Introduction to Lattice QCD

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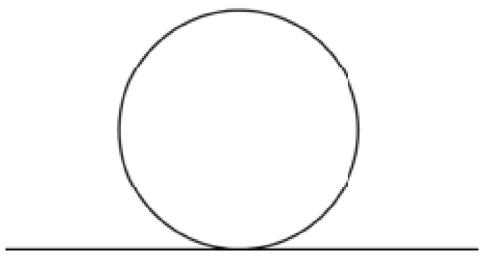
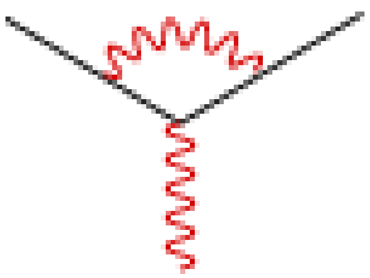
Prelude



ϕ^4: mass diverges with cutoff ?



QED: e diverges with cutoff ?

changes with gauge ?

$\Longrightarrow$ Renormalization

The lattice is the only known gauge-invariant, non-perturbative regulator of QFT

Outline

- Lattice field theory:
  - Quantum Mechanics with Path Integral (demo)
  - Lattice ϕ^4
  - Scalar QED $\rightarrow$ QCD
- Monte Carlo
- Finite temperature: Y-M deconfinement transition
- Fermions:
  - Continuum symmetries
  - Species doubling
  - Numerical simulation
  - Finite temperature
- Finite chemical potential: → Seminar
  - Expectations
  - Sign problem
  - Imaginary chemical potential

1-particle Quantum Mechanics

- Wavefunction $\psi(x,t):\ \mathcal{R}\times\mathcal{R}\to\mathcal{C}$, State $|\psi(t)\rangle = \int dx\ \psi(x,t)|x\rangle$

- Schroedinger eq. $i\hbar\frac{d|\psi\rangle}{dt} = H|\psi\rangle\ \rightarrow\ |\psi(t)\rangle = \exp[-\frac{i}{\hbar}Ht]|\psi(0)\rangle$

- Define Green's fctn / transition amplitude / transfer matrix elt.

$$G(x',t';x,t) \equiv \langle x'|\exp[-\frac{i}{\hbar}H(t'-t)]|x\rangle$$

- Then $\psi(x,t) = \int dx_0\ G(x,t;x_0,0)\psi(x_0,0)$ eq.(*)

Check: eq.(*) $\Rightarrow |\psi(t)\rangle = \int dx\ |x\rangle \int dx_0\ G(x,t;x_0,0)\psi(x_0,0)$

$$= \int dx \int dx_0\ |x\rangle\langle x|\exp[-\frac{i}{\hbar}Ht]|x_0\rangle\psi(x_0,0)\ =\ \exp[-\frac{i}{\hbar}Ht]|\psi(0)\rangle$$

- Crucial property: $G(x,t;x_0,0) = \int dx_1\ G(x,t;x_1,t_1)G(x_1,t_1;x_0,0)$

Trotter-Suzuki: $\langle x|\exp[-\frac{i}{\hbar}Ht]|x_0\rangle = \lim_{N\to\infty}\int dx_1..dx_{N-1}\prod_{k=1}^{N}\langle x_k|\exp[-\frac{i}{\hbar}H\frac{t}{N}]|x_{k-1}\rangle$

Evaluating $\langle x_k|\exp[-\frac{i}{\hbar}H\frac{t}{N}]|x_{k-1}\rangle,\quad \frac{t}{N}\equiv\delta t$

- Difficulty: $H=T+V,\ [T,V]\neq 0$

  $T=\frac{p^2}{2m}$ diagonal in momentum space, $V=V(x)$ diagonal in coordinate space

- Change of basis: $\langle x|p\rangle=\langle p|x\rangle^*=\exp[i\frac{px}{\hbar}]$; completeness: $\int dx\ |x\rangle\langle x|=\int\frac{dp}{2\pi}|p\rangle\langle p|=1$

- Baker-Campbell-Hausdorff: $\exp[-\frac{i}{\hbar}(T+V)\delta t]=\exp[-\frac{i}{\hbar}T\delta t]\times\exp[-\frac{i}{\hbar}V\delta t]\times(1+\mathcal{O}(\delta t^2))$

$$\Rightarrow\ \langle x_k|\exp[-\frac{i}{\hbar}(T+V)\delta t]|x_{k-1}\rangle\approx\langle x_k|\exp[-\frac{i}{\hbar}T\delta t]|x_{k-1}\rangle\exp[-\frac{i}{\hbar}V(x_{k-1})\delta t]$$

$$=\iint\frac{dp_k}{2\pi}\frac{dp_{k-1}}{2\pi}\langle x_k|p_k\rangle\langle p_k|\exp[-\frac{i}{\hbar}T\delta t]|p_{k-1}\rangle\langle p_{k-1}|x_{k-1}\rangle\exp[-\frac{i}{\hbar}V(x_{k-1})\delta t]$$

$$=\iint\frac{dp_k}{2\pi}\frac{dp_{k-1}}{2\pi}\exp[i\frac{p_kx_k}{\hbar}]\delta(p_k-p_{k-1})\exp[-\frac{i}{\hbar}\frac{p_k^2}{2m}\delta t]\exp[-i\frac{p_{k-1}x_{k-1}}{\hbar}]\exp[-\frac{i}{\hbar}V(x_{k-1})\delta t]$$

$$=\int\frac{dp_k}{2\pi}\exp\left[\frac{i}{\hbar}\left(p_k(x_k-x_{k-1})-\frac{p_k^2}{2m}\delta t\right)\right]\exp[-\frac{i}{\hbar}V(x_{k-1})\delta t]$$

$$=\int\frac{dp_k}{2\pi}\exp\left[-\frac{i}{\hbar}\left(p_k\sqrt{\frac{\delta t}{2m}}-(x_k-x_{k-1})\sqrt{\frac{m}{2\delta t}}\right)^2+\frac{i}{\hbar}(x_k-x_{k-1})^2\frac{m}{2\delta t}\right]\exp[-\frac{i}{\hbar}V(x_{k-1})\delta t]$$

$$= \int \frac{dp_k}{2\pi} \exp\left[-\frac{i}{\hbar}\left(p_k\sqrt{\frac{\delta t}{2m}} - (x_k - x_{k-1})\sqrt{\frac{m}{2\delta t}}\right)^2 + \frac{i}{\hbar}(x_k - x_{k-1})^2 \frac{m}{2\delta t}\right] \exp[-\frac{i}{\hbar}V(x_{k-1})\delta t]$$

$$\Rightarrow \langle x_k| \exp[-\frac{i}{\hbar}(T+V)\delta t]|x_{k-1}\rangle \approx \mathbf{C} \exp\left[\frac{i\delta t}{\hbar}\left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\delta t}\right)^2 - V(x_{k-1})\right)\right]$$

$$\langle x| \exp[-\frac{i}{\hbar}Ht]|x_0\rangle = \lim_{N\to\infty} \int \prod_{k=1}^{N} (C dx_k)\delta(x_N, x) \exp\left[\frac{i}{\hbar}\delta t \sum_k \left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\delta t}\right)^2 - V(x_{k-1})\right)\right]$$

$$= \text{"}C^\infty\text{"} \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}x(t') \exp\left[\frac{i}{\hbar}\int dt' \left(\frac{m\dot{x}(t')^2}{2} - V(x(t'))\right)\right]$$

- Integral over paths $x(t')$, with weight $\exp[\frac{i}{\hbar}S]$, $S = T - U$, S *action of path*

- Wick rotation: $\tau = it$, Euclidean / "imaginary" time ($\tau \in \mathcal{R}$)

  $it' \to \tau', \quad \dot{x}(t')^2 \to -\dot{x}(\tau')^2$

$$\langle x| \exp[-\frac{1}{\hbar}H\tau]|x_0\rangle = \int_{x(0)=x_0}^{x(\tau)=x} \mathcal{D}x(\tau') \exp[-\frac{1}{\hbar}S_E], \quad S_E = \int d\tau' \left(\frac{m\dot{x}(\tau')^2}{2} + V(x(\tau'))\right)$$

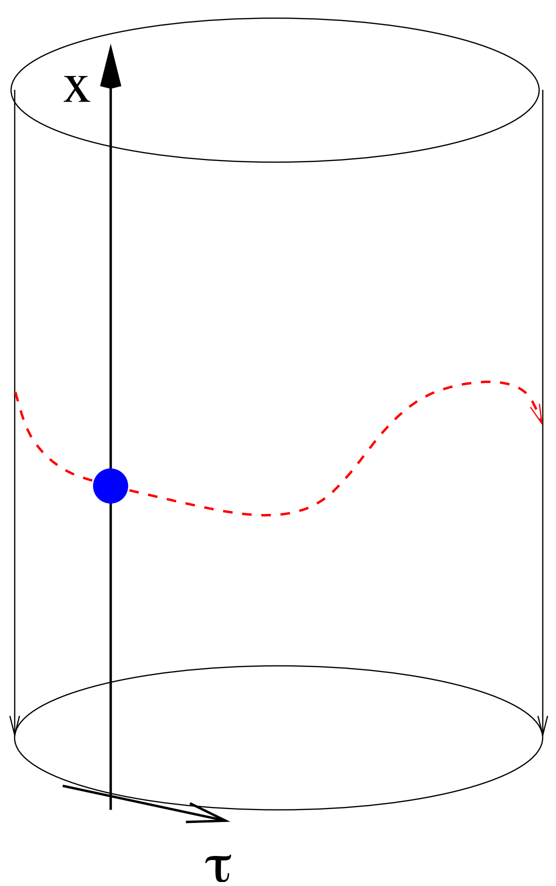
$$\langle x|\exp[-\frac{1}{\hbar}H\tau]|x_0\rangle = \int_{x(0)=x_0}^{x(\tau)=x} \mathcal{D}x(\tau')\exp[-\frac{1}{\hbar}S_E], \quad S_E = \int d\tau' \left(\frac{m\dot{x}(\tau')^2}{2} + V(x(\tau'))\right)$$

$S_E = T + U$ is *Euclidean action* (cf. *Hamiltonian* in Eucl. time)

- Classical limit: $\hbar \to 0 \;\Rightarrow$ *minimum action* (others exponentially suppressed)

  $\hbar \neq 0 \;\to$ *quantum fluctuations* around minimal action path

- **Finite temperature**: $x = x_0$ (periodic paths), $\frac{\tau}{\hbar} = \frac{1}{T} \equiv \beta$



$$Z = \mathrm{Tr}[\exp(-\beta H)] = \int_{x(\beta)=x(0)} \mathcal{D}x(\tau')\exp[-\frac{1}{\hbar}S_E]$$

$1/T \;\leftrightarrow$ extent of compact direction

$\hbar \;\leftrightarrow$ quantum fluctuations around classical path

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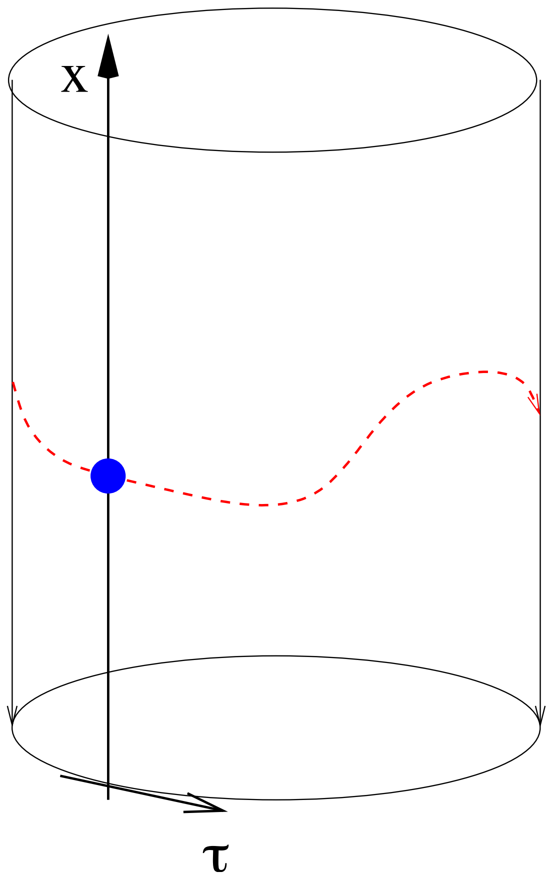

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Expand Z in eigenstates of H : $H|n\rangle = E_n|n\rangle, \; E_0 < E_1 < \cdots$

$$Z = \sum_n \langle n|\exp(-\beta H)|n\rangle = \sum \exp(-\beta E_n)$$

$$\underset{T\to 0}{=} \exp(-\beta E_0)(1 + \exp(-\beta(E_1 - E_0)) + \cdots)$$

Propagation in Euclidean time suppresses excited states, isolates groundstate

Observables: $\langle W \rangle = \frac{1}{Z}\mathrm{Tr}[W\exp(-\beta H)] = \frac{1}{Z}\int_{\text{paths}} \mathcal{D}x(\tau)\; W(x(\tau))\exp[-S_E(x(\tau))]$

- local in time: groundstate wavefunction $|\psi(x_0)|^2 \;\propto\; \langle \delta(x - x_0)\rangle$

Count the proportion of paths passing through x_0 (divide x-axis into bins and count hits)

- unequal-time correlator: $C(\tau) \equiv \langle x(\tau)x(0)\rangle$

$$C(\tau) = \frac{1}{Z}\sum_k \langle k|\exp[-H(\beta-\tau)]x\exp[-H\tau]x|k\rangle \;\; = \frac{1}{Z}\sum_{k,l}\langle k|\exp[-H(\beta-\tau)]x\exp[-H\tau]|l\rangle\langle l|x|k\rangle$$

$$= \frac{1}{Z}\sum_{k,l}|\langle k|x|l\rangle|^2\exp[-E_k(\beta-\tau)]\exp[-E_l\tau]$$

$$\underset{T\to 0}{=} \frac{1}{Z}\left(|\langle 0|x|0\rangle|^2\exp[-\beta E_0] + |\langle 0|x|1\rangle|^2\exp[-\beta E_0]\exp[-\tau(E_1-E_0)] + \cdots\right)$$

$$\langle x(\tau)x(0)\rangle - \langle x\rangle^2 \underset{T\to 0}{=} |\langle 0|x|1\rangle|^2\exp[-\tau(E_1-E_0)] + \cdots$$

Extract "mass gap" $(E_1 - E_0)$ from decay of *connected* 2pt-fct

Numerical simulation

- Go back to discretized Euclidean time:

$$Z = \mathrm{Tr}[\exp(-\beta H)] \approx \int_{x_0=x_N} \prod_{k=1}^{N} dx_k \exp\left[-\frac{\delta\tau}{\hbar}\sum_k \left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\delta\tau}\right)^2 - V(x_{k-1})\right)\right]$$

- Draw successive paths $(x_1, x_2, .., x_N)$ from distribution $\frac{1}{Z}\exp[-S_E(\mathrm{path})]$

- At each Monte Carlo step, update only ONE d.o.f.: $x_{k_0}^{\mathrm{old}} \to x_{k_0}^{\mathrm{new}}$

- Metropolis recipe: - candidate $x_{k_0}^{\mathrm{cand}} = x_{k_0}^{\mathrm{old}} + \eta,\ \eta$ random, $\mathrm{Prob}(+\eta) = \mathrm{Prob}(-\eta)$

  - accept (ie. $x_{k_0}^{\mathrm{new}} = x_{k_0}^{\mathrm{cand}}$) with probability $\min\left(1, \frac{\mathrm{Prob(candidate\ path)}}{\mathrm{Prob(old\ path)}}\right)$

  (if reject, then keep old value: $x_{k_0}^{\mathrm{new}} = x_{k_0}^{\mathrm{old}}$)

- Crucial points: Z not needed (cancels in acceptance probability)

  Change in $S_E(\mathrm{path})$ limited to 2 terms ($k = k_0$ and $k = k_0 + 1$)

Technical details

$$Z = \mathrm{Tr}[\exp(-\beta H)] \approx \int_{x_0=x_N} \prod_{k=1}^{N} dx_k \exp\left[-\frac{\delta\tau}{\hbar}\sum_k \left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\delta\tau}\right)^2 - V(x_{k-1})\right)\right]$$

- Change to dimensionless variables: $\delta t = a, \ \hat{m} = am, \ \hat{x} = \frac{x}{a}, \ \hat{V} = aV \quad (\hbar = 1)$

$$S_E = \sum_k \left(\frac{\hat{m}}{2}(\hat{x}_k - \hat{x}_{k-1})^2 + \hat{V}(\hat{x}_k)\right)$$

- η- distribution: not too narrow (no change), not too wide (no acceptance)

  adjust for average acceptance around 1/2

- Systematic errors:

  - discretization errors $\mathcal{O}(ma)^2$: want $ma \ll 1$ + continuum extrapolation

  - finite-size (temperature) errors $\mathcal{O}\left(\exp(-\frac{E_1 - E_0}{T})\right)$: want $N(\hat{E}_1 - \hat{E}_0) \gg 1$

    + thermodynamic extrapolation

Classic reference

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A Statistical Approach to Quantum Mechanics*

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A Monte Carlo method is used to evaluate the Euclidean version of Feynman's sum over particle histories. Following Feynman's treatment, individual paths are defined on a discrete (imaginary) time lattice with periodic boundary conditions. On each lattice site, a continuous position variable x_i specifies the spacial location of the particle. Using a modified Metropolis algorithm, the low-lying energy eigenvalues, $|\psi_0(x)|^2$, the propagator, and the effective potential for the anharmonic oscillator are computed, in good agreement with theory. For a deep double-well potential, instantons were found in our computer simulations appearing as multi-kink configurations on the lattice.

I. INTRODUCTION

Feynman's path integral formulation of quantum mechanics reveals a deep connection between classical statistical mechanics and quantum theory. Indeed, in an imaginary time formalism the Feynman integral is mathematically equivalent to a partition function. Using this analogy, particle physicists have recently employed a well-known technique of statistical mechanics in using Monte Carlo simulation to study gauge field theories [1, 2]. The simulations are a means of numerical evaluation of the path integrals. This has yielded new non-perturbative insight into the behavior of quantized Yang–Mills fields.

A gauge system is a rather complicated quantum theory with many degrees of freedom. This masks the connection between a Euclidean Monte Carlo treatment and a more traditional Hilbert space formulation of quantum mechanics. In this paper we search for such connections by studying a considerably simpler model, a one-degree-of-freedom Schrödinger system. We will see how Monte Carlo methods can provide information on the ground and first excited states of this problem. We do not advocate these methods for accuracy, rather we hope they may lead to better understanding of the workings of the Monte Carlo method. Furthermore, these methods are rather easily generalizable to systems with many degrees of freedom.

This paper is organized as follows. In Section II we review the Feynman formalism and present the formulas we will use in our numerical studies. Section III presents and

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