Physics 127c: Statistical Mechanics

Path Integral Methods

The Trotter quantum Monte Carlo method leads easily into a discussion of path integral methods in statistical mechanics. Feynman introduced a "sum over histories" approach to quantum mechanics that provides a nice intuitive approach to many problems, as well as a new systematic formal approach. With very little effort these ideas can be transferred to the formalism of statistical mechanics. This is often the approach used in research on statistical mechanics of many body quantum systems, and my main motivation for introducing the ideas is to connect with this modern literature. The method, and its Monte Carlo implementation, also provides an informative way of understanding and calculating interacting Boson systems such as superfluid He^4, an approach introduced by Feynman in the early 1950s.

Quantum Mechanics and Statistical Mechanics

In quantum mechanics much can be learnt by focusing on the matrix elements of the evolution operator

$$U(\mathbf{x}, \mathbf{x}'; t) = \left\langle \mathbf{x} \left| e^{-iHt/\hbar} \right| \mathbf{x}' \right\rangle. \tag{1}$$

(I will formulate the argument in terms of the position of a single particle, but the ideas apply generally.) In statistical mechanics the (unnormalized) density matrix

$$\bar{\rho}(\mathbf{x}, \mathbf{x}'; \beta) = \left\langle \mathbf{x} \left| e^{-\beta H} \right| \mathbf{x}' \right\rangle \tag{2}$$

can be used to calculate the partition function and other averages.

There is clearly a close analogy between these two quantities. In fact we can think of $\bar{\rho}$ as being given by the *imaginary time evolution* $t \to -i\tau$

$$\hbar \frac{\partial \bar{\rho}}{\partial \tau} = -H\bar{\rho} \tag{3}$$

and the density matrix is given by evolving for imaginary time $\tau = \beta\hbar$. This analogy is very useful, and is the basis in many formal methods in statistical mechanics. It is sometimes known as *Wick rotation*.

The basic idea of the path integral approach was already introduced in the previous lecture: split the time evolution up into small pieces. The evolution between states becomes simple over small time intervals, and the full evolution is given by the product of the small steps. Taking the limit of the time step to zero, and the number of steps to infinity, gives the path integral. Feynman formulated the path integral method in terms of Eq. (1), but we can transfer his methods over to Eq. (2). In fact, the text books say that the expressions are better defined mathematically for the statistical mechanics application.

The path integral approach has a number of advantages in complicated problems. It leads to compact formal expressions involving integrals over numbers, rather than operators. This allows the application of familiar approximation techniques, such as the method of steepest descents or stationary phase, giving mean field approximations valid when fluctuations are small. In addition, it often gives nice intuitive pictures for the different "classical" possibilities that make up the quantum state. Finally there is a close connection with the quantum Monte Carlo implementation, which is just a discretization of the integral expressions.

I will first introduce the path integral representation of the quantum evolution operator, since the resulting expressions may be familiar to you from other courses.

Feynman's Path Integral Method

As in the last lecture we split up the evolution into a number of steps M, but now let $M \to \infty$. We insert the completeness relation for some convenient choice of basis states between each evolution step.

$$U(\mathbf{x}, \mathbf{x}'; t) = \lim_{M \to \infty} \int \cdots \int \prod_{n=1}^{M-1} d\mathbf{x}_n \left\langle \mathbf{x} \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}_{M-1} \right\rangle \left\langle \mathbf{x}_{M-1} \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}_{M-2} \right\rangle \ldots \left\langle \mathbf{x}_1 \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}' \right\rangle, \quad (4)$$

with $\varepsilon = t/M$. We now want some approximation to $\left\langle \mathbf{x}_n \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}_{n-1} \right\rangle$ taking advantage of the small ε. This approximation must be chosen so that the product of all the terms gives the correct evolution. Suppose the Hamiltonian is

$$H = \frac{p^2}{2m} + V(\mathbf{x}). \quad (5)$$

Since H depends on $\mathbf{p}$ and $\mathbf{x}$ it is convenient to introduce the complete set of momentum states $\mathbf{p}_n$ and write

$$\left\langle \mathbf{x}_n \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}_{n-1} \right\rangle = \sum_{\mathbf{p}_n} \langle \mathbf{x}_n | \mathbf{p}_n \rangle \left\langle \mathbf{p}_n \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}_{n-1} \right\rangle, \quad (6a)$$

$$= \sum_{\mathbf{p}_n} \langle \mathbf{x}_n | \mathbf{p}_n \rangle \langle \mathbf{p}_n | \mathbf{x}_{n-1} \rangle \, e^{-i\varepsilon[p_n^2/2m + V(\mathbf{x}_{n-1})]/\hbar} \quad (6b)$$

Two different ways of treating this expression lead to a "Lagrangian" or a "Hamiltonian" formulation.

In the first, we introduce the explicit x representation of the momentum state

$$\langle \mathbf{x} | \mathbf{p} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{p} \cdot \mathbf{x}/\hbar} \quad (7)$$

and do the momentum sum using $\sum_{\mathbf{p}} \to V/(2\pi\hbar)^3 \int d^3p$ as usual, to give

$$\left\langle \mathbf{x}_n \left| e^{-iH\varepsilon/\hbar} \right| \mathbf{x}_{n-1} \right\rangle = \int \frac{d^3 p_n}{(2\pi\hbar)^3} e^{i\mathbf{p}_n \cdot (\mathbf{x}_n - \mathbf{x}_{n-1})/\hbar} e^{-i\varepsilon[p_n^2/2m + V(\mathbf{x}_{n-1})]/\hbar} \quad (8)$$

$$= \left(\frac{m}{2\pi i \varepsilon \hbar} \right)^{3/2} \exp \left\{ \frac{i\varepsilon}{\hbar} \left[\frac{m}{2} \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})^2}{\varepsilon^2} - V(\mathbf{x}_{n-1}) \right] \right\}. \quad (9)$$

Now when we take the product of the M evolution steps, and let $M \to \infty$, we can write

$$(\mathbf{x}_n - \mathbf{x}_{n-1})/\varepsilon \to \dot{\mathbf{x}}(t), \quad (10)$$

$$V(\mathbf{x}_{n-1}) \to V(\mathbf{x}(t)), \quad (11)$$

$$\sum_{n=1}^{M-1} \varepsilon \ldots \to \int_0^t dt \ldots. \quad (12)$$

We also have to integrate over the intermediate $\mathbf{x}_n$ and have M factors of $(m/2\pi i\varepsilon\hbar)^{3/2}$, which we lump together into a formal expression for the "measure"

$$\left(\frac{m}{2\pi i \varepsilon \hbar} \right)^{3M/2} \int \cdots \int \prod_{n=1}^{M-1} d\mathbf{x}_n \to \int \mathcal{D}\mathbf{x}(t). \quad (13)$$

Thus we get

$$U(\mathbf{x}, \mathbf{x}'; t) = \int_{\substack{\mathbf{x}(0)=\mathbf{x}' \\ \mathbf{x}(t)=\mathbf{x}}} \mathcal{D}\mathbf{x}(t) e^{iS/\hbar}, \quad (14)$$

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where the "action" S is

$$S = \int_0^t dt \, L(\mathbf{x}(t)), \tag{15}$$

with L the usual Lagrangian

$$L = \frac{1}{2} m \dot{\mathbf{x}}^2 - V(\mathbf{x}(t)). \tag{16}$$

The path variables $\mathbf{x}(t)$ are integrated over all values consistent with the boundary conditions $\mathbf{x}(0) = \mathbf{x}'$, $\mathbf{x}(t) = \mathbf{x}$. This is undoubtedly a pretty expression, although the symbol $\int \mathcal{D}\mathbf{x}(t)$ contains mathematical difficulties that are in practice resolved by returning to the discrete expression, and taking $M \to \infty$ after the calculation is done.

Alternatively we can keep the $\mathbf{p}_n$ sum introduced in Eq. (6) and write

$$\langle \mathbf{x}_n | \mathbf{p}_n \rangle \langle \mathbf{p}_n | \mathbf{x}_{n-1} \rangle \exp \left\{ -\frac{i\varepsilon}{\hbar} \left[\frac{p_n^2}{2m} + V(\mathbf{x}_{n-1}) \right] \right\} = \frac{1}{V} \exp \left\{ \frac{i\varepsilon}{\hbar} \left[\mathbf{p}_n \cdot \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})}{\varepsilon} - \frac{p_n^2}{2m} - V(\mathbf{x}_{n-1}) \right] \right\}, \tag{17}$$

which on taking the limits gives

$$U(\mathbf{x}, \mathbf{x}'; t) = \int_{\substack{x(0)=x' \\ x(t)=x}} \mathcal{D}\mathbf{x}(t) \mathcal{D}\mathbf{p}(t) \exp \left\{ \frac{i}{\hbar} \int_0^t \left[\mathbf{p} \cdot \dot{\mathbf{x}} - H(\mathbf{p}, \mathbf{x}) \right] \right\}, \tag{18}$$

where $\mathcal{D}\mathbf{p}(t)$ stands for

$$\int \cdots \int \prod_n \frac{d^3 p_n}{(2\pi\hbar)^3} \to \mathcal{D}\mathbf{p}(t). \tag{19}$$

The momenta $\mathbf{p}(t)$ are integrated over all values.

Application to Statistical Mechanics

For simple particle problems with the standard $p^2/2m$ term in the Hamiltonian the "Lagrangian" expression is usually used. Repeating the derivation with $t \to -i\tau$ leads to

$$\bar{\rho}(\mathbf{x}, \mathbf{x}'; \beta) = \int_{\substack{\mathbf{x}(0)=\mathbf{x}' \\ \mathbf{x}(\beta\hbar)=\mathbf{x}}} \mathcal{D}\mathbf{x}(t) \exp \left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left[\frac{m}{2} \dot{\mathbf{x}}^2 + V(\mathbf{x}(\tau)) \right] \right\} \tag{20}$$

with $\dot{\mathbf{x}}$ now $d\mathbf{x}/d\tau$ and the measure

$$\mathcal{D}\mathbf{x}(t) = \lim_{M \to \infty} \left(\frac{m}{2\pi\varepsilon\hbar} \right)^{3M/2} \int \cdots \int \prod_{n=1}^{M-1} d\mathbf{x}_n. \tag{21}$$

According to the text books this is better defined mathematically than for the real time case. The partition function involves setting $\mathbf{x}' = \mathbf{x}$ and then integrating over $\mathbf{x}$, which is often written as

$$Z = \int_{\mathbf{x}(0)=\mathbf{x}(\beta\hbar)} \mathcal{D}\mathbf{x}(t) \exp \left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left[\frac{m}{2} \dot{\mathbf{x}}^2 + V(\mathbf{x}(\tau)) \right] \right\}, \tag{22}$$

implying the integration over all paths with periodic boundary condition in imaginary time.

For a many particle system in the particle coordinate representation the same expression apply with $\mathbf{x}$ the $3N$ coordinate vector $\mathbf{x} = (\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \ldots \mathbf{x}^{(N)})$. For indistinguishable particles we do not care which particle

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is at each final position, and must implement the symmetry or antisymmetry requirement. Thus for Bosons we must include all possible permutations of the paths, and the density matrix becomes

$$\bar{\rho}_B(\mathbf{x}, \mathbf{x}'; \beta) = \frac{1}{N!} \sum_P \bar{\rho}(\mathbf{x}, P\mathbf{x}'; \beta). \tag{23}$$

Often we prefer the second quantized representation in terms of particle creation and annihilation operators. For Bosons we can generate a convenient path integral representation by using *coherent states* as the complete set of states at each time step. (Coherent states actually form an over-complete set, but the completeness relation is all that is required, so this is not a problem.) The coherent states are defined as eigenfunctions of the particle annihilation operator

$$\hat{\psi}_\alpha |\psi_a\rangle = \psi_\alpha |\psi_a\rangle. \tag{24}$$

Here $\hat{\psi}_\alpha$ is the annihilation operator for state α (which might be a momentum state, position state, or some other choice), $|\psi_a\rangle$ is the coherent state eigenvector corresponding to the eigenvalue ψ_α which is a complex number. Without going through all the algebra of coherent states, we can motivate the resulting expression by noting the commutation rule

$$\left[\psi_\alpha, \psi_\alpha^+\right] = 1 \tag{25}$$

is like the $\mathbf{x}$, $\mathbf{p}$ commutation rule if we think of $i\hbar\psi_\alpha^+$ as the momentum conjugate to ψ_α. Using the Hamiltonian version of the path integral Eq. (18) then gives (with $t \to -i\tau$) for the grand canonical partition function

$$Z = \int \mathcal{D}\psi_\alpha \mathcal{D}\psi_\alpha^* \exp\left\{-\int_0^{\beta\hbar} d\tau \left[\sum_\alpha \psi_\alpha^*(\tau)\left(\frac{\partial}{\partial\tau} - \mu\right)\psi_\alpha(\tau) + H\left(\psi_\alpha(\tau), \psi_\alpha^*(\tau)\right)\right]\right\}. \tag{26}$$

Remember that here ψ_α is just a complex number for each label α ($\mathbf{x}$ or $\mathbf{k}$, etc.).

Fermions are significantly harder, because the anticommutation properties mean we have to introduce "anticommuting numbers" known as Grassmann variables. I will leave you to consult texts (e.g. *Negele and Ormand*) if you are interested in this.

Further Reading

A classic introduction to the application of path integral methods to statistical mechanics is *Statistical Mechanics* by *Feynman*. Section 11.10 discusses his application of the method to the λ-transition leading to superfluid He. More modern books that go *much* deeper into the applications to many body physics are *Quantum Many-Particle Systems* by Negele and Ormand (§2.2 is a nice, if terse, introduction including the Fermion case) and *Field Theories of Condensed Matter Systems* by *Fradkin*. The review article by *Ceperley* Rev. Mod. Phys. **67**, 279 (1995) has a colloquial discussion of path integrals in statistical mechanics emphasizing the connection to quantum Monte Carlo methods, and also the application to superfluid He[4] which I will talk about in the next lecture.