Lattice Quantum Field Theory Lectures

Lecture 1: quantum mechanics and path integral

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Outline

• A short review of quantum mechanics (with Dirac notation and Harmonic Oscillator)
• Classical mechanics by the principle of least action
• Quantum mechanical evolution, as a path integral.
• Numerical calculations: Monte Carlo and imaginary-time evolution.
• Setting up calculating the ground state energy and wave function, etc.
Review of quantum mechanics (with Dirac notation and harmonic oscillator)
Quantum states

A quantum mechanical state is represented by a vector in Hilbert space (usually infinite dimensional complex space):

\[ |\psi\rangle, \text{ or } \langle\psi| \]

All states form a linear vector space which obeys all the rule about the linear vector space.

ps. Vectors with different phases (called ray) represent the same state.

(Dirac Notation: bra and ket)
Quantum dynamics

• Assume the system has a Hamiltonian $H$.

• A quantum mechanical state at $t=0$ as $|\psi(0)\rangle$ will evolve in the following way:

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

or the state obey the Schrödinger eq.

• The evolution is unitary:

$$U(t_2, t_1) = e^{-iH(t_2-t_1)/\hbar}$$
Mechanical observables

- All observables, such as position \( x \), momentum \( p \), etc., are represented by linear Hermitian operators in the Hilbert space.
  \[
  \hat{x}, \hat{p}, \hat{O}
  \]
- They have real eigenvalues, \( x, p, o \)
  \[
  \hat{x}|x\rangle = x|x\rangle
  \]
- The corresponding eigenvectors are orthogonal
  \[
  \langle x|x'\rangle = \delta(x - x')
  \]
- The eigenvectors are complete
  \[
  \int dx \ |x\rangle\langle x| = 1 \text{ (unit operator)}
  \]
Measurements

• A measurement of an observable \( \hat{O} \) always produces its eigenvalue \( O_i \),

• The probability amplitude (PA) of yielding \( O_i \) in a state \( |\psi\rangle \) is,

\[ C_i = \langle O_i |\psi\rangle \]

which is a complex number.

• Any state can be expanded in the basis of \( \hat{O} \),

\[ |\psi\rangle = \sum_i \langle O_i |\psi\rangle |O_i\rangle \]

and the modulus of the PA is 1.
Quantization condition

• In Quantum Mechanics, the conjugate mechanical observables \{x, p\} are postulated to have the following commutation relation

\[ [p, x] = i \hbar \]

where \( \hbar = h/2\pi \) is the reduced Planck constant.

• It is often stated in the textbooks that the classical limit is recovered when

\[ \hbar (\hbar = h/2) \rightarrow 0 \]

in this case, the commutation relation vanishes and the operators become real-number.
1D Harmonic oscillator

• Hamiltonian

\[ H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \]

eigenfunction,

\[ H|n\rangle = E_n|n\rangle \quad n = 0, 1, 2, \ldots \]
eigenvalues,

\[ E_n = \left( n + \frac{1}{2} \right) \frac{\hbar\omega}{\pi} \]

In coordinate space, the ground state has a wave function look like (length parameter: \( b^2 = \frac{\hbar}{m\omega} \))

\[ \langle x | 0 \rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \exp\left( -\frac{m\omega}{2\hbar} x^2 \right) = \frac{1}{\sqrt{b\sqrt{\pi}}} e^{-x^2/2b^2} \]
Quantum Oscillator wave functions

Coherent State
Principle of least action
Classical mechanics

• Classical mechanics is usually represented by Newton’s three laws (1687).

• However, Hamilton reformulated the mechanics problems using the variational principle. Define the lagrangian as,

\[ L = T - V = \frac{1}{2}mv^2 - \frac{1}{2}m\omega^2x^2 \]

when particle moves from \((x_1, t_1)\) to \((x_2, t_2)\) along a path \(x=x(t)\), we calculate the action,

\[ S(x(t)) = \int_{t_1}^{t_2} L dt \]
- The action is different for different path
- The physical path is the one for which the action is minimum!
Using the principle of the least action, one can derive the well-known Euler-Lagrange equation

\[ \int_{t_1}^{t_2} \delta L \, dt = 0. \]

\[ \delta L = \sum_{j=1}^{n} \left( \frac{\partial L}{\partial q_j} \delta q_j + \frac{\partial L}{\partial \dot{q}_j} \delta \dot{q}_j \right), \quad \delta \dot{q}_j \equiv \delta \frac{dq_j}{dt} = \frac{d(\delta q_j)}{dt}, \]

\[ \int_{t_1}^{t_2} \delta L \, dt = \sum_{j=1}^{n} \left[ \frac{\partial L}{\partial \dot{q}_j} \delta q_j \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \sum_{j=1}^{n} \left( \frac{\partial L}{\partial q_j} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_j} \right) \delta q_j \, dt. \]

\[ \frac{\partial L}{\partial q_j} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_j} = 0. \]
EL equation for oscillator

• The EL equation for the oscillator is just
\[ \frac{d^2x}{dt^2} + \omega^2 x = 0 \]
This is the same as Newton’s equation.
• Action principle completely covers the Newton’s mechanics.
• This is usually called Analytical Mechanics, which starts with lagrangian.
Quantum mechanics using classical action
Quantum amplitude

• Consider now a particle at $x_a$ when time $t=t_a$. The quantum state is $|x_a\rangle$.

• At time $t=t_b$, the particle can be at $x_b$, with a certain probability amplitude (also called Propagator or Green’s function)

$$\langle x_b t_b | x_a t_a \rangle = \langle x_b | e^{-iH(t_b-t_a)/\hbar} | x_a \rangle$$

• It was shown by Feynman that this PA can be expressed in terms of path integral

$$\langle x_b t_b | x_a t_a \rangle = \int [Dx(t)] e^{iS/\hbar}$$

where integration sums up all paths.
Summing up all paths

• All paths satisfying the boundary condition need be included
• Every path defines an action $S$
• Every path contribution is weighted with a phase factor $e^{iS/\hbar}$
• In the classical limit, $\hbar \to 0$, one gets the least action principle.
Classical limit

• By taking $\hbar \to 0$ limit, one shall recover classical mechanics.

• In this case the path integral is dominated by one path for which $S$ is minimum, or
  \[ \delta S = 0 \]
  this is just the least-action principle.

• Any path deviating from this with a finite action difference $\Delta S$, will have a phase difference $\Delta S/\hbar \to \infty$, which contributes 0 to the path integral.
Derivation of the path integral in QM

\[ U(q_a, q_b; T) = \langle q_b | e^{-iHT/\hbar} | q_a \rangle. \]

Break the time interval into \( N \) short slices of duration \( \epsilon \).

\[ e^{-iHT} = e^{-iH\epsilon} e^{-iH\epsilon} e^{-iH\epsilon} \cdots e^{-iH\epsilon}. \]

So \( U(q_a, q_b; T) = \langle q_b | e^{-iH\epsilon} e^{-iH\epsilon} e^{-iH\epsilon} \cdots e^{-iH\epsilon} | q_a \rangle. \) Insert a complex of intermediate states,

\[ 1 = \left( \prod_i \int dq_k^i \right) |q_k\rangle \langle q_k| \cdot \]
Completing the derivation

\[ \langle q_{k+1} | e^{-iH\epsilon} | q_k \rangle = \langle q_{k+1} | e^{-iH\epsilon} \int \frac{dq_k}{2\pi} |p_k\rangle \langle p_k | q_k \rangle = \int \frac{dp_k}{2\pi} e^{-iH\epsilon} e^{i\epsilon p_k(q_{k+1} - q_k)}. \]

This \( q_{k+1} - q_k \) can be written as \( \frac{q_{k+1} - q_k}{\epsilon} \epsilon \rightarrow \dot{q}_k \epsilon. \)

\[ \langle q_{k+1} | e^{-iH\epsilon} | q_k \rangle = \int \frac{dp_k}{2\pi} e^{i\epsilon(p_k\dot{q}_k - H)}. \]

The transition amplitude can be written

\[ U(q_a, q_b; T) = \int \mathcal{D}q(t)\mathcal{D}p(t) e^{i \int_0^T dt (p\dot{q} - H)} = \int \mathcal{D}q(t) e^{i \int_0^T dt L}. \]
Analytical example: free particle

• In this case, the action is very simple.

\[ K(x - y; T) = \int_{x(0)=x}^{x(T)=y} \exp \left( -\int_0^T \frac{\dot{x}^2}{2} \, dt \right) \, Dx. \]

Splitting the integral into time slices:

\[ K(x, y; T) = \int_{x(0)=x}^{x(T)=y} \prod_t \exp \left( -\frac{1}{2} \left( \frac{x(t + \varepsilon) - x(t)}{\varepsilon} \right)^2 \varepsilon \right) \, Dx, \]

• Integration yields \((x_a=x, \ x_b=y)\)

\[ K(x - y; T) \propto e^{\frac{i(x-y)^2}{2T}} \]
Harmonic oscillator

\[ x_c(t) = x_i \frac{\sin \omega(t_f - t)}{\sin \omega(t_f - t_i)} + x_f \frac{\sin \omega(t - t_i)}{\sin \omega(t_f - t_i)}. \]

This trajectory yields the classical action

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

\[ = \frac{1}{2} m \omega \left( \frac{x_i^2 + x_f^2}{\sin \omega(t_f - t_i)} \cos \omega(t_f - t_i) - 2x_i x_f \right) \]

Next, expand the non-classical contribution to the action \( \delta S \) as a Fourier series, which gives

\[ S = S_c + \sum_{n=1}^{\infty} \frac{1}{2} a_n^2 \frac{m}{2} \left( \frac{(n\pi)^2}{t_f - t_i} - \omega^2(t_f - t_i) \right). \]

This means that the propagator is

\[ K(x_f, t_f; x_i, t_i) = Q e^{\frac{i s_c}{\hbar}} \prod_{j=1}^{\infty} \frac{j \pi}{\sqrt{2}} \int d\alpha_j \exp \left( \frac{i}{2\hbar} a_j^2 \frac{m}{2} \left( \frac{(j\pi)^2}{t_f - t_i} - \omega^2(t_f - t_i) \right) \right) \]

\[ = e^{\frac{i s_c}{\hbar}} Q \prod_{j=1}^{\infty} \left( 1 - \left( \frac{\omega(t_f - t_i)}{j\pi} \right)^2 \right)^{-\frac{1}{2}} \]
Let $T = t_f - t_i$. One may write this propagator in terms of energy eigenstates as

$$K(x_f, t_f; x_i, t_i) = \left( \frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}} \exp \left( \frac{i}{\hbar} \frac{1}{2} m\omega \frac{(x_i^2 + x_f^2) \cos \omega T - 2x_i x_f}{\sin \omega T} \right)$$

$$= \sum_{n=0}^{\infty} \exp \left( -\frac{iE_n T}{\hbar} \right) \psi_n(x_f)^* \psi_n(x_i).$$
Numerical calculation

• For more complicated system, one has to resolve to numerical calculation.
• For few degrees of freedom (d.o.f), one can directly solve the Schrodinger equation.
• However, for a quantum system with a large number (often $\infty$) of d.o.f, solving Schrodinger eq. is no longer an option. Path-integral becomes useful
  • Strongly-coupled relativistic quantum field theory such as Quantum Chromodynamics (QCD)
  • Non-relativistic quantum many-body systems (many electrons or large nuclei with many protons and neutrons)
Numerical calculation: Monte Carlo and imaginary-time evolution
Difficulties with path integral

• For non-trivial quantum systems, one needs to make calculations of the path integral numerically using a large computer.

• There are two paramount difficulties with numerical integrals
  • There are infinite number of integrals.
  • The integrand can change sign. Therefore, there will be a large number of cancellations.
Approximate infinite number of integral with finite number

• When doing numerical integration, one often approximate an integral by a finite sum.

\[ \int_{b}^{a} f(x)\,dx = \sum_{i} f(x_{i})\Delta x \]

• Is it possible that one may approximate the continuous infinite number of integrals by a discrete, finite number?
  
  • Not always
  • For simple quantum systems, yes.
Getting ready for numerical calculations

For a particle in a smooth potential, the path integral is approximated by zigzag paths, which in one dimension is a product of ordinary integrals. For the motion of the particle from position \( x_a \) at time \( t_a \) to \( x_b \) at time \( t_b \), the time sequence

\[
t_a = t_0 < t_1 < \cdots < t_{n-1} < t_n < t_{n+1} = t_b
\]

can be divided up into \( n + 1 \) smaller segments \( t_j - t_{j-1} \), where \( j = 1, \ldots, n + 1 \), of fixed duration

\[
\varepsilon = \Delta t = \frac{t_b - t_a}{n + 1}.
\]

This process is called time-slicing.

An approximation for the path integral can be computed as proportional to

\[
\int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \exp \left( \frac{i}{\hbar} \int_{t_a}^{t_b} L(x(t), v(t)) \, dt \right) \, dx_1 \cdots dx_n,
\]

where \( L(x, v) \) is the Lagrangian of the one-dimensional system with position variable \( x(t) \) and velocity \( v = \dot{x}(t) \) considered (see below), and \( dx_j \) corresponds to the position at the \( j \)th time step, if the time integral is approximated by a sum of \( n \) terms.\(^{[nb \ 2]}\)
the abovementioned "zigzagging" corresponds to the appearance of the terms

\[
\exp \left( \frac{i}{\hbar} \varepsilon \sum_{j=1}^{n+1} L \left( \tilde{x}_j, \frac{x_j - x_{j-1}}{\varepsilon}, j \right) \right)
\]

in the Riemann sum approximating the time integral, which are finally integrated over \( x_1 \) to \( x_n \) with the integration measure \( dx_1 \ldots dx_n \). \( \tilde{x}_j \) is an arbitrary value of the interval corresponding to \( j \), e.g. its center, \( \frac{x_j + x_{j-1}}{2} \).

For example, for a 1D particle, the lagrangian,

\[
L = \sum_{j=1,n+1}^{1} \frac{1}{2} m \left[ \frac{(x_j - x_{j-1})}{\varepsilon} \right]^2 - v(\tilde{x}_j)
\]

Hopefully, systematic error for the path integral goes like \( \varepsilon \).
Large number of integrals: Monte Carlo method

• One killer method to do a large number of integral is to use Monte Carlo method.

• Simple examples of Monte carlo integration will be introduced in the afternoon, in which the calculation of $\pi$ is determined by the number of shootings in the right region.
Methodology

\[ I = \int_{\Omega} f(\mathbf{x}) \, d\mathbf{x} \]

where \( \Omega \), a subset of \( \mathbb{R}^m \), has volume

\[ V = \int_{\Omega} d\mathbf{x} \]

The naive Monte Carlo approach is to sample points uniformly on \( \Omega \): \(^4\) given \( N \) uniform samples,

\[ \mathbf{x}_1, \ldots, \mathbf{x}_N \in \Omega, \]

\( I \) can be approximated by

\[ I \approx Q_N \equiv V \frac{1}{N} \sum_{i=1}^{N} f(\mathbf{x}_i) = V(f). \]

This is because the \underline{law of large numbers} ensures that

\[ \lim_{N \to \infty} Q_N = I. \]
Statistical error estimation: the secret of why it is powerful

\[ \text{Var}(f) \equiv \sigma_N^2 = \frac{1}{N-1} \sum_{i=1}^{N} (f(x_i) - \langle f \rangle)^2. \]

which leads to

\[ \text{Var}(Q_N) = \frac{V^2}{N^2} \sum_{i=1}^{N} \text{Var}(f) = V^2 \frac{\text{Var}(f)}{N} = V^2 \frac{\sigma_N^2}{N}. \]

As long as the sequence

\[ \{\sigma_1^2, \sigma_2^2, \sigma_3^2, \ldots\} \]

is bounded, this variance decreases asymptotically to zero as \(1/N\). The estimation

\[ \delta Q_N \approx \sqrt{\text{Var}(Q_N)} = V \frac{\sigma_N}{\sqrt{N}}, \]

which decreases as \(1/\sqrt{N}\). This is standard error of the mean multiplied with \(V\).
Example of calculating $\pi$ with

A paradigmatic example of a Monte Carlo integration is the estimation of $\pi$. Consider the function

$$H(x, y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{else} \end{cases}$$

and the set $\Omega = [-1,1] \times [-1,1]$ with $V = 4$. Notice that

$$I_\pi = \int_\Omega H(x, y) \, dx \, dy = \pi.$$

Thus, a crude way of calculating the value of $\pi$ with Monte Carlo integration is to pick $N$ random numbers on $\Omega$ and compute

$$Q_N = 4 \frac{1}{N} \sum_{i=1}^{N} H(x_i, y_i)$$

In the figure on the right, the relative error $\frac{Q_N - \pi}{\pi}$ is measured as a function of $N$, confirming the $\frac{1}{\sqrt{N}}$. 

Relative error as a function of the number of samples, showing the scaling $\frac{1}{\sqrt{N}}$.
```c
int i, throws = 99999, circleDarts = 0;
long double randX, randY, pi;

srand(time(NULL));

for (i = 0; i < throws; ++i) {
    randX = rand() / (double)RAND_MAX;
    randY = rand() / (double)RAND_MAX;
    if (1 > ((randX*randX) + (randY*randY))) ++circleDarts;
}

pi = 4 * (circleDarts/throws);
```
Imaginary-time evolution

• For real-time evolution, even the Monte Carlo method does not produce reliable answer.
• This is become the action phase can be both positive and negative. After summing over a large number of positive and negative numbers, the result can be exponentially small.
• However, the Monte Carlo approach works for imaginary time evolution!
1D Statistical Mechanics?!

• Define the imaginary time, 
\[ \tau = it \]

One can consider propagator in imaginary time. 
\[ \langle x_b \tau_b | x_a \tau_a \rangle = \langle x_b | e^{-H(\tau_b-\tau_a)/\hbar} | x_a \rangle \]

In this case, the weighting factor \( e^{iS/\hbar} \) becomes \( e^{-S_E/\hbar} \), which is the action in Euclidean space 
\[ S_E = \int d\tau [T + V] \sim H\beta \]

• Thus the problem becomes 1D statistical mechanics!
Calculating ground state energy and wave function, with imaginary time evolution
Calculate the g.s. energy

- To calculate the g.s. energy, one can start with the imaginary time propagator

\[
\langle x_b | e^{-HT/\hbar} | x_a \rangle = \sum_i e^{-E_i T/\hbar} \psi_i(x_b) \psi_i(x_a)^* 
\]

at large time t, it is dominated by the ground state, i= 0, or

\[
\rightarrow e^{-E_0 T/\hbar} \psi_0(x_b) \psi_0(x_a)^*
\]

Plotting the log of this as a function of T, the slope gives the g.s. energy.

Varying \( x_b \) or \( x_a \) will generate the ground state wave function. (or let \( x_a=x_b \), will give \( |\psi_0(x)|^2 \))
Practical consideration for HO

• For a piratical H.O. problem, we consider a time lattice,

\[ T \gg \frac{2\pi}{\omega} = \tau_0 \]

• To have large enough \( T \), one has to have

\[ \Delta t = a \] much smaller than \( \frac{2\pi}{\omega} \), the classical period.
Practical consideration

• Thus, choosing \(2\pi/\omega=1\),
  then \(a = 0.1\)
  one can choose \(T = 10\) forming a hierarchy
  \[ T \gg \frac{1}{\hbar \omega} \gg a \]
  correspondingly, \(T\) can also be 9, 8, 7, 6, 5, 4...
• Then, \(N = 100, 90, 80, 70, 60, \text{ etc.}\)
Rescale coordinates

- As to calculate the action, one can rescale $x$ by
  \[ \hat{x} = \sqrt{\frac{m}{\hbar}} x = \sqrt{\omega} x / b \]
  and the rescaled action is
  \[ \frac{S}{\hbar} = \sum_{j=1,n+1} \left\{ \frac{1}{2\omega} \left[ (\hat{x}_j - \hat{x}_{j-1}) / \epsilon \right]^2 + \frac{\omega}{2} \hat{x}_j^2 \right\} \]
- Each configuration consists of $N \{ \hat{x}_j \}$
- One needs a large number of configuration $C$ to calculate the two-point function.
First excited state

• To calculate the first excited state, one can project out the odd part of the wave function by making combination

\[ \langle x_2 | e^{-HT} | x_1 \rangle - \langle -x_2 | e^{-HT} | x_1 \rangle \]

this part is odd in \( x_2 \)

• At large \( T \), the first excited state contributes to the energy and wave function.
Goal of numerical work

- Important Sampling
- Metropolis formalism
- VERGAS Monte Carlo
- Calculate the grand state of H. O.
- Calculate the wave function
- Calculate the excited state energy and wave function