EM sea effects in hadron polarizabilities through reweighting

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The background field method

- Expect a mass shift equal to $\alpha_E E^2$ in the presence of a uniform background field
- Determine polarizability by measuring neutron correlators with $\vec{E} = 0$ and $\vec{E} = \pm i E_0 \hat{x}$, then fitting them to determine the mass shift
- When fitting correlators, the zero-field and nonzero-field correlators are correlated
- This results in a much smaller error on ΔM than on the mass measurements themselves

Reweighting approach

How do we include the effects of the sea quark charges in the background field approach?

- In principle it's easy: just generate two otherwise identical ensembles, one with a background field and one without
- But this requires unaffordably high statistics, since our two mass measurements now no longer have correlated errors
  - Lose all the information in the "cross-correlation" terms of the covariance matrix
- Reweighting is a technique for extracting physics from a different action than the one used in generation: "retroactively change the ensemble parameters"
- We can use it to generate two correlated ensembles, one with and one without the electric field

Reweighting

Reweighting is just a modification to the standard quantum Monte Carlo, where only a part of the factor $e^{-\mathcal{S}}$ is absorbed into a Monte Carlo weight:

Standard

$$\frac{\int [dU] \mathcal{O} e^{-S_0}}{\int [dU] e^{-S_0}} \to \frac{\sum \mathcal{O}_i}{\sum 1}$$

Reweighted

$$\frac{\int [dU] \mathcal{O} e^{-S_E}}{\int [dU] e^{-S_E}} = \frac{\int [dU] \mathcal{O} e^{-(S_E - S_0)} e^{-S_0}}{\int [dU] e^{-(S_E - S_0)} e^{-S_0}} \to \frac{\sum \mathcal{O}_i w_i}{\sum w_i}$$

where $w_i = e^{-(S_E - S_0)_i}$.

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

- Otherwise, the weight factor will fluctuate wildly, and the ensemble will be dominated by a few configs with large weights

Determining the weight factors

- In order to do reweighting, need the weight factors $w_i = e^{-\Delta\mathcal{S}} = \det^{-1} \mathbf{M}_\eta^{-1}\mathbf{M_0}$
  - There is a standard stochastic estimator for the inverse determinant
  - Several improvement techniques, like low-mode separation and determinant breakup, are very successful in reducing stochastic noise when reweighting in m_q
  - They don't work at all when reweighting in the background field
- The fluctuations in this standard stochastic estimator are awful (and it is expensive)
  - So long as the estimator is unbiased, the result will be too – just with larger error bars
  - Useful yardstick: ideally stochastic fluctuations ("noise") less than gauge fluctuations ("signal")
  - We are so far away from this benchmark that it looks hopeless

A new pseudo-perturbative approach

- The standard improvement techniques (determinant breakup, low mode separation) used for mass reweighting don't work
- Can't distinguish the value of the weight factor from 1 with any sane number of noises on a production lattice
- 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?
- Expand w_i in a power series in η up to second order, about $\eta = 0$
    - 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 η we choose to get $w_i(\eta)$
- Sea contributions taken into account in a way that is similar in practice to the current-insertion approach of Engelhardt

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

The second derivative proceeds similarly:

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

Unfortunately, stochastic estimators of the traces here are still too noisy.

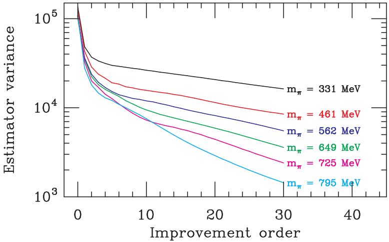
Hopping-parameter expansion improvement

- We want to estimate $\mathrm{Tr}\,\mathcal{O}$ as $\langle \xi^\dagger \mathcal{O} \xi \rangle$, but that estimator is too noisy
- We can always add and subtract the same thing, so we can also write:

$$\mathrm{Tr}\,\mathcal{O} = \left\langle \xi^\dagger \left(\mathcal{O} - \sum_i \mathcal{O}'_i \right) \xi \right\rangle + \sum_i \mathrm{Tr}\,\mathcal{O}'_i$$

- Identify other operators $\mathcal{O}'_i$ with the following properties:
  - $\mathrm{Tr}\,\mathcal{O}'_i$ can be computed exactly
  - Stochastic estimators of $\mathrm{Tr}\,O'_i$ have correlated fluctuations with that of $\mathcal{O}$
- Construct such operators by making a hopping parameter expansion of each $\mathbf{M}^{-1}$ that appears
- Computing exact traces is possible, but quite messy
- Do as many orders as you can afford (cost goes as $O(14^n)$)

- Yields substantial improvement
- Exact traces computed up to $\mathcal{O}(\kappa^7)$



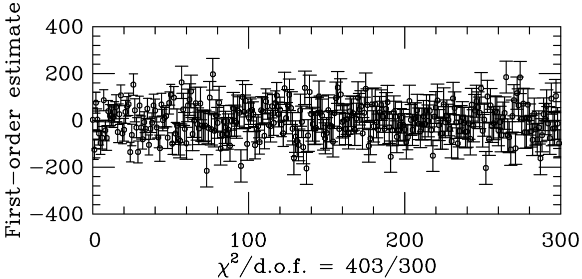
Calculation parameters, first try

- $24^3 \times 48$ lattice, 2 flavors of dynamical nHYP-clover fermions with $m_\pi \simeq 300 MeV$, 300 configs
- At least 3000 stochastic estimators of first-order term and 1000 estimators of each second-order term (and often more) per config

- Normally, the effect of reweighting on the statistical power of a calculation can be determined pretty easily:
  - Fluctuations of weight factor decrease effective number of configs: $N_{\text{eff}} = N \frac{\langle w \rangle^2}{\langle w^2 \rangle}$
- But we rely on correlations between zero-field and nonzero-field correlators to reduce error on ΔE
- These correlations are very strong and get stronger for low η: for $\eta = 10^{-4}$, $\sigma_E = 9 * 10^{-8}$, $\sigma_{\Delta E} = 6 * 10^{-3}$
- Reweighting only the nonzero-field correlators may spoil these correlations, even if all the weight factors are $\mathcal{O}(1)$
- No way to know how well reweighting will work until the end of the calculation

Stochastic estimator statistics

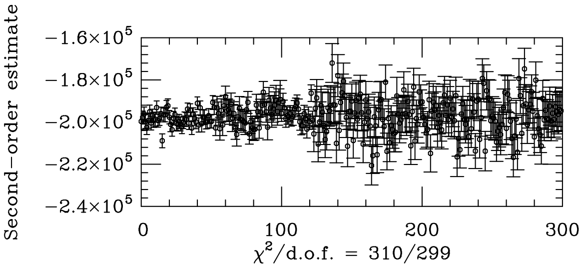
- Even with all of this effort, the first-order estimates are just barely distinguishable from random noise:
- To see if we can resolve the gauge fluctuations through the noise, do a zero-parameter fit to $\mathrm{Tr}\,\frac{\partial M}{\partial \eta} M^{-1} = 0$:



- This is still dominated by stochastic fluctuations, but the gauge fluctuations (signal) are evident – barely
- What about the second-order term?

Stochastic estimator statistics

- Here the gauge average is not zero, so fit to a constant:

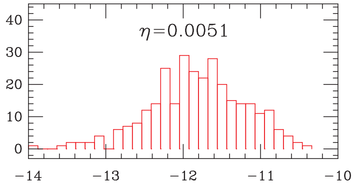


- This is indistinguishable from pure noise
- Ran extra noise sources on the first hundred configs to see if a signal would appear, to no effect

Weight factors

- Need to choose a particular η at which to evaluate the expansion to finish the calculation
- Valence correlators computed mostly with $\eta = 0.0051$
- This value of η is too big for a naïve reweighting:

- Large constant shift in the action from **E** causes expansion to break down ($\Delta\mathcal{S} > 1$)
- Still small enough that the effects of **E** on hadron are perturbative (only quadratic valence behavior seen)
- Solve this by using valence correlators "rescaled" to $\eta = 10^{-4}$
  - Effect on valence correlators is nearly perfectly quadratic, so this is okay



- Then, everything is nice and perturbative

The full reweighting calculation

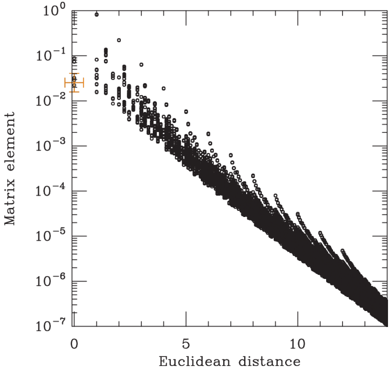
- Combine these with the "rescaled" valence correlators and do the reweighting order by order
- Fitting from $t = 9$ to $t = 21$ gives the following for ΔE:

0^{th} order (unreweighted)	6.01(88) * 10^{-7}
1^{st} order	2.86(2.32) * 10^{-7}
2^{nd} order	17.8(10.9) * 10^{-7}

- Clearly we need to beat down the stochastic noise further, especially at second order
- Would like a gain of roughly a factor of ten in error!

Origin of stochastic noise

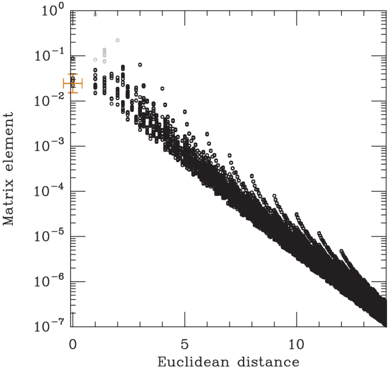
- Variance of stochastic estimator proportional to sum of off-diagonal matrix elements
- Can't study them all, but we can map out a representative set grouped by offset



- For most uses of this stochastic estimator (to get, say, $\mathrm{Tr}\,\mathbf{M}^{-1}$), the matrix is diagonally dominant
- Not the case here: $\frac{\partial \mathbf{M}}{\partial \eta}\mathbf{M}^{-1}$ has large offdiagonal elements
- This is a stark depiction of why this problem is so hard

Origin of stochastic noise

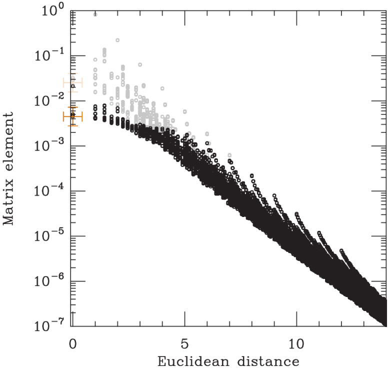
- How does hopping parameter expansion help things?
- Improvement operators are ultralocal; only expect reduction near diagonal



- Exactly what is expected: improvement up to radius 2
- Suppresses large near-diagonal elements which dominate the noise, but doesn't eliminate them

Origin of stochastic noise

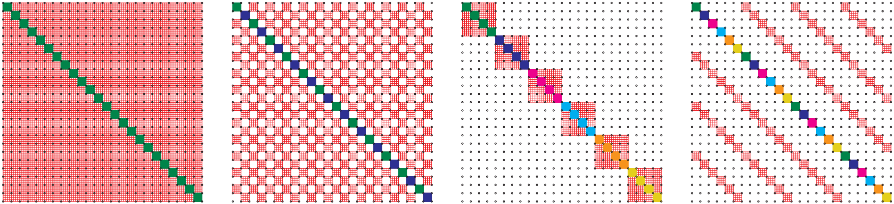
- To seventh order there is more reduction in offdiagonal elements
- Improvement up to radius 7, as expected



- Shift in value of diagonal elements comes from traces of improvement operators which are added back in the full calculation
- This is as far as the hopping-parameter expansion can realistically take us
- What else can we do?

Dilution

- Dilution separates the matrix dimension into N subsets and stochastically estimates the trace over each separately
  - Advantage: eliminates noise contributions from offdiagonal terms from different subsets
  - Disadvantage: Requires N operations to cover the lattice; could have reduced noise by factor of $\sqrt{N}$ by simple repetition
  - Only outperforms simple repetition if the offdiagonal matrix elements "kept" are lower than the average



- We should choose a (four-dimensional generalization) of the rightmost scheme to eliminate the large near-diagonal elements

Dilution, for us

- Spin-color dilution on its own actually makes things worse
- Spatial dilution is somewhat redundant with hopping parameter expansion improvement
- Until you get to very aggressive (N large) dilution schemes, dilution in the presence of HPE improvement makes things worse
- Best dilution schemes are gridding with an additional "8-way hypercubic checkerboard" pattern overlaid, along with standard spin-color dilution
  - Nearest neighbor in a grid with spacing x is Manhattan distance $2x$ away
- Using a 4^4 grid along with spin-color dilution (24,576 subspaces) breaks even with 24,576 HPE-improved undiluted noises
- Using a 6^4 grid (124,416 subspaces!) seems to gain roughly a factor of 2 in error per inversion for first-order term
  - One such 6^4 diluted estimate per config will give us a signal/noise ratio of about 1 on the first-order terms
  - Still not sure what the signal strength for the second-order terms is; haven't been able to resolve it yet
- How many inversions are we willing to dedicate to each configuration?

Performance improvements and proposed future run

- Have already done some things that will improve performance on a subsequent run
  - Inversion reuse: save result of $\mathbf{M^{-1}}\psi$ and use it for all three operators that need estimators (factor of 3)
  - Decreased inverter precision: using 10^{-5} rather than 10^{-10} gives a three-fold speedup (and negligible penalty)
    - Need to investigate "sloppy CG": can perhaps wring another factor of 2 or 3 out of it
- 6^4 grid + spin-color dilution + 8-way "checkerboard" for the whole ensemble is 75 million inversions = 300k GPU-hours
  - This should buy us the factor of ten we need so that the total error in the polarizability isn't dominated by the sea contribution

Conclusions

- Stochastic estimates of weight factor expansion terms are very noisy
- Much, much worse than many common stochastic estimates ($\mathrm{Tr}\,\mathbf{M^{-1}}$) because of strong nondiagonal dominance
- Hopping-parameter expansion helps some, but not enough
- Need very strong dilution ($N = 124416$) to show gains over repeated undiluted HPE-improved estimator
- Combined effect of various optimizations means that such a run is possible, and should give the needed decrease in error
- If we see a significant shift in the polarizability from the sea effect, we can then attack the ensemble with lighter m_π (for which deflation will pay dividends) or the ensemble with a larger n_x