New Finite Temperature Methods for Strongly Correlated Systems

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Telluride
Stochastic Methods in Electronic Structure Theory
Caveats

- Not ab-initio
- Simplified models
  - (some even in 1D)

**Stochastic Methods in Electronic Structure Theory**
Many Body Localization

One-dimension
Interaction + Disorder (W)

with:
Xiongjie Yu,
Benjamin Corregea
David Pekker
Finding chunks of spectrum...

Many Body Localization

One-dimension Interaction + Disorder (W)

with:
Xiongjie Yu,
David Pekker
Bosonic Wave-Functions: Beyond Jastrows

with:
Hassan Shapourian

\[ H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i \sum_{\langle\langle ik \rangle\rangle} \Delta_{ik} c_{ik}^\dagger c_k + \sum_i m_i c_i^\dagger c_i \]

\[ \Psi(\{r_i\}) = \text{det}_1(\{r_i\}) \times \text{det}_2(\{r_i\}) \]
Strange Metals

ok...some actual electrons

with:
Katie Hyatt
Matthew Fisher

No sign problem

Done with reputation + DMC

Worse forward walking + population bias I’ve ever seen.
Done with advertisement
Ground State Methods

Variational Monte Carlo
  Variational Error

Diffusion Monte Carlo
  Statistical Error

Fixed-Node Diffusion Monte Carlo
  `Better' Variational Error
Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Error

Restricted Path Integral Monte Carlo

`Better’ Variational Error

Path Integral Monte Carlo

Statistical Error
In this talk, we will consider the question: *What are the some algorithms to compute finite temperature properties of fermionic, strongly correlated systems?*

We will discuss three algorithms:

- **VAFT** $\leftrightarrow$ A new (*implicit*) Variational Density Matrix
- **RPIMC** with (morally) the new VDM as the restriction

**Variational Finite T PI**
Variational Density Matrices

Choose a class of trial density matrices $\rho[\beta, \bar{\alpha}]$

Select the one with the lowest free energy. 

This optimization is not straightforward.

Choice 1

Compute Free Energy by thermodynamic integration.

Need all $\rho(\tau)$ for $0 < \tau < \beta$

How are you going to optimize this?

Choice 2

Use a Monte Carlo move to swap between density matrices and measure time at each spot.
Trial Density Matrices

\[ \rho(R^*, R) \]

\[ \rho(R^*, R) = \det[\exp[-k(r_i^* - r_j)^2]] \]

Free fermion density matrix

\[ k = 1/(4\lambda \tau) \]
\[ \tau = 1/T \]

Outer product of wave-functions

\[ \rho(R^*, R) = \langle R^* | \left( \sum_{i,j} \alpha_{ij} |\Psi_i\rangle \langle \Psi_j | \right) |R\rangle \]

Ground state

\[ \rho(R^*, R) = \langle R^* | \Psi_0 \rangle \langle \Psi_0 | R \rangle \]

eigenstates

\[ \rho(R^*, R) = \langle R^* | \left( \sum_i \exp[-\tau E_i] |\Psi_i\rangle \langle \Psi_i | \right) |R\rangle \]
\[ \rho(R^*, R) = \langle R^* \mid \left( \sum_i \exp[-\tau E_i] \mid \Psi_i \rangle \langle \Psi_i \mid \right) \mid R \rangle \]

This is the right answer and an appealing start for an approximation.

Just need to

Guess a wave-function for each excitation

Guess an energy for each excitation

(but at least we have experience in wave-functions)
\[
\rho(R^*, R) = \langle R^* | \left( \sum_i \exp[-\tau E_i] |\Psi_i\rangle \langle \Psi_i | \right) |R\rangle
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This is the right answer and an appealing start for an approximation.

Just need to

- Guess a wave-function for each excitation
- Guess an energy for each excitation

*(but at least we have experience in wave-functions)*

Write the right answer and approximate is a good approach.

Need a different representation of the right answer.
A Different Representation

(Sneakily) an exponential sum of outer products that we can compute with.

VAFT

**Input:** Variational Manifold of wave-functions

**Output:** Approximate samples from a variational many-body density matrix.

**High level approach:** Write down a Markov chain (not metropolis) which samples configurations from the many body density matrix.

Discover you can’t do the Markov chain.

Write down a new Markov chain which hopefully has a stationary distribution close to the actual one.

Notice that this is also sampling from some many-body density matrix.
A Markov chain whose fixed point probability distribution is the diagonal of the finite temperature many-body density matrix.

Proof: Two slice PIMC with an exact action of inverse temperature $\beta/2$.

Select $|R'\rangle$ with prob $|\langle R' | \exp[-\beta/2H]|R\rangle|^2$
Proof by PIMC

Typical PIMC: move $R$, move $R'$, move $R$, move $R'$, ...

Atypical PIMC 1: move $R$ a lot, move $R'$ a lot, move $R$ a lot, ....

Atypical PIMC 2:

Select $R$ with prob $|\langle R | \exp[-\beta H/2] | R' \rangle|^2$

Select $R'$ with prob $|\langle R' | \exp[-\beta H/2] | R \rangle|^2$

Select $R$ with prob $|\langle R | \exp[-\beta H/2] | R' \rangle|^2$

....
A Markov chain whose fixed point probability distribution is the diagonal of the finite temperature many-body density matrix.

| $R\rangle$ | \[ \exp[-\beta/2H]|R\rangle \]
| $|R\rangle$ \[ \rightarrow |R\rangle \]

**How?**

**Select $|R\rangle$ with prob $|\langle R'|\exp[-\beta/2H]|R\rangle|^2$**

Sample using VMC
Imaginary time evolution of arbitrary variational wave-functions

**High level approach**

\[
\exp[-\tau H] \exp[-\tau H] \exp[-\tau H]|R\rangle \\
P \exp[-\tau H] P \exp[-\tau H] P \exp[-\tau H]|R\rangle
\]

**Low level approach: Stochastic reconfiguration**

Schrodinger equation in the tangent space of local variational subspace.

Tangent space of \( \Psi[\vec{\alpha}] \):
\[
\frac{\partial \psi[\vec{\alpha}]}{\partial \alpha_0}, \frac{\partial \psi[\vec{\alpha}]}{\partial \alpha_1}, \frac{\partial \psi[\vec{\alpha}]}{\partial \alpha_2}, \ldots
\]

\[
H_{ij} \equiv \langle \partial \psi[\alpha_i] | \hat{H} | \partial \psi[\alpha_j] \rangle \quad \text{Run VMC on } |\Psi[\alpha]\rangle \\
S_{ij} \equiv \langle \partial \psi[\alpha_i] | \partial \psi[\alpha_j] \rangle \\
(1 - \tau HS^{-1})|\Psi[\alpha]\rangle
\]

Measure \( H \) and \( S \)
Q: Is the approximation a variational density matrix?

Yes…implicitly (at least for a fixed $\beta$)

$$\sum_c \frac{|\tilde{\Psi}[\beta/2; c]\rangle \langle \tilde{\Psi}[\beta/2; c]|}{\langle \tilde{\Psi}[\beta/2; c]|\tilde{\Psi}[\beta/2; c]\rangle} \tilde{p}(c)$$

*Ideal*  \[ \tilde{p}(c) = \frac{\langle c| e^{-\beta' H} |c\rangle}{Tr(e^{-\beta' H})} \]

*Reality*  \[ \tilde{p} \] is defined implicitly by the markov chain
A prototypical variational wave-function: Essentially a fancy Jastrow

**Huse-Elser States** (aka correlated product states, entangled plaquette states, graph tensor networks states, ... )

A prototypical Hamiltonian: **Heisenberg Model**

\[ H = \sum_{\langle i,j \rangle} \sigma_i \cdot \sigma_j \]

On a bipartite lattice can do exactly with SSE to compare new method against.
Via thermodynamic integration
Free energy variational principle
Gives best variational manifold*

*Free energy of “all DM”
4 x 4 bipartite Heisenberg
via thermodynamic integration
Free energy variational principle (tells you which variational manifolds are ‘better’)
Can compute arbitrary properties of the “variational density matrix.”
We have versions of this with projector Monte Carlo (sign problem but you can beat it down with FCIQMC)

A better (in some ways) DMQMC

Also developing fixed-phase AFQMC version
Advantages…

No `optimization’

Exact when variational ansatz gets sophisticated enough.

Probably a better density matrix.

No stochasticity or sign problem

Consistent approach for all temperatures.

Disadvantages..

Variational Error

Slow….

Question (not answered yet): How does VAFT compare to RPIMC with simple trial density matrix.
Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Error

not explicitly representable

Can this be used?

Restricted Path Integral Monte Carlo

`Better' Variational Error

Path Integral Monte Carlo

Statistical Error
Path Integrals for Fermions (without approximations)

\[
\rho_F(R^*, R; \beta') = \frac{1}{N!} \sum_{\pi} (-1)^\pi \int_{R^*}^{\pi(R)} dR_t \exp[-S(R(t)]
\]

Sample all paths + permutations

Odd permutations count negative

\[\begin{align*}
\text{positive} & \quad \text{negative}
\end{align*}\]
Path Integrals for Fermions (with approximations)

Restricted Path Integral Monte Carlo

\[ \rho_F(R^*, R; \beta') = \frac{1}{N!} \sum_{\pi} (-1)^\pi \int \rho_F(R^*, R; \beta') \ dR_t \ exp[-S(R(t))] \]

Removes all negative and some positive
Restricted Path Integral Monte Carlo needs to know for $R^*$, $R$ if

$$\rho(R^*, R) \equiv \langle R^* | \exp[-k\tau H] | R \rangle > 0$$

**Typical Approach**

Pick some variational density matrix (*free fermions*)

$$\rho_T(R^*, R; k\tau) > 0$$

**Improved Approach**

Pick some class of variational density matrices

$$\{ \rho_T(\tau) \}$$

Optimize over them

Optimization is hard :(

Writing down compact density matrices is hard :(
Q: Can we mirror VAFT?

Write the right answer and approximate is a good approach.
Q: Can we mirror VAFT?

Write the right answer and approximate is a good approach.

\[ \rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0 \]

If we could just evaluate this matrix element, we would be done.
(of course, then we wouldn’t have to do PIMC then)
Q: Can we mirror VAFT? Write the right answer and approximate is a good approach.

\[ \rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0 \]

If we could just evaluate this matrix element, we would be done. 
(of course, then we wouldn’t have to do PIMC then)

So, we want to approximate it.

\[ \rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0 \]

This highlighted region is a wave-function.

We just need to have a wave-function \( |\Psi_{R^*, \tau} \rangle \) for every \((R^*, \tau)\)

Then we can do \( \langle \Psi_{R^*, \tau} | R \rangle \)

This naïvely looks worse then a wave-function per excitation just generate it variationally.

Not quite the same density matrix
Also breaks time symmetry (data still coming but probably not a problem)
Do any of these ideas help us here?
Do any of these ideas help us in PIMC?

If my propagation to $\beta/2$ is exact then so is this.

But my propagation probably isn’t exact that far.
Do any of these ideas help us in PIMC?

Yes!

Removes all sign-incoherent paths which start from R and go beta of 1. Attenuates the sign problem…
An alternative approximation

If my propagation to $\beta/2$ is not exact then this is VAFT.
An alternative approximation

Two Slices

Worse Sign Problem

Variational Error

Where do you want to sit at fixed computer time?
Finite Temperature Methods

Variational Density Matrices (VDM)

Variational Approximate Path Integrals

Path Integral Monte Carlo
  Statistical Error

Restricted Path Integral Monte Carlo
  `Better' Variational Error
Q: Can you combined restricted with this better density matrices?

In principle, it should be possible.

In practice there is a nodal error I don’t know how to deal with.
Conclusion…

An implicit variational density matrix (VAFT)

Eats class of variational ansatz

\[ \rho(R^*, R; \tau) \equiv \langle R^* | \exp[-\tau H] | R \rangle > 0 \]

Can (morally) use this for RPIMC

New approach combining variational and PIMC