Infinite Variance in Fermionic Systems[1]

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[1] Work done with William Detmold

Outline

1. Exceptional configurations in QCD
2. A Toy Model
3. Discrete Hubbard-Stratonovich transformation
4. Test for Toy Model and Gross-Neveu
5. Reweighting

Exceptional Configurations in QCD

In QCD, one frequently calculates multiplication of N propagators:

$$\left\langle \prod_{n=1}^{N} \bar{\Psi}_{i_n} \Psi_{j_n} \right\rangle = \frac{\int \mathcal{D}[U] e^{-S[U]} \det\left(D[U]\right) \prod_{n=1}^{N} D[U]^{-1}_{i_n j_n}}{\int \mathcal{D}[U] e^{-S[U]} \det\left(D[U]\right)} \tag{1}$$

One can choose a linear combination of the propagators such that they will give inverses of the eigenvalues of the Dirac operator:

$$\left\langle \prod_{n=1}^{N} \sum_{m} c_{n,m} \bar{\Psi}_{i_{n,m}} \Psi_{j_{n,m}} \right\rangle = \frac{\int \mathcal{D}[U] e^{-S[U]} \prod_a \lambda_a[U] \prod_{n=1}^{N} \frac{1}{\lambda_n[U]}}{\int \mathcal{D}[U] e^{-S[U]} \prod_a \lambda_a[U]} \tag{2}$$

Expcetional Configurations in QCD

Natural estimator:

$$\hat{\mathcal{O}}_{1,\cdots,N} = \frac{1}{S}\sum_{i=1}^{S} \frac{1}{\prod_{n=1}^{N} \lambda_n[U_i]}$$

Issues arise when one of the eigenvalues, $\lambda_1[U]$, vanishes at $U = U^*$. The probability of sampling U^* is 0. The configurations around $U = U^*$ will be sampled with very small frequency $\propto \lambda_1[U]$ but the measurements there will have a large size $\propto \frac{1}{\lambda_1[U]}$ with the net contribution is finite.
The estimator has infinite variance!

$$var\left(\hat{\mathcal{O}}_1\right) \supset \frac{1}{S}\left\langle \mathcal{O}_1[U]^2 \right\rangle \propto \int \mathcal{D}[U] \frac{1}{\lambda_1[U]} (\cdots)$$

A Toy Model

We introduce a 0-d QFT with the partition function:

$$Z = \int \left[d\Psi d\bar{\Psi}\right] e^{-m\bar{\Psi}\Psi + \frac{g}{2}(\bar{\Psi}\Psi)^2}$$

with $\Psi \equiv \Psi_a^s | a \in \{1,2\}, s \in \{\uparrow, \downarrow\}$ and $g > 0$. One can apply the usual Hubbard-Stratonovich transformation

$$e^{\frac{1}{2}\Phi^2} = \frac{1}{2\pi} \int d\sigma e^{-\frac{1}{2}\sigma^2 + \sigma\Phi}$$

where $\Phi = \bar{\Psi}\Psi$ to write the partition function in terms of the auxiliary field σ:

$$Z = \int d\sigma e^{-\frac{1}{2}\sigma^2} (m + \sqrt{g}\sigma)^4$$

A Toy Model

$$Z = \int d\sigma e^{-\frac{1}{2}\sigma^2} (m + \sqrt{g}\sigma)^4$$

Morally speaking, this model should be though as having a Dirac operator with the eigenvalues:

$$\lambda_{1,2,3,4} = m + \sqrt{g}\sigma$$

The observable we want to construct is:

$$\mathcal{O} = \prod_{a=1,2} \prod_{s=\uparrow,\downarrow} \bar{\Psi}_a^s \Psi_a^s \equiv \frac{1}{\prod_{i=1}^4 \lambda_i} = \frac{1}{\left(m + \sqrt{g}\sigma\right)^4}$$

The estimator $\hat{\mathcal{O}} = \frac{1}{S} \sum_{i=1}^{S} \frac{1}{\left(m+\sqrt{g}\sigma_i\right)^4}$ has infinite variance due to configurations near $\sigma^* = -\frac{m}{\sqrt{g}}$.

Two Proposals

1. A Discrete Hubbard-Stratonovich Transformation
2. A Reweighting Method

A Discrete Hubbard-Stratonovich Transformation

Continuous Hubbard-Stratonovich transformation is satisfied at every order in Φ:

$$e^{\frac{1}{2}\Phi^2} = \frac{1}{2\pi}\int d\sigma e^{-\frac{1}{2}\sigma^2+\sigma\Phi}$$

However, since $\Phi = \bar{\Psi}\Psi$ is constructed out of fermions, a certain power of Φ vanishes:

$$\Phi^{2N_f+1} = 0$$

Therefore, such an auxiliary field transformation needs to be satisfied only up to $\mathcal{O}\left(\Phi^{2N_f+1}\right)$. We ask: can we find a finite sum

$$e^{\frac{1}{2}\Phi^2} = \sum_k w_k e^{t_k \Phi}$$

such that $\underbrace{w_k > 0}_{\text{needed for probability interpretation}}$ and $\underbrace{t_k \in \mathbb{R}}_{\text{needed to avoid sign problem}}$.

Discrete Hubbard-Stratonovich Transformation

Hope: if all t_k are far away from the exceptional configuration $\sigma^* = -\frac{m}{\sqrt{g}}$, then the variance of $\hat{\mathcal{O}}$ will be small.
Let $\Phi \to i\Phi$ and reinterpret the equation as equality of moment generating functions of some probability distributions up to some power of Φ:

$$e^{-\frac{1}{2}\Phi^2} = \sum_k w_k e^{i t_k \Phi} + \mathcal{O}\left(\Phi^{2N_f+1}\right)$$

In terms of the probability distributions $e^{-\frac{1}{2}t^2}$ and $\sum_k w_k \delta(t - t_k)$, this means that:

$$\int_{-\infty}^{\infty} dt\, e^{-\frac{1}{2}t^2} f(t) = \sum_k w_k f(t_k)$$

for all polynomials $f(t)$ of degree equal or less than $2N_f$.

Discrete Hubbard-Stratonovich Transformation

This problem is solved with the method of Gauss-Hermite quadrature. Let $He_j(t)$ to be the (probabilist's) Hermite polynomials:

$$He_j(t) = (-1)^j e^{\frac{1}{2}t^2} \left(\frac{d}{dt}\right)^j e^{-\frac{1}{2}t^2}$$

then t_k are the roots of $He_N(t)$ such that $N \geq N_f + 1$ and $w_k > 0$ are given by:

$$w_k = \frac{(N!)^2}{He'_N(t_k) He_{N-1}(t_k)}$$

Two remarks:

1. Infinitely many choices for a given N_f.
2. In the limit $N \to \infty$, it gives the continuous version.

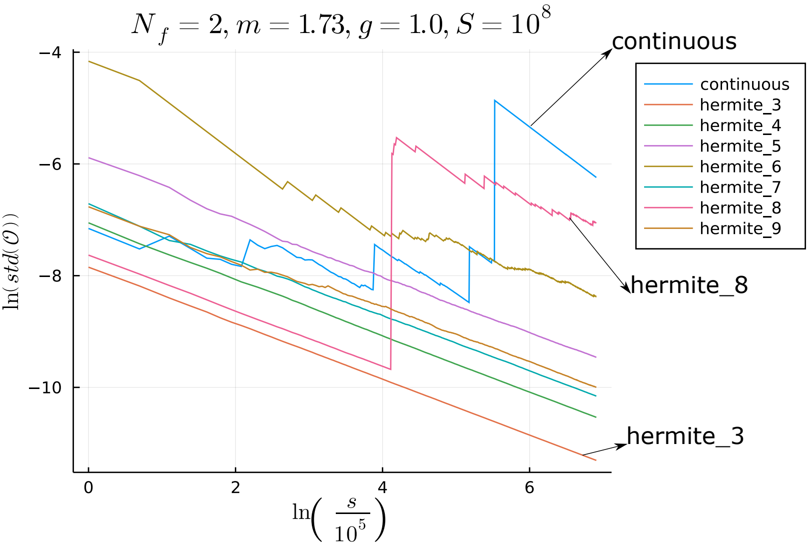
Comparison for the Toy Model

Normally, the standard deviation of an estimator has the scaling relation:

$$\sigma\left(\hat{\mathcal{O}}\right) \propto \frac{1}{\sqrt{s}}$$

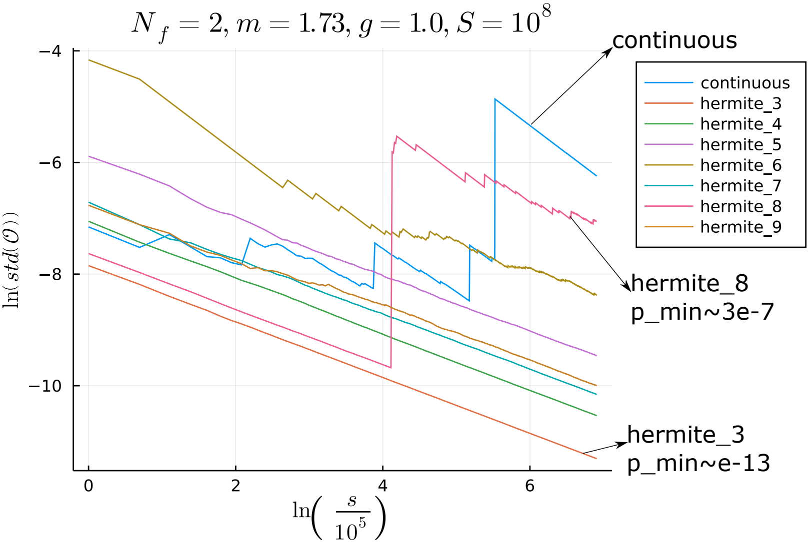
where s is the sample size.
We expect this relation to be invalid for estimators with infinite variance.

Comparison for the Toy Model

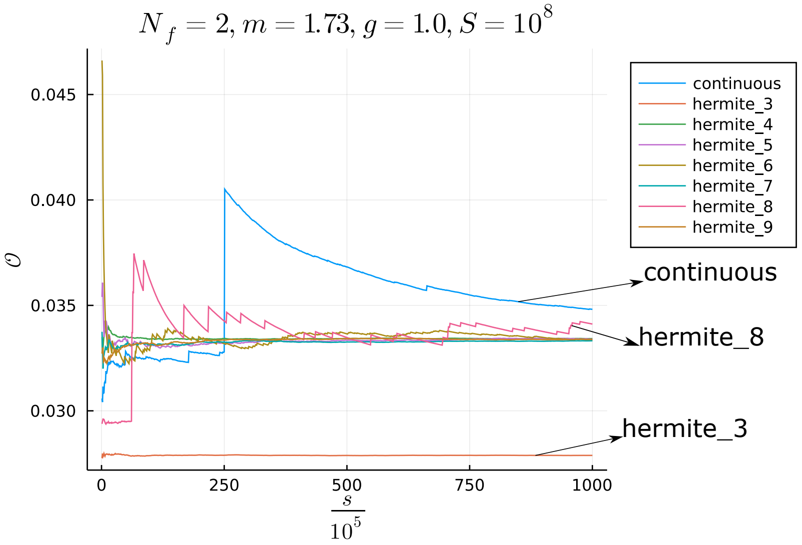


Jumps happen due to configurations close the exceptional configuration.

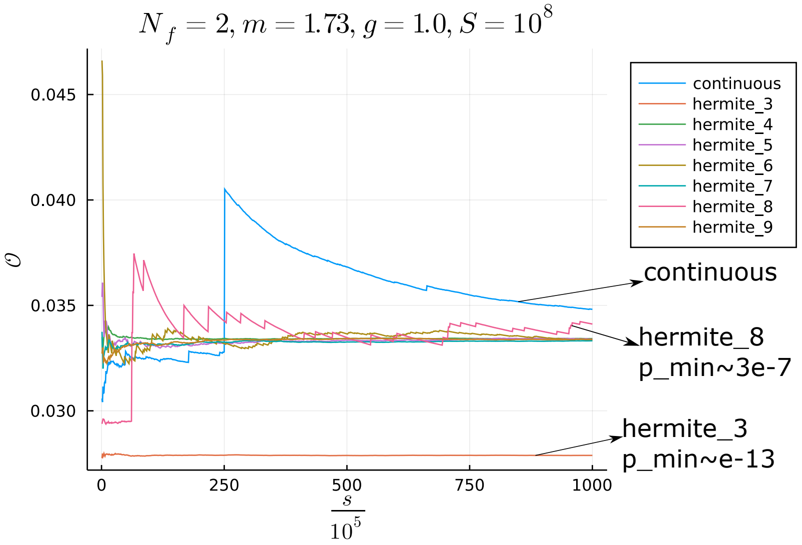
Comparison for the Toy Model



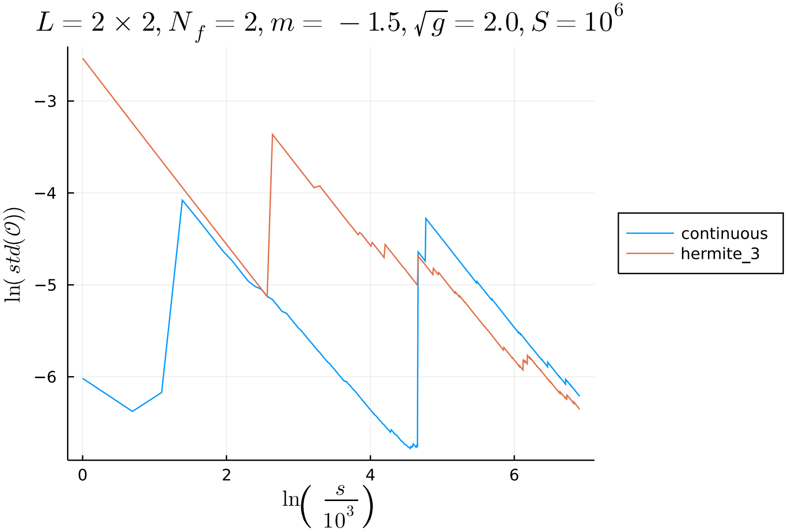
Comparison for the Toy Model



Comparison for the Toy Model

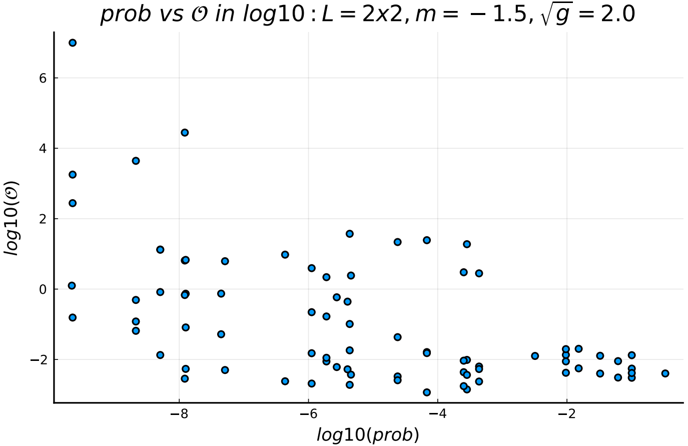


Comparison for the Gross-Neveu Model



Comparison for the Gross-Neveu Model

Spectrum for He_3:



The problem is much worse for larger lattices.

Reweighting

The observable $\mathcal{O}$ is highly fluctuating. Try to make less fluctuating by calculating $\mathcal{O}$ in steps by absorbing $\mathcal{O}$ into the probability distribution P:

$$\langle \mathcal{O} \rangle = \frac{\int d\sigma \, [P(\sigma)] \cdot \mathcal{O}(\sigma)}{\int d\sigma \, [P(\sigma)]}$$

$$= \frac{\int d\sigma \left[P(\sigma)\mathcal{O}^{\frac{1}{2}}(\sigma)\right] \cdot \mathcal{O}^{\frac{1}{2}}(\sigma)}{\int d\sigma \left[P(\sigma)\mathcal{O}^{\frac{1}{2}}(\sigma)\right]} \frac{\int d\sigma \, [P(\sigma)] \cdot \mathcal{O}^{\frac{1}{2}}(\sigma)}{\int d\sigma \, [P(\sigma)]}$$

Reweighting

To generalize to N steps we define the probability distributions:

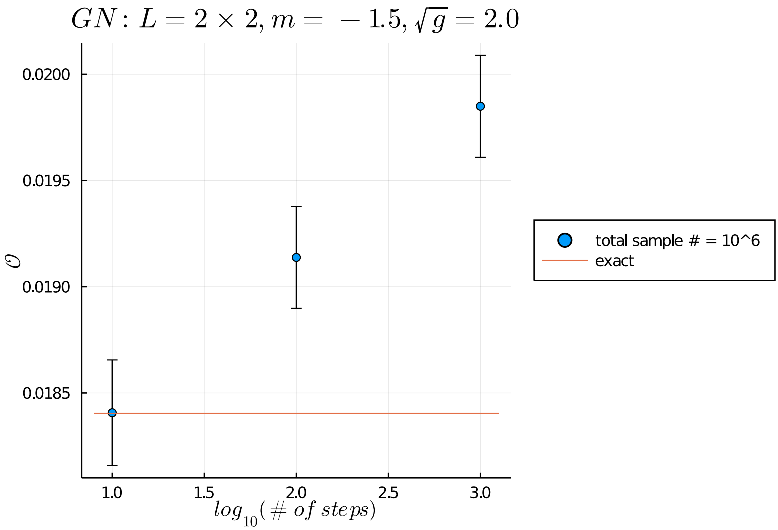
$$P_\mu(\sigma) \propto P(\sigma)\mathcal{O}^\mu(\sigma)$$
$$\langle X \rangle_\mu = \int d\sigma \left[P_\mu(\sigma)\right] \cdot X(\sigma)$$

Then we obtain:

$$\langle \mathcal{O} \rangle = \prod_{n=0}^{N-1} \left\langle \mathcal{O}^{\frac{1}{N}} \right\rangle_{\mu=\frac{n}{N}}$$

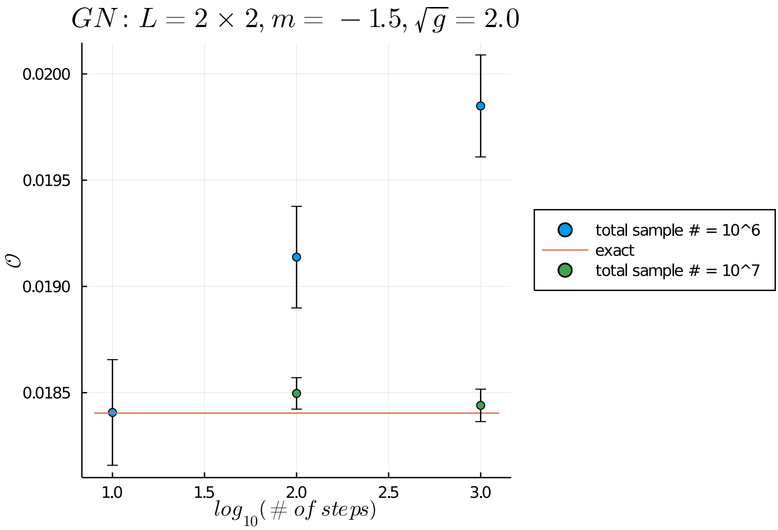
One expects that for large enough N each term should have finite variance.

Testing for Gross-Neveu



Higher # of steps may give worse results because sample size per step decreases.

Testing for Gross-Neveu



Choose the smallest N that makes every term finite.

Takeaway

1. Observables with infinite variance occurs in some fermionic systems due to zero eigenvalues of the Dirac operator
2. Discrete Hubbard-Stratonovich works in principle but is not useful for realistic problems
3. Reweighting works however one should choose smallest number of steps possible

Future Work

1. $N \to \infty$:
$$\langle \mathcal{O} \rangle = e^{\int_0^1 d\mu \langle \log(\mathcal{O}) \rangle_\mu}$$
2. Application to higher dimensional theories

Thank you!