Short Takes 331

Toward QMC: Spacetime determinant identities

Toward finite-temperature Quantum Monte Carlo (QMC):

Spacetime determinant identities

- Last video...

fermions: $\det(\mathbb{1} + e^{\lambda_1} e^{\lambda_2} \dots e^{\lambda_N})$

bosons: $\det{}^{-1}(\mathbb{1} - e^{\lambda_1} e^{\lambda_2} \dots e^{\lambda_N})$

$e^{\lambda_k} = U_k \qquad U = U_1 U_2 \dots U_N$

- I will show that

$$\det(\mathbb{1} + U) = \det \begin{pmatrix} \mathbb{1} & 0 & & +U_N \\ -U_1 & \mathbb{1} & 0 & \\ & -U_2 & \ddots & 0 \\ 0 & & \ddots & \\ & 0 & -U_{N-1} & \mathbb{1} \end{pmatrix}$$

$$\det(\underbrace{\mathbb{1} - U}) = \det \begin{pmatrix} \mathbb{1} & 0 & & -U_N \\ -U_1 & \mathbb{1} & 0 & \\ & -U_2 & \ddots & 0 \\ 0 & & \ddots & \\ & 0 & -U_{N-1} & \mathbb{1} \end{pmatrix}$$

Space x Space

each entry is of size space x space

L^d

d: spatial dimension

L^d: size of s.p. basis.

Spacetime x Spacetime

- We know that the det does not change if we add to a row (or column) a multiple of another row (or column).

E.g. $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \longrightarrow \det A = 4 - 6 = -2$

$$A' = \begin{pmatrix} 1-3 & 2-4 \\ 3 & 4 \end{pmatrix} = \begin{pmatrix} -2 & -2 \\ 3 & 4 \end{pmatrix} \longrightarrow \det A' = -8 + 6 = -2$$

$$A'' = \begin{pmatrix} 1 & 2 \\ 3-2 & 4-4 \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 1 & 0 \end{pmatrix} \longrightarrow \det A'' = -2$$

This also works with matrix blocks.

E.g. $$\det \begin{pmatrix} \mathbb{1} & A \\ 0 & \mathbb{1} \end{pmatrix} = \det \begin{pmatrix} \mathbb{1}-0 & A-A \\ 0 & \mathbb{1} \end{pmatrix} = \det \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}$$

↓ mult second block row by A & subtract from 1st block

- In our case,

$$\begin{pmatrix} 1 & 0 \dots & 0 & +u_N \\ -u_1 & 1 & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & & -u_{N-1} & 1 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 0 & & u_{N-1}u_N & 0 \\ -u_1 & 1 & \ddots & 0 & 0 \\ \vdots & \ddots & & \vdots & \vdots \\ 0 & & & 1 & 0 \\ & & & -u_{N-1} & 1 \end{pmatrix} \longrightarrow \dots$$

$\times u_N$; $\times u_{N-1}u_N$

$$\longrightarrow \begin{pmatrix} 1+u_1u_2\dots u_N & 0 & 0 \dots & 0 \\ -u_1 & \ddots & 1 & \ddots \\ 0 & & -u_2 & \ddots \\ \vdots & & & -u_{N-1} \; 1 \end{pmatrix} \longleftarrow \det = \det\left(1 + u_1u_2\dots u_N\right)$$

- Proceed identically in the bosonic case.

- These identities have many uses.
  - space formulation ⟷ spacetime formulation
  - connect to relativistic QFT
  - simplify entanglement calculations ..

Entanglement, noise, and the cumulant expansion

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We put forward a simpler and improved variation of a recently proposed method to overcome the signal-to-noise problem found in Monte Carlo calculations of the entanglement entropy of interacting fermions. The present method takes advantage of the approximate lognormal distributions that characterize the signal-to-noise properties of other approaches. In addition, we show that a simple rewriting of the formalism allows circumvention of the inversion of the restricted one-body density matrix in the calculation of the n-th Rényi entanglement entropy for $n > 2$. We test our technique by implementing it in combination with the hybrid Monte Carlo algorithm and calculating the $n = 2, 3, 4, \ldots, 10$ Rényi entropies of the 1D attractive Hubbard model. We use that data to extrapolate to the von Neumann ($n = 1$) and $n \to \infty$ cases.

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INTRODUCTION

Recently [1], we proposed an algorithm to compute the Rényi entanglement entropy S_n of interacting fermions. Many algorithms have been proposed to this effect in the last few years [2–8]. Our proposal, based on the free-fermion decomposition approach of Ref. [10], overcomes the signal-to-noise problem present in that approach and is compatible with the hybrid Monte Carlo (HMC) method [9] widely used in the context of lattice quantum chromodynamics. The core idea of our method is that, by differentiating with respect to an auxiliary parameter λ, one may carry out a Monte Carlo (MC) calculation of $dS_n/d\lambda$ with a probability measure that includes entanglement properties explicitly. [This was not the case in the approach of Ref. [10], where the probability measure factored across auxiliary field replicas; we identified this as the cause of the signal-to-noise problem (see below)]. Once the MC calculation is done, integration with respect to λ returns the desired entanglement entropy relative to that of a noninteracting system (which is easily computed separately).

In this work, we describe and implement a variation on that Monte Carlo algorithm which, while sharing the properties and core idea mentioned above, differs from it in two important ways; the new method, in fact, is different enough that we advocate its use over our original proposal. First, the new method takes advantage of the approximate lognormal shape of the underlying statistical distributions of the fermion determinants, which we already noted in Ref. [1] and which we explain in detail below. Second, and more importantly, the present method is simpler than our original proposal: whereas in the latter the parameter λ multiplied the coupling constant g (thus generating a rather involved set of terms upon differentiation of the fermion determinant), here λ is coupled to the number of fermion species N_f. As we show below, this choice not only simplifies the implementation, but also exposes the central role of the logarithm of the fermion determinant in our calculation of S_n, and thus brings to bear the approximate lognormality property mentioned above.

Below, we present the basic formalism, review the evidence for approximate lognormal distributions, and explain our method. Besides the points mentioned above, in our calculations we have found the present method to be more numerically stable than its predecessor. We explain this in detail in our Results section.

In addition to the new method, we show that it is possible to rewrite part of the formalism in order to bypass the calculation of inverses of the restricted density matrix (see e.g. [1, 6, 7]) in the determination of Rényi entropies of order $n > 2$. To test our method, we computed the $n = 2$ Rényi entropy of the 1D attractive Hubbard model using the previous as well as the new formalism, and checked that we obtained identical results. Going beyond the $n = 2$ case, we present results for the $n = 2, 3, 4, \ldots, 10$ Rényi entropies and find that higher Rényi entropies display lower statistical uncertainty in MC calculations.

BASIC FORMALISM

As in our previous work, we set the stage by briefly presenting the formalism of Ref. [10]. The n-th Rényi entropy S_n of a sub-system A of a given system is

$$S_n = \frac{1}{1-n} \ln \mathrm{tr}(\hat{\rho}_A^n), \tag{1}$$

where $\hat{\rho}_A$ is the reduced density matrix of sub-system A. For a system with density matrix $\hat{\rho}$, the reduced density matrix is defined via a partial trace over the Hilbert space corresponding to the complement $\bar{A}$ of our sub-system:

$$\hat{\rho}_A = \mathrm{tr}_{\bar{A}} \hat{\rho}. \tag{2}$$

An auxiliary-field path-integral form for $\hat{\rho}_A$, from which S_n can be computed using MC methods for a wide