Quantum Monte Carlo in momentum space and on the Lefschetz thimble

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Advances in quantum Monte Carlo techniques for non-relativistic many-body systems, INT, Seattle
Collaborators

- Configuration interaction Monte Carlo
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    A. Roggero, AM & F. Pederiva, in preparation

- Lefschetz thimble Monte Carlo
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    AM, M. Cristoforetti & L. Scorzato, in preparation
Configuration Interaction Monte Carlo

- QMC *a la* fixed-node DMC in CI/k-space
- QMC with non-local ($\chi$ EFT) forces

- Variational energies from CC wave functions
  Standard CC theory is non-variational

- Momentum distribution in QMC
The rise of second quantization

We want to solve:

\[ H = \Omega \sum_i \epsilon_i a_i^\dagger a_i + \Omega \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \ldots \]

Full-CI diagonalization possible only for small systems

![Graph showing the relationship between dimension and \( \Omega \) for different values of N and \( \Omega \).]
The rise of second quantization

We want to solve:

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \ldots$$

- A general $V_{ijkl}$ leads to a non-local interaction in $r$-space
- Cannot apply standard $r$-space fixed-node DMC
- Formulate DMC in CI space?
Configuration interaction Monte Carlo

- Use the power method

\[ |\Psi_{\text{Ground State}}\rangle = \lim_{N \to \infty} P^N |\Psi_{\text{Initial State}}\rangle \]

- Occupation number basis: \( |n\rangle = |\ldots0101\ldots\rangle \)
- Interpret \( P_{mn} \) as transition probabilities

- Propagator
  - Simplest choice: \( P = (1 - \Delta \tau H) \)
  - In reality we use more efficient propagators: \( e^{-\Delta \tau (H - E_T)} \)
Configuration interaction Monte Carlo

\[ \mathcal{P} = 1 - \Delta \tau \mathcal{H} \rightarrow |\Psi_{\tau+\Delta \tau}\rangle = \mathcal{P}|\Psi_\tau\rangle \]

\[ \Psi_{\tau+\Delta \tau}(m) = \sum_n \langle m|\mathcal{P}|n\rangle \psi_\tau(n) \]

\[ = \sum_n \left( \frac{\langle m|\mathcal{P}|n\rangle}{\sum_m \langle m|\mathcal{P}|n\rangle} \right) \left( \sum_m \langle m|\mathcal{P}|n\rangle \right) \psi_\tau(n) \]

\[ = \sum_n p(m, n) w(n) \psi_\tau(n) \]

Transition probability Branching

MC sampling not possible if \( p(m, n) < 0 \)

\[ \Rightarrow \langle m|\mathcal{H}|n\rangle > 0 \rightarrow \text{sign problem} \]
Configuration interaction Monte Carlo

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- There is a sign problem for the generic case
- We need to somehow construct non-negative propagators

Transition probability Branching

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Non-negative propagator

How to choose a non-negative propagator?

Borrow from lattice-GFMC (discrete, finite Hilbert space) \textit{ten Haaf et al PRB (1995)}

- Use \textit{importance sampling} to circumvent the sign problem
  \[ \mathcal{P} \rightarrow \mathcal{P}_{\text{new}}(\Phi_G) \geq 0 \]

- But there is a price

  \begin{align*}
  \text{Variational upper bound} \\
  \text{Exact GS energy}
  \end{align*}

- Better \( \Phi_G \Rightarrow \) tighter bound

- \( E_{\text{CIMC}} \leq \langle \Phi_G | H | \Phi_G \rangle \)

\textit{AM \& Alhassid, arXiv:1304.1645 (2013)}
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How to choose a non-negative propagator?

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- Use importance sampling to circumvent the sign problem
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How to choose the importance function $\Phi_G$?

- Better $\Phi_G \implies$ tighter bound
- $E_{\text{CIMC}} \leq \langle \Phi_G | H | \Phi_G \rangle$

\[ AM \ & Alhassid, \ arXiv:1304.1645 \ (2013) \]
Good CI wave functions

The importance function should be:

- **Accurate/Flexible**: Should be able to include the major correlations in the system
- **Calculable**: Need a fast algorithm to calculate it on a computer (fast = at most polynomial in $N$ and/or $\Omega$)

- Plenty of experience in $r$-space ($\sim 50$ years)
- Very little is CI/$k$-space
- ‘Fourier’ transform of $r$-space wave functions (e.g. Jastrow-Slater) does not work
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**Can we get known CI w.f.s to work with MC?**

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Antisymmetric geminal power

- For even $N$

$$|\Phi_{AGP}\rangle = \left(\phi_{ij} a_i^\dagger a_j^\dagger\right)^{N/2} |0\rangle$$

- For odd $N$, we put the additional particle in a general sp orbital

- Fast algorithms: $\langle n|\Phi_G\rangle$ is a Pfaffian ($\sim N^3$).

- Very flexible: can include different kinds of 2b correlations

- HFB, BCS, HF are special cases
Trapped unitary fermi gas

- Atoms in a harmonic trap
- Contact interaction among $\uparrow$ and $\downarrow$ spins only
- In this case $\langle n|\Phi_G\rangle$ is a determinant!

Coupled Cluster wave functions

\[ |\Phi_{CC}\rangle = e^T |\Phi_0\rangle \]

\[ T = \sum t_i^a a_a^\dagger a_i + \sum t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \ldots \]

- Different truncations for \( T \) lead to different approximations \( \text{CCD, CCSD, CCSDT} \ldots \)
- Accurate: \( \text{CCSD}(T) \) is ‘gold standard’ in chemistry ✓
- Energies not variational in the standard approach ✗

Can we calculate \( \langle n | \Phi_{CC} \rangle \) quickly?
The magic formula

Start with Coupled Cluster Doubles (good for uniform systems):

\[ \Phi_{\text{CCD}}^m (p_1 p_2 \cdots p_m h_1 h_2 \cdots h_m) = \Phi_{\text{CCD}}(n) \]

for

\[ |n\rangle = a_{p_1}^\dagger \cdots a_{p_m}^\dagger a_{h_1} \cdots a_{h_m} |\Phi_{\text{HF}}\rangle \]

Recursive formula:

\[ \Phi_{\text{CCD}}^m (\cdots) = \sum_{\gamma=2}^m \sum_{\mu<\nu} (-)^{\gamma+\mu+\nu} t_{h_1 h_\gamma}^{\mu \nu} \Phi_{\text{CCD}}^{m-2} (\cdots) \]

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- Can be easily generalized to CCSD, CCSDT ...
- Scaling only with \# \( ph \)
- No scaling with particle number or basis size!

Results for 3DEG

- The 3d electron gas is the canonical long range Hamiltonian.
- Good benchmark, many calculations available

How to do CIMC?

- Lattice in momentum space
- Single particle basis = plane waves
- Include all sp states up to some $k^2 \leq k_{\text{max}}$

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- CCD + CIMC captures $\sim 95\%$ of the correlation energy
- No adjustable parameters in the wf
- Accuracy comparable to $r$-space MC
- Can improve systematically: CCDT, …

What have we achieved, so far?

- Formulated ‘Fixed-node’ DMC in CI/k-space ✔
- Shown how to use two well known classes of accurate wave functions as importance functions ✔
- Supervariational energies from CC wave functions
  Remember
  \[ E_{GS} \leq E_{CIMC} \leq \langle \Phi_G | H | \Phi_G \rangle \]
  when \( \Phi_G \equiv \Phi_{CC} \)
  \[ E_{GS} \leq E_{CIMC} \leq \langle \Phi_{CC} | H | \Phi_{CC} \rangle \quad \text{✔✔✔!!!} \]
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\[ E_{GS} \leq E_{\text{CIMC}} \leq \langle \Phi_{\text{CC}} | H | \Phi_{\text{CC}} \rangle \ ✓ ✓ ✓ !!! \]
But, we can do better . . .

Sign-structure important, not exact amplitudes

- \( \text{CCD(1)} = \text{CCD wf with amplitudes taken from 2nd order perturbation theory} \)
- \textbf{Huge} saving in computational time
- Can be very important for CCSD(T)
Fringe benefits: momentum distribution

- Difficult in r-space MC
- However, its diagonal in k-space ✓
- We can even calculate pure estimators ✓
  - Typically in DMC/GFMC one calculates $\langle \Phi_G | O | \Psi \rangle$
  - Not the same as $\langle \Psi | O | \Psi \rangle$, if $[O, H] \neq 0$
  - But in CIMC we can calculate $\langle \Psi | O | \Psi \rangle$ using the Feynman-Hellmann theorem

$$\langle \Psi | n_k | \Psi \rangle = \left. \frac{\partial \langle H + \alpha n_k \rangle}{\partial \alpha} \right|_0 = \langle \Phi_G | n_k | \Psi \rangle - \text{const.} \times \text{cov}(E, n_k)$$

No need to calculate numerical derivatives! ✓

Gaudin & Pitarke, PRL (2007)
Roggero, AM & Pederiva, in preparation
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Rogero, AM & Pederiva, in preparation
We want to calculate quantities like this

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathbb{R}^n} d\phi \mathcal{O}(\phi) e^{-S(\phi)}}{\int_{\mathbb{R}^n} d\phi e^{-S(\phi)}}$$

If $S(\phi)$ is not real, we have a sign problem.

Can we do better by letting $\phi$ venture into the complex plane?
Successive complexification of life
Successive complexification of life

\[ S(\phi) \]

Saddle point of \( S(\phi) \)

\[ \Re \phi \quad \Im \phi \]
Successive complexification of life

Saddle point of $S(\phi)$
Successive complexification of life

Saddle point of $S(\phi)$
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Steepest descent

\[ d_{\tau} \phi = -\overline{\partial_{\phi} S} \]

Saddle point of \( S(\phi) \)
Successive complexification of life

Steepest descent

\[ d_{\tau}\phi = -\overline{\partial_{\phi} S} \]

Saddle point of \( S(\phi) \)

- \( \Im S(\phi) \) is constant on SD path
- No sign problem from the action! ✓
- \( \Re S(\phi) \) is bounded below on SD path ✓
Life and times on the Lefschetz thimble

- A Lefschetz thimble is a many dimensional generalization of the paths of steepest descent
- It is the union of all paths of steepest descent which end at the saddle point at $\tau \to \infty$
- It is a $n$-dimensional object ✓
- On the Lefschetz thimble

$$\langle O \rangle = \frac{e^{-i\mathcal{S}} \int_{\mathcal{J}} d\phi \mathcal{O}(\phi) e^{-\mathcal{RS}(\phi)}}{e^{-i\mathcal{S}} \int_{\mathcal{J}} d\phi e^{-\mathcal{RS}(\phi)}}$$

Constant

Non-trivial measure
One-link model: \( S(\phi) = -i\beta \cos(\phi) \)
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$\cos(\text{arg} \{J_\eta e^{-\mathcal{S}}\})$

$|J_\eta e^{-\mathcal{S}}|$

Gaussian
$N_\tau = 6$
$N_\tau = 20$
$N_\tau = 200$

$A M, M. \text{ Cristoforetti \& L. Scorzato, in preparation}$
Complex $\phi^4$ theory

$\langle e_{S_I} \rangle$

$4^4$ $6^4$ $8^4$

$0.5$ $0.6$ $0.7$ $0.8$ $0.9$ $1$ $1.1$ $1.2$ $1.3$

$0$ $0.1$ $0.2$ $0.3$ $0.4$ $0.5$ $0.6$ $0.7$ $0.8$ $0.9$ $1$


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Complex $\phi^4$ theory

\begin{center}
\includegraphics[width=\textwidth]{complex.phi4_theory.png}
\end{center}

Details

Q How to sample on the Lefschetz thimble?
We have used two different algorithms
- Langevin dynamics, improved version in progress
- Mapping Lefschetz thimble $\rightarrow$ flat manifold + Metropolis

Q What about the measure?
Need to calculate the Jacobian of the tangent space

Q Does the measure lead to a sign problem?
We cannot prove that it does not, but
- Leading order = 1
- Fluctuations small where $e^{-\Omega S}$ large

Q Enough to integrate on one (or a small #) thimble(s)?
Strong arguments in favor, but no rigorous proof
THE END
Fixing the sign problem in Fock space

- Comes from the Hamiltonian (if $H_{mn} > 0$ for $m \neq n$)
- Carrying walker sign leads to a null state
- No concept of ‘continuity’ in discrete Fock space
- Node fixing not possible 😞

Fixed ‘sign’ Hamiltonian

$$[H_\gamma]_{mn} = \delta_{mn} \{H_{mn} + (1 + \gamma) \sum_{s_{nn'} > 0} \Phi_G(n')H_{n'n}\Phi_G(n)^{-1}\}$$

$$+ (1 - \delta_{mn})\{\gamma \Theta(s_{mn}) + \Theta(-s_{mn})\}H_{mn}$$

where $s_{mn} = \text{sign}\{\Phi_G(m)H_{mn}\Phi_G(n)^{-1}\}$
Fixing the sign problem in Fock space

\[
[\mathcal{P}_\gamma]_{mn} = \Phi_G(m) \left\{ \delta_{mn} - \Delta \tau \left( [\mathcal{H}_\gamma]_{mn} - E_T \delta_{mn} \right) \right\} \Phi_G^{-1}(n)
\]

- \( \mathcal{H}_{\gamma=-1} = \mathcal{H} \)
- \( \mathcal{H}_{0\leq\gamma\leq1} \) has no sign problem by construction
- GS energies of \( \mathcal{H}_{0\leq\gamma\leq1} \) provide upper bounds for the GS energy of \( \mathcal{H} \)
- So does any linear extrapolation to \( \gamma = -1 \)

*ten Haaf et al., PRB (1995); Sorella & Capriotti, PRB (2000); Beccaria, PRB (2001)*


Our tightest upper bound for GS energy of \( \mathcal{H} \) is:

\[
E_{\text{CIMC}} = 2E_{\text{GS}[\mathcal{H}_{\gamma=0}]} - E_{\text{GS}[\mathcal{H}_{\gamma=1}]}
\]