Solving Quantum Chromodynamics numerically: overview and selected details

BY ULLI WOLFF (HU Berlin)

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Abstract

While in QCD many high-energy questions can be answered by perturbation theory, low energy features are non-perturbative and leave simulation as the only systematic computational method

Scalar Quantum Field Theory

- degrees of freedom: $\phi(\vec{x}) \in \mathbb{R}$
- for numerical (even classical) FT calculations this is truncated to a (dense, large) grid

$$\vec{x} = \vec{n}a, \quad n_i = 0, 1, \ldots, L/a \in \mathbb{N}$$

- UV and IR cutoffs in place, scales a, L
- two special choices have been made: cubic lattice + torus
- only $a \ll \text{phys. scale} \ll L$ usually of interest '($a \to 0$, $L \to \infty$)' (unless solid state physics or finite size scaling...)

$$\hat{H} = \frac{1}{2} \sum_{\vec{n}} \hat{\pi}^2(\vec{n}a) + V[\hat{\phi}]$$

with momenta $\hat{\pi}(\vec{n}a)$ conjugate to $\hat{\phi}(\vec{n}a)$. Typical case (ϕ^4 theory)

$$V[\phi] = \frac{1}{2} a^3 \sum_{\vec{n}} \{(\partial_i \phi)^2 + m^2 \phi^2\} + \frac{\lambda}{4!} a^3 \sum_{\vec{n}} \phi^4 \quad (\text{discrete}\, \partial_i)$$

- for $\lambda = 0$, H is quadratic $\leftrightarrow$ harmonic oscillators
- modes $\omega(\vec{k}) = \sqrt{m^2 + \vec{\hat{k}}^2}$, $\quad \hat{k}_i = \frac{2}{a} \sin(\frac{a k_i}{2}) \approx k_i$ if $a k_i \ll 1$
- relativistic free particles associated with long wavelength modes

- $\lambda > 0$: interactions between particles; this is a perturbative picture, in principle for large λ the free particles may not appear as asymptotic states and physics maybe completely different, 'other quasiparticle dgf'.

Path integral formulation

The partition function may be written as a path integral:

$$Z(\beta) = \mathrm{tr}\left[\mathrm{e}^{-\beta \hat{H}}\right] = \int D\phi \, \mathrm{e}^{-S[\phi]}$$

- $\beta/\tau \times (L/a)^3$ fold integration over discretized field paths ('histories') $\phi(t = k\tau, \vec{x} = \vec{n}a)$; $D\phi \equiv \prod_{\tau,\vec{n}} d\phi(t, \vec{x})$

- nonperturbative definition; small λ expansion $\rightarrow$ Feynman diagrams

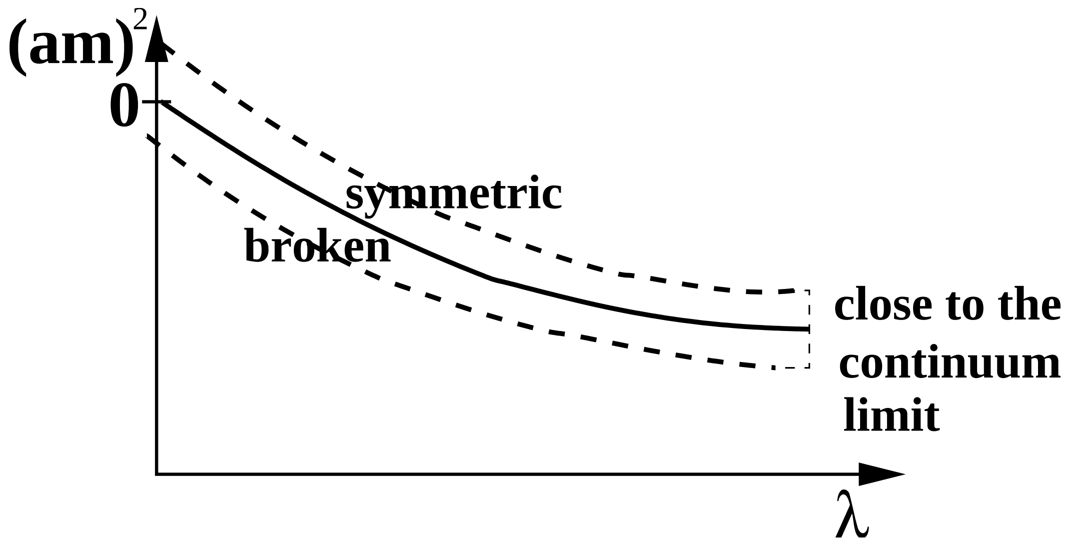
$$S[\phi] = \tau a^3 \sum_{t,\vec{x}} \left\{ \frac{1}{2}(\partial_\mu \phi)^2 + \frac{m^2}{2}\phi^2 + \frac{\lambda}{4!}\phi^4 \right\}$$

correlation functions:

$$\langle \phi(x_1)\phi(x_2)\cdots\phi(x_n)\rangle = \frac{1}{Z}\int D\phi \, \mathrm{e}^{-S[\phi]}\, \phi(x_1)\phi(x_2)\cdots\phi(x_n)$$

- allow to extract lots of information on H, states, matrix elements
- ground state ('vacuum') expectation value as $\beta \to \infty$ (zero temp.)
- can be Monte Carlo estimated
- the lattice is artificial: only universal properties at critical points are related to particle physics ($\leftrightarrow$ renormalization, continuum limit)

phase diagram of ϕ^4 theory



QCD has gauge fields (gluons) and Dirac fermions (quarks), not scalars.....

Discretizing gauge theories

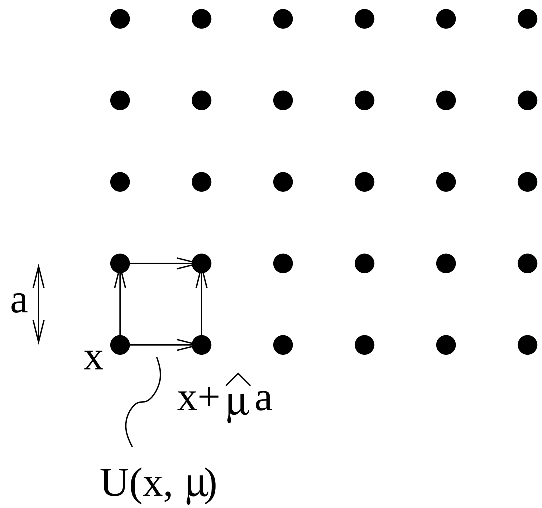
continuum:

$$D_\mu \psi = \partial_\mu \psi + i A_\mu \psi$$

is a gauge covariant derivative.
Lattice covariant difference $\Rightarrow$

$$D_\mu \psi(x) = \frac{U(x,\mu)\psi(x+a\hat{\mu}) - \psi(x)}{a}$$

lattice field $U(x,\mu)$: group valued parallel transporter ($\in \mathrm{SU}(3)$ for QCD)
gauge invariant action for the field $U(x,\mu)$?



$$U(x,\mu)U(x+a\hat{\mu},\nu)-U(x,\nu)U(x+a\hat{\nu},\mu)=i\,a^2F_{\mu\nu}(x)+O(a^3)$$

$$S_{\mathrm{Wilson}}=\frac{2}{g_{\mathrm{bare}}^2}\sum_{\mathrm{Plaquettes}}\mathrm{Re}\,\mathrm{tr}(1-U_{\mathrm{Pl.}})$$

$$Z=\int\prod_{\mathrm{links}}dU\,\mathrm{e}^{-S_{\mathrm{Wilson}}(U)}$$

- continuum limit at $g_{\mathrm{bare}}^2\to 0\leftrightarrow$ asymptotic freedom

- $U(x,\mu) \approx \exp(i a A_\mu(x))$
- confinement of static quarks $\leftrightarrow$ area decay of Wilson loop observable
- possible to show analytically for large lattice spacing
- very precise numerical 'proof' close to the continuum (Yang Mills)

Fermions on the lattice

free 'first quantized' Dirac Hamiltonian:

$$h = i\vec{\alpha}\vec{\nabla} + \beta m$$

continuum eigenfunctions $e^{i\vec{p}\cdot\vec{x}}$, eigenvalues $\pm\sqrt{\vec{p}^{\,2} + m^2}$ (two-fold each), negative $\leftrightarrow$ antiparticles
'Second quantization' leads to QFT (many-particle theory)

$$H = a^3 \sum_{\vec{x}} \psi^\dagger h \psi, \quad \{\psi(\vec{x}), \psi^\dagger(\vec{y})\} = \frac{1}{a^3}\delta_{\vec{x},\vec{y}}, \quad \{\psi,\psi\} = 0 = \{\psi^\dagger, \psi^\dagger\}$$

and partition function

$$Z(\beta) = \mathrm{tr}\, \mathrm{e}^{-\beta H}$$

- interaction with a gauge field: $\partial_k \to D_k$ in h
- Path integral representation via Grassmann integrals

$$Z(\beta) = \int D\psi D\bar{\psi}\, \mathrm{e}^{-S(\psi,\bar{\psi},U)}$$

$$S(\psi,\bar{\psi}) = a^4 \sum_x \bar{\psi}(\gamma_\mu D_\mu + m)\psi$$

- careful discretization required to obtain the desired dgf. (spectral doubling, Nilson Ninomija no-go-theorem)
- Gaussian Grassmann integral $\rightarrow$ fermion determinant:

$$\int D\psi D\bar{\psi}\, \mathrm{e}^{-a^4 \sum_x \bar{\psi}(\gamma_\mu \tilde{D}_\mu + m)\psi} = \det(\gamma_\mu \tilde{D}_\mu + m)$$

Monte Carlo Simulation

$$Z = \int DU \mathrm{e}^{-S_{\text{eff}}(U)}, \qquad \langle \mathcal{O} \rangle = \frac{1}{Z} \int DU \mathrm{e}^{-S_{\text{eff}}(U)} \mathcal{O}(U)$$

$$S_{\text{eff}}(U) = S_{\text{Wilson}}(U) - \log |\det(\not{D} + m)|^2$$

- two (light) quark flavors, $\det(\not{D} + m)$ real positive

most simulation algorithms employ stochastic pseudofermion repesentation

$$|\det(\not{D} + m)|^2 = \int D\varphi D\varphi^* \, \mathrm{e}^{-a^4 \sum_x |(\not{D}+m)^{-1}\varphi|^2}$$

- the sampling of a nonlocal action is very costly
- main stumbling block for QCD simulation at phenomenologically realistic parameters (e.g. light quarks)
- precision results sofar in the (unsystematic) quenched approximation: $\det(\not{D} + m) \to \text{constant}$
- many experimental results like the hadron spectrum $\sim 10\%$ accurate
- intense algorithm development to go beyond this