Developments in wave function-based approaches to two-dimensional materials

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An enduring legacy of lattice model research...

Hubbard model in infinite dimensions

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Hubbard model in infinite dimensions

Density Matrix Formulation for Quantum Renormalization Groups

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A generalization of the numerical renormalization-group procedure used first by Wilson for the Kondo problem is presented. It is shown that this formulation is optimal in a certain sense. As a demonstration of the effectiveness of this approach, results from numerical real-space renormalization-group calculations for Heisenberg chains are presented.
Wavefunction (ground state) approaches to lattice models:

- **Long history:** Gutzwiller, RVB, ...

- **More recently:**
  - Tensor Networks: **MPS, PEPS**
    (White, Cirac, Verstrate, Corboz,...)
  - Wfn-QMC: **VMC, AFQMC, GFMC**
    (Sorella, Becca, Zhang,...)

\[
|\psi\rangle = \sum_{q_1q_2q_3...q_m} C^{q_1q_2q_3...q_m} |q_1q_2q_3...q_m\rangle
\]
\[ |\psi\rangle = \sum_{q_1 q_2 q_3 \ldots q_r} C^{q_1 q_2 q_3 \ldots q_m} |q_1 q_2 q_3 \ldots q_m\rangle \]

Choose subset?

- Linear problem
- Zero correlation in thermodynamic limit
\[ |\psi\rangle = \sum_{q_1 q_2 q_3 \ldots q_m} C^{q_1 q_2 q_3 \ldots q_m} |q_1 q_2 q_3 \ldots q_m\rangle \]

**Projector QMC**

- Stochastically apply projector
- Discretize and sample from amplitudes

\[ \Psi = e^{-\beta H} |\psi_0\rangle \]

**Various flavors**

(Choice of projector, Hilbert space):

- AFQMC, GFMC, FCIQMC, DMC, ...

**Sign problem**
\[ |\psi\rangle = \sum_{q_1q_2q_3\ldots q_m} C^{q_1q_2q_3\ldots q_m} |q_1q_2q_3\ldots q_m\rangle \]

Variational QMC

\[ |\psi\rangle = \sum_{q_1q_2q_3\ldots q_m} f(q_1q_2q_3\ldots q_m; X)|q_1q_2q_3\ldots q_m\rangle \]

- Choose an explicit non-linear parameterization
- Optimize parameters via Metropolis sampling

• How to choose parameterization?
• How to optimize variables with MC?
• How to reduce parameter space?
**Correlator Product States / Entangled Plaquette States**

$$\psi = \sum_{q_1q_2q_3} C^{q_1q_2q_3} |q_1q_2q_3\rangle$$

$$|\psi\rangle = \sum_{q_1q_2q_3\ldots q_m} C^{q_1q_2q_3} C^{q_2q_3q_4} C^{q_3q_4q_5} \ldots |q_1q_2q_3\ldots q_m\rangle \times \phi_{HF/DFT}$$

- Linear parameters with system size
- Exponential growth of parameters with correlator size
Non-linear projector Monte Carlo

Overlapping 5-site correlators x Slater determinant for 98-site, 2D Hubbard (U=8t)

Similar problems found in optimization of non-linear neural networks...

\[
\frac{\partial \Psi}{\partial \beta} = - (H - E) \Psi
\]

\[
\frac{\partial^2 \Psi}{\partial \beta^2} = -b \frac{\partial \Psi}{\partial \beta} - (H - E) \Psi
\]

- Chebyshev expansion of optimal projection operator
Non-linear projector Monte Carlo

Overlapping 5-site correlators × Slater determinant for 98-site, 2D Hubbard (U=8t)

Non-linear projector Monte Carlo

Overlapping 5-site correlators x Slater determinant for 98-site, 2D Hubbard (U=8t)

Million+ parameter VMC...
Non-linear projector Monte Carlo

4 x 4 Graphene sheet
Local p-space Gaussian functions from VASP

Low-energy correlated spin-fluctuations
• How to choose parameterization?
• How to optimize variables with MC?
• How to reduce parameter space?

Modern fitting of Potential Energy Surfaces

\[ E(r_1, r_2, r_3, \ldots, r_N) \]

Statistical inference
*(Gaussian Process Regression)*
\( f(\text{plaquette parameters}) \)

- Explicit parameters
- Iterative Non-linear fitting
- Restricted to ‘small’ numbers of parameters
- Optimize parameters

\( f(\text{distance from data points}) \)

- Implicit parameters (never referenced directly)
- Analytic optimal fitting without expanding in variables
- No restriction in number of parameters
- Optimize datapoints
<table>
<thead>
<tr>
<th>Parameter-space’</th>
<th>‘Data-space’</th>
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\[ \Psi(r) = e^{\left( \sum_d k r_d \alpha_d \right)} \phi_{SD}(r) | r \rangle \]

- Independent of number of underlying parameters
- Linear with number of “data” configurations

“Distance” to data points

Weight of data points
Data:

Subset of configurations and their amplitudes
  e.g. All configurations on ‘small’ system, then infer amplitudes on ‘large’ system

Distance “Covariance Kernel”:

Quantify ‘similarity’ (covariance) between two configurations:
  How likely is it that their amplitudes are similar?
**K1:** How many unoccupied (Holons), up, down, Doubly-occupied (Doublons)?

\[
\begin{pmatrix}
\#\text{unocc} \\
\#\text{up} \\
\#\text{down} \\
\#\text{doub}
\end{pmatrix}
\]
K1: How many unoccupied (Holons), up, down, Doubly-occupied (Doublons)?

\[ k_{1,2} = \begin{pmatrix} \#unocc \\ \#up \\ \#down \\ \#doub \end{pmatrix}_1 \cdot \begin{pmatrix} \#unocc \\ \#up \\ \#down \\ \#doub \end{pmatrix}_2 \]

Does not need to refer to the same sized system
K1: How many unoccupied (Holons), up, down, Doubly-occupied (Doublons)?

K2: Start to build in (local) anti-ferromagnetic correlation, Holon-Doublon binding

16-dimensional ‘feature’ space
K1: How many unoccupied (Holons), up, down, Doubly-occupied (Doublons)?

K2: Start to build in (local) anti-ferromagnetic correlation, Holon-Doublon binding

K3: 3-site descriptors
Gutzwiller Projection:

= 1.0

= 1.0

= 1.0

= 0.0
Extrapolation errors: Can we reproduce 10-site wave function from 6-site data?

All 6-site fluctuations with all symmetries conserved
1D Hubbard Model, U=8t

400 linear coefficients from 6-site model
1D Hubbard Model, $U=8t$

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1D Hubbard Model, U=8t

400 linear coefficients from 6-site model
1D Hubbard Model, $U=8t$

- Variational
- Size-extensive, $N_t M^4$ cost
- 97% correlation in TDL

400 linear coefficients from 6-site model
1D Hubbard Model, U=2t

400 linear coefficients from 6-site model
1D Hubbard Model, U=2t

Variational, Size-extensive, \( N_t M^4 \) cost, 95% correlation in TDL

400 linear coefficients from 6-site model
How to we avoid constructing these vectors...?
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\[ L^2 \text{ cost} \text{ to evaluate contribution to kernel function } \text{between any two configurations, for any plaquette topology, independent of size} \]
How to we avoid constructing these vectors...?

$L^2$ cost to evaluate contribution to kernel function **between any two configurations**, for any plaquette topology, independent of size
How to we avoid constructing these vectors...

- **L³ cost** to evaluate *all* possible plaquettes of *all* topology to quantify configurational similarity ($k_d$)
- **Exponentially** large ‘feature’ space of implicit plaquette parameters
- **Exact results with exact data**
- Beware of *overfitting*... (Hyperparameters avoid this)
Exact results for data with complete plaquette space
MF energy for 32 sites

Bethe Ansatz

GP extrapolation from 8 to 32 sites
96-99% correlation in TDL with data-driven, zero parameter wavefunction
Optimize parameters

Optimize Data

Graph showing the variation of energy with epoch, comparing exact energy, ED of variational WF, and MC of variational WF.
Conclusions

• **Accelerated Gradient Descent** technique for combining projector and variational QMC

• **Data-driven wavefunctions** as an intriguing new approach to formulations of lattice models
  – Early development, but clear extension to 2D systems
Thanks

Non-linear stochastic optimizations:
Lauretta Schwarz

Gaussian Process Wavefunctions:
Aldo Glielmo, Sandro de Vita, Gabor Csanyi

PhD and Postdoc positions available in the group!