Infinite Variance in Fermionic Systems

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Outline

1. Exceptional configurations in QCD
2. Discrete Hubbard-Stratonovich transformation
3. Empirical Bias

Exceptional Configurations in QCD

In QCD, one frequently calculates the expectation values of propagators:

$$\left\langle \bar{\Psi}_i \Psi_j \right\rangle = \frac{\int \mathcal{D}[U] e^{-S[U]} \det\big(D[U]\big) D[U]^{-1}_{ij}}{\int \mathcal{D}[U] e^{-S[U]} \det\big(D[U]\big)} \tag{1}$$

Natural estimator:

$$\hat{\mathcal{O}} = \frac{1}{N_S} \sum_{i=1}^{N_S} D[U]^{-1}_{ij}$$

Exceptional Configurations in QCD

Issues arise when one of the eigenvalues, $\lambda_1[U]$, vanishes at $U = U^*$.

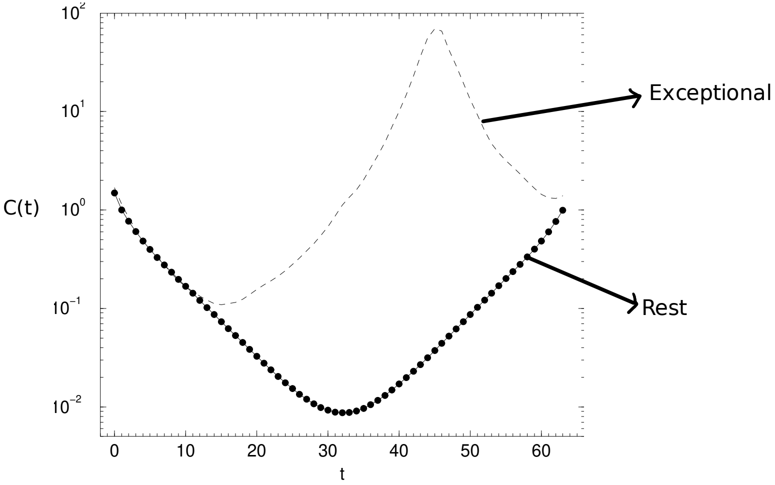
The probability of sampling U^* is 0.

The configurations around $U = U^*$ will be sampled with very small frequency $\propto \lambda_1[U]$, however there will be propagators whose (standard) estimators diverge at $U = U^*$ as $\propto \frac{1}{\lambda_1[U]}$.

These estimators have infinite variances!

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

Pion Correlator



Source: Göckeler et al., arXiv:hep-lat/9809165

Inadequacy of the Standard Estimator

Central Limit Theorem is not applicable.

Theorem

Let $X_{n\geq 1}$ to be a sequence of independent and identically distributed random variables with finite mean μ and infinite variance. Then, for any given $L > 0$, the number of the random variables s_n that satisfies $s_n > L$ is infinite almost surely where s_n is the sample variance.

Discrete Hubbard-Stratonovich Transformation

For theories where bosons are auxiliary fields that are obtained through the Hubbard-Stratonovich transformation,

$$e^{\frac{1}{2}\left(\bar{\Psi}\Psi\right)^2} = \frac{1}{2\pi}\int d\sigma\, e^{-\frac{1}{2}\sigma^2+\sigma\bar{\Psi}\Psi}$$

exceptional configurations can be eliminated by using a discrete version of the Hubbard-Stratonovich transformation.

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(s) , 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:

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

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.
3. $N = 1$ gives the original Discrete Hubbard Stratonovich Transformation due to Hirsch.

Discrete Hubbard-Stratonovich Transformation

Discrete Hubbard-Stratonovich transformations solve the issues due to the exceptional configurations formally when they are applicable.
However...

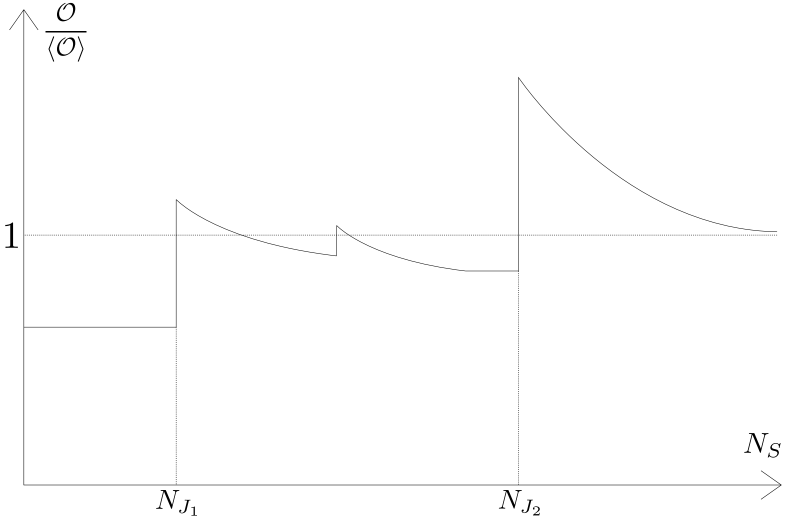
Empirical Bias

Even though there are no exceptional configurations, there may be roots that are almost exceptional. If that is the case unless one has a very large sample size, the sample mean will have a bias with very large probability.

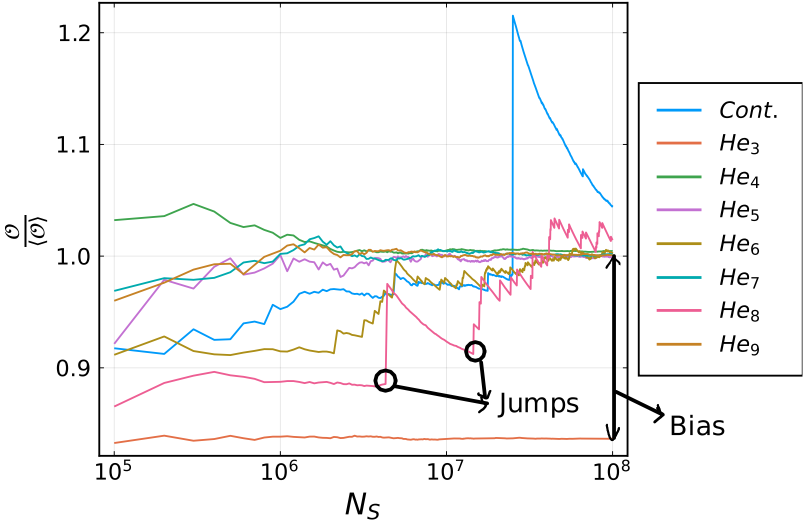
If the almost exceptional configuration has the weight p and contributes to the mean by $\frac{\Delta}{p}$, a bias of Δ will be observed unless $N_s \gtrsim \frac{1}{p}$.

There will be large "jumps" when the almost exceptional configuration is first sampled.

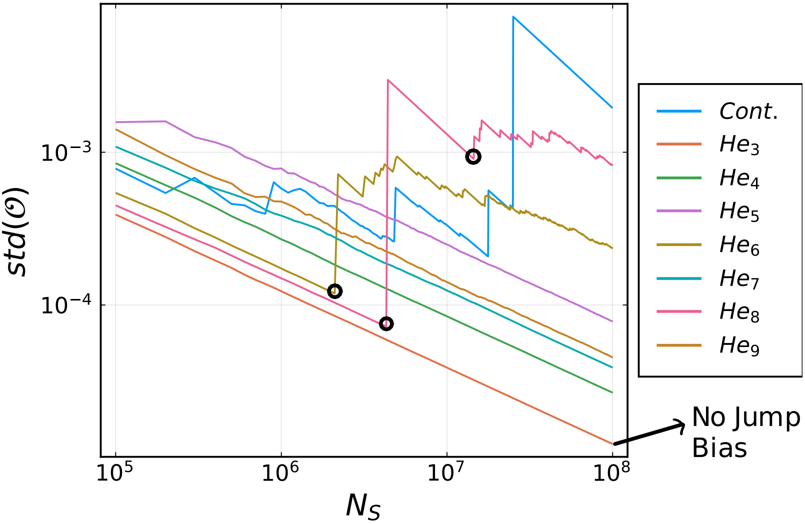
Empirical Bias



Empirical Bias



Empirical Bias



Empirical Bias

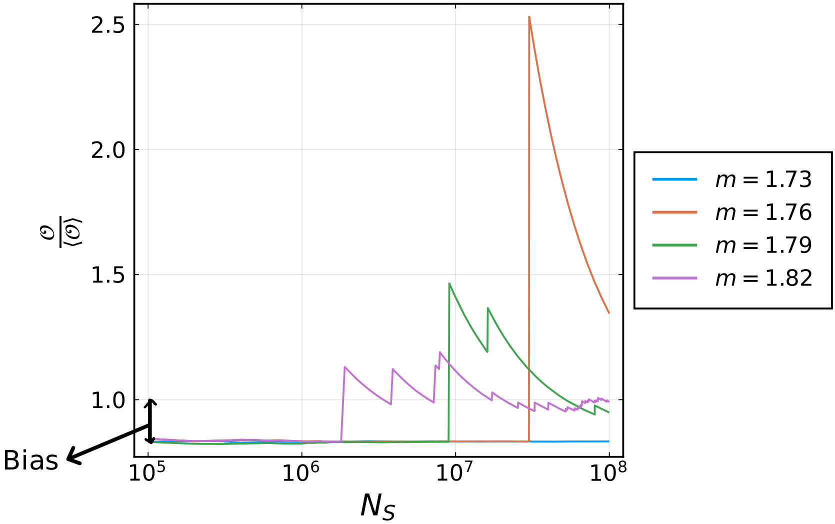
Let t be a parameter of theory such that at $t = 0$ the almost exceptional configuration becomes an exceptional configuration.

Theorem

Let $\delta, \epsilon > 0$. There is an integer $N(\delta, \epsilon)$ such that for all $N \geq N(\delta, \epsilon)$:

$$\lim_{t \to 0} P^t\left(\left|\hat{\mathcal{O}}_N - (\mu - \Delta)\right| \leq \delta \right) \geq 1 - \epsilon$$

Empirical Bias



Takeaway

1. Observables with infinite variance occurs in some fermionic systems due to zero eigenvalues of Dirac operator
2. Discrete Hubbard-Stratonovich works in principle but is not useful for realistic problems