpha_1}e^{-H\tau_1} \tag{17}$$

If we proceed as usual and introduce complete sets of states after splitting the imaginary time evolution into infinitesimal bits of size ϵ, we see that in both cases we obtain the *same* expression:

$$\frac{1}{Z}\int \mathcal{D}\phi(\tau)\mathcal{D}\phi^*(\tau)e^{-\int d\tau\left[\phi^\star\frac{\partial\phi}{\partial\tau}+H[\phi^\star\phi]\right]}\phi^\star_{\alpha_2}(\tau_2)\phi_{\alpha_1}(\tau_1) \tag{18}$$

Thus, the path integral automatically incorporates the imaginary time ordering. Also, at equal times $\tau_1=\tau_2$, $\phi^\star_{\alpha_2}$ will still be calculated at $\tau_2+\epsilon$ if we go back to our discrete expression that underlies this formal path integral formula.

To appreciate this formula better, we now calculate this quantity using the explicit discrete form that we have been using thus far in this lecture. But first a small digression: If we consider the integral

$$I=\int\prod_i\frac{d\mathrm{Re}x_i d\mathrm{Im}x_i}{\pi}e^{-\sum_{ij}x_i^\star K_{ij}x_j+\sum_i J_i^\star x_i+\sum_i J_i x_j^\star} \tag{19}$$

we see that

$$\int\prod_i\frac{d\mathrm{Re}x_i d\mathrm{Im}x_i}{\pi}x_i^\star x_j e^{-\sum_{ij}x_i^\star K_{ij}x_j+\sum_i J_i^\star x_i+\sum_i J_i x_j^\star}=\frac{\partial^2 I}{\partial J_i\partial J_j^\star}\Big|_{J=0} \tag{20}$$

Using our earlier explicit formula for this integral, we see that this equals

$$\frac{1}{\det K}K^{-1}_{ji} \tag{21}$$

Therefore, we see that

$$\langle x_i^\star x_j\rangle = K^{-1}_{ji}. \tag{22}$$

where the angular brackets denote averaging with respect to the Gaussian measure whose integral is I.

We may now use this result in conjunction with the discrete form of the path integral expression for the imaginary-time ordered Green function to obtain

$$\mathcal{G}(\alpha_1\tau_j|\alpha_2\tau_i)=\delta_{\alpha_1\alpha_2}(S^{\alpha_1})^{-1}_{ji} \tag{23}$$

Now, we note that

$$(S^\alpha)^{-1} \quad = \quad \frac{1}{1-a_\alpha^M}\begin{bmatrix} 1 & a_\alpha^{M-1} & a_\alpha^{M-2} & \cdots & a_\alpha \\ a_\alpha & 1 & a_\alpha^{M-1} & \cdots & a_\alpha^2 \\ a_\alpha^2 & a_\alpha & 1 & \cdots & a_\alpha^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_\alpha^{M-1} & a_\alpha^{M-2} & a_\alpha^{M-3} & \cdots & 1 \end{bmatrix} \tag{24}$$

For $\tau_j \equiv \epsilon j > \tau_i \equiv \epsilon i$, we have

$$(S^\alpha)^{-1}_{ji} = \frac{a_\alpha^{j-i}}{1-a_\alpha^M} \tag{25}$$

Taking the limit $M \to \infty, \epsilon \to 0$ with $M\epsilon = \beta$ fixed, we therefore obtain the following expression for for $\tau_j > \tau_i$:

$$\begin{aligned}
\frac{(1-\epsilon E_\alpha)^{j-i}}{1-(1-\epsilon E_\alpha)^M} &= \frac{(1-\epsilon E_\alpha)^{\frac{\tau_j-\tau_i}{\epsilon}}}{1-(1-\epsilon E_\alpha)^{\frac{\beta}{\epsilon}}} \\
&= \frac{e^{-(\tau_j-\tau_i)E_\alpha}}{1-e^{-\beta E_\alpha}} \\
&= e^{-E_\alpha(\tau_j-\tau_i)}\left[1+\frac{1}{e^{\beta E_\alpha}-1}\right] \\
&= e^{-E_\alpha(\tau_j-\tau_i)}(1+n_\alpha).
\end{aligned}$$

On the other hand, for $\tau_j < \tau_i$, we have

$$(S^\alpha)^{-1}_{ji} \quad = \quad \frac{a_\alpha^{M-(i-j)}}{1-a_\alpha^M} \tag{26}$$

Taking the limit $M \to \infty, \epsilon \to 0$ with $M\epsilon = \beta$ fixed, we now obtain

$$\begin{aligned}
\frac{e^{-E_\alpha(\beta-(\tau_1^0-\tau_j))}}{1-e^{-\beta E_\alpha}} &= \frac{e^{-E_\alpha(\tau_j-\tau_i)}}{e^{-\beta E_\alpha}-1} \\
&= e^{-E_\alpha(\tau_j-\tau_i)}n_\alpha
\end{aligned} \tag{27}$$

Finally, for $\tau_j = \tau_i$, we need to take the expression for $\tau_i > \tau_j$ and set the two times equal.

All of this is summarized in the expression

$$\mathcal{G}(\alpha\tau_j|\alpha\tau_i) \;=\; e^{-E_\alpha(\tau_j-\tau_i)}[(1+n_\alpha)\theta(\tau_j-\tau_i-\eta)+n_\alpha\theta(\tau_i-\tau_j+\eta)] \tag{28}$$

where $\eta = 0^+$ is a positive infinitesimal quantity.

By taking repeated derivatives with respect to the sources in Eqn. (10), we see that it is possible to relate $\langle x_i x_j \ldots x_k^* x_l^* \ldots\rangle$ to a sum of products of expectation values of the form $\langle x_i x_k^*\rangle$. This property of averages taken in a Gaussian probability distribution is called "Wick's theorem" in the context of many-body theory, and allows us to compute more complicated correlation functions in terms of sums of products of Green functions. It is in this sense that the Green functions are the basic building blocks of many computations including those of response functions defined earlier.

This completes our discussion of path integrals for bosonic systems. In the next couple of lectures we will discuss the possible phases of some simple bosonic systems, as well as the nature of phase transitions between these phases—this discussion will be greatly facilitated by thinking in the path integral language developed here.