30+ years on the Lattice

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Lattice QCD

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Introduction

I discuss the history of Lattice QCD from a personal perspective.

In 1973, the work of Gross, Wilczek and Politzer showed that Yang-Mills theories – in particular $SU(3)$ Yang-Mills theory – were asymptotically free. This convinced people that the $SU(3)$ Yang-Mills theory – quantum chromodynamics (QCD) – was the theory of the strong interactions. The $SU(3)$ charge became known as COLOUR.

The Lagrangian density for QCD is:

$$\mathcal{L} = -\frac{1}{2}\mathrm{Tr}F^{\mu\nu}F_{\mu\nu} + \bar{\psi}(i\not{D} - m)\psi$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - g[A_\mu, A_\nu]$ and $D_\mu = \partial_\mu + igA_\mu$.

Since asymptotic freedom means that QCD is weakly coupled at short distances (large momenta), this regime is accessible to perturbation theory. Because the known hadrons are all colourless states, this suggests that the theory is strongly interacting at long distances. Hadrons are states of quarks (and antiquarks) bound by gluons. This long distance behaviour is clearly non-perturbative.

Within a year, Wilson and Polyakov had ported QCD to a discrete space-time lattice in a way that preserved gauge invariance, and lattice QCD was born. This afforded access to non-perturbative phenomena in QCD, including insights into colour (and hence quark and gluon) confinement.

Non-perturbative phenomena in QCD include:

- Hadron masses
- Hadronic matrix elements and form factors
- Nuclear physics
- QCD thermodynamics (early universe, neutron stars and relativistic heavy-ion collisions)

Lattice QCD is a theory analogous to lattice spin models and other systems encountered in condensed matter physics, and the methods used for studying such systems can be applied to study its non-perturbative behaviour.

Strong coupling expansions

Shortly after Wilson formulated Lattice QCD, strong coupling expansions emerged as a way of calculating hadronic properties. Kogut and Susskind studied the Hamiltonian of QCD defined on a 3-dimensional spatial lattice. Balian, Drouffe and Itzykson started from Wilson's functional integral quantization of QCD in Euclidean space-time on a 4-dimensional space-time lattice.

In lattice QCD, the quark fields ψ reside on the sites of the lattice, the gauge (gluon) fields $U_\mu = \exp[igA_\mu]$ lie on the links. The simplest gauge invariant action for Lattice QCD is

$$S = \beta \sum{}_{\square} \left(1 - \frac{1}{3}\mathrm{ReTr}_{\square} UUUU\right) + \sum{}_{sites} \bar{\psi}(\not{D} + m)\psi$$

where $\beta = 6/g^2$ and $\not{D} = \gamma_\mu D_\mu$ with

$$D_\mu \psi(n) = \frac{1}{2}\left[U_\mu(n)\psi(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu})\psi(n-\hat{\mu})\right].$$

Local gauge transformations are implemented by a set of $SU(3)$ matrices $V(n)$, viz.,

$$U_\mu(n) \rightarrow V(n+\hat{\mu})U_\mu(n)V^\dagger(n)$$

and

$$\psi(n) \to V(n)\psi(n).$$

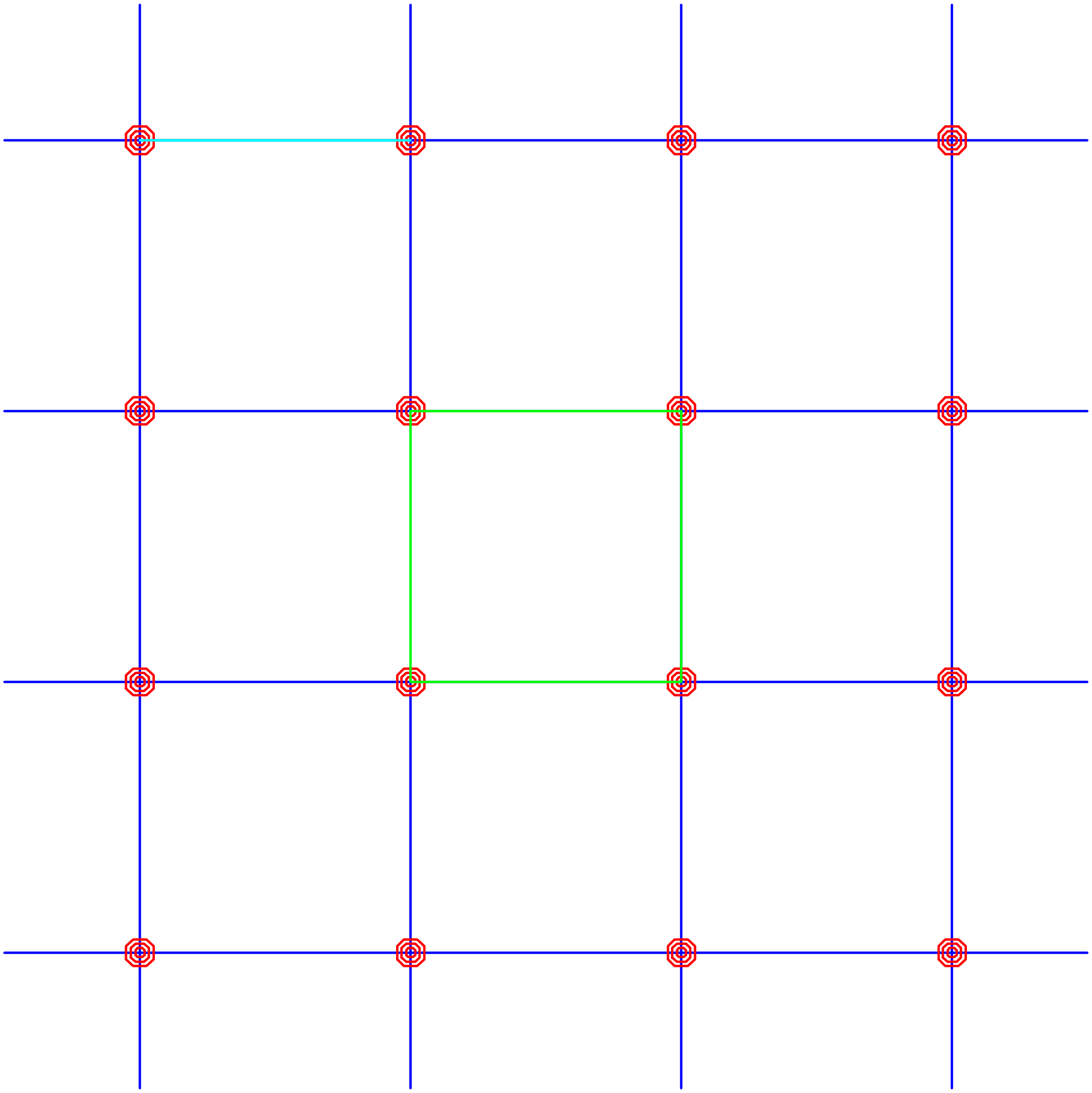


Figure 1: 2-dimensional slice of the lattice.

Quantization is now achieved through the functional integral formalism. On the lattice, the functional integral becomes a regular integral, analogous to a partition function:

$$Z = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}U e^{-S}$$

The strong coupling expansion in powers of $\beta = 6/g^2$ is the analogue of a high temperature expansion in statistical mechanics.

To see confinement at strong coupling, we replace the quarks by static colour charges. Writing $n = (\boldsymbol{x}, t)$, a static quark introduces a factor

$$W(\boldsymbol{x}) = \mathrm{Tr}[U_4(\boldsymbol{x},1)U_4(\boldsymbol{x},2).....U_4(\boldsymbol{x},N_t)]$$

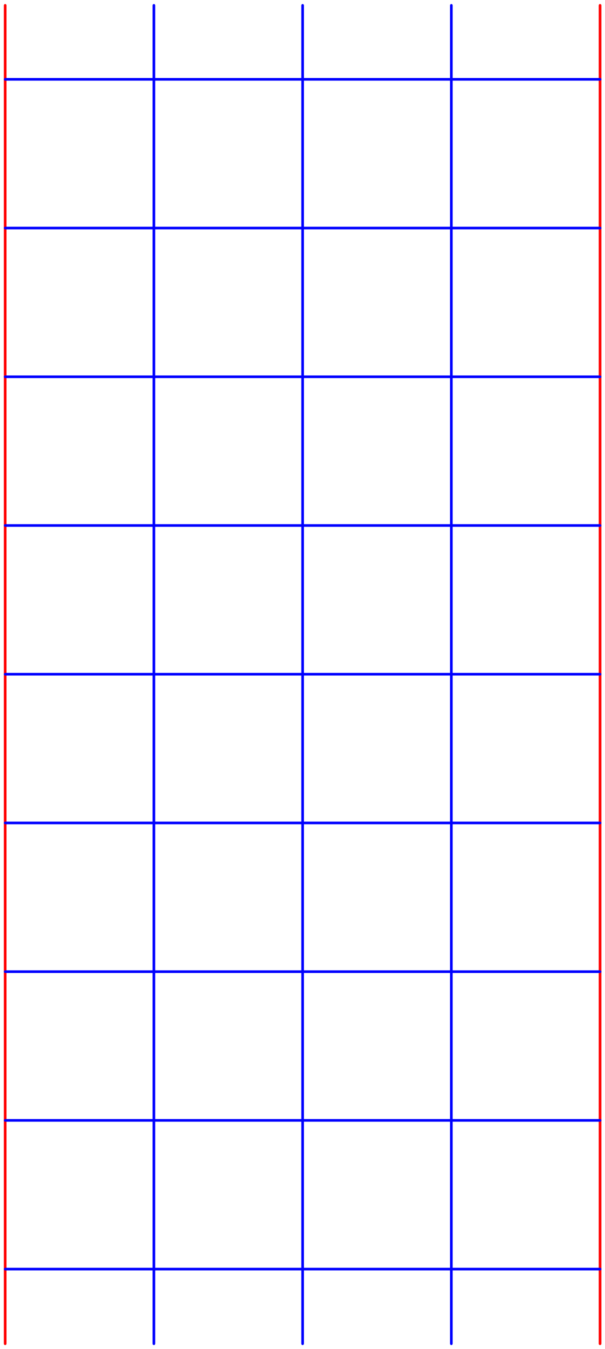
into the functional integral.

Now let us consider a quark and an antiquark at separation X on the lattice. At strong coupling the leading contribution comes from paving the plane between the quark and antiquark with plaquettes. Thus the contribution of the quark-antiquark pair

$$\exp(-E_{q\bar{q}}N_t) = const \left(\frac{c}{g^2}\right)^{XN_t} ;$$

the area law for confinement. In particular, we see that the energy $E_{q\bar{q}} = A + BX$. This indicates a linear potential and hence confinement. If we can reach the continuum limit $a \longrightarrow 0$ and $g(a) \longrightarrow 0$ without encountering a phase transition then confinement is a property of QCD. Note that the cutoff in momenta provided by the discrete lattice is crucial in allowing a strong coupling expansion.

Strong coupling expansions in lattice QCD were eventually abandoned, because it was only practical to calculate a few terms in the series – too few to reliably continue to weak coupling.



Monte-Carlo Methods

In 1980 Creutz introduced Monte-Carlo methods (again from condensed matter) to Lattice Gauge Theories. These numerical methods were applied to Lattice QCD without quarks.

Defining QCD on a space-time lattice reduces the functional integral to an integral over a countable number of variables. Using a (large but) finite lattice reduces this to a finite number of variables. On lattice sizes of interest, the number of variables can be in the millions. Hence numerical evaluations which divide the interval for each variable into a finite number of discrete steps are impractical.

Since the integrand is positive, one can use Monte-Carlo methods. If one randomly chooses N points in this large-dimensional space, it is known that this gives an estimate of the integral with error $\mathcal{O}(1/\sqrt{N})$.

Since, however, it is known that the integrand is strongly peaked over a region that is vanishingly small in the large volume limit, the most naive Monte-Carlo would also be impractical. What is done, is to design a Markov process which (after equilibration) samples the fields with the Boltzman probability. For the pure Yang-Mills theory one chooses an updating scheme which updates the gauge fields sequentially. Since the action is local, each of these updates only involves a few terms (6 plaquettes).

Unfortunately, when we include the quarks, such methods cannot be applied directly, since there is no numerical method of approximating integrals over non-commuting objects directly. Integrating out these fermi fields we have:

$$Z = \int \mathcal{D}U e^{-S_g} \det(\not{D} + m)$$

Such a determinant is difficult to calculate on any sizable lattice. It is also non-local.

As a first attempt to circumvent these difficulties people introduced pseudo-fermions – bosons with the same indices as the fermions. Since doing this produces the inverse of the determinant, we must replace the Dirac operator by its inverse. For simplicity let us consider the case where we have 2 such fermion species. We can write Z as

$$Z = \int \mathcal{D}\phi \mathcal{D}\phi^\dagger \mathcal{D}U e^{-S}$$

with

$$S = S_g + S_\phi$$

and

$$S_\phi = \phi^\dagger[(\not{D} + m)^\dagger]^{-1}[(\not{D} + m)]^{-1}\phi.$$

Here it is clear that we can perform the integral over ϕ by choosing $(\not{D} + m)^{-1}\phi$ to be a set of gaussianly distributed random numbers. Updating the gauge fields for a fixed set of pseudo-fermions remains a problem requiring a new inverse for each link update. What one needs is a small-change algorithm where only one inverse is required per update.

Molecular-Dynamics methods

The Lattice QCD partition function Z can be converted to that for a classical many-body system by introducing momenta p_μ^α conjugate to the gluon fields, writing:

$$Z = \int \mathcal{D}p\mathcal{D}\phi\mathcal{D}\phi^\dagger\mathcal{D}U e^{-(\frac{1}{2}\sum_{links} p^2 + S)}$$

and interpreting

$$H = \frac{1}{2}\sum{}_{links} p^2 + S$$

as the classical Hamiltonian describing motion in some new fictitious 'time'.

We can now obtain all the physics of the partition function by numerically integrating the equations of motion defined by H. Periodically bringing this system in contact with a heat-bath (refreshing p and $(\not{D}+m)^{-1}\phi$ with gaussian random numbers) enforces ergodicity and a canonical distribution.

Because this is a small-change algorithm, only one inversion of the Dirac operator needs to be performed each update. This can be performed efficiently using iterative schemes such as the conjugate gradient algorithm.

Variants of this method of simulation continue to be used for lattice QCD simulations.

To calculate the mass of the lightest meson with given quantum numbers, one calculates the (zero momentum) meson propagator:

$$S(T = x_4 - y_4) = \sum{}_{\boldsymbol{x}} \langle \mathrm{Tr}[\Gamma^\dagger G(x,y) G^\dagger(x,y)] \rangle$$

where $\langle\rangle$ represents an average over an ensemble of gauge configurations produced in ones simulations. $G(x,y)$ is the fermion greens function calculated in the gauge configuration under consideration, obtained by solving

$$(\not{D} + m) G(x,y) = \delta(x-y)$$

numerically. Γ is a product of γs and flavour matrices which project on to states with the desired quantum numbers. The mass M of the lightest meson in this channel is given by

$$S(T) \longrightarrow const \times [\exp(-MT) + \exp(-M(N_t - T)]$$

as $T \rightarrow \infty$.

Subtleties and Improvements

Here I mention a few subtleties associated with Lattice QCD and indicate some improvements which, in addition to the increase in computer power since the '80s, have enabled serious calculations of physical quantities from lattice QCD.

Many of the subtleties are associated with the difficulties in porting femions (quarks) to the lattice. Subtleties associated with fermions include:

- One flavour of naive lattice fermions corresponds to 16 continuum fermions.
- It is impossible to preserve exact flavour and chiral symmetry for lattice fermions.
- The best compromise which has exact flavour symmetry and only short distance chiral symmetry breaking (Ginsparg-Wilson fermions) is not ultra local.
- Tuning the number of flavours of naive (or staggered) fermions leads to a non-local formulation.
- The Dirac operator becomes singular when the quark mass is zero.

Improvements which have occurred in simulating lattice QCD and extracting physics include:

- Modifications which remove all errors associated with discretization of the equations of motion in molecular-dynamics ‘time’, even where one needs fractional powers of the determinant.
- Use of improved lattice actions which decrease the lattice spacing dependence thus allowing coarser lattices.
- Introduction of a class of actions where the Dirac operator is non-singular in the massless quark limit.
- Introduction of algorithms which allow the use of Ginsparg-Wilson fermions.
- Introduction of improved methods for heavy quarks such as NRQCD, allowing precise calculations involving heavy quarks on relatively coarse lattices.
- Use of better sources and sinks, including using multiple sources and sinks to improve the extraction of masses (including excited states) and matrix elements.

- Systematic extraction of continuum matrix elements from their lattice counterparts, including perturbative and non-perturbative matching.
- Use of chiral perturbation theory to continue down to the physical u and d quark masses.
- Further improvements to updating.

Physics – Zero Temperature

- Lattice QCD has been successful in extracting low lying hadron masses with errors of a few percent.
- For charmonium and bottomonium, spectrum calculations predict the hyperfine splitting to around 10% or better.
- Lattice QCD has produced accurate values for the strong coupling constant $\alpha_s^{\overline{MS}}$.
- Quark masses have been extracted.
- Lattice QCD predicts the strong coupling contributions to weak and electromagnentic decays. Removing these effects allows extractions of the weak interaction parameters – CKM matrix.
- The strong interaction contributions to $K\bar{K}$, $D\bar{D}$ and $B\bar{B}$ mixing have been calculated.
- Certain simple strong decay rates and form factors have been calculated.
- Decay rates of charmonium and bottomonium have been calculated. The colour octet and colour singlet contributions have been isolated.

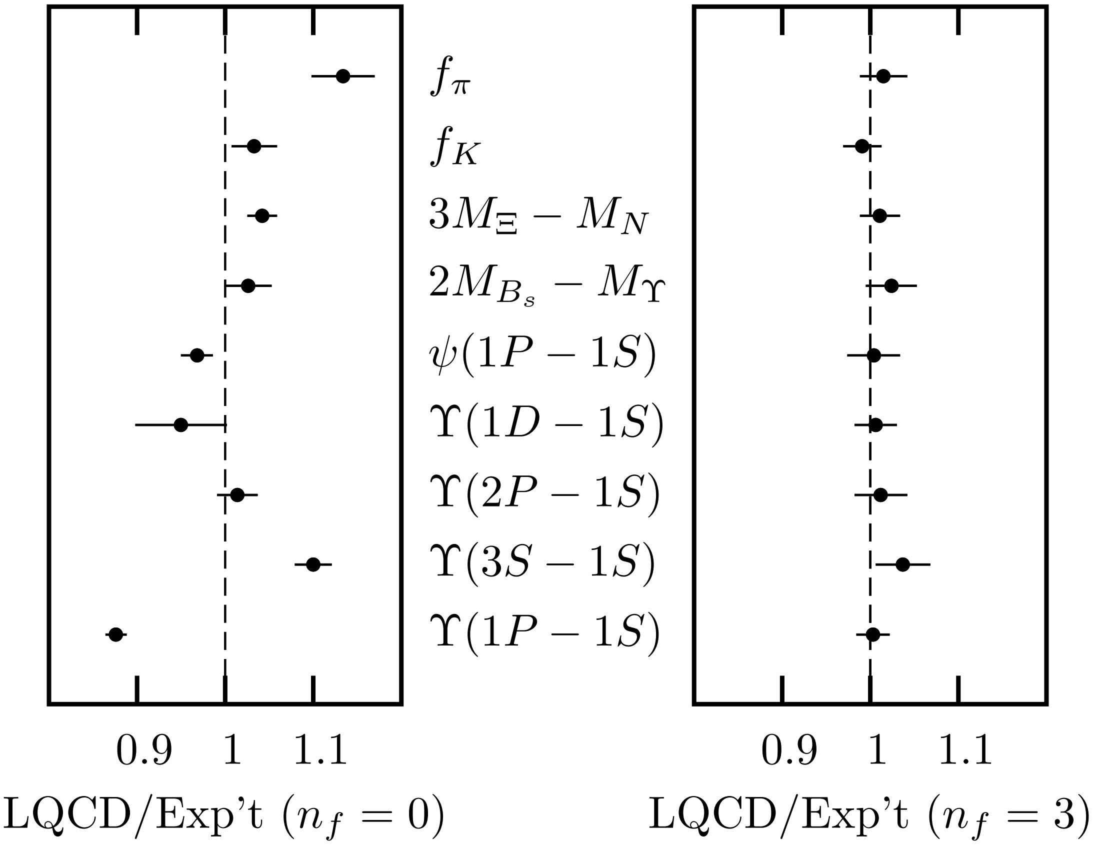


Figure 2: "Goldplated" measurements: From C. T. H. Davies *et al.* "High-precision lattice QCD confronts experiment," Phys. Rev. Lett. **92**, 022001 (2004) [arXiv:hep-lat/0304004].

Higher precision calculations need to be performed. Methods need to be found to calculate more matrix elements and decay rates. More work is needed on glueballs and other exotic states.

QCD at finite temperature

QCD at finite temperature describes hot hadronic matter and, in particular, the transition from hadronic matter to a quark-gluon plasma. This is relevant to the early universe and to the physics of relativistic heavy-ion collisions (RHIC and the LHC heavy-ion program).

Finite temperature T is obtained by simulating on a lattice with temporal extent $1/T$ and spatial dimensions $>> 1/T$.

Lattice QCD yields estimates of the transition temperature and the nature of the transition – a crossover for physical quark masses, a second order transition for massless u and d quarks.

Lattice QCD enables studies of the 'melting' of charmonium and bottomonium in the quark-gluon plasma.

The equation-of-state, which affects the evolution of the system after a relativistic heavy-ion collision, can be obtained from lattice QCD.

It is hoped that lattice QCD will eventually give useful mea-

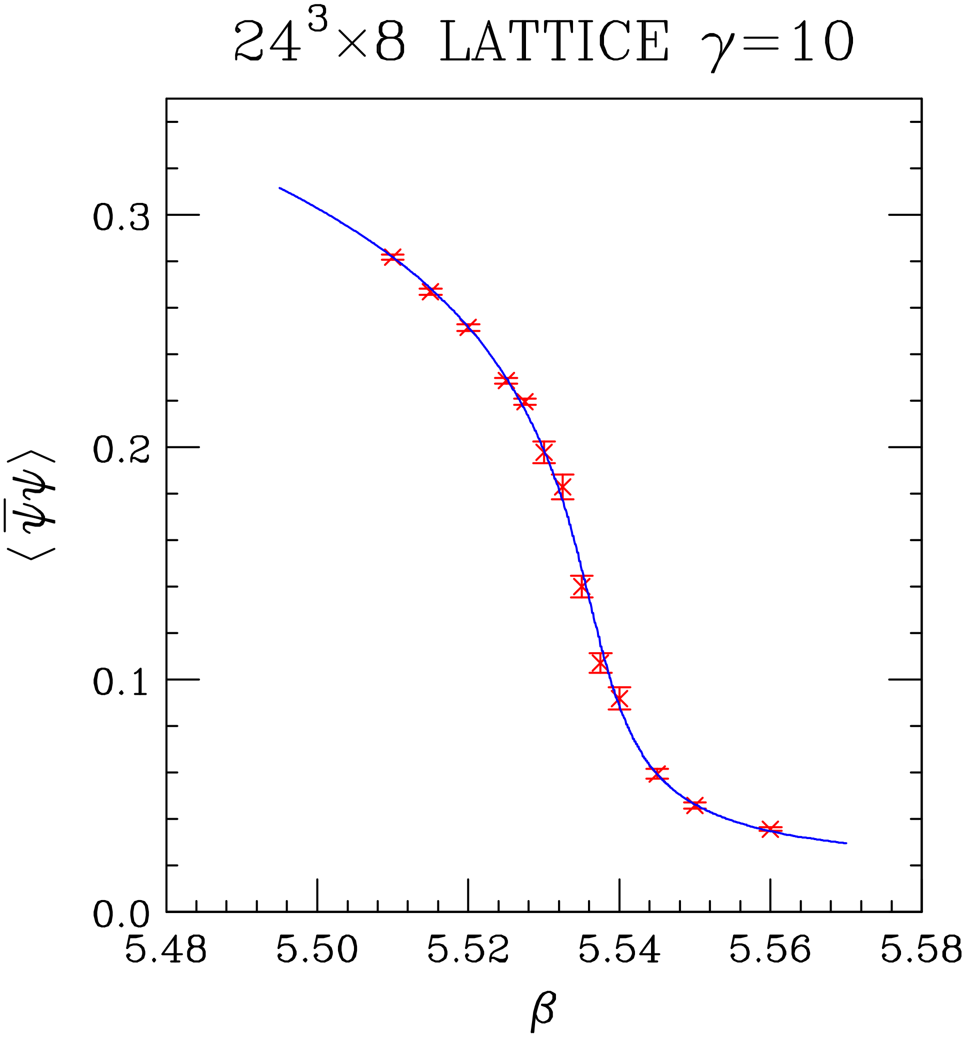


Figure 3: Chiral condensate (points) near the chiral phase transition for lattice QCD, fitted to the magnetization (solid line) for the $O(2)$ spin model {J. B. Kogut and D. K. Sinclair, Phys. Rev. D **73**, 074512 (2006) [arXiv:hep-lat/0603021]. }.

surements of the transport coefficients which describe the hydrodynamic evolution of the aftermath of a relativistic heavy-ion collision.

Nuclear Matter

QCD at finite baryon-number density describes nuclear matter. Studies of finite density QCD are relevant to the physics of neutron stars and superheavy nuclei. QCD at finite temperature and baryon-number density describes the physics of (lower-energy) relativistic heavy-ion collisions.

QCD with a finite chemical potential for quark-(and hence baryon-)number has a complex determinant and cannot be simulated with current algorithms, which are based on importance sampling. QCD at fixed baryon-number also has a sign problem associated with taking a Fourier transform.

Limited progress has been made at high temperatures and low baryon-number density.

Summary

- Lattice QCD is the only known way to perform first-principles calculations of the non-perturbative properties of hadrons and hadronic matter.
- Precision measurements of hadron masses, matrix elements and form-factors are now possible. Higher precision results will be forthcoming.
- Lattice QCD can now study hadronic matter at finite temperatures. Precision studies are needed. Relevant to RHIC and the LHC heavy-ion program.
- Nuclear matter (hadronic matter at finite baryon-number density) remains an unsolved challenge. Similar challenges currently prevent us from using lattice QCD for nuclear physics.
- Algorithms for handling fermions need improvement.
- The performance of computers available for simulations has increased by at a factor of $10^{6\pm2}$ since Lattice QCD simulations began.