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

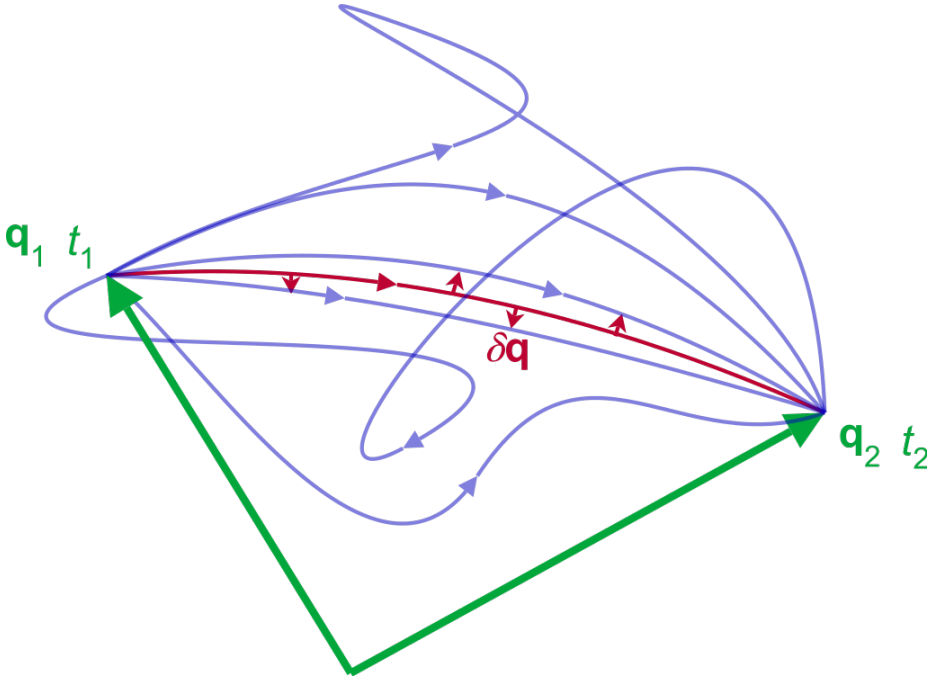
- Classical mechanics is usually represented by Newton's three laws (1687).
- However, Hamilton reformulated the mechanics problems using the variational principle. Define the lagrangian as,

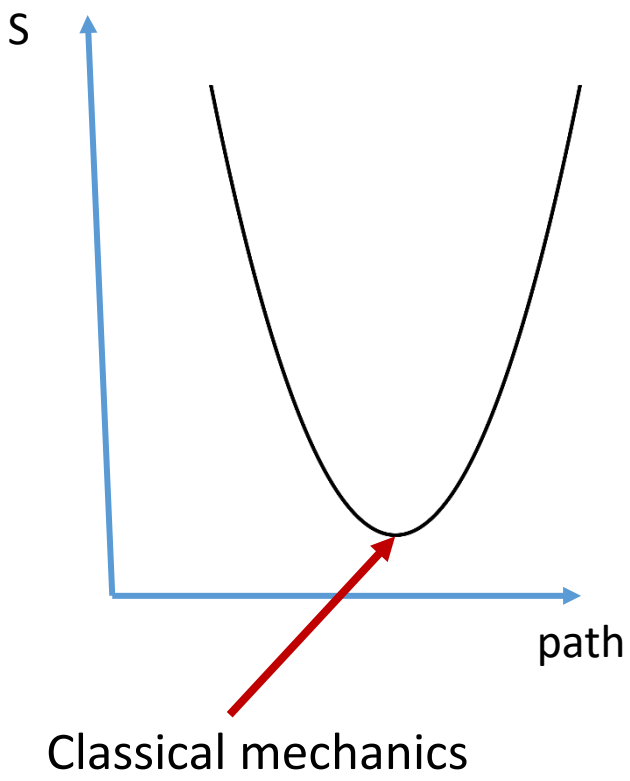
$$L = T - V = \frac{1}{2}mv^2 - \frac{1}{2}m\omega^2 x^2$$

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)

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

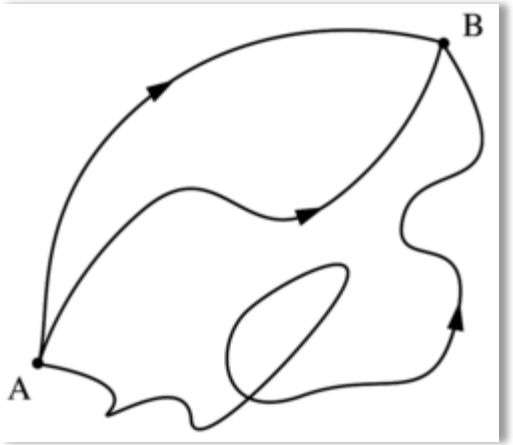
- It was shown by Feynman that this PA can be expressed in terms of path integral

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

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.

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

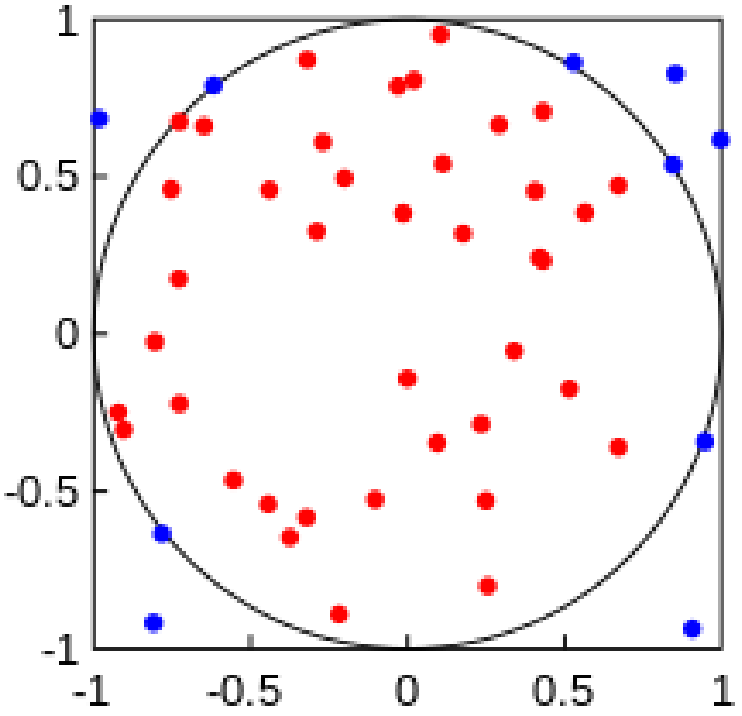
For example, for a 1D particle, the lagrangian,

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

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 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

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

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

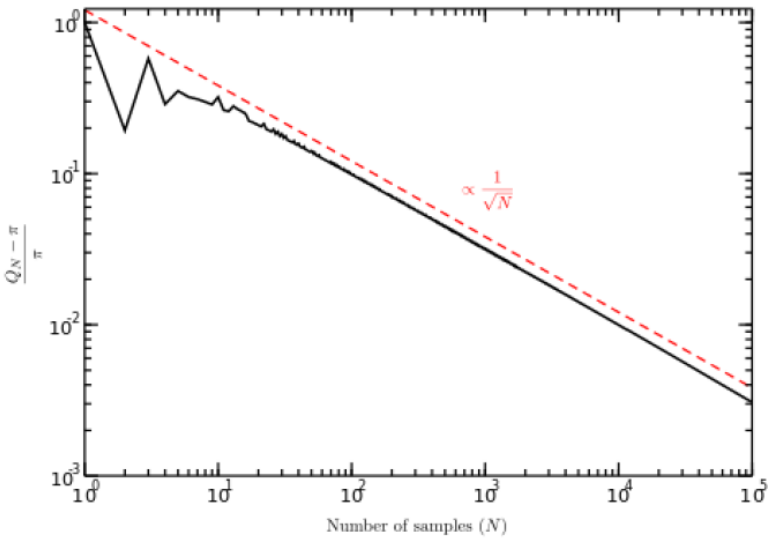
$$H(x,y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{else} \end{cases}$$

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 $\frac{1}{\sqrt{N}}$.

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.

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

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 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

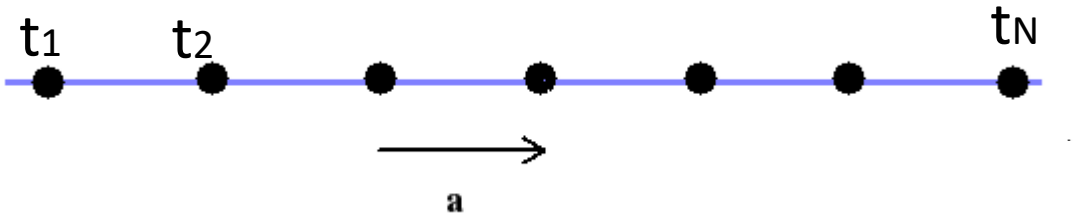
$$\rightarrow e^{-E_o T/\hbar} \psi_0(x_b) \psi_0(x_a)^*$$

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

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

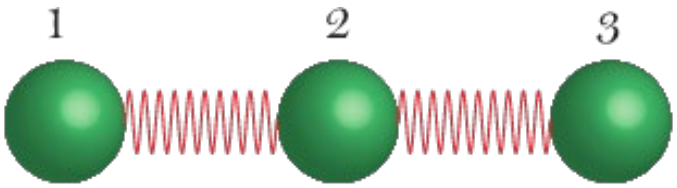
and the rescaled action is

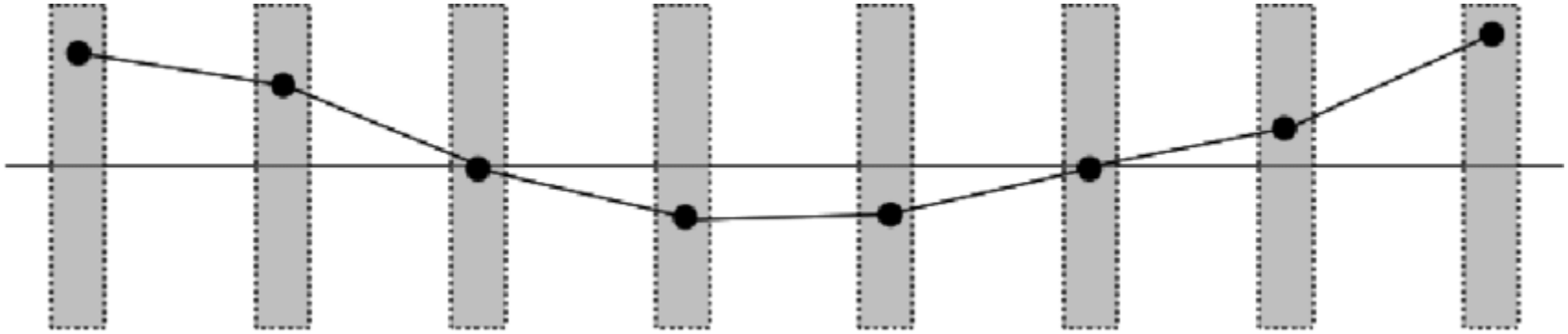
$$S/\hbar = \sum_{j=1,n+1}\{\frac{1}{2\omega}[(\hat{x}_j - \hat{x}_{j-1})/\epsilon]2 + \omega/2\ \tilde{x}_j{}^2)\}$$

- 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,

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

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

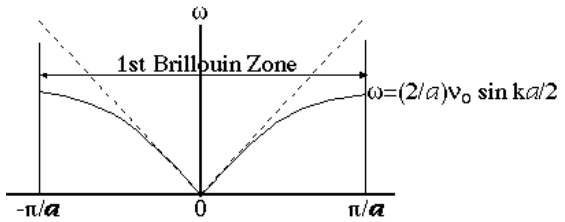
- New Hamiltonian is a sum of non-interacting normal modes

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

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

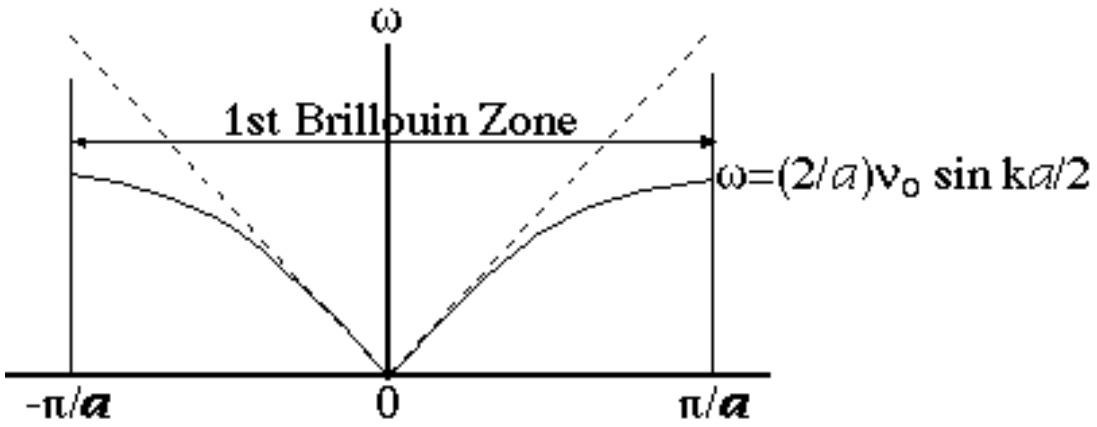
$$\hat{a}_{k_l} = \sqrt{\frac{m\omega_{k_l}}{2\hbar}}\left(\hat{u}_{-k_l} + \frac{i}{m\omega_{k_l}}\hat{p}_{k_l}\right)$$

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

- 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

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

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)

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

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

Only the excitation energy is measurable experimentally!

Taking continuum limit

- Let a$\to$0 and N$\to\infty$, 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$\rightarrow$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

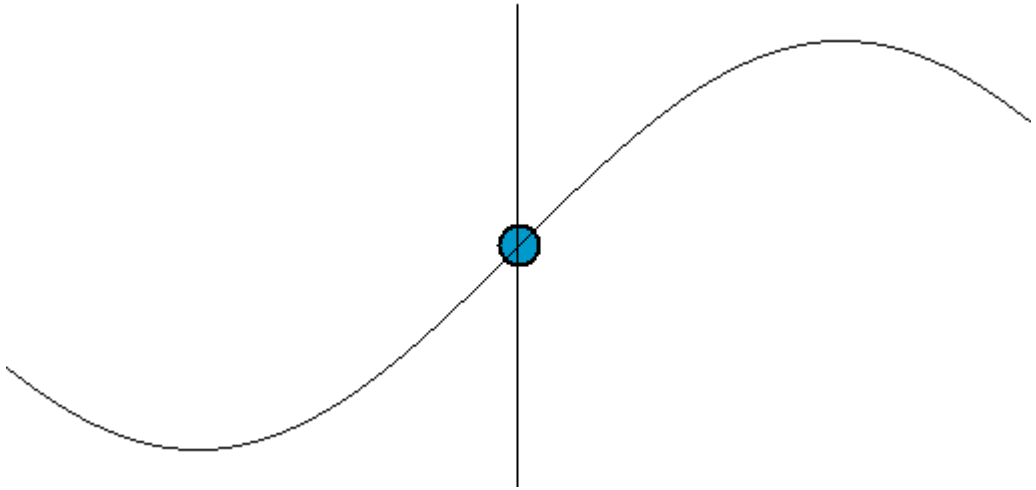
$$\left(\frac{1}{v_s^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) q(x,t) = 0,$$

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

$$\mathrm{L} = \int L dx$$

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

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

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

$$\mathrm{C}_2(k,T) = \langle 0 \left| \hat{\phi}(x, \tau = T) \hat{\phi}_k(\tau = 0) \right| 0 \rangle$$

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

$$\mathrm{C}_2(k,T,E) \sim e^{-E(k)T}$$

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

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

where again λ is positive and dimension-2.

Lattice calculation

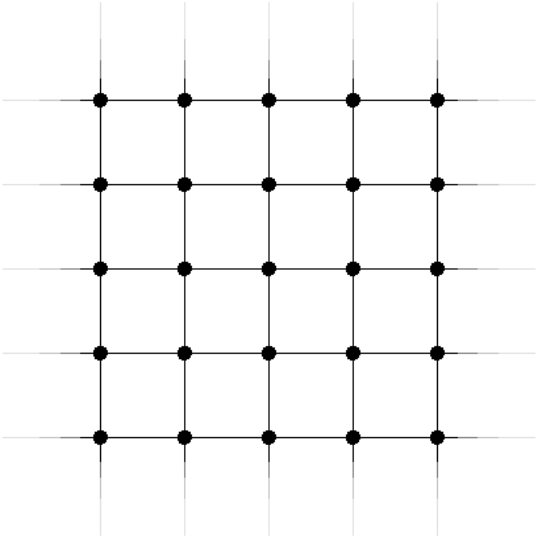
- We consider field configurations in 2-D lattice, with N points in "time" as well as space directions, N^2.
- Assume the lattice spacing is a in both directions.

  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.

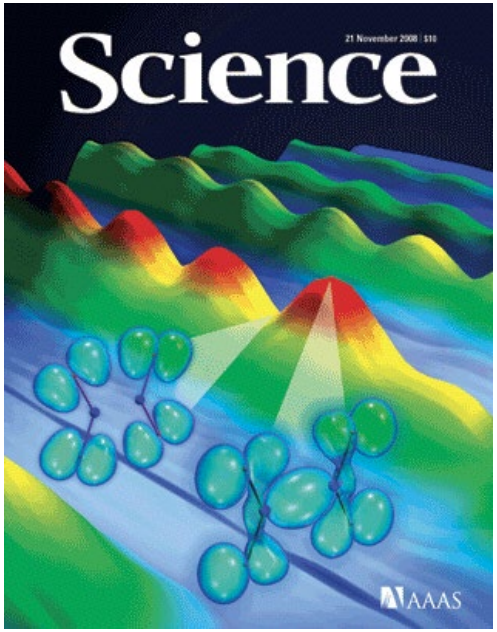
Thus mass M will have lna-dependence, which can be computed in pert. theory.

- 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



(2008)

Ab Initio Determination of Light Hadron Masses

S. Dürr, Z. Fodor, C. Hoelbling, R. Hoffmann, S.D. Katz, S. Krieg, T. Kuth, L. Lellouch, T. Lippert, K.K. Szabo and G. Vulvert

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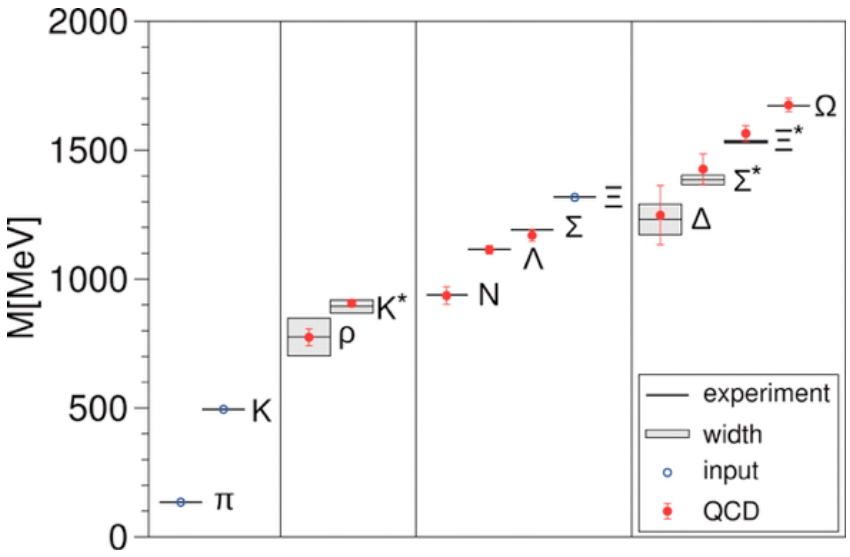
589 citations



Neutron-Proton Mass Difference in Lattice QCD

Ab initio calculation of the neutron-proton mass difference

Sz. Borsanyi, S. Durr, Z. Fodor,
C. Hoelbling, S.D. Katz,S. Krieg,
L. Lellouch, T. Lippert, A. Portelli,
K. K. Szabo, and B.C. Toth

Science **347** (6229), 1452-1455
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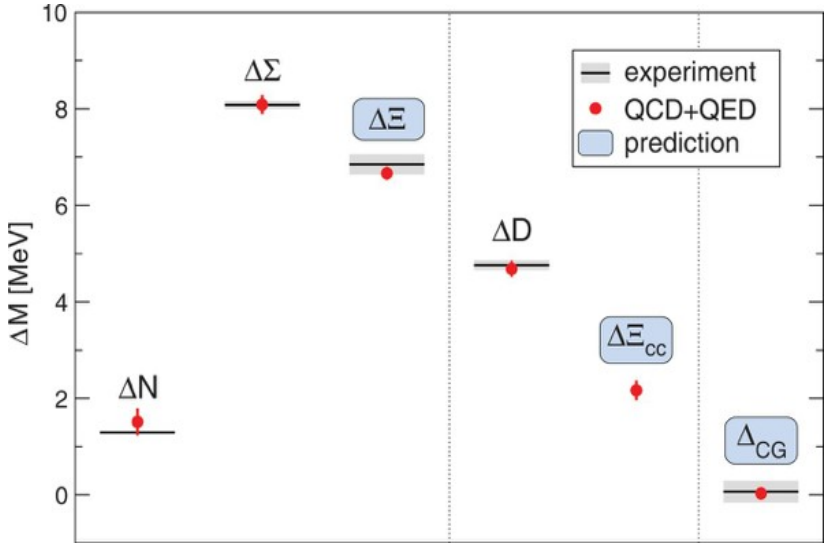
281 Citations



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