Lecture 2: An amateur's guide to lattice field theory

Outline

- 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.
- Example of 1+1 dimensional field theories.

Principle of least action

Classical mechanics

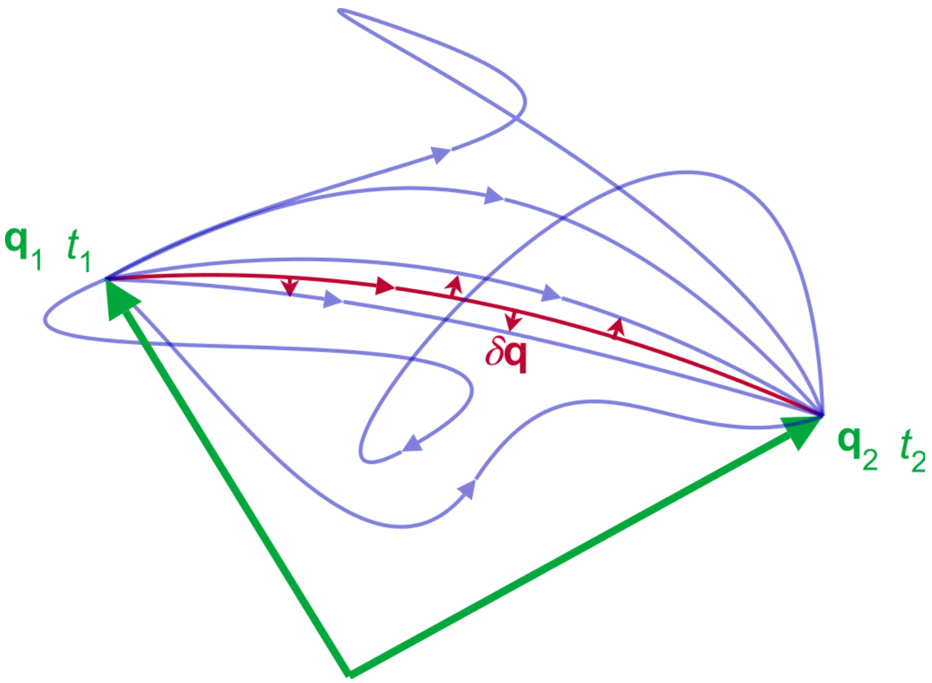
- Classical mechanics is usually represented by Newton's three laws (1687).
- However, Hamilton reformulated the mechanics problems using the variational principle. Define the lagrangian as,

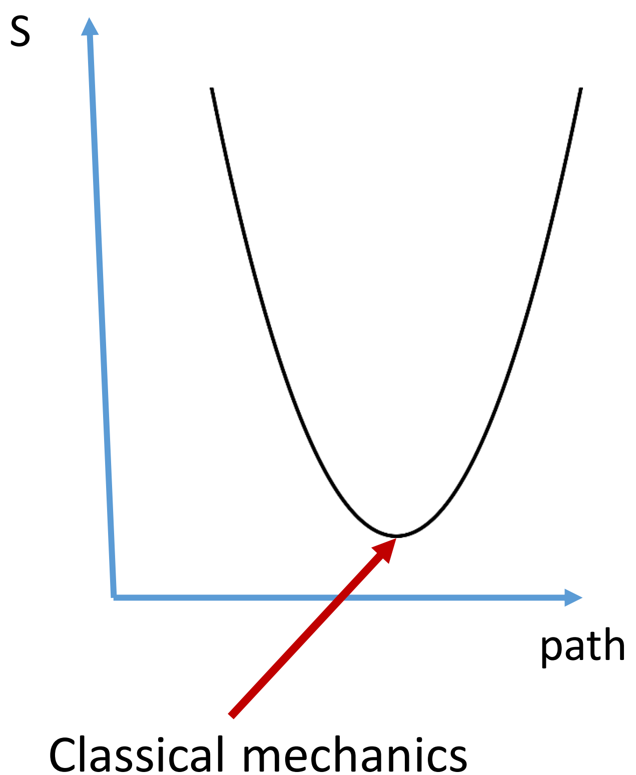
$$L = T - V = \frac{1}{2}mv^2 - \frac{1}{2}m\omega^2 x^2$$

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

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

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

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

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

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)

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

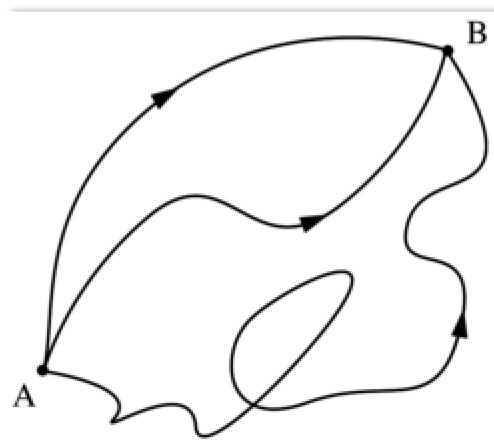
- It was shown by Feynman that this PA can be expressed in terms of path integral

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

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 ΔS, 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 ϵ.

$$e^{-iHT} = e^{-iH\epsilon} e^{-iH\epsilon} e^{-iH\epsilon} \cdots e^{-iH\epsilon} \, .$$

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

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

This trajectory yields the classical action

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

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

Next, expand the non-classical contribution to the action δS as a Fourier series, which gives

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

This means that the propagator is

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

$$= e^{\frac{iS_c}{\hbar}} Q \prod_{j=1}^{\infty} \left(1 - \left(\frac{\omega(t_f - t_i)}{j\pi} \right)^2 \right)^{-\frac{1}{2}}$$

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 ∞) 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.
  - In QFT, this is possible only for asymptotically free theories, for which the UV is perturbative.

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

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

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 jth 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 $dx_1...dx_n$, $\tilde{x}_j$ is an arbitrary value of the interval corresponding to j, e.g. its center, $\frac{x_j+x_{j-1}}{2}$.

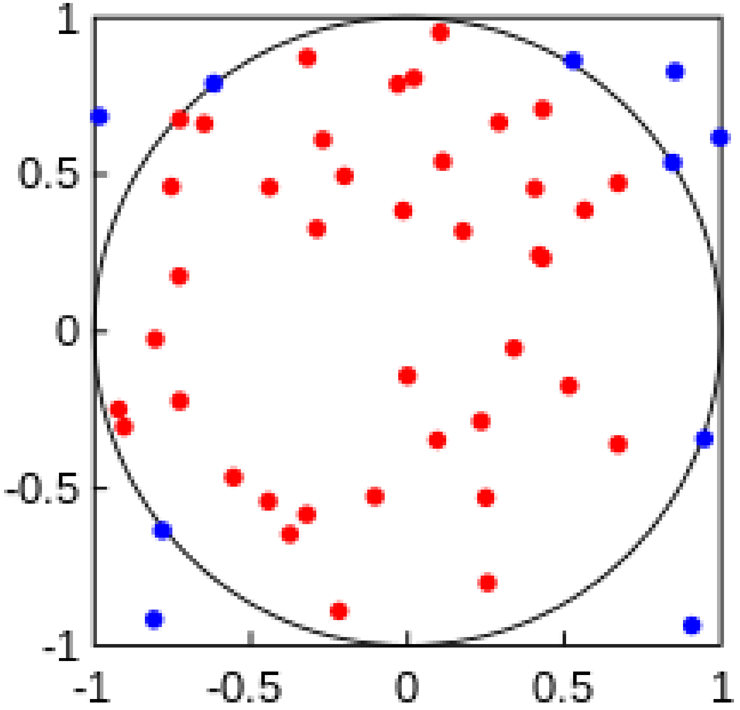
For example, for a 1D particle, the lagrangian,

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

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 integrals is to use Monte Carlo method.
- Example: the calculation of π is determined by the number of shootings in the right region.



Methodology

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

where Ω, 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 Ω:[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

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

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

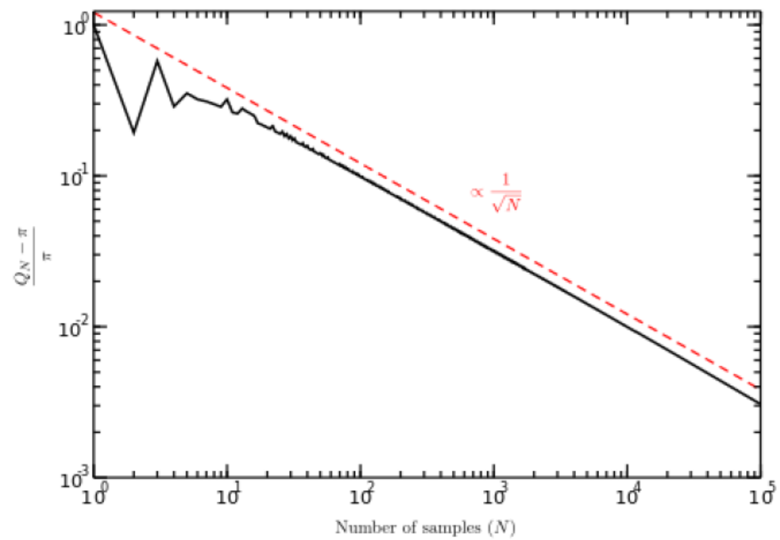
$$H(x,y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{else} \end{cases}$$

and the set Ω = [−1,1] × [−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 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 $\frac{1}{\sqrt{N}}$.

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 (sign problem, NP-hard problem)
- 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.

$$\langle x_b \tau_b | x_a \tau_a \rangle = \langle x_b \left| e^{-H(\tau_b - \tau_a)/\hbar} \right| x_a \rangle$$

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 one-DOF QM problem becomes 1D statistical mechanics problem.

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

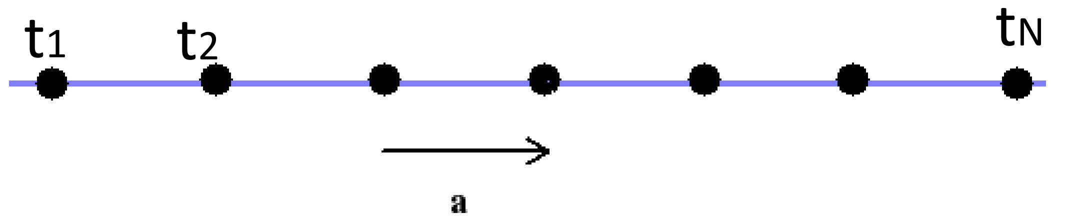
$$\rightarrow e^{-E_o T/\hbar}\, \psi_0(x_b) \psi_0(x_a)^*$$

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

$$\hat{x} = \sqrt{\frac{m}{\hbar}}x = \sqrt{\omega}x/b$$

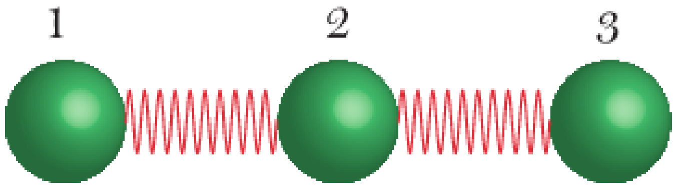
and the rescaled action is

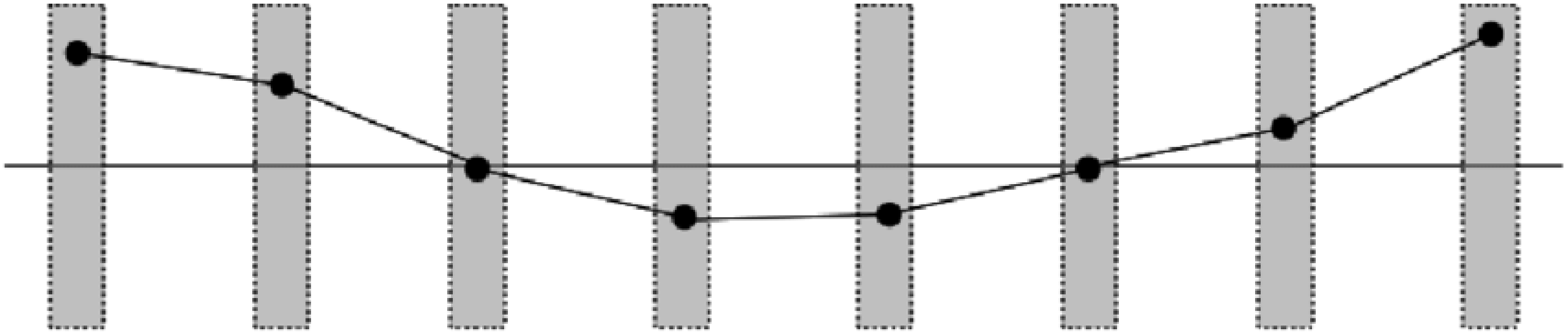
$$S/\hbar = \sum_{j=1,n+1}\{\frac{1}{2\omega}[(\hat{x}_j - \hat{x}_{j-1})/\epsilon]2 + \omega/2\ \tilde{x}_j{}^2\ )\}$$

- Each configuration consists of N $\{\hat{x}_j\}$
- One needs a large number of configuration C to calculate the two-point function.

Solving one dimensional QFT

N coupled oscillators





1D chain (ring)

- We label oscillators by i = 1, 2,…., N, with periodic condition such that i=0 and N are identical.
- Each oscillator has 1D coordinate $x_i = ia$, where a can be viewed as the basic length unit.
- The total kinetic energy,

$$T = \frac{1}{2} m \sum_{i=1,N} \dot{q}^2(ia)$$ where dot is the t-derivative

- The total potential energy ([N+1]=1)

$$V = \frac{1}{2}\kappa \sum_{n=1}^{N_a} \left(q(na) - q([n+1]a)\right)^2 ,$$

Equations of motion (E.O.M)

- The EOM are coupled linear differential equations

$$\begin{aligned} m\ddot{q}(na) &= -\frac{\partial V}{\partial q(na)} \\ &= -\kappa\left(2q(na) - q([n-1]a) - q([n+1]a)\right). \end{aligned}$$

- We can diagonalize these Eqs by introducing the normal coordinates,

$$q(na) = \frac{1}{\sqrt{N_\mathrm{a}}} \sum_{k_l} e^{ik_l na} u_{k_l},$$

$$k_l = \frac{2\pi}{N_\mathrm{a} a} l \text{ with } l = 0, \pm 1, \pm 2, \cdots, \frac{N_\mathrm{a}}{2}.$$

ℓ must be integer
$\ell = 0$ is zero − mode

Zero mode etc

- The periodic boundary condition is satisfied.
- There is always one zero mode. Zero-mode $l=0$ corresponds all coordinates move together. The potential energy is zero. It is a free motion.
- For $N=3$, there are two additional modes corresponds to $l=\pm 1$.
- For $N=4$, there are three additional modes, correspond to $l=\pm 1, 2$. The mode $l=-2$ is the same as $l=2$.
- Positive and negative l's are complex conjugate of each other, with opposite chirality.

Normal mode dynamics

- The lagrangian of the normal modes are

$$L = \frac{m}{2}\sum_{k_l}\dot{u}_{k_l}\dot{u}_{-k_l} - \frac{\kappa}{2}\sum_{k_l}2\left(1-\cos(k_l a)\right)u_{k_l}u_{-k_l}$$

- Introduce the canonical coordinates,

$$p_{k_l} = \frac{\partial L}{\partial \dot{u}_{k_l}} = m\dot{u}_{-k_l}$$
$$p_{-k_l} = \frac{\partial L}{\partial \dot{u}_{-k_l}} = m\dot{u}_{k_l}.$$

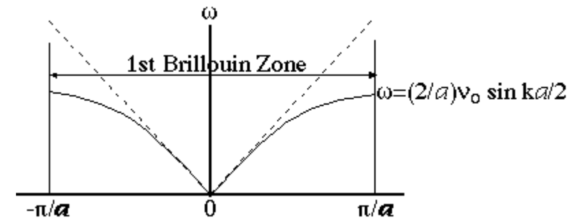
- New Hamiltonian is a sum of non-interacting normal modes

$$\text{H} = \sum_{k_l}\left(\frac{1}{2m}p_{k_l}p_{-k_l} + \frac{1}{2}m\omega_{k_l}^2 u_{k_l}u_{-k_l}\right),$$

Dispersion relation and quantization

- Dispersion relation: Frequency related to different k

$$\omega_{k_l} = \sqrt{\frac{2\kappa\left(1-\cos(k_l a)\right)}{m}} = 2\sqrt{\frac{\kappa}{m}}\left|\sin(\frac{k_l a}{2})\right|$$



- Introduce creation and annihilation operators

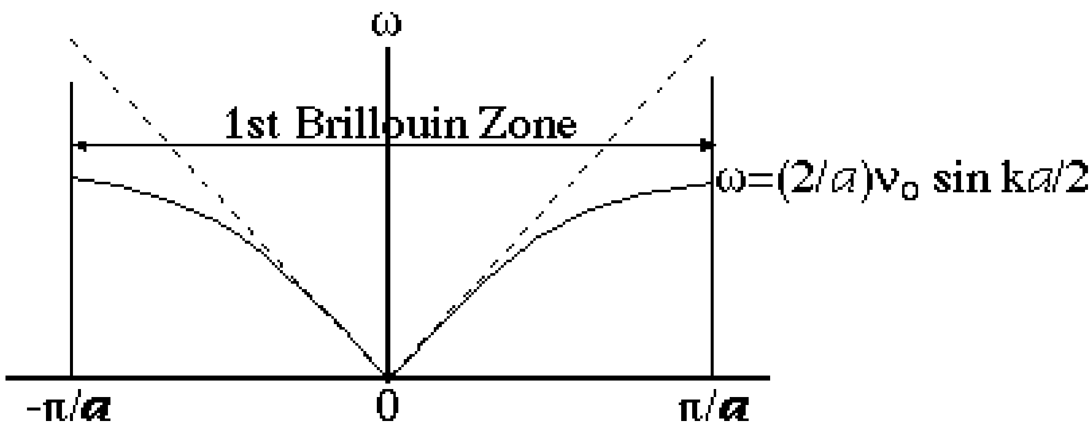
$$\hat{a}_{k_l} = \sqrt{\frac{m\omega_{k_l}}{2\hbar}}\left(\hat{u}_{-k_l} + \frac{i}{m\omega_{k_l}}\hat{p}_{k_l}\right)$$

$$\hat{a}^\dagger_{k_l} = \sqrt{\frac{m\omega_{k_l}}{2\hbar}}\left(\hat{u}_{k_l} - \frac{i}{m\omega_{k_l}}\hat{p}_{-k_l}\right).$$

- Now we have N-non-interacting harmonic oscillators,

$$H = \sum_{k_l}\mathcal{H}_{k_l} \qquad \mathcal{H}_{k_l} = \hbar\omega_{k_l}\left(\hat{a}^\dagger_{k_l}\hat{a}_{k_l} + \frac{1}{2}\right)$$

- It is interesting to note that even though every term of pot. energy seems to support an oscillator with angular frequency $\omega=\sqrt{\{\frac{k}{m}\}}$, the normal modes can have a range of angular frequency, going from 0 to 2ω.



Quantum states

- The ground state of the system is when all oscillators are the ground state

$|0,0,\ldots.,0\rangle$ with $E_0 = \frac{\hbar}{2}\sum \omega_{k_l}$ (vacuum energy)

The w. f. is $\Pi_{kl}\, \varphi_0(u_{kl})$ which is a complicated function of the original coordinates.

- The first excited state is a set of states with one quantum in one of the oscillators (kl)

$|0,1,\ldots.,0\rangle$ with energy $E(kl)=E_0+\hbar\omega_{k_l}$

which has the excitation energy $\Delta E(kl)= \hbar\omega_{k_l}$.

Only the excitation energy is measurable experimentally!

Taking continuum limit

- Let a→0 and N→∞, Na=L finite, we have infinite number of quantum mechanical degrees of freedom (field theory!)

  we define a field through

$$q(x,t) = \lim_{\substack{a\to 0\\ N_a\to\infty}} \frac{q_n(t)}{\sqrt{a}} = \lim_{\substack{a\to 0\\ N_a\to\infty}} \frac{1}{\sqrt{N_a a}} \sum_k u_k(t) e^{ikx} = \frac{1}{\sqrt{L}} \sum_k u_k(t) e^{ikx}$$

$$p(x,t) = \lim_{\substack{a\to 0\\ N_a\to\infty}} \frac{p_n(t)}{\sqrt{a}} = \lim_{\substack{a\to 0\\ N_a\to\infty}} \frac{1}{\sqrt{N_a a}} \sum_k p_k(t) e^{-ikx} = \frac{1}{\sqrt{L}} \sum_k p_k(t) e^{-ikx},$$

More on the limit

- In the $a \to 0$, we pack ∞ number of dof in the finite line segment L.
- Correspondingly, there are infinite number of non-interacting normal modes corresponding to

$$k = \frac{2\pi}{L} l \quad \text{with } l = 0, \pm 1, \pm 2, \ldots, \infty$$

Now $\omega = (\omega_0 a)\, k$ (k is still discrete)

now $\omega_0 a$ has a unit of velocity, v_s it is the sound speed in this one dimensional medium.

Thus $\omega = v_s k,$

Wave equation

- The classical e.o.m now becomes the wave equation

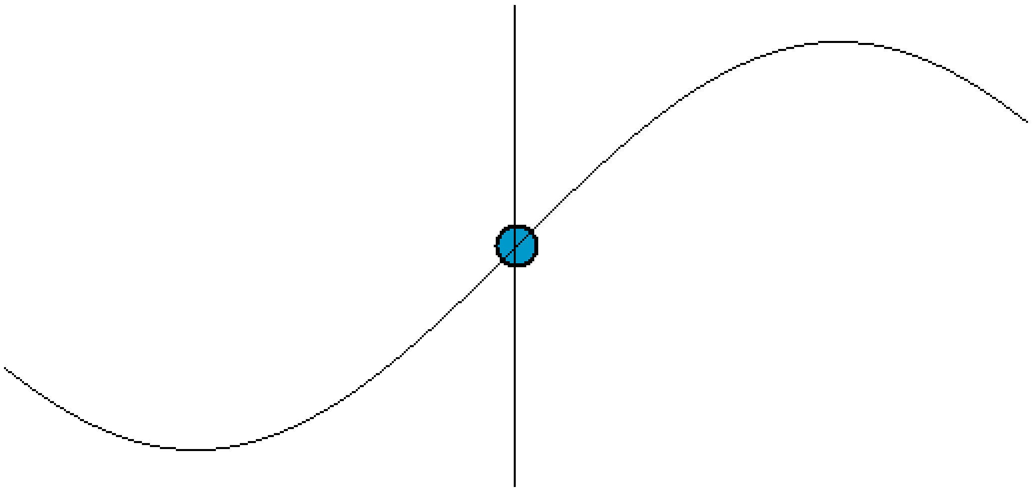
$$\left(\frac{1}{v_s^2}\frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2}\right)q(x,t)=0,$$

whereas $k=\frac{\omega}{v_s}=2\pi/\lambda$ where λ is the wavelength.

- Thus in this finite-length L, 1D system (a string), with ∞ number of h.o., one equivalently can represent the system by infinite number of waves with variable k.

q is the wave field. Large k means small w.l. (UV mode), small k means large w.l. (IR mode), smallest are $\pm\frac{2\pi}{L}$ and 0.

Single oscillator and continuous wave (classical)



1D classical field theory

- 1D field theory deals with this 1D systems of waves.
- In the above example, we have free waves, i.e., the waves do not interact.
- However, more meaningful examples deals with waves that interact.
- We can easily add interactions when using Lagrangian dynamics for the field theory.

Quantum mechanical wave

- In QM, particles are described by QM waves, just like that the electron is described by electron wave. For non-relativistic particles, they are described by waves satisfying Schrodinger eq. which corresponds to $E = p^2/2m$
- For a relativistic QM particle, it shall satisfy the relativistic wave equation.
- For a free particle, relativistic w.e. shall be derived from $E^2 = p^2c^2 + c^4m^2$, where m is the rest mass.

Klein-Gordon equation

For the relativistic energy-momentum relation, one can derive the following wave equation

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi - \nabla^2\psi + \frac{m^2c^2}{\hbar^2}\psi = 0.$$

This is famous Klein-Gordon equation. Comparing to our earlier example, one has an extra mass term

$$\frac{m^2c^2}{\hbar^2}$$

which has the Planck constant $\hbar$, indicating it is a Quantum w.e.

It reduced to the Schrodinger eq. in small velocity limit.

Quantum field theory: quantized theory of waves

- In relativistic theories, the mass and energy can convert into each other.
- Thus, particles can disappear into energy, and reversely energy can create particles.
- The single particle quantum mechanics as described by Klein-Gordon eq. is useless. One needs a theory which can create and annihilate particles.
- For this, one needs to discuss the quantized wave systems (coupled h.o.) or quantum ∞ dof systems or quantum field theory.

Quantization of 1+1 wave system

- One needs to quantize 1+1 dimensional wave system, which is in a sense already quantum mechanical (it contains Planck const).
- One can quantize by assuming the field $\varphi(x,t)$ is an operator and find the conjugate field operator $\pi(x,t)$

  and postulate commutation relations among quantum field

- However, for a numerical approach, the above strategy is of little use. One can again, however, use Feynman's path integral approach. To do this, we need to start with a lagrangian.

Lagrangian for a field

- The lagrangian is a sum over all modes, thus

$$L = \int L dx$$

where the lagrangian density can be written as

$$L = \frac{1}{2}\phi_t^2 - \frac{1}{2}\phi_x^2 - \frac{1}{2}m^2\phi^2.$$

One can verify that EL eq. reproduces KG eq.

When quantized, the first excited state of the system with a set of h.o. angular frequency,

$$\omega^2 = k^2 + m^2$$

describes a particle of mass m and momentum k.

Introducing interactions

- 1D interaction-free field theory is very simple and not interesting.
- To make a non-trivial field theory, we can introduce an interaction term

$$L = -\frac{\lambda}{4!}\phi^4$$

with $\lambda > 0$, so that the total energy has a lower bound.

- It can be shown that the system still supports a free propagating wave as the first excited state of the system, corresponding to a "physical particle" with non-trivial internal structure.

Euclidean time

- Again to make numerical calculation possible, one has to use Euclidean time
- One needs to consider evolution in imaginary time.
- 1D quantum wave system has a similar formulation as 2D statistical mechanics system.

Ground state and filtering

- Again label the exact ground state of 1+1 field theory as

$$|0\rangle$$

- A quantum wave with momentum k=0 can be generated by

$$\hat{\phi}_{k=0}(\tau = 0) \ \ |0\rangle$$

which can be expanded into a set of exact eigenstates. After long "time" T,

$$e^{-TH}\hat{\phi}_{k=0}(\tau = 0)|0\rangle \sim e^{-TM}|k = 0\rangle$$

Only the first excited with k=0 remains.

Two-point correlation function

- Now define the two-point correlation function

$$\langle 0 \big| \hat{\phi}(x, T) \hat{\phi}_{k=0}(\tau = 0) \big| 0 \rangle$$

which reduces to at large T,

$$C_2(T, M) \sim c e^{-TM}$$

Thus by studying the large-T behavior of the of the two-point correlation function, one can get the physical mass M, as the energy or frequency corresponding to k=0.

Calculating "dispersion" relation

- To find the dispersion relation, E(k), one can calculate the two-point correlation function

$$C_2(k,T) = \langle 0 \big| \hat{\phi}(x, \tau = T)\hat{\phi}_k(\tau = 0) \big| 0 \rangle$$

- At large T, the first excited state with momentum k dominates, which produces the following exponential

$$C_2(k,T,E) \sim e^{-E(k)T}$$

one can get the E(k) by checking the leading large-T behavior

Lattice implementation

- Two-point function as a functional integral

$$C_2 \ (k, T) = \int [D\phi(x,\tau)]\phi(x,T)\int dy\phi(y,0)e^{-S_E}$$

where the action is

$$S_E = \int dx d\tau [\frac{1}{2}\phi_t^2 + \frac{1}{2}\phi_x^2 + \frac{1}{2}m^2\phi^2 + \frac{1}{4!}\lambda\phi^4]$$

where again λ is positive and dimension-2.

Lattice calculation

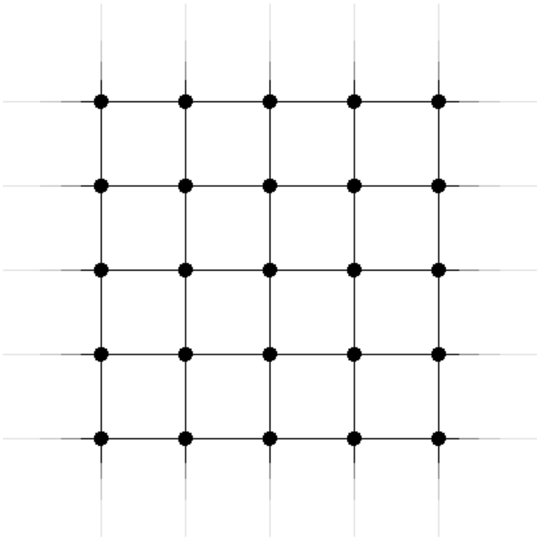
- We consider field configurations in 2-D lattice, with N points in “time” as well as space directions, N^2.
- Assume the lattice spacing is a in both directions.

  Thus， the size of the box is L=Na.
- To simulate the theory well, one needs to have

$$\frac{1}{L} \ll m, \quad \sqrt{\lambda} \ll \frac{1}{a}$$

where 1/a is the UV cut-off and 1/L is IR cutoff.

Lattice implementation



- On the lattice, one has ϕ_{ij} degrees of freedom with I, j = 1, …., N with periodic boundary condition

$$\phi_{i+N,j+N} = \phi_{ij}$$

- One generate configuration $\{\phi_{ij}\}$ using Monte Carlo method

$$C_2(k,m,T) = \sum \phi(x\,,T) \sum_y e^{iky}\, \phi(y,0)$$

Actual consideration

- For 2D simulation, a reasonable choice is N=100.

  If we one choose, m=1, λ=1, a=0.1, L=10.

- Finite-volume effect

one can do the same simulation, but with N=500, L=50 with the same a, m, λ.

- Finite-a effect: one can do the same simulation with a=0.05, N=200, or a=0.02, N=500.

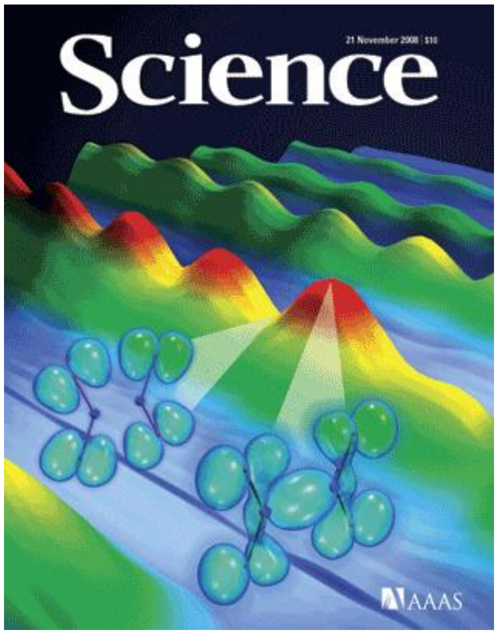
Thus mass M will have lna-dependence, which can be computed in pert. theory.

- The continuum limit exists when all physical observables are expressed in terms of M and λ.

Consideration in lattice QCD

- Hadron has sizes about 1fm. One needs at least 10 point in each direction, a = 0.1fm.
- One needs to have an hadron moving freely in a box, L=3~4 fm. Thus lattice size can be L=32,64,96,128 points in each direction.
- The simplest will be 32^4.
- One needs to put quarks and gluons on the lattice in a gauge-invariant way (K. Wilson)
- Fermions must be integrated out (as classically they are grassmann numbers)
- Small fermion mass calculations present a great challenge.

Hadron Masses from Lattice QCD



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Ab Initio Determination of Light Hadron Masses

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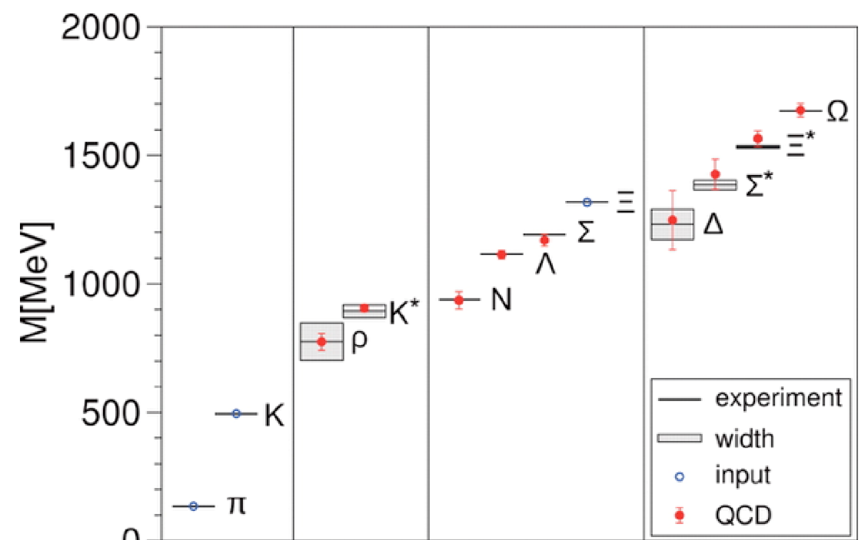

Neutron-Proton Mass Difference in Lattice QCD

Ab initio calculation of the neutron-proton mass difference

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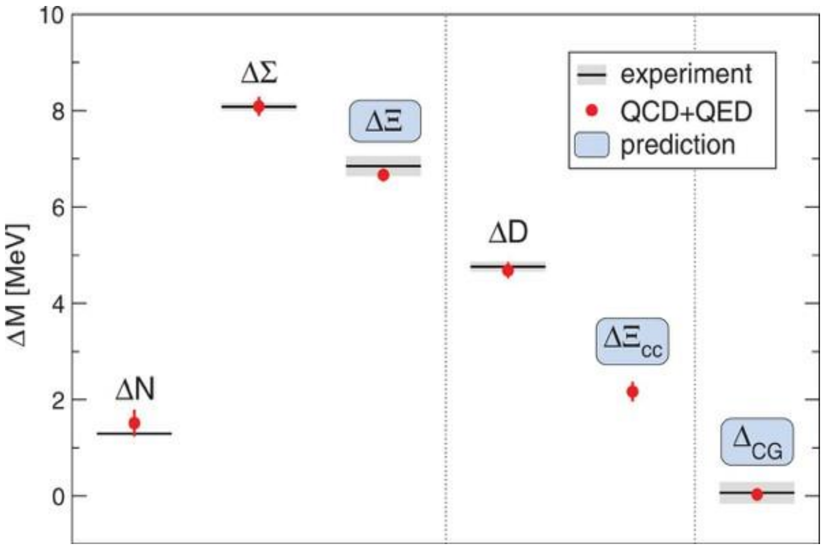

How does QCD generate this? The role of quarks and of gluons?