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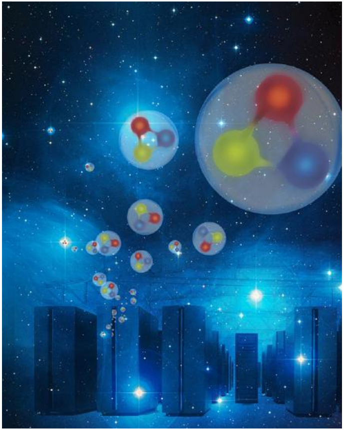
Advancements in Simulations of Lattice Quantum Chromodynamics

Highlights in Computational Quantum Field Theory 5th Vienna Central European Seminar on Particle Physics and Quantum Field Theory

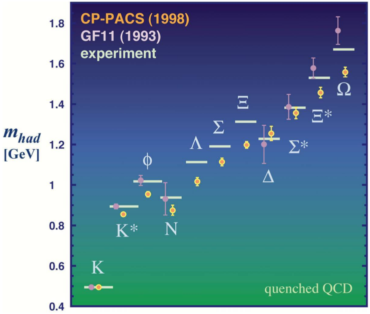
28. November 2008 | Thomas Lippert, Institute for Advanced Simulation

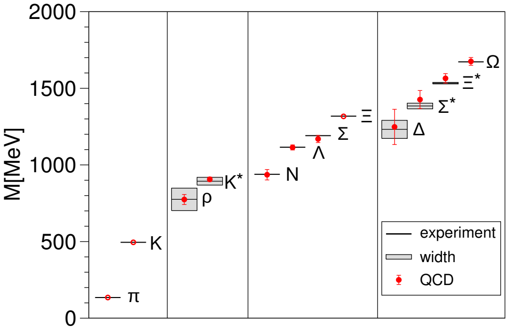
Highlight



- “The weight of the world is quantum chromodynamics”
- S. Dürr, Z. Fodor, J. Frison, C. Hoelbling, R. Hoffmann, S. D. Katz, S. Krieg, T. Kurth, L. Lellouch, T. Lippert, K. K. Szabo, G. Vulvert
- $2 + 1$ dynamical flavours
- Full agreement with experimental observations for the first time
- Fully controlled uncertainties
- QCD is validated in light hadron sector

From Quenched to $2+1$-flavor QCD





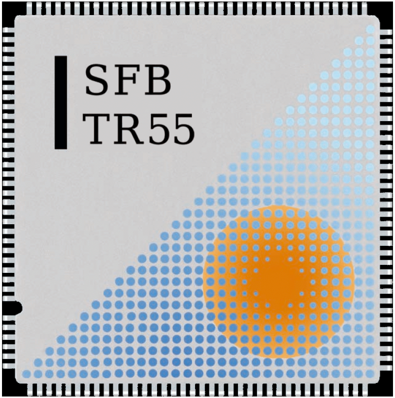
The most patient coworker

More Details...

More Details...

$\Rightarrow$ ...talk by Stefan Krieg

Algorithm Group Wuppertal-Jülich-Regensburg



Nigel Cundy, Andreas Frommer, Stefan Krieg, Th. L.,
Andreas Schäfer

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Outline

Basics of Lattice QCD

Fermion Discretization Schemes

- Wilson fermions
- Overlap fermions
- Numerical representation

HMC for OF

- Partition function
- Step function

Advancements

- I. Small mode mixing problem
- II. Low tunneling rate problem

Status of Simulation and Outlook

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Status of Simulation and Outlook

Physics goals of Lattice-QCD

Hadron spectrum:	Verification of QCD
Quark masses:	Input for standard model
CKM-matrix:	CP-violation, physics beyond SM
Interquark-potential:	Confinement
String breaking:	Heavy meson decay
Structure functions:	Hadron structure
Quark gluon plasma:	GSI-FAIR, LHC, FNAL, BNL, etc.
Glueballs:	Exotic matter
Topology:	η', UA(1)-problem, chiral symmetry

Elements of lattice QCD

Lagrangian

$$L_{QCD} = -\frac{1}{4} F_{\mu\nu a} F^{a\mu\nu} + i \sum_{q=1}^{n_f} \bar{\psi}^i{}_q \gamma^\mu (D_\mu)_{ij} \psi^j{}_q - \sum_{q=1}^{n_f} m_q \bar{\psi}^i{}_q \psi_{iq}$$

$$F_{\mu\nu}{}^a = \partial_\mu A^a{}_\nu - \partial_\nu A^a{}_\mu + g_s f^a{}_{bc} A^b{}_\mu A^c{}_\nu$$

$$(D_\mu)_{ij} = \delta_{ij}\partial_\mu - i g_s \sum_a \frac{\lambda^a{}_{ij}}{2} A^a{}_\mu = \delta_{ij}\partial_\mu - i g_s \mathcal{A}_{ij\mu}$$

Quantization through Path Integral

$$Z = \int [dA][d\bar{\psi}][d\psi] e^{i \int d^4 x \, L_{QCD}}$$

Fermions: ψ are Grassmann variables, $\{\psi_i, \psi_j\} = \delta_{ij}$

Lattice computation

- Euclidean space $t \to i\tau \Rightarrow L_{QCD}$ real positiv definite $\Rightarrow$ partition function
- Discretize space-time $\Rightarrow$ 4-d lattice
- Monte Carlo evaluation on supercomputer $\Rightarrow$ HMC

Stochastic Simulation

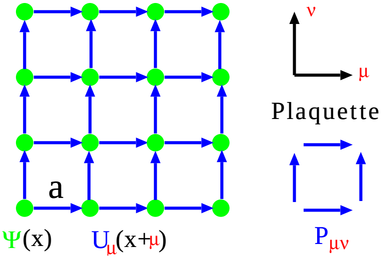
- Gauge action: $e^{-\beta S_g}$ is positiv definit $\Rightarrow$ Boltzmann weight
- Fermions: Gauss integrate over Grassmann variables $\Rightarrow$ det M

$$Z = \int \prod_{x,\mu} [dU_\mu(x)] \det(M) e^{-\beta S_g}$$

- Importance sampling: Generate canonical ensemble according to Boltzmann weight $\rightarrow$ Markov process

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^{N} O_i[U_i], \qquad \sigma_O^2 = \frac{1}{N} \left(\frac{1}{N} \sum_{i=1}^{N} |O_i[U_i]|^2 - \bar{O}^2 \right)$$

Discretization



- Gauge links U: $\psi'(x) = U_\mu(x)\psi(x+\mu) = \mathbf{P}e^{ig_s\int_x^{x+\mu} dx_\mu A_\mu}\psi(x+\mu)$
- Wilson gauge action: $\beta S = \frac{2N_c}{{g_s}^2}\sum_{x,\mu,\nu}\left[1 - \frac{1}{2}Tr(P_{\mu\nu}(x) + P^\dagger_{\mu\nu}(x))\right]$

$$\underset{a\to 0}{\longrightarrow} -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

Fermions and doubling

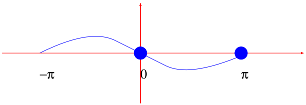
$$S_f = \int_{d^4x} \bar{\psi}\gamma^\mu \partial_\mu \psi + m\bar{\psi}\psi \rightarrow \sum_x \bar{\psi}_x \gamma_\mu \frac{\psi_{x+\mu} - \psi_{x-\mu}}{2a} + m\bar{\psi}_x \psi_x$$

$$= \sum_x \bar{\psi}_x M_{x,y} \psi_y$$

- Doubling — Dirac fermions $\Rightarrow$ 16 fold degeneracy
- Mom. space — Greens function $\propto \sin^{-1}$:

$$\partial_\mu \psi \rightarrow \frac{1}{2a}[\psi_{x+\mu} - \psi_{x-\mu}] \rightarrow i \sin p_\mu a.$$

- Mass — poles of propagator $\Rightarrow$ 16 poles



Nielsen-Ninomiya-No-Go Theorem

A lattice fermion action with

- hermiticity
- discrete translation invariance
- locality: $||D(x, y; U_\mu)|| \leq c_1 \exp(-c_2|x - y|)$
- chiral symmetry

is not possible!

- Non-local action — Either break Lorentz-invariance on quantum level or violate important axial anomaly (quantum effect)
- Ways out: — Wilson fermions
Overlap fermions

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- Advancements
  - I. Small mode mixing problem
  - II. Low tunneling rate problem
- Status of Simulation and Outlook

Wilson fermions

- Add 2nd order derivative $\bar{\psi}_x \frac{\psi_{x+\mu} - 2\psi_x + \psi_{x-\mu}}{2a}$

$$
\begin{aligned}
D_{W\,x,y} &= (m+4)\delta_{x,y} \\
&- \frac{1}{2a}\sum_{\mu=1}^{4}(1-\gamma_\mu)U_\mu(x)\,\delta_{x,y-\mu} + (1+\gamma_\mu)U^\dagger_\mu(x-\mu)\delta_{x,y+\mu}
\end{aligned}
$$

- $m \to 0$

The remaining diagonal term together with the Dirac diagonal parts break chiral symmetry explicitly but should become irrelevant with $a \to 0$

Explicit breaking of chiral symmetry

- Chirality: Action

$$S_{wf} = \sum_{i=1}^{3} \bar{\psi}_i \, D_w^i \, \psi_i,$$

not invariant under chiral transforms even for $m = 0$. Wilson fermions violate CS on the lattice explicitly

- Consequence: The chirally symmetric point of the theory is not at $m = 0 \Rightarrow$ additive renormalization $\Rightarrow$ complicated tuning and extrapolation procedure to $m_c(\beta) < 0$

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$\Rightarrow$ talk by Stefan Krieg

Overlap fermions for lattice QCD– Advantages

Overlap Fermions (Neuberger) are the formulation of lattice QCD closest to the continuum

- Overlap fermions show lattice variant of chiral symmetry
- Consistent quark mass definition
- No mixing of operators under renormalisation $\Rightarrow$ analysis greatly simplified
- The Overlap chiral symmetry is connected to the ABJ Anomaly exactly as in the continuum
- The Overlap ABJ anomaly gives a precisely defined topological index on the lattice
- Overlap fermions are *automatically* $O(a)$ improved: Better scaling towards the continuum

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Problems

- The Overlap operator is defined via the matrix sign function of a kernel matrix
- Implementation of the sign function requires the repeated computation of the multiplication of the kernel operator and a vector
- Advanced simulation algorithms require “inversion” of the overlap operator and thus very frequent computation of the multiplication of the Overlap operator and a vector
- Efficient solvers for the overlap operator have to be found
- Simulation algorithms (HMC) require the derivative of the sign function with respect to the kernel (during MD) $\Rightarrow$ Problems with discontinuity of the sign function

Definiton of the Overlap operator

The (massless) Overlap (Dirac) operator is defined as:

$$D_o = 1 + \gamma_5 \, \mathrm{sign}(Q)$$

with the hermitian Q given by $Q = \gamma_5 M$.

Ginsparg-Wilson Relation

- ?

  D_o violates chiral symmetry, however, violation is mild!!

- Locality

  The overlap operator fulfills the Ginsparg-Wilson-Relation

$$\gamma_5 D_o^{-1} + D_o^{-1} \gamma_5 = a \gamma_5 R$$

R is a local matrix, its matrix elements vanish exponentially with the distance

Chirality is violated only locally for the physically relevant propagator

Implementation of the matrix sign function

- Definition of the sign function

$$\text{sign}(Q) = \sum_i |\psi_i\rangle\langle\psi_i| \, \text{sign}(\lambda_i)$$

- Practical implementation: treat lowest EVs using this definition, employ rational approximation for higher EVs

$$\gamma_5 \, \text{sign}(Q) = \frac{M}{M^\dagger M} = M \sum_{j=0}^{N} \frac{\omega_j}{Q^2 + \tau_j}$$

with the ω_i and τ_i given via the Zolotarev procedure

v.d. Eshof, Frommer, Lippert, Schilling, v.d. Vorst,2001

- Shifted inverersions: Muli-Mass solver

Frommer, Nöckel, Güsken, Lippert, Schilling, 1995, 1996

Optimal solver: SUMR

- In HMC simulations of lattice QCD with overlap fermions

$$b = D_o x$$

  has to be solved repeatedly
- SUMR is the optimal solver in this case

  Arnold, Cundy, v.d. Eshof, Krieg, Lippert, Schäfer 03

- Further gains by optimizing the nested system:
  - (*inner* system) sign function has to be constructed via repeated applications of the kernel matrix M.
  - (*outer* system) to solve the system the above multiplication (and thus the sign function) has to be carried out repeatedly

Relaxation – GMRESR

Relaxation strategies for the (inner) precision of the sign function while keeping the residual gap under control

$$\| \underbrace{b - Ax^k}_{\text{true residual}} \| \leq \| \underbrace{r^k - (b - Ax^k)}_{\text{residual gap}} \| + \| \underbrace{r^k}_{\text{computed residual}} \|.$$

Cundy, v.d.Eshof, Frommer, Krieg, Lippert, Schäfer 04

With relaxation the optimal solver for overlap fermions for a large range of lattice sizes is the GMRESR(SUMR) algorithm

SUMR is (single precision) preconditioner to the (double precision) inversion in the GMRESR scheme.

Outline

Hybrid Monte Carlo

- Generate an ensemble of gauge field configurations weighted by the function (2 flavors)

$$e^{-S_g[u]}\,\mathrm{det}(H^2)$$

with

$$H = \gamma_5 D_o$$

- Estimate determinant using pseudo-fermion fields generated by a heatbath

$$\mathrm{det}(H^2) = \int [d\phi][d\phi^\dagger]\,\mathrm{exp}\left(-\phi^\dagger \frac{1}{H^2}\phi\right)$$

Step Function Problem

- HMC contains
  1. A Molecular dynamics evolution of the gauge links
  2. A Metropolis accept reject step
- In 1: discontinuity of the sign function when a kernel matrix eigenvalue changes sign

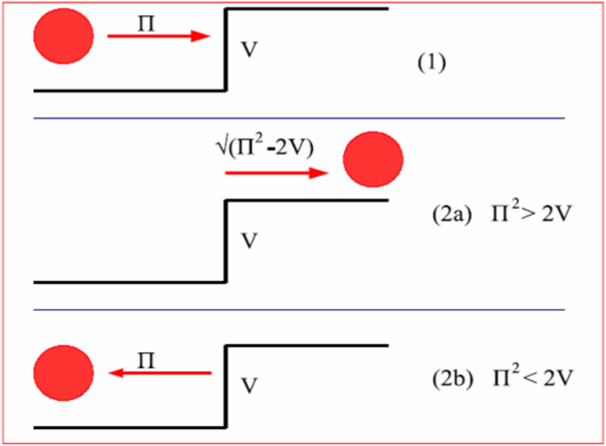
$$\Delta S = \langle\phi|\frac{1}{{H_-}^2}({H_-}^2 - {H_+}^2)\frac{1}{{H_+}^2}|\phi\rangle$$

- This is equivalent to a Dirac δ contribution to the MD force

Solution of the step function problem

- Solution to the step function problem (Fodor et al, Cundy et al):
  When encountering a step during MD evolution
  - Integrate to the exact hyper-surface where the crossing eigenvalue is zero
  - If the conjugate momentum is large enough, transmit through hypersurface
  - If the conjugate momentum is too small, reflect of the hypersurface
- Schemes differ by the level of energy conservation
  Cundy et al. allows for $O(\tau^2)$ and is guaranteed to fulfill detailed balance

Solution in the classical particle picture



Does this scheme really work?

- The scheme works on very small lattices at larger quark masses
- For larger lattices and smaller quark masses:
  - The density of small eigenmodes of the kernel matrix increases
  - The small eigenmodes can mix and produce a close-to-zero mode
  - The dynamical system becomes stiff and refuses to change the (precisely defined) topological sector frequently enough or at all
- Cundy, Frommer, Krieg, Lippert, Arnold, Schilling 08

Outline

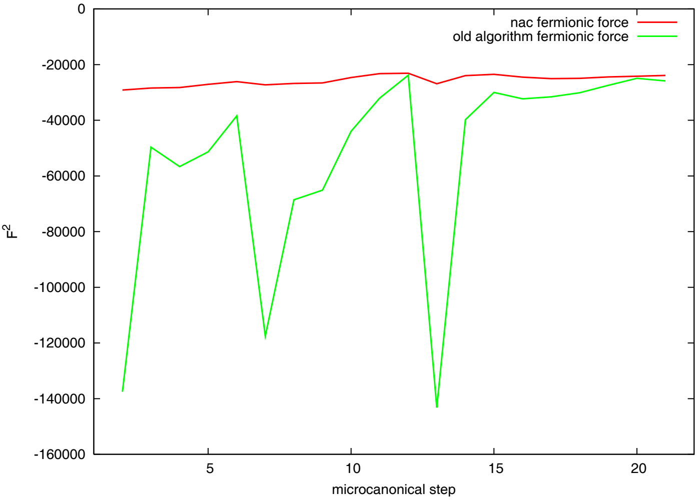
I. Small mode mixing problem

- Small eigenmodes are treated explicitely in MD evolution
- Small eigenmodes can mix
- $\Rightarrow$ spikes in the MD force $\Rightarrow$ low acceptance rate
- Reason: by differentiation of EV, relevant part of the force contains

$$F = \ldots + \langle A|\psi\rangle\langle\psi|\frac{d}{d\tau}Q|\psi\rangle\langle\psi|B\rangle\,\frac{\text{sign}(\lambda_1) - \text{sign}(\lambda_2)}{\lambda_1 - \lambda_2}$$

- Small eigenmodes occur more frequently when lattice size is increased

Solution (Cundy et al. 07)



The Problem

- Matrix sign function is calculated in terms of Zolotarev, with the smallest eigenvalues of Q deflated (q generically stands for U):

$$\begin{aligned}\mathrm{sign}\big(Q(q)\big) &= Q(q)\sum_i \frac{\omega_i}{Q(q)^2+\sigma_i}(1-\sum_i P_i) \\ &+ \sum P_i \epsilon(\lambda_i) \\ P_i x &= \psi_i(\psi_i, x)\end{aligned}$$

- Differentiating the rational approximation with respect to q is easy; differentiating the eigenvectors is difficult ...
- ...a straightforward procedure does not work!

The Trick

- Expand the eigenvectors as follows:

$$|\delta\psi_i\rangle = \sum_{j\neq i} \left[(\cos\theta_{ij} - 1)|\psi_i\rangle + e^{i\phi_{ij}} \sin\theta_{ij}|\psi_j\rangle\right]$$

- Insert this into the eigenvalue equations

$$\tan 2\theta_{ij} = \frac{2\sqrt{\langle\psi_i|\delta Q|\psi_j\rangle\langle\psi_j|\delta Q|\psi_i\rangle}}{\lambda_i - \lambda_j + \langle\psi_i|\delta Q|\psi_i\rangle - \langle\psi_j|\delta Q|\psi_j\rangle}$$

$$e^{i\phi_{ij}} = \sqrt{\frac{\langle\psi_j|\delta Q|\psi_i\rangle}{\langle\psi_i|\delta Q|\psi_j\rangle}}$$

Challenges sui generis

- Algorithm violates area conservation and is not exact
  $\Rightarrow$ Update Jacobian must be included in Metropolis step to correct the area problem
- Fermionic force becomes a horrid function of the momenta
- Naive momentum update is not reversible. This can be fixed by an iterative procedure
- Resulting algorithm albeit complex does *not* require substantially more resources

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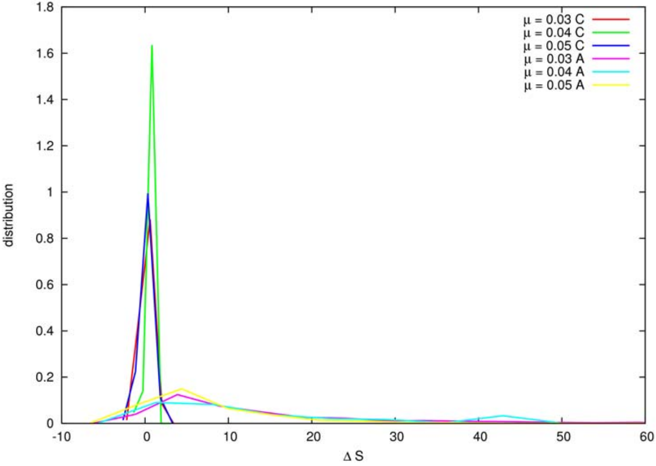
And it works!!!

II. Low tunnelling rate problem

- Note: Transmission $\Rightarrow$ top. index changes
  Reflection $\Rightarrow$ no change
- Autocorrelation: for topological observables $\Rightarrow$ tunnelling rate must be high
- !! Generic for all descretizations! With overlap fermions problem visible for the first time

- Size of discontinuity critical for the transmission rate
- A pseudo-fermion estimate of the determinant badly handles the discontinuity (large ΔS)
- Idea:
  - Split the determinant in terms of EVs
  - Calculate the small eigenvalue determinant exactly
  - Treat large eigenvalue determinant with pseudo-fermions

Solution (Cundy 2008)



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Transmission/Reflection

- Original proposal (Fodor et al. / Cundy et al.) analogous to classical mechanics case
- Update the gauge field to the $\lambda = 0$ surface; introduce a discontinuity ΔS in the kinetic energy $\Rightarrow$ transmit

$$\begin{aligned} \frac{1}{2}\pi_{new}^2 &= \frac{1}{2}\pi_{old}^2 + \Delta S \\ (\pi_{new}, \hat{\eta}) &= (\pi_{old}, \hat{\eta})\sqrt{1 + \frac{2\Delta S}{(\pi_{old}, \hat{\eta})^2}} \end{aligned}$$

- When $1 + \frac{2\Delta S}{(\pi_{old},\hat{\eta})^2} < 0 \Rightarrow$ reflect

$$(\pi_{new}, \hat{\eta}) = -(\pi_{old}, \hat{\eta})$$

First step: Improved Proposal

$$
\begin{aligned}
e^{-(\pi_{new},\hat{\eta})^2} &= e^{-(\pi_{old},\hat{\eta})^2-\Delta S} + (1-e^{-\Delta S}) \\
e^{-(\pi_{new},\hat{\eta}_1)^2-(\pi_{new},\hat{\eta}_2)^2} &= e^{-(\pi_{old},\hat{\eta}_1)^2-(\pi_{old},\hat{\eta}_2)^2} \\
&\quad e^{-\tau c[(\pi_{old},\hat{\eta})(F_{old},\hat{\eta})-(\pi_{new},\hat{\eta})(F_{new},\hat{\eta})]} \\
(\pi_{new}, F_{old}-\hat{\eta}(\hat{\eta},F_{old})) &= (\pi_{old}, F_{old}-\hat{\eta}(\hat{\eta},F_{old}))+ \\
&\quad (F_{old}-\hat{\eta}(F_{old},\hat{\eta}), F_{old}-\hat{\eta}(F_{old},\hat{\eta}))
\end{aligned}
$$

Probability of transmission increased by about a factor of 3 for a given ΔS, improvement of energy conservation

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\begin{aligned}
e^{-(\pi_{new},\hat{\eta})^2} &= e^{-(\pi_{old},\hat{\eta})^2-\Delta S} + (1 - e^{-\Delta S}) \\
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&\quad e^{-\tau_c[(\pi_{old},\hat{\eta})(F_{old},\hat{\eta})-(\pi_{new},\hat{\eta})(F_{new},\hat{\eta})]} \\
(\pi_{new}, F_{old} - \hat{\eta}(\hat{\eta}, F_{old})) &= (\pi_{old}, F_{old} - \hat{\eta}(\hat{\eta}, F_{old})) + \\
&\quad (F_{old} - \hat{\eta}(F_{old}, \hat{\eta}), F_{old} - \hat{\eta}(F_{old}, \hat{\eta}))
\end{aligned}
$$

Probability of transmission increased by about a factor of 3 for a given ΔS, improvement of energy conservation

This is not sufficient

Second step: Fighting pseudo fermion action noise

- Estimate via EVs for a single pseudo fermion term shows a scaling with the quark mass of

$$\Delta S = \mathcal{O}(\mu^{-2}).$$

- $\Rightarrow$ The rate of topological charge change scales at low mass as

$$e^{-1/\mu^2}.$$

- But ΔS from the fermion determinant is

$$\Delta S = \mathcal{O}(1).$$

- Low tunneling rate is obviously an artefact of the pseudo fermions

Procedure

- The fermion determinant is factorized

$$
\begin{aligned}
\det H =& \det(\frac{H}{\tilde{H}})\det(\tilde{H}) \\
\tilde{H} =& (1+\mu)\gamma_5 + (1-\mu)\tilde{\epsilon}(Q) \\
S =& -\phi^\dagger \frac{1}{\tilde{H}^2}\phi + 2\log\ \det\left[\delta_{ij} + \langle\psi_i|\frac{1}{\tilde{H}}|\psi_j\rangle(\epsilon(\lambda_i) - \tilde{\epsilon}(\lambda_i))\right]
\end{aligned}
$$

- As long as $(\epsilon(\lambda_i) - \tilde{\epsilon}(\lambda_i)) = 0$ for all but a few eigenvalues, one can calculate the additional log term and the force for this log term easily.
- Still have to remove zero modes!!
- $\Rightarrow$ Factorize overlap operator similar to Bode et al. (1999)

Action used

$$S = S_g[q] + \left(\phi_1, \frac{1}{\tilde{D}_+(\mu+\Delta)}\phi_1\right) + \left(\phi_2, \frac{\tilde{D}_+(\mu+\Delta)}{\tilde{D}_+(\mu)}\phi_2\right) +$$
$$\left(\phi_3, \frac{1}{\tilde{D}_+(\mu+\Delta)}\phi_3\right) + \left(\phi_4, \frac{\tilde{D}_+(\mu+\Delta)}{\tilde{D}_+(\mu)}\phi_4\right) +$$
$$2\mathrm{Tr}\log\left[\delta_{ij} + \left(\psi_i, \frac{1}{\gamma_5 \tilde{D}}\psi_j\right)(\tilde{\epsilon}(\lambda_i) - \epsilon(\lambda_i))\right]$$

- S_g =Tadpole Improved Lüscher Weisz gauge action,
- Wilson kernel with one flavour of modified over improved stout smearing
- Improved transmission/reflection and NAC eigenvalue differentiation

This appears to be a viable algorithm!

Outline

Status of Simulation and Outlook

- Currently we work on a $16^3 \times 48$-lattice on the Jülich Blue Gene/P.
- We aim at a lattice spacing of around 0.12 fm; $m_\pi \sim 350$ MeV.
- The 16^3 run is currently taking about 6 hours/trajectory on 2048 processors
- Simulations with dynamical Overlap fermions will steadily approach physical lattice sizes and quark masses
- The next generation of supercomputers will allow overlap fermions to run as fast as Wilson fermions today

...

Enjoy the next talk!