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 Schrodinger 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

$$h\ (\hbar = h/2\quad) \rightarrow 0$$

in this case, the commutation relation vanishes and the operators become real-number.

# 1D Harmonic oscillator

- Hamiltonian

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

eigenequation,

$$H|n\rangle = E_n|n\rangle \qquad\qquad n = 0, 1, 2, \ldots.$$

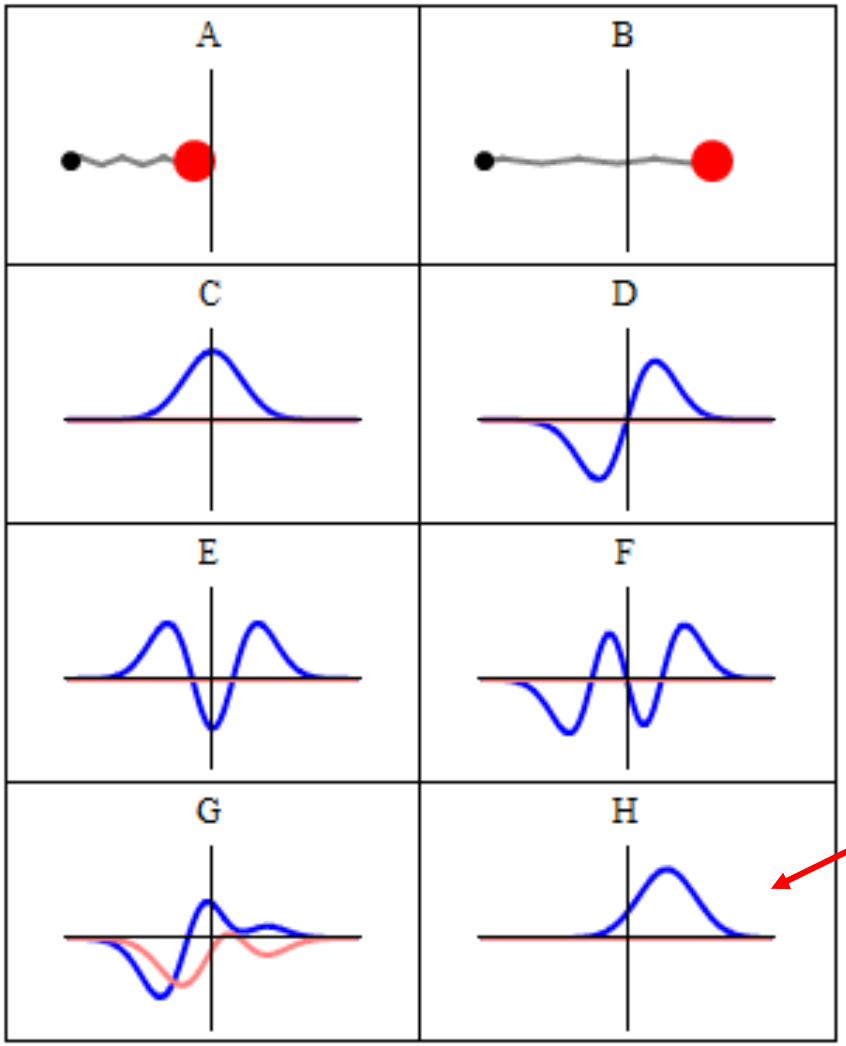
eigenvalues,

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

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

$$\langle x \mid 0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \qquad = \frac{1}{\sqrt{b\sqrt{\pi}}} e^{-x^2/2b^2}$$

# Quantum Oscillator wave functions




Coherent State

# Principle of least action

# Classical mechanics

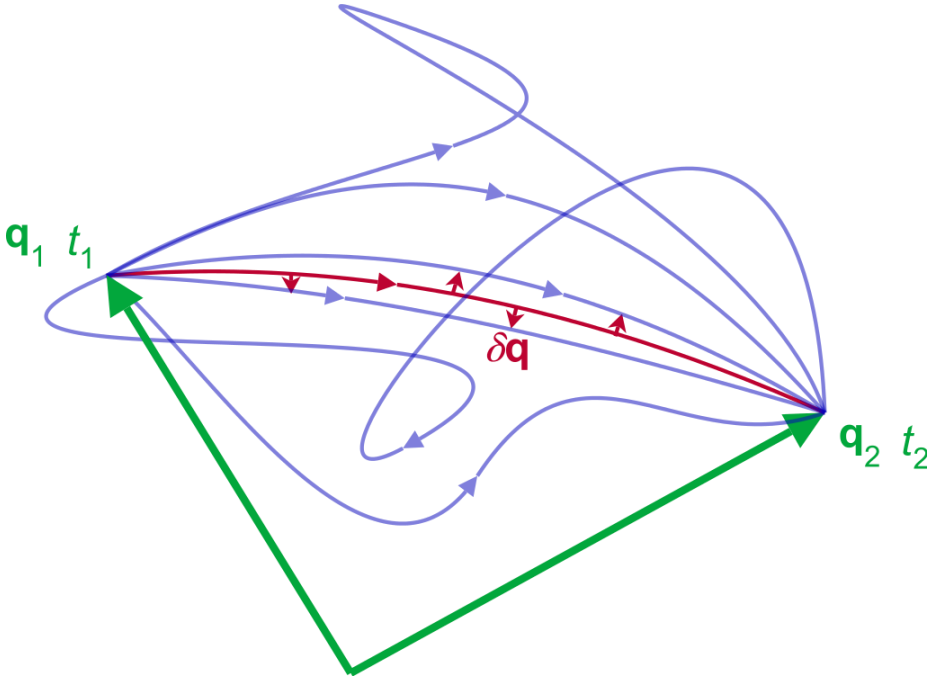
- Classical mechanics is usually represented by Newton's three laws (1687).
- However, Hamilton reformulated the mechanics problems using the variational principle. Define the lagrangian as,

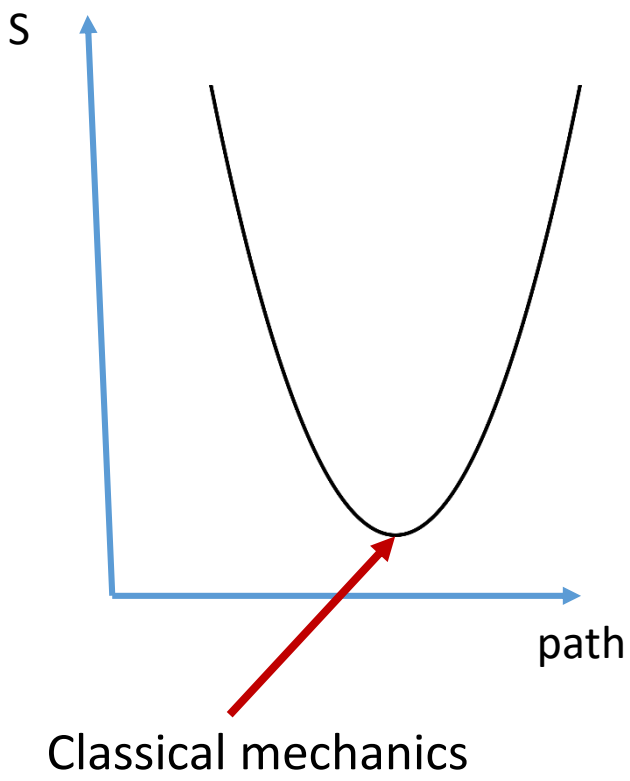
$$L = T - V = \frac{1}{2}mv^2 - \frac{1}{2}m\omega^2 x^2$$

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!



# Euler-lagrange equation

- Using the principle of the least action, one can derive the well-known Euler-Lagrange equation

$$\int_{t_1}^{t_2} \delta L \, \mathrm{d}t = 0 \,.$$

$$\delta L = \sum_{j=1}^{n} \left( \frac{\partial L}{\partial q_j} \delta q_j + \frac{\partial L}{\partial \dot{q}_j} \delta \dot{q}_j \right) , \quad \delta \dot{q}_j \equiv \delta \frac{\mathrm{d}q_j}{\mathrm{d}t} \equiv \frac{\mathrm{d}(\delta q_j)}{\mathrm{d}t} ,$$

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

$$\frac{\partial L}{\partial q_j} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_j} = 0 \,.$$

# 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)

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

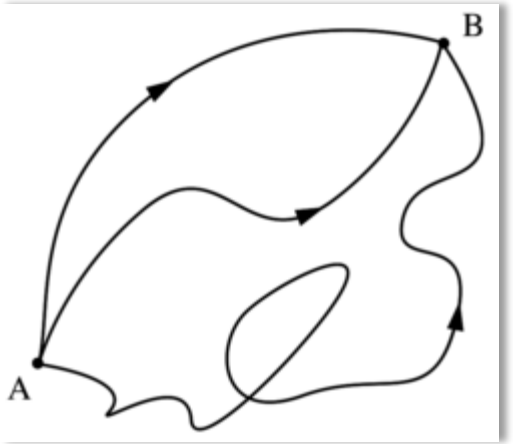
- It was shown by Feynman that this PA can be expressed in terms of path integral

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

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 comple of intermediate states,

$$1 = \left( \Pi_i \int dq_k^i \right) |q_k\rangle\langle q_k| \, .$$

# Completing the derivation

$$\begin{aligned}\langle q_{k+1}|e^{-iH\epsilon}|q_k\rangle &= \langle q_{k+1}|e^{-iH\epsilon}\int\frac{dq_k}{2\pi}|p_k\rangle\langle p_k|q_k\rangle \\ &= \int\frac{dp_k}{2\pi}e^{-iH\epsilon}e^{ip_k(q_{k+1}-q_k)}\,.\end{aligned}$$

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

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

The transition amplitude can be written

$$\begin{aligned}U(q_a,q_b;T) &= \int\mathcal{D}q(t)\mathcal{D}p(t)e^{i\int_0^T dt(p\dot{q}-H)} \\ &= \int\mathcal{D}q(t)e^{i\int_0^T dtL}\,.\end{aligned}$$

# 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:

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

- Integration yields ($x_a$=x, $x_b$=y)

$$K(x-y;T) \propto e^{\frac{i(x-y)^2}{2T}}$$

# Harmonic oscillator

$$x_{\mathrm{c}}(t) = x_i \frac{\sin\omega(t_f - t)}{\sin\omega(t_f - t_i)} + x_f \frac{\sin\omega(t - t_i)}{\sin\omega(t_f - t_i)}.$$

This trajectory yields the classical action

$$\begin{aligned} S_{\mathrm{c}} &= \int_{t_i}^{t_f} \mathcal{L}\, dt = \int_{t_i}^{t_f} \left(\tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2 x^2\right) dt \\ &= \frac{1}{2}m\omega \left( \frac{(x_i^2 + x_f^2)\cos\omega(t_f - t_i) - 2x_i x_f}{\sin\omega(t_f - t_i)} \right) \end{aligned}$$

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

$$S = S_{\mathrm{c}} + \sum_{n=1}^{\infty} \tfrac{1}{2} a_n^2 \frac{m}{2} \left( \frac{(n\pi)^2}{t_f - t_i} - \omega^2 (t_f - t_i) \right).$$

This means that the propagator is

$$\begin{aligned} K(x_f, t_f; x_i, t_i) &= Q e^{\frac{iS_{\mathrm{c}}}{\hbar}} \prod_{j=1}^{\infty} \frac{j\pi}{\sqrt{2}} \int da_j \exp\left( \frac{i}{2\hbar} a_j^2 \frac{m}{2} \left( \frac{(j\pi)^2}{t_f - t_i} - \omega^2 (t_f - t_i) \right) \right) \\ &= e^{\frac{iS_{\mathrm{c}}}{\hbar}} Q \prod_{j=1}^{\infty} \left( 1 - \left( \frac{\omega(t_f - t_i)}{j\pi} \right)^2 \right)^{-\frac{1}{2}} \end{aligned}$$

# Propagator for oscillator

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

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

There are n integrals :

$x_1, x_2, \ldots, x_n$

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, $\frac{x_j + x_{j-1}}{2}$.

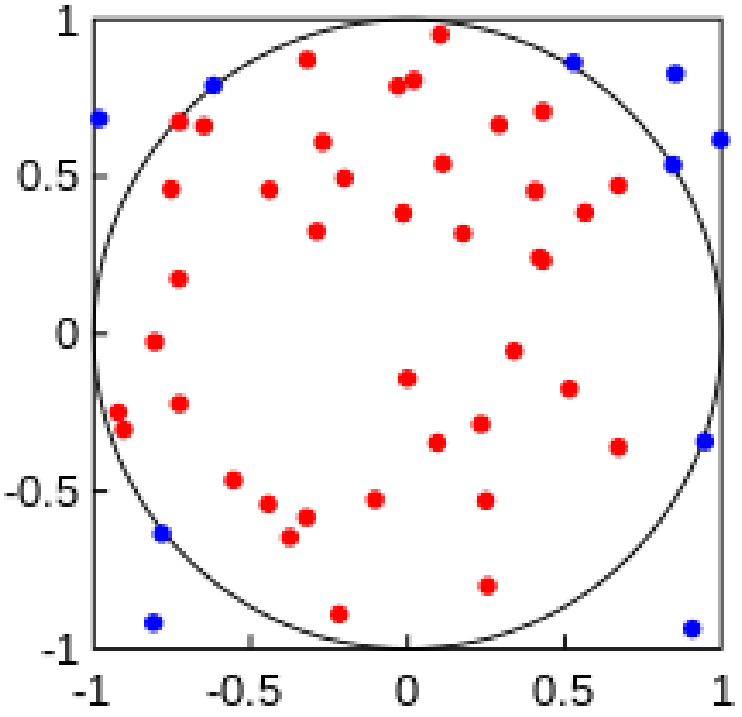
For example, for a 1D particle, the lagrangian,

$$L = \sum_{j=1,n+1}\{\frac{1}{2}m[(x_j - x_{j-1})/\epsilon]2 \ - v(\tilde{x}_j)\}$$

Hopefully, systematic error for the path integral goes like ε.

# 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

$$I = \int_{\Omega} f(\overline{\mathbf{x}})\, d\overline{\mathbf{x}}$$

where $\Omega$, a subset of $\mathbf{R}^m$, has volume

$$V = \int_{\Omega} d\overline{\mathbf{x}}$$

The naive Monte Carlo approach is to sample points uniformly on $\Omega$:[4] given $N$ uniform samples,

$$\overline{\mathbf{x}}_1, \cdots, \overline{\mathbf{x}}_N \in \Omega,$$

$I$ can be approximated by

$$I \approx Q_N \equiv V \frac{1}{N} \sum_{i=1}^{N} f(\overline{\mathbf{x}}_i) = V\langle f \rangle.$$

This is because the law of large numbers ensures that

$$\lim_{N \to \infty} Q_N = I.$$

# Statistical error estimation: the secret of why it is powerful

$$\mathrm{Var}(f) \equiv \sigma_N^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(f(\overline{\mathbf{x}}_i) - \langle f\rangle\right)^2.$$

which leads to

$$\mathrm{Var}(Q_N) = \frac{V^2}{N^2}\sum_{i=1}^{N}\mathrm{Var}(f) = V^2\frac{\mathrm{Var}(f)}{N} = V^2\frac{\sigma_N^2}{N}.$$

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

$$\delta Q_N \approx \sqrt{\mathrm{Var}(Q_N)} = V\frac{\sigma_N}{\sqrt{N}},$$

which decreases as $\frac{1}{\sqrt{N}}$. This is standard error of the mean multiplied with $V$. T

# Example of calculating π with

A paradigmatic example of a Monte Carlo integration is the estimation of π. Consider the function

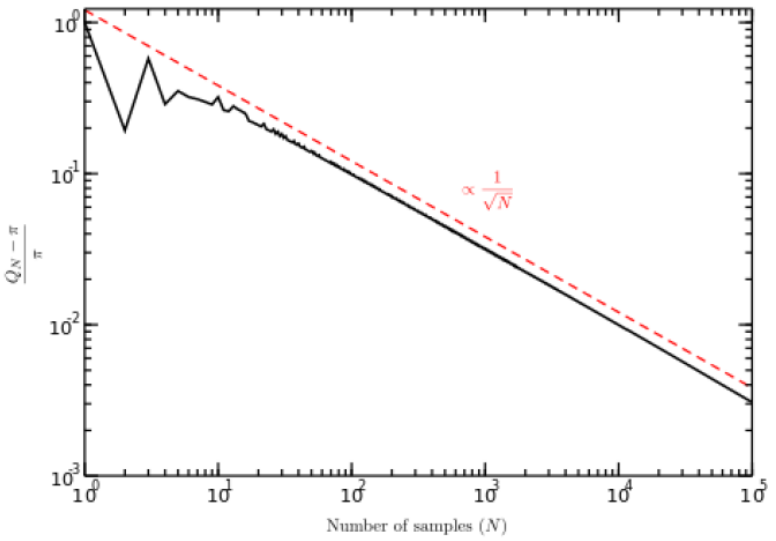
$$H(x,y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{else} \end{cases}$$

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

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

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

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




Relative error as a function of the number of samples, showing the scaling $\frac{1}{\sqrt{N}}$

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

# C-code

```
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

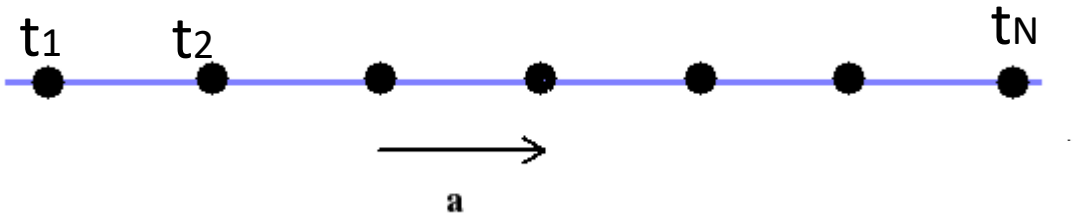
$$\rightarrow e^{-E_o T/\hbar} \psi_0(x_b) \psi_0(x_a)^*$$

Plotting the log of this as a function of T, the slop 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,




- To have large enough T, one has to have

$$T \gg \frac{2\pi}{\omega} = \tau_0$$

- On the other hand, time-interval $\Delta t = a$ shall be much smaller than $2\pi/\omega$, 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, 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

$$S/\hbar = \sum_{j=1,n+1} \{ \frac{1}{2\omega} [(\hat{x}_j - \hat{x}_{j-1}) / \epsilon] 2 + \omega/2 \, \tilde{x}_j{}^2 ) \}$$

- 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 excite 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