Signal-to-noise issues in entanglement entropy calculations of ultracold fermions...

...and other demons

Joaquin E. Drut
University of North Carolina
at Chapel Hill
Motivation: Why ultracold atoms? Why entanglement?

Challenge: A signal-to-noise problem in MC calculations

Solution: A new algorithm

Results: Entanglement entropy for strongly coupled fermions

+ [Bonus track]
Based upon...

*The entanglement spectrum and Rényi entropies of non-relativistic conformal fermions*
William J. Porter, Joaquín E. Drut

*Entanglement, noise, and the cumulant expansion*
Joaquín E. Drut, William J. Porter

*A hybrid Monte Carlo approach to the entanglement entropy of interacting fermions*
Joaquín E. Drut, William J. Porter
Disclaimer

Lots of great work out there that I won’t get to directly (short talk!), but that you can find in excellent review articles.

See e.g.:
L. Amico, R. Fazio, A. Osterloh, and V. Vedral,

R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki,
Rev. Mod. Phys. 81, 865 (2009).

J. Eisert, M. Cramer, and M. B. Plenio,
Rev. Mod. Phys. 82, 277 (2010).

N. Laflorencie

And also:
D. J. Luitz, X. Plat, N. Laflorencie, and F. Alet,

F. F. Assaad, T. C. Lang, and F. P. Toldin,

F. F. Assaad,
Motivation: why ultracold atoms?

For the purposes of this talk…

**Ultracold atoms** = extremely **clean**
**malleable**
**non-relativistic** particles with
**short-range, controllable interactions**

**Controllable parameters**: temperature, coupling, polarization, mass imbalance, trap shape (harmonic, “flat bottom”, lattices);
Motivation: why entanglement?

• Quantum information: cryptography, computation, teleportation, etc.
• Quantum phase transitions (esp. topological)
• It is challenging to compute and it tells us something new!
**Motivation: entanglement**

Qualitatively: **Entanglement** is the property that makes a state of a two-(or more-) component quantum system **unfactorizable**.

For example: \( N \) non-interacting fermions (or bosons)…

\[
\Psi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\chi_1(x_1) & \chi_2(x_1) & \cdots & \chi_N(x_1) \\
\chi_1(x_2) & \chi_2(x_2) & \cdots & \chi_N(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\chi_1(x_N) & \chi_2(x_N) & \cdots & \chi_N(x_N)
\end{vmatrix}
\]

… clearly not factorizable into single-coordinate functions.
Motivation: entanglement

Quantitatively: Entanglement entropy!

Density matrix
\[ \rho = |\Psi\rangle \langle \Psi| \]

“Reduced” density matrix
\[ \rho_A = \text{Tr}_B \rho \]

Von Neumann version
\[ S_A = -\text{Tr} \left[ \rho_A \ln \rho_A \right] \]

Rényi version
\[ S_{A,n} = \frac{1}{1-n} \ln \text{Tr} \left[ \rho_A^n \right] \]

Note: The entropy of the full system (A+B) vanishes; The entropy of the subsystem does not vanish, unless the state factorizes! The resulting entropy is purely quantum mechanical!
Motivation: quantum phase transitions

Spin chains (XY, XXZ)

Non-critical: saturation
Critical: log divergence

Motivation: area laws and their violation

For bosons,

\[ S_{A,n} \sim L^{d-1} \]

but...

Gapless fermions:

\[ S_{A,n} \sim L^{d-1} \log L \]

Dependent on having a well-defined Fermi surface...

...but what about strongly coupled systems?

The replica “trick”
(or: How to take powers of the reduced density matrix and not die in the attempt)

\[ S_{A,n} = \frac{1}{1 - n} \ln \text{Tr} [\rho_A^n] \]

Rényi version of the entanglement entropy

\[ \text{Tr} [\rho_A^n] = \frac{Z_{A,n}}{Z^n} \]

Partition function of the system (to the n-th power)

Partition function of n copies of the system, glued together in region A
Path-integral formulation

Auxiliary-field (i.e. Hubbard-Stratonovich) representation of the interacting density matrix…

\[ \hat{\rho} = \frac{e^{-\beta \hat{H}}}{\mathcal{Z}} = \int \mathcal{D}\sigma \ P[\sigma] \ \hat{\rho}_\sigma \]

Non-interacting density matrix in external field

Fermion determinant, etc.

Any review on AFQMC
J. of Any Computational Methods (20XX)
Path-integral formulation

Auxiliary-field (i.e. Hubbard-Stratonovich) representation of the interacting reduced density matrix...

\[ \hat{\rho}_A = \int D\sigma P[\sigma] \hat{\rho}_{\sigma,A} \]

Non-interacting reduced density matrix in external field (see also work by I. Peschel)

Fermion determinant, etc.

T. Grover
PRL 111, 130402 (2013).
Path-integral formulation

Auxiliary-field (i.e. Hubbard-Stratonovich) representation of the interacting reduced density matrix...

\[ \hat{\rho}_A = \int \mathcal{D}\sigma P[\sigma] \hat{\rho}_{\sigma,A} \]

Taking powers...

\[ \rho^n_A = \int \mathcal{D}\{\sigma_i\} \prod_i^n P[\sigma_i] \prod_i^n \rho_{\sigma_i,A} \]

\[ e^{(1-n)S_{A,n}} = \text{Tr}_A \hat{\rho}_A^n = \int \mathcal{D}\sigma P[\{\sigma\}] \det M_{A,n}[\{\sigma\}] \]

Probability measure

Observable

\[ S_{A,n} = \frac{1}{1 - n} \ln \langle \det M_{A,n} \rangle \]

T. Grover
PRL 111, 130402 (2013).
Path-integral formulation

\[ M_{A,n}[\{\sigma\}] = \prod_{i=1}^{n} \left( 1 - G_{A,\sigma_i} \right) \left[ 1 + \prod_{i=1}^{n} \frac{G_{A,\sigma_i}}{1 - G_{A,\sigma_i}} \right] \]

“Restricted” one-body density matrix

\[ G_{A,\sigma} \]

From the one-body density matrix of the full system, take rows and columns that belong in the subsystem A.

**E.g.:** If A is made of points \( x = \{2, V-1, V\} \), then:

\[ G_\sigma(x, x') = \begin{pmatrix}
    G_{1,1} & G_{1,2} & \cdots & G_{1,V-1} & G_{1,V} \\
    G_{2,1} & G_{2,2} & \cdots & G_{2,V-1} & G_{2,V} \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    G_{V-1,1} & G_{V-1,2} & \cdots & G_{V-1,V-1} & G_{V-1,V} \\
    G_{V,1} & G_{V,2} & \cdots & G_{V,V-1} & G_{V,V}
\end{pmatrix} \]
The challenge: A signal-to-noise problem

**Problem:** determinant fluctuations grow exponentially with sub-system size…

Broecker and Trebst
Solved StN problem differently!

10-site Hubbard chain at half filling
The challenge: A signal-to-noise problem

**Diagnosis:** overlap problem
Probability measure does not capture correlations across auxiliary-field replicas

\[ e^{(1-n)S_{A,n}} = \text{Tr}_A \hat{\rho}_A^n = \int D\sigma \ P[\{\sigma\}] \ \det M_{A,n}[\{\sigma\}] \]

This heavy-tail behavior was seen before in correlation functions!

In cold atoms

Endres, Kaplan, Lee, Nicholson,

In QCD

DeGrand,
The solution: Differentiate and integrate

\[ e^{(1-n)S_{A,n}} = \int \mathcal{D}\{\sigma\} \ P[\{\sigma\}]Q[\{\sigma\}] \]

\[ Q[\{\sigma\}] = \det M_{A,n}[\{\sigma\}] \]

\[ \Gamma(\lambda) = \int \mathcal{D}\{\sigma\} \ P[\{\sigma\}]Q^\lambda[\{\sigma\}] \]

\[ \ln \Gamma(0) = 0 \]

\[ \frac{1}{1-n} \ln \Gamma(1) = S_{A,n} \]

\[ \frac{d \ln \Gamma}{d\lambda} = \int \mathcal{D}\{\sigma\} \ \tilde{P}_\lambda[\{\sigma\}] \ln Q[\{\sigma\}] \]

\[ = \langle \ln Q[\{\sigma\}] \rangle_\Gamma \]

\[ S_{A,n} = \frac{1}{1-n} \int_0^1 d\lambda \ \langle \ln Q[\{\sigma\}] \rangle_\Gamma \]

\[ \tilde{P}_\lambda[\{\sigma\}] = \frac{1}{\Gamma(\lambda)}P[\{\sigma\}]Q^\lambda[\{\sigma\}] \]
An interpretation: The ratio “trick”

\[ e^{(1-n)S_{A,n}} = \frac{\mathcal{Z}_{A,n}}{\mathcal{Z}^n} = \frac{\mathcal{Z}_{A,n}}{\mathcal{Z}_{A',n}} \frac{\mathcal{Z}_{A'',n}}{\mathcal{Z}_{A''',n}} \cdots \frac{\mathcal{Z}_{A^{(m)},n}}{\mathcal{Z}^n} \]

Our “trick” is similar:

\[ e^{(1-n)S_{A,n}} = \frac{1}{\prod_{\lambda=0}^{1}} e^{\langle \ln Q[\{\sigma\}] \rangle_{\Gamma(\lambda)}} \]

Broecker and Trebst

Wang and Troyer,

Assaad, Lang, Toldin,

Hastings, González, Kallin, Melko,
Results: 1D Half-filled Hubbard Model

Second Rényi entropy: integrand

10-site Hubbard chain at half filling

Integrand behavior. 20 \( \lambda \) points.
Results: 1D Half-filled Hubbard Model

Second Rényi entropy
10-site Hubbard chain at half filling

Our algorithm (data) vs. Exact solution (solid lines)

vs.
Non-interacting (dashed)

Graph showing $S_2(L_A)$ as a function of $L_A/L$ for different values of $U/t$: $0.5$, $1.0$, $2.0$, and $4.0$.
Results: Unitary Fermions  
(Spin-1/2 at scale-invariant point)

Second Rényi entropy: integrand

Integrand behavior. 10 $\lambda$ points.  
250 samples per point

$$\langle \ln Q[\sigma] \rangle_\lambda$$

$L_A/L = 2/12$  
$L_A/L = 3/12$  
$L_A/L = 4/12$  
$L_A/L = 5/12$

$N_x = 12, \ n = 2, \ N = 136$
Results: Unitary Fermions  
(Spin-1/2 at scale-invariant point)

Rényi entropies $n = 2, .., 5$

Scaling of $S_n$ with sub-system size and comparison with non-interacting case
Conclusions: Yes, we can!

Entanglement entropy of non-relativistic fermions

Algorithm

- Designed new algorithm based on auxiliary-parameter differentiation and post-MC integration;
- Solved signal-to-noise problem by exploiting log-normal behavior;
- Found algebraic simplifications that enable high-order Rényi entropy calculations.

Results

- Known results reproduced in simple cases (1D Hubbard);
- First calculation of the entanglement of fermions at unitarity: universal result. Answers surprisingly close to non-interacting result (!?)
Other demons…

…Complex Langevin for non-relativistic many-fermion systems

Third-order perturbative lattice and complex Langevin analyses of the finite-temperature equation of state of non-relativistic fermions in one dimension
Andrew C. Loheac, Joaquín E. Drut
arXiv:1702.04666

Thermal equation of state of polarized fermions in one dimension via complex chemical potentials
A. C. Loheac, J. Braun, J. E. Drut, D. Roscher

Also in collaboration with:
J. Braun, L. Rammelmüller, W. J. Porter, C. R. Shill, J. R. McKenney
**Results:** 1D fermions attractively & repulsively interacting

**Density EoS**
(in units of non-interacting result $n_0$)

Lattice: $N_x = 80; N_t = 160$

Complex Langevin (diamonds) vs. Hybrid MC (data) vs. PT: NLO, N2LO, N3LO (lines)

Complex Langevin (diamonds) vs. PT: NLO, N2LO, N3LO (lines)
Results: Polarized 1D fermions

Density EoS

Lattice: \( N_x = 60; N_t = 160 \)

Complex Langevin (black squares) vs. Imaginary polarization (data) vs. PT: N3LO (lines)
Results: Polarized Unitary Fermions (3D)

Density EoS

Lattice: $N_x = 7; \ N_t = 160$

Complex Langevin (data) vs. Virial expansion (black lines) vs. MIT Experiment (red circles; unpolarized)
Results: Particle projection

CL running average of projection onto:

2+1 particles (blue)

4+6 particles (red)
Conclusions: Exciting times! Stay tuned!

Complex Langevin for non-relativistic systems with a sign problem

**STATUS REPORT**

**Repulsive interactions**
Looks great (1D) compared with PT @ N3LO.

**Polarized systems**
Very promising (1D) compared with PT @ N3LO and imaginary polarization.

**Polarized unitary fermions**
Need larger volumes but looks promising too!

**Particle-number projection**
Looks OK. Stay tuned!
Thank you!
Path-integral formulation

Auxiliary-field (i.e. Hubbard-Stratonovich) representation of the interacting reduced density matrix...

\[
\rho_A = \int D\sigma P[\sigma] \rho_{\sigma, A}
\]

(Non-interacting) density matrix in external field

\[
\rho_{\sigma, A} = D_{\sigma, A} e^{-\hat{b}_i^\dagger B_{ij}[\sigma, A] \hat{b}_j}
\]

Normalization

\[
D_{\sigma, A} = \det \left( 1 - e^{-B[\sigma, A]} \right)
\]

B matrix

\[
B[\sigma, A] = \log(G_{\sigma, A}^{-1} + 1)
\]

“Restricted” correlation function

\[
\text{Tr} \left[ \rho_{\sigma, A} \hat{b}_i^\dagger \hat{b}_j \right] = G_{\sigma, A}^{ij}
\]

Great!

Got path-integral rep of the reduced density matrix!

T. Grover
Results: Unitary Fermions  (Spin-1/2 at scale invariant point)

Second Rényi entropy  
Approach to the continuum and scaling with sub-system size
Results: 1D fermions CL stabilization

Stabilization: modified action

$$S[\sigma] \rightarrow S[\sigma] + \xi \sum_{x, \tau} \sigma^2$$

Complex evolution equation

$$\delta \sigma = -\frac{\delta S[\sigma]}{\delta \sigma} \delta t - 2\xi \sigma \delta t + \eta \sqrt{\delta t}$$

Lattice: $N_x = 80; N_t = 160$