EM sea effects in hadron polarizabilities through reweighting

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Overview

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  - Boundary condition considerations
  - Sea contributions
- Background on reweighting
- Simulation details
- The traditional stochastic estimator
  - Failed improvement approaches
- "Perturbative reweighting"
  - Hopping parameter expansion and improvement
- Preliminary results
- Next steps

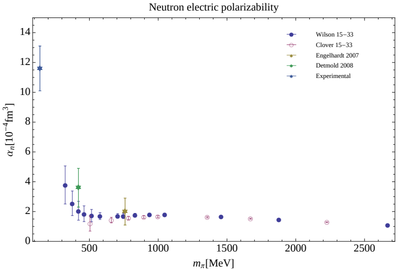
Status of polarizability calculations

This work is part of a long-term project to attack the polarizability of the neutron (or other hadrons).

A "basic" computation of the neutron polarizability is not too hard to do.

Multiple challenging issues required to make contact with experiment:

- Approach to the chiral limit
  - EFT's predict very strong dependence on m_q near chiral limit
  - Lighter quark masses and expensive chiral actions
  - Good probe of chiral behavior on lattice
- Finite volume corrections
- Continuum limit



- Sea effects (this project): simulating interactions between sea quarks and background field is less straightforward

Long-term goal: understand these effects one by one, then put them together

Background on polarizability measurements

Variety of polarizabilities parametrize mass shift in the presence of EM fields:

$$H_{\rm EM} = -\boldsymbol{\mu}\cdot\mathbf{B} - \frac{1}{2}\alpha\mathbf{E}^2 - \frac{1}{2}\beta\mathbf{B}^2 - \frac{1}{2}\gamma_{\rm E1}\boldsymbol{\sigma}\cdot\mathbf{E}\times\dot{\mathbf{E}} - \frac{1}{2}\gamma_{\rm M1}\boldsymbol{\sigma}\cdot\mathbf{B}\times\dot{\mathbf{B}} + \ldots$$

Background field method: measure M_N without and with uniform electric field, examine difference

- Apply electric field by applying appropriate U(1) phase to links in x_4 direction
- Error on mass shift can be much less than error on each mass separately: use extended covariance matrix (error on M_N is 13 MeV; error on ΔM_N is 0.7 MeV)
- Consider fields of both $\vec{E}$ and $-\vec{E}$ to eliminate first-order effects and reduce noise

Apply field by multiplying gauge links by U(1) phases:

Make substitution $U_\mu \to e^{-iqaA_\mu} U_\mu$ with $A = (0, 0, 0, iEx_1)$

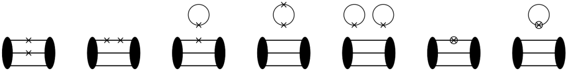
Issues with the background field

- Should really use true exponential rather than linearizing the phase factor ($\exp \alpha = 1 + \alpha$)
- In Euclidian time, U(1) phases represent an *imaginary* electric field!
  - Something of a non-issue: this just flips sign of ΔM
  - Tests on quenched: this works just fine
- Need to address discontinuities at edges of lattice:
- Use Dirichlet boundary conditions in time
- Three options in spatial direction:
  - Just deal with discontinuity at edge of lattice
  - Use larger value of η, well out of perturbative regime
  - Use Dirichlet boundary conditions in x_1, too
    - Avoid multi-valued electric potential, issues with quarks winding around lattice
    - Any effect can be treated as "another finite volume effect": vanishes as $n_x \to \infty$ (we have elongated lattices...)
    - Potentially more important for sea effects
    - Effect of DBC's needs further study: comparison with PBC's as a function of n_x

EM sea contributions to neutron polarizability: status

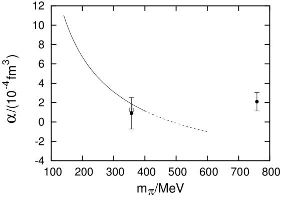
Only aware of one other calculation for the neutron polarizability including sea effects: M. Engelhardt, [0706.3919] and [1011.5044]:

- Uses explicit expansion of the path integral up to order E^2
- Mixed-action calculation: DWF valence on MILC Asqtad 2+1 sea ($a = 0.12$ fm)
- Sea effects appear naturally in list of diagrams that must be evaluated



- Calculation done relatively far from chiral limit: $m_\pi = 357, 759$ MeV

	α_E, $10^{-4} fm^3$	
M_π	Valence	Valence + sea
759 MeV	1.5(3)	2.1(1.0)
357 MeV	0.5(5)	0.9(1.6)



- Ensembles far enough from chiral limit that result expected to be small
- Effect of sea contributions not yet distinguished from zero

EM sea contributions to neutron polarizability: status

- Related calculation (another plenary at this conference): T. Ishikawa *et al.*[1202.6018], using reweighting to look at EM sea effects on EFT LEC's
  - A bit different, as they are using reweighting to get dynamical QED, rather than a background field
- Conclusions:
  - Reweighting method successful
  - Sea effects not distinguishable from zero
  - Future work can bring down uncertainties
- Both this work and Engelhardt's work unable to resolve effect of charged sea
- It may well be that sea EM effects are not that important, but we'd like to put a smaller error bar on them
  - Zero, after all, is a perfectly reasonable result, if it comes with small errors...

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- Problem: requires unaffordably high statistics, since our two mass measurements now no longer have correlated errors

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... yes!

Reweighting, in general

In general, a technique for extracting physics from a different action than the one used in generation: "retroactively change the ensemble parameters"

Standard	Reweighted
$\frac{\int [dU] \mathcal{O} e^{-S_1}}{\int [dU] e^{-S_1}} \to \frac{\sum \mathcal{O}_i}{\sum 1}$	$\frac{\int [dU] \mathcal{O} e^{-S_2}}{\int [dU] e^{-S_2}} = \frac{\int [dU] \mathcal{O} e^{-(S_2 - S_1)} e^{-S_1}}{\int [dU] e^{-(S_2 - S_1)} e^{-S_1}} \to \frac{\sum \mathcal{O}_i w_i}{\sum w_i}$ where $w_i = e^{-(S_2 - S_1)_i}$.

This will only work well if the two ensembles overlap sufficiently.

- If they don't, this manifests as large fluctuations in w_i's (over many orders of magnitude!)
- Large fluctuations decrease the statistical power of the ensemble: can compute the "effective number of configurations": $N_{\rm eff} = N \frac{\overline{w}^2}{\overline{w^2}}$ (Liu et al., [1206.0080])
- Not a problem for reweighting in E, since in principle we are only after perturbatively small changes

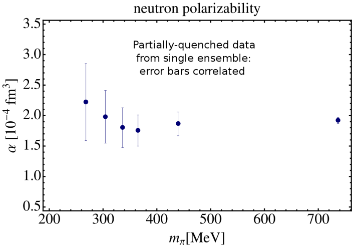
Very useful for us, generate two correlated ensembles with different parameters!

$\to$ Taking advantage of this property of reweighting is nothing new: used by H. Ohki *et al.* to compute $\frac{\partial M_N}{\partial m_s}$ by reweighting in m_s [0910.3271]

Plan of attack

We already know how to do the valence contribution:

- Measure the zero-field neutron correlator as usual
- Compute the link variables with the field: $U_\mu \to e^{-iqaA_\mu} U_\mu$ (different for u and d quarks)
- Use these links to measure the neutron correlator with $\vec{E} = \pm E_0 \hat{x}$
- Do correlated fit to correlators to determine dependence of M_N on E^2



To include the sea contribution:

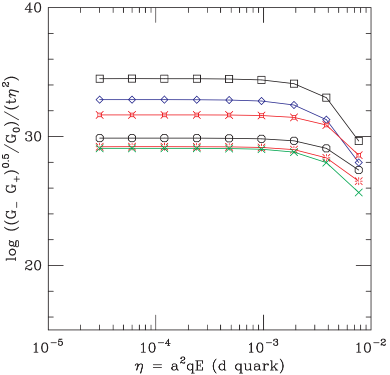
- Determine weight factor $w_i = \frac{\det M_0}{\det M_\eta}$ for each configuration
  - Different for u, d quarks – multiply weight factors together.
- Compute valence propagators as before, using reweighted ensemble

Choosing a value of η

What value of the electric field shall we use?

- Use of Dirichlet boundary conditions in x_1 allows use of arbitrarily small fields
  - Choosing $\eta = a^2 qE$ too large will provoke $\mathcal{O}(E^4)$ effects
  - Choosing η too small will run into numerical precision issues

- Plot $\Delta M_N/\eta^2$ against η for a handful of configurations



- Large intermediate area in the middle where correlator response is almost perfectly quadratic
- Some calculations (including ours!) have gotten dangerously close to the edge of the perturbative region
- Have the freedom to choose η at whatever point makes the reweighting easier

Estimating weight factors

Can't compute $w_i = e^{-(S_2 - S_1)_i} = \det \frac{M_2}{M_1}$ exactly

Standard stochastic estimator: $w_i = \left\langle \exp(-\xi^\dagger(\Omega - 1)\xi) \right\rangle_{e^{-\xi^\dagger \xi}}$ where $\det \Omega = \det M_1 M_2^{-1}$ and Ω is explicitly Hermitian

- For reweighting two identical flavors at once, this is easy: $\Omega = M_2^{\dagger -1} M_1^\dagger M_1 M_2^{-1}$
- For us, must take the square root: $\Omega = \sqrt{M_2^{\dagger -1} M_1^\dagger M_1 M_2^{-1}}$
- Use a rational function approximation to the square root
- Somewhat expensive: requires inverting a matrix that itself contains inversions
  - It has been suggested by J. Finkenrath *et al.* that one can just abandon Hermiticity and discard the imaginary part of the estimator
  - This saves all the work associated with the rational function approximation
  - See their talk at this conference for details on more ways to improve estimators
- Stochastic estimator not a problem as far as bias: the average over noises commutes with the gauge average (A. Hasenfratz, [0805.2369])
- How much work should you do for the stochastic estimator, then?
- Rough yardstick: $\sigma_{\mathrm{stoc}} \simeq \sigma_{\mathrm{gauge}}$

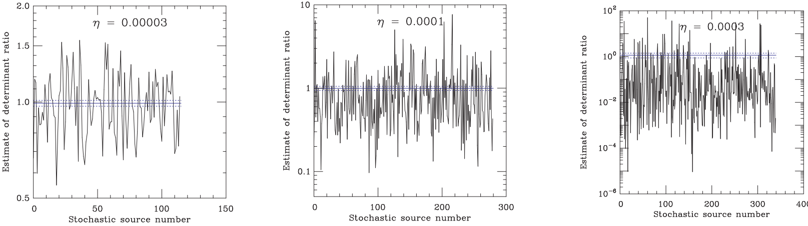
Gauge ensembles and analysis code

- 2 flavors of nHYP-smeared clover fermions, $m_\pi \approx 300$ MeV
- Standard Symanzik-improved gauge action, $\beta = 7.1$
- $24^3 \times 48$, $32 \times 24^2 \times 48$, $48 \times 24^2 \times 48$ volumes; $a = 0.1255$ fm
  - Elongated boxes originally generated for a scattering study; we reuse them here
- $24^3 \times 64$, $m_\pi \approx 230$ MeV in progress
- 300 minimally-autocorrelated configurations per ensemble
- Analysis done with the GWU-QCD general-purpose library
  - Most notable feature: multi-GPU support for many things

Estimating weight factors

Problem: this estimator is tremendously noisy!

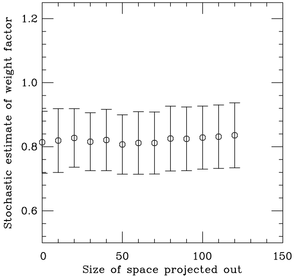
- This is not a problem *per se*: the average over noises commutes with the gauge average (A. Hasenfratz *et al.*, [0805.2369])
- However, too much variance in the stochastic estimator will kill the signal
- Distribution of estimators is log-normal, as you might expect
  - Extreme difficulties in sampling the "long tail" for $\eta = aqE$ large ($\eta \gtrsim 10^{-4}$)
  - Weight factors indistinguishable from unity for smaller η for a "sane" number of noises
  - Can't even estimate how many noises we will need to see a "signal"!



- On a 4^4 test lattice we confirmed that the estimator gives the right result... but it takes $10^5 - 10^6$ noises!
- The "signal-to-noise ratio" is essentially independent of η

Variance reduction techniques that don't work, I

- Common technique in mass reweighting: separate out low modes
  - Low modes: compute determinant exactly
  - Remaining high modes: use stochastic estimator
  - Easier for mass reweighting, since eigenvectors of **M** (and thus Ω) don't depend on m_q
  - ... they *do* depend on η, so we must explicitly compute eigensystem of Ω (expensive!)
  - For us Ω close to **1**; might as well extract extremal modes on both ends



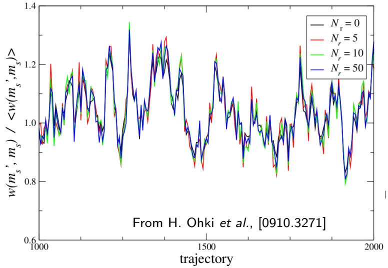
Projecting out extremal modes doesn't reduce the noise at all, unlike for mass reweighting (see A. Hasenfratz *et al.*, [0805.2369] and others)

What is going on?

Variance reduction techniques that don't work, I

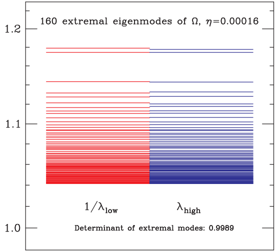
For mass reweighting, most of the signal is carried by the low modes:

- Shown analytically by F. Palombi and M. Lüscher [0810.0946]
- Shown very starkly by H. Ohki *et al.* in their reweighting in m_s – low modes had no effect at all!
- Similar behavior seen by T. Kaneko (talk at this conference), using reweighting to retune m_s



Low and high extremal eigenvalues are very nearly paired
→ Extremal sector contributes very little to $\det \Omega$ for reweighting in the background field!

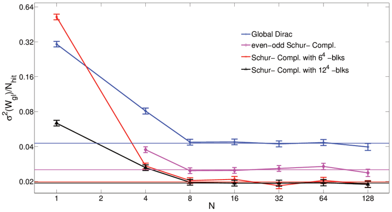
The mechanism that protects the mass reweighting weight factor from high-mode fluctuations does not seem to apply to our problem!



Variance reduction techniques that don't work, II

- Another common technique for improving stochastic estimators is "determinant breakup"
- Instead of reweighting from $\mathcal{S}_0$ to $\mathcal{S}'$ in one step, do it in several

- Used by T. Ishikawa *et al.* [1202.6018] to reweight in α_E
- Investigated in detail by Liu *et al.* [1206.0080] and used by J. Finkenrath *et al.* (Tuesday's talk) for mass reweighting



- Reduces the tendency to underestimate the error associated with highly skew log-normal distributions
- Makes possible "macroscopic" shifts by breaking them into "microscopic" steps
- Not terribly useful for us, since we already want a perturbatively-small change
  - We tried it anyway: using more "steps" is no better than using more "hits"
- Can't be paired efficiently with determinant breakup, since eigenvectors of our Ω change each step

A new pseudo-perturbative approach

- Can we make use of the fact that we only need perturbatively small η?
- Perhaps it is easier to estimate $\left.\frac{\partial w_i}{\partial \eta}\right|_{\eta=0}$ and $\left.\frac{\partial^2 w_i}{\partial \eta^2}\right|_{\eta=0}$ than w_i itself?
- Need to compute form of w_i up to second order in η
  - Linear term in weight factor can combine with linear dependence of $G_N(t)$ on η to give quadratic effect
  - Quadratic term in weight factor by itself can give quadratic effect
- If we can estimate these derivatives instead we can evaluate at any sufficiently-small η we like to get $w_i(\eta)$

Derivation of the estimator

For the first derivative, we want $\frac{\partial}{\partial\eta} \left. \frac{\det M_\eta}{\det M_0} \right|_{\eta=0}$. Rewrite $\det M_\eta$ as a Grassman integral:

$$
\begin{aligned}
\frac{\partial}{\partial\eta} \left. \frac{\det M_\eta}{\det M_0} \right|_{\eta=0} &= \frac{1}{\det M_0} \frac{\partial}{\partial\eta} \int d\psi d\bar{\psi}\, e^{-\bar{\psi} M \psi} \\
&= \frac{1}{\det M_0} \int d\psi d\bar{\psi}\, -\bar{\psi} \frac{\partial M_0}{\partial\eta} e^{-\bar{\psi} M_0 \psi} \\
&= \mathrm{Tr} \left(\frac{\partial M_0}{\partial\eta} M_0^{-1} \right).
\end{aligned}
$$

- This trace still must be evaluated stochastically; perhaps it can be made more tractable?
- It certainly seems cheaper (no square root)

The second derivative proceeds similarly:

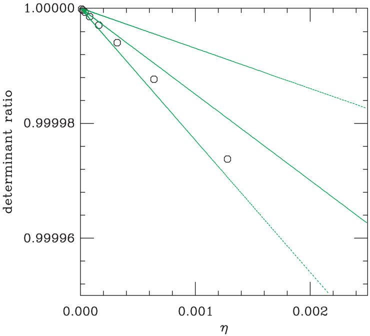
$$
\frac{\partial^2}{\partial\eta^2} \left. \frac{\det M_\eta}{\det M_0} \right|_{\eta=0} = -\mathrm{Tr} \frac{\partial^2 M}{\partial\eta^2} M_0^{-1} + \left(\mathrm{Tr} \frac{\partial M}{\partial\eta} M_0^{-1} \right)^2 - \mathrm{Tr} \left(\frac{\partial M}{\partial\eta} M_0^{-1} \right)^2
$$

Fluctuations in the new stochastic estimator

Estimate the traces in the conventional way: $\mathrm{Tr}\mathcal{O} = \left\langle \xi^\dagger \mathcal{O} \xi \right\rangle$ with either Gaussian or Z(4) noises

- The bad news: the new estimator is still awfully noisy!
- As before, use a coarse 4^4 lattice as a test
  - Can actually afford the statistics needed to get a "signal"
  - Can also do the determinant exactly to test the estimator

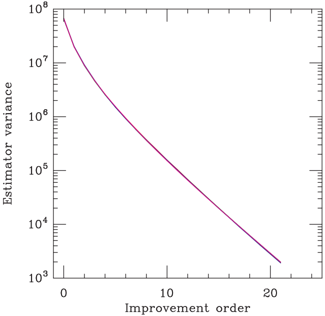
- Estimate for $\left.\frac{\partial w_i}{\partial \eta}\right|_{\eta=0}$: $-0.015(8)$
- ... using 5×10^6 Gaussian noises!
- Good agreement with exact calculation
- ... so what have we gained?



(Possible) salvation: estimator improvement

- Key idea of improvement technique: traceless parts of $\frac{\partial M}{\partial \eta} M^{-1}$ contribute only noise
- Identify and subtract them
- Do this by making hopping parameter expansion of M^{-1}:
  - $AM^{-1} = A + \kappa A\Gamma + \kappa^2 A\Gamma^2 + \kappa^3 A\Gamma^3 + \ldots$, where $A = \frac{\partial M}{\partial \eta}$ and Γ incorporates both the hopping and (if included) clover terms
  - Subtract these terms from the stochastic estimator (cheap)
  - Many have zero trace already and can be just ignored
  - Compute the trace of the rest exactly and add it back in (maybe not cheap)

- Can examine improvement in estimator without doing exact traces
- Estimator is much (much!) faster: no square root
- Examine improvement on several $24^3 \times 48$ lattices
- Improvement of roughly a factor of ten in statistics per two orders!
- How many orders can we compute exactly?



Computing exact traces: Wilson quarks

- Need to compute traces exactly of the $A\Gamma^n$ terms subtracted from estimator
- Problem much simpler without clover term: then A and Γ only contain hopping terms
- Even powers ($\mathrm{Tr} A$, $\mathrm{Tr} A\Gamma^2$) are trivially zero
- $\mathrm{Tr} A\Gamma^2 = 0$ as well due to Dirac structure
- Lowest nonzero contribution is $\mathrm{Tr} A\Gamma^3$ – works out to be the sum of imaginary parts of (1,4) plaquettes
- In general, trace over loops of a given shape proportional to the product of links times electric flux through them

Computing exact traces: clover quarks

- Problem much more difficult once clover term is added
  - Now $\Gamma = \not{D} + \mathcal{C}$, $A = \frac{\partial \not{D}}{\partial \eta} + \frac{\partial \mathcal{C}}{\partial \eta}$, where $\mathcal{C}$ is the clover term
  - Can no longer discard half of the orders outright, and only look at loop shapes
- Problem: How can we compute this efficiently?
- Solution: separate Γ into hopping (in each of eight directions) and clover term
- Further separate clover term into its six "leaves":
  $\mathcal{C} = c_{sw} \left(\sigma_{12} C_{12} + \sigma_{13} C_{13} + \sigma_{14} C_{14} + \sigma_{23} C_{23} + \sigma_{24} C_{34} + \sigma_{12} C_{34} \right)$
- Expand $A\Gamma^n$, giving 3×14^n terms – each has a simple spatial and Dirac structure
  - Only need to evaluate SU(3) products for terms that are both closed and have nonzero Dirac trace
  - Example:
    $\mathrm{Tr} A\Gamma^2 = \sum \mathrm{Tr}_{SU(3)} \left(4i \frac{\partial C_{14}}{\partial \eta} C_{12} C_{24} + 4i \frac{\partial C_{14}}{\partial \eta} C_{13} C_{34} - 4i \frac{\partial C_{14}}{\partial \eta} C_{24} C_{12} - 4i \frac{\partial C_{14}}{\partial \eta} C_{34} C_{13} \right)$
  - For $A\Gamma^7$: 316M terms, 7M of them closed, 0.5M nonzero Dirac trace
  - Evaluation of loop products: 40 CPU-hours/config (to this order)

→ This variance reduction method can be applied to other estimators on other actions:

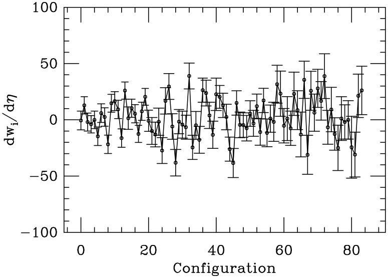
- Estimators of ex. charm quark condensate, which are very noisy
- May be simpler on "pure hopping" actions, like staggered

Finally, a signal

Applying this technique allows extraction of a signal with "modest" amounts of work.

Preliminary data:

- ~ 5000 noises per configuration (10 GPU-hours on "slower" GPU cluster)
- 7th-order improvement (40 CPU-hours)
- Can easily do better than this; this is just a proof-of-concept



- Estimates for $\frac{\partial w_i}{\partial \eta}$ significantly different than zero: success!
- For values of η we are interested in, w_i close to unity $\rightarrow$ ensembles will be highly correlated. This suggests reweighting won't increase error on ΔM_N too much.

Completing the calculation to get α_E

- Need to do the second derivative term too
  - Exact computations of weight factors on 4^4 lattice suggest it doesn't matter that much
  - Same sort of estimator and improvement technique can be used; cost should be comparable
  - Same technology can be used to compute the exact traces
  - Modify stochastic estimator for $(\mathrm{Tr}\mathcal{O})^2$
- Evaluate form for $w_i(\eta)$ for both $\eta = \eta_0$ and $\eta = -2\eta_0$ to get overall sea weight factor
- Use ensemble of weight factors to compute hadron correlators for $\eta \neq 0$
- Construct jackknife estimator for extended covariance matrix and fit to determine ΔM_N as before

Next steps

- Further refine the technique:
  - Port exact trace code to GPU's (take advantage of GWU-QCD code and GPU resources)
  - Exact trace code can be further optimized (at the cost of memory)
- Focusing on α_E:
  - May still be unable to resolve sea effect on polarizability from zero if it is small, but that's okay
  - Fold technique into broader GWU-QCD program for polarizability: approach to chiral limit, higher statistics, bigger volumes, finer lattices
  - New ensemble currently being generated: sea effects predicted to be larger for lower m_π
- Investigate other applications of improvement technique
  - Can be applied to many things involving a trace of an operator containing M^{-1}
  - Charm quark estimators come to mind – estimator noise a major factor in large error in nucleon charm
  - May be difficult to apply to more complicated actions: DWF, overlap?

Conclusions

Reweighting becoming an increasingly-popular technique. Two main uses:

- Make small shift in a parameter (m_q, $\vec{E}$...) to study effect (this work, Ohki's strangeness study) or finetune parameters
- Make large shift as a way of *e.g.* getting closer to chiral limit

Determinant breakup only useful to turn large shifts into small ones (J. Finkenrath's talk)

Low-mode subtraction tremendously powerful for mass reweighting (H. Ohki *et al.*'s work on strangeness, T. Kaneko's talk at Latt2012, useless for us

Estimator for background field reweighting tremendously noisy, can't be tamed by common techniques

New pseudo-perturbative method shows promise:

- Compute $\frac{\partial w_i}{\partial \eta}$ and $\frac{\partial^2 w_i}{\partial \eta^2}$ instead
- Hopping parameter expansion of M^{-1} and exact trace calculations improves estimator drastically
- Preliminary studies show this allows affordable calculation of weight factors
- Potentially broadly applicable