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Joint DEMOCRITOS - ICTP School on
CONTINUUM QUANTUM MONTE CARLO METHODS
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AUXILIARY FIELD QUANTUM MONTE CARLO

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These are preliminary lecture notes, intended only for distribution to participants.

Quantum Monte Carlo methods using auxiliary fields

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OUTLINE

1) Introduction to auxiliary-field (AF) methods

- What is the relation with diffusion Monte Carlo? Why are they useful?
- Toy problem to set up “the language”
- Standard AF QMC and sign problem

2) Branching random walks in Slater determinant space

- Connection with DMC
- Bosons?

3) Sign problem for model Hamiltonians and how to control it

4) Phase problem for realistic Hamiltonians and how to control it

5) Finite-temperature formulation

6) Illustrative results

Overview of QMC methods

QMC methods *loosely* divide into two categories according to primary applications:

	Continuum	Lattice
<i>Applications</i>	<ul style="list-style-type: none">• electronic structure• quantum chemistry• ^3He• few-body nuclei	<ul style="list-style-type: none">• correlated electron models• nuclear shell model• quantum field theory
	GROUND-STATE:	
<i>Algorithm</i>	Diffusion MC	auxiliary-field/projector QMC ← (1)
<i>Description</i>	<ul style="list-style-type: none">- random walks- 1st quantized form- in configuration space	<ul style="list-style-type: none">- auxiliary-fields- 2nd quantized form
<i>Sign problem</i>	fixed-node approximation	constrained path MC ← (2) + (3)

Overview of QMC methods

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<hr/> FINITE-TEMPERATURE: <hr/>		
<i>Algorithm</i>	Path-Integral MC	QMC/BSS \leftarrow (1)
<i>Description</i>	- Mapping to classical ring-polymer system.	- related to above - grand canonical ensemble
<i>Sign problem</i>	restricted path appr.	“new” finite- T method \leftarrow (5)

- Cross-fertilization: e.g., GFMC \Rightarrow lattice models (*Ceperley, Sorella, ...*)
- The reverse: auxiliary-field \Rightarrow continuum (realistic systems) has appealing features but had *phase problem* \leftarrow a new method now makes this practical (2) + (4)

Standard ground-state QMC methods

To project ground state $|\Psi_0\rangle$ of many-body Hamiltonian \hat{H} ,

$$|\Psi^{(n+1)}\rangle = e^{-\tau\hat{H}} |\Psi^{(n)}\rangle \xrightarrow{n \rightarrow \infty} |\Psi_0\rangle$$

τ : small positive cnsnt $|\Psi^{(0)}\rangle$: arbitrary

Difference in methods:

different ways of realizing above process **stochastically** **1/sqrt scaling of MC**

- Diffusion Monte Carlo (DMC)
- Auxiliary-field methods

Diffusion Monte Carlo (DMC)

Summary

- $\Psi_0(R) = \langle R | \Psi_0 \rangle$ obtained by random walks in electronic configuration space
 $|R\rangle = |\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\rangle$
- Has been applied to atoms, molecules, clusters, solids, etc
- Is the more mature and more established method for continuum systems

Issues

- Reducing systematic errors — we would like the calculation to find the right answer even when we can't be as sure about the quality of the trial w.f.
 - Fermion sign problem:
fixed-node approximation depends on trial w.f.
 - Technical problem with treating core electrons:
locality approximation — used to deal with non-local pseudo-potentials — depends on overall quality of trial w.f. (not just the node)
- Calculations of off-diagonal observables and correlation functions
- Efficiency: human (e.g., trial w.f. optimization) and machine

Auxiliary-field quantum Monte Carlo (AF QMC)

Why study it?

- It is a different QMC method, applied to many “lattice” problems, with interesting and useful connections to DMC/PIMC
- It is developing into a method for continuum systems also, *complementary* to DMC. Early results show much promise in addressing some of the issues of DMC.

What is the basic idea?

- For any given single-particle basis, the Hamiltonian of a many-body system with 2-body interactions can be written as

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_{i,j} T_{ij} c_i^\dagger c_j + \sum_{i,j,k,l} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

where i, j, k, l run through the basis, and all matrix elements are known.

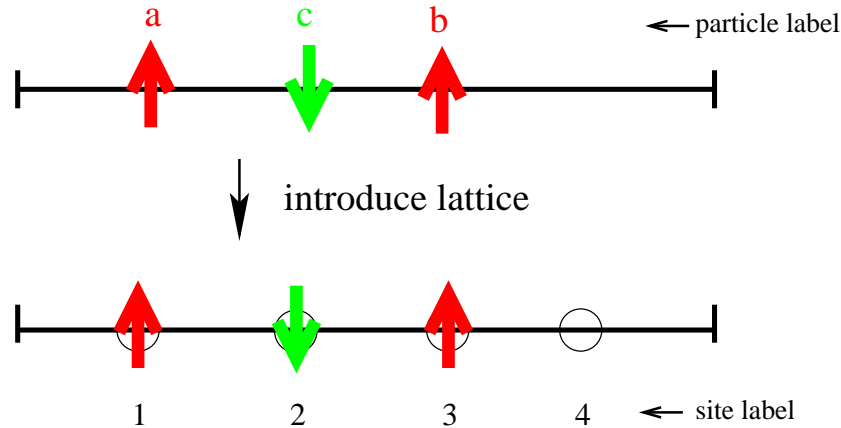
- The QMC method calculates the ground-state (or finite- T) properties of \hat{H} .
- The “walker” in this case is a Slater determinant formed by single-particle orbitals, i.e., it looks like the occupied manifold of a DFT or HF solution, except the orbitals undergo random walks.

AF QMC — introduction

A toy model of trapped alkali fermion atoms:

- 3 fermions in a box, two with \uparrow spin and one with \downarrow spin;
contact interaction $V(R) = a_s \delta(r_a - r_c) + a_s \delta(r_b - r_c)$

(no s -wave bt. **a** & **b**)



- Use a crude lattice basis with $i = 1, 2, 3, 4$ sites (circles). In second quantized form:

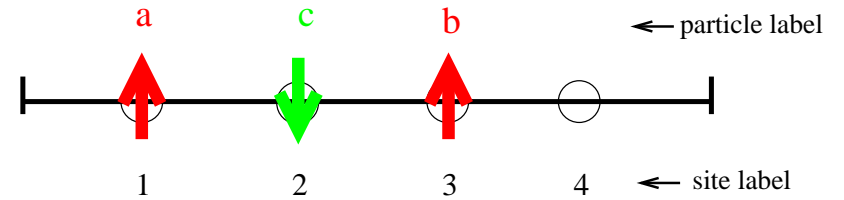
$$H = K + V = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

\swarrow near-neighbor

- Parameters: t ; $U \propto a_s$

A toy problem

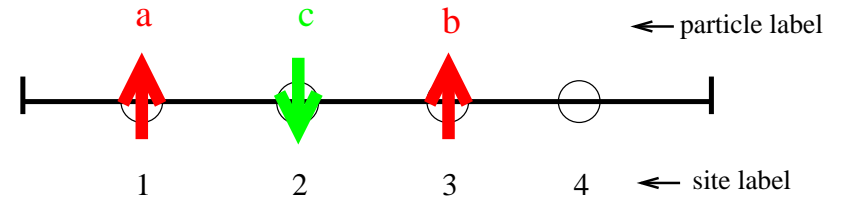
Hubbard model of trapped atoms:



- What is the ground state when $U = 0$, *i.e.*, *without interaction*?
 - Diagonalize single-particle Hamiltonian directly

A toy problem

Hubbard model of trapped atoms:



- What is the ground state when $U = 0$, *i.e.*, *without interaction*?
 - Diagonalize single-particle Hamiltonian directly
 - Alternatively, use power method to obtain $|\Psi_0\rangle$

$$e^{-\tau H} : \quad \left(4 \times 4 \right) \otimes \left(4 \times 4 \right) \equiv B_K \text{ operate on any } |\Psi^{(0)}\rangle \text{ repeatedly} \Rightarrow |\Psi_0\rangle$$

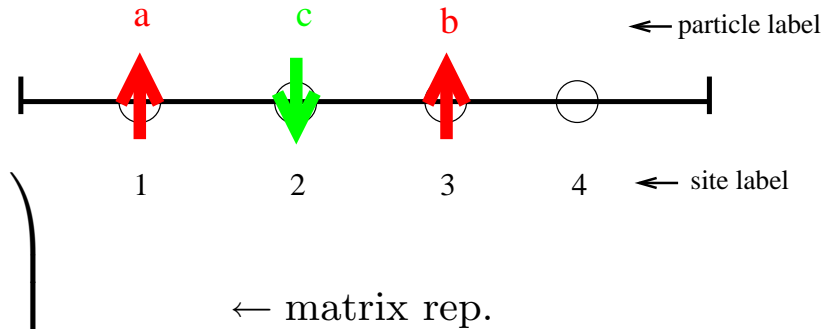
Theorem: For any $\hat{v} = \sum_{ij} v_{ij} c_i^\dagger c_j$,
 $e^{\hat{v}} |\phi\rangle = |\phi'\rangle$ where $\Phi' \equiv e^v \Phi$ in matrix form

- * Note re-orthogonalizing the orbitals prevents fermions from collapsing to the bosonic state — eliminates DMC sign problem for non-interacting systems

AF QMC — introduction

Properties of Slater determinants:

$$|\phi\rangle : \Phi = \begin{pmatrix} 0.37 & -0.60 \\ 0.60 & -0.37 \\ 0.60 & 0.37 \\ 0.37 & 0.60 \end{pmatrix} \otimes \begin{pmatrix} 0.37 \\ 0.60 \\ 0.60 \\ 0.37 \end{pmatrix}$$

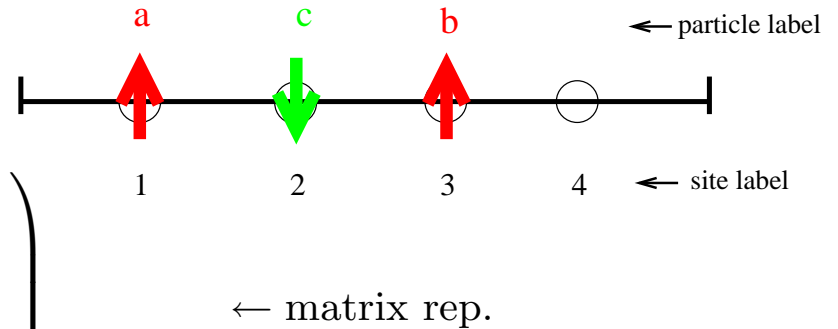


- What is the probability to find the electron configuration shown in the picture?
That is, how to calculate $\langle R|\phi\rangle$?
- How to calculate $E_0 = \langle \phi|H|\phi\rangle$ from the wave function?
- How to calculate the density matrix? The spin-spin correlation function?

AF QMC — introduction

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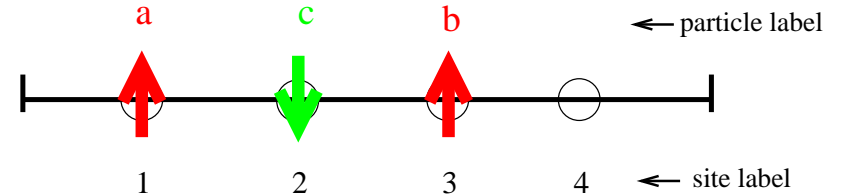


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A: Simple matrix manipulations (See Lab exercises)

A toy problem

Hubbard model of trapped atoms:



- What is the ground state when $U = 0$, *i.e.*, *without interaction*?
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$$e^{-\tau H} : \quad \left(4 \times 4 \right) \otimes \left(4 \times 4 \right) \equiv B_K \quad \text{operate on any } |\Psi^{(0)}\rangle \text{ repeatedly} \quad \Rightarrow |\Psi_0\rangle$$

- What is the ground state, now $U \neq 0$, *i.e.*, *with interaction*?
 - Diagonalizing many-body H involves a matrix whose size grows rapidly with N and M_\uparrow or M_\downarrow (Lanczos method)
 - Can we still write $e^{-\tau H}$ in one-body form?
Yes — **Hubbard-Stratonovich transformation**

AF QMC — introduction

Hubbard-Stratonovich transformation

- Interacting two-body problem can be turned into a **linear combination** of **non-interacting problems** living in **fluctuating external fields** ('completion of square'):

$$e^{\tau \hat{v}^2} \xrightarrow{\text{Hubbard-Stratonovich transformation}} \int e^{-\sigma^2/2} e^{\sigma \sqrt{\tau} \hat{v}} d\sigma \quad \sigma : \text{auxiliary field}$$



$$\hat{v} = \sum v_{ij} c_i^\dagger c_j : \text{one-body operator}$$

- Illustration of HS transformation — Hubbard-like interaction:

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} \rightarrow e^{\tau U (n_{i\uparrow} - n_{i\downarrow})^2 / 2} = \text{factor} \times \int e^{-\frac{1}{2} x^2} e^{\sqrt{\tau U} x (n_{i\uparrow} - n_{i\downarrow})} dx$$

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} \rightarrow e^{-\tau U (n_{i\uparrow} + n_{i\downarrow})^2 / 2} = \text{factor} \times \int e^{-\frac{1}{2} x^2} e^{\sqrt{\tau U} i x (n_{i\uparrow} + n_{i\downarrow})} dx$$

Or trick by Hirsch:

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} = e^{-\tau U (n_{i\uparrow} + n_{i\downarrow}) / 2} \cdot \sum_{x=\pm 1} \frac{1}{2} e^{\gamma x (n_{i\uparrow} - n_{i\downarrow})} \quad \cosh \gamma = e^{\tau U / 2}$$

AF QMC — introduction

Back to toy problem

Hubbard-Stratonivich transformation

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} = \text{factor} \times \sum_{x=\pm 1} \frac{1}{2} e^{\gamma x n_{i\uparrow}} e^{-\gamma x n_{i\downarrow}} \quad \cosh \gamma = e^{\tau U/2}$$

$$e^{-\tau H} = \int d\mathbf{x} p(\mathbf{x}) \begin{pmatrix} e^{\gamma x_1} & 0 & 0 & 0 \\ 0 & e^{\gamma x_2} & 0 & 0 \\ 0 & 0 & e^{\gamma x_3} & 0 \\ 0 & 0 & 0 & e^{\gamma x_4} \end{pmatrix} \cdot B_{K,\uparrow} \\ \otimes \begin{pmatrix} e^{-\gamma x_1} & 0 & 0 & 0 \\ 0 & e^{-\gamma x_2} & 0 & 0 \\ 0 & 0 & e^{-\gamma x_3} & 0 \\ 0 & 0 & 0 & e^{-\gamma x_4} \end{pmatrix} \cdot B_{K,\downarrow}$$

$B(\mathbf{x})$ 1-particle propagator

$$e^{-\tau H} = \int p(\mathbf{x}) B(\mathbf{x}) d\mathbf{x}$$

$$\mathbf{x} \equiv \{x_1, x_2, x_3, x_4\}$$

$U \neq 0$ is the same as $U = 0$, except integral/sum over \mathbf{x} — Monte Carlo!

Auxiliary-field quantum Monte Carlo (AF QMC)

Standard ground-state AF QMC

Sugiyama & Koonin '86

$$\langle \hat{O} \rangle = \frac{\langle \Psi^{(0)} | e^{-\tau H} \dots e^{-\tau H} \hat{O} e^{-\tau H} \dots e^{-\tau H} | \Psi^{(0)} \rangle}{\langle \Psi^{(0)} | e^{-\tau H} \dots e^{-\tau H} e^{-\tau H} \dots e^{-\tau H} | \Psi^{(0)} \rangle}$$

↓

$$e^{-\tau H} = \int p(\mathbf{x}) B(\mathbf{x}) d\mathbf{x}$$

$$\frac{\int p(\mathbf{x}^{(1)}) \dots p(\mathbf{x}^{(2L)}) \langle \Psi^{(0)} | B(\mathbf{x}^{(2L)}) \dots B(\mathbf{x}^{(L+1)}) \hat{O} B(\mathbf{x}^{(L)}) \dots B(\mathbf{x}^{(1)}) | \Psi^{(0)} \rangle d\mathbf{x}^{(1)} \dots d\mathbf{x}^{(2L)}}{\int p(\mathbf{x}^{(1)}) \dots p(\mathbf{x}^{(2L)}) \langle \Psi^{(0)} | B(\mathbf{x}^{(2L)}) \dots B(\mathbf{x}^{(L+1)}) B(\mathbf{x}^{(L)}) \dots B(\mathbf{x}^{(1)}) | \Psi^{(0)} \rangle d\mathbf{x}^{(1)} \dots d\mathbf{x}^{(2L)}}$$

Choose $|\Psi^{(0)}\rangle$ as a Slater determinant

$$B(\mathbf{x})|\phi\rangle = |\phi'\rangle$$

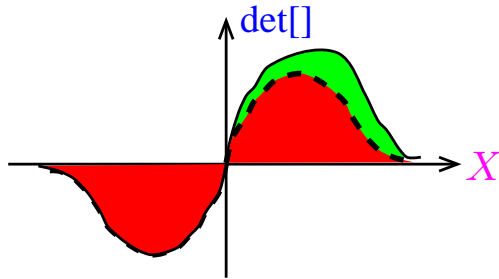
Many-dim integral can be done by Monte Carlo: $\frac{\int O_{\text{Gr}}(\mathbf{X}) p(\mathbf{X}) \det[\mathbf{X}] d\mathbf{X}}{\int p(\mathbf{X}) \det[\mathbf{X}] d\mathbf{X}} \quad \mathbf{X} \equiv \{\mathbf{x}^{(l)}\}$

Applications mostly to “simple models”:

- Hubbard model, impurity models in condensed matter
- nuclear shell model
- lattice QCD

Auxiliary-field quantum Monte Carlo (AF QMC)

Sign problem in standard AF QMC:



As system size grows, average sign of $\det[] \rightarrow 0$ exponentially.

\Rightarrow exponential scaling

- Sign problem is often most severe where the physics is most interesting, for example, in 2-D Hubbard model when number of electrons $\sim 85\%$ number of lattice sites, where it is thought to model the CuO planes of high- T_c cuprates
- In fact, a **phase (not just sign) problem** appears for general 2-body interactions.

Random walks in Slater determinant space:

Zhang, Carlson, Gubernatis, '97; Zhang & Krakauer, '03

- Reformulate ground-state projection as random walks in Slater determinant space
- Necessary to control the sign/phase problem \leftarrow subtlety of projection in AF space

Random walks in Slater determinant space: preliminaries

- In general, we can choose any single-particle basis $\{|\chi_i\rangle\}$, with $i = 1, 2, \dots, N$
- A single-particle orbital (labeled by m) is given by $\hat{\varphi}_m^\dagger|0\rangle \equiv \sum_{i=1}^N \varphi_{i,m}|\chi_i\rangle$
- If we have M identical fermions ($M \leq N$), a Slater determinant $|\phi\rangle$ is given by:

$$|\phi\rangle \equiv \hat{\varphi}_1^\dagger \hat{\varphi}_2^\dagger \cdots \hat{\varphi}_M^\dagger |0\rangle$$

- $|\phi\rangle$ is represented by an $N \times M$ matrix:

$$\Phi \equiv \begin{pmatrix} \varphi_{1,1} & \varphi_{1,2} & \cdots & \varphi_{1,M} \\ \varphi_{2,1} & \varphi_{2,2} & \cdots & \varphi_{2,M} \\ \vdots & \vdots & & \vdots \\ \varphi_{N,1} & \varphi_{N,2} & \cdots & \varphi_{N,M} \end{pmatrix}$$

- E.g., $\langle\phi|\phi'\rangle = \det(\Phi^T \Phi')$; $G_{ij} \equiv \frac{\langle\phi|c_i^\dagger c_j|\phi'\rangle}{\langle\phi|\phi'\rangle} = [\Phi'(\Phi^T \Phi')^{-1} \Phi^T]_{ij}$;
any 2-body correlation $\leftarrow \{G_{ij}\}$

Random walks in Slater determinant space: preliminaries II

For example in electronic systems:

$$H = K + V_{e-I} + V_{e-e} + V_{I-I}$$

In plane-wave one-particle basis $|k\rangle \equiv \frac{1}{\sqrt{\Omega}} e^{i\mathbf{G}_k \cdot \mathbf{r}}$:

$$V_{e-I} = \sum_{i \neq j} V_{\text{local}}(\mathbf{G}_i - \mathbf{G}_j) c_i^\dagger c_j + \sum_{i,j} V_{\text{NL}}(\mathbf{G}_i, \mathbf{G}_j) c_i^\dagger c_j$$

$$V_{e-e} = \frac{1}{2\Omega} \sum_{i,j,\mathbf{Q} \neq 0} \frac{4\pi}{|\mathbf{Q}|^2} c_{\mathbf{G}_i + \mathbf{Q}}^\dagger c_{\mathbf{G}_j - \mathbf{Q}}^\dagger c_{\mathbf{G}_j} c_{\mathbf{G}_i}$$

$$\rightarrow -\frac{1}{2\Omega} \sum_{\mathbf{Q} \neq 0} \frac{4\pi}{|\mathbf{Q}|^2} \rho^\dagger(\mathbf{Q}) \underline{\rho(\mathbf{Q})}$$

↖ $\sum_i c_{\mathbf{G}_i + \mathbf{Q}}^\dagger c_{\mathbf{G}_i}$

$$\rightarrow \sum_{\mathbf{Q} \neq 0} \sqrt{\frac{4\pi}{|\mathbf{Q}|^2}} \left(\underbrace{[\rho^\dagger(\mathbf{Q}) + \rho(\mathbf{Q})]}_{i \hat{v}}^2 - \underbrace{[\rho^\dagger(\mathbf{Q}) - \rho(\mathbf{Q})]}_{\hat{v}'}^2 \right)$$

Random walks in Slater determinant space

For any given one-particle basis: $\hat{H} = H_1 + H_2 = \sum_{i,j} T_{ij} c_i^\dagger c_j - \sum \hat{v}^2$

$$\hat{v} = \sum v_{ij} c_i^\dagger c_j \quad \text{or} \quad \mathbf{i} \sum v_{ij} c_i^\dagger c_j$$

$$|\Psi^{(n+1)}\rangle = e^{-\tau H} |\Psi^{(n)}\rangle \rightarrow |\Psi_0\rangle$$

Write $e^{-\tau \hat{H}}$ in non-interacting form: $e^{-\tau \hat{H}} \propto e^{-\tau \hat{H}_1} \prod \int e^{-\sigma^2/2} e^{\sigma \sqrt{\tau} \hat{v}} d\sigma$

For any 1-body \hat{h} : $e^{\hat{h}} |\phi\rangle \longrightarrow |\phi'\rangle$

Random walk in Slater determinant space:

$$|\Psi^{(0)}\rangle \xrightarrow{e^{-\tau \hat{H}}} |\Psi^{(1)}\rangle \quad \dots \quad \rightarrow |\Psi_0\rangle$$

sample σ from $e^{-\frac{\sigma^2}{2}}$;

$$|\phi^{(0)}\rangle \xrightarrow{\text{apply 1-body propag.'s}} |\phi^{(1)}(\sigma)\rangle \rightarrow |\phi\rangle$$

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$$|\Psi_0\rangle \doteq \sum_{\phi} |\phi\rangle$$

New QMC method: Random walks in Slater determinant space

Standard DMC

$$|R\rangle = |\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\rangle$$

$$|\Psi_0\rangle = \sum_R \Psi_0(R) |R\rangle$$



$$|\Psi_0\rangle \doteq \sum_{\text{MC}} |R\rangle$$

Slater determinant RW

$$|\phi\rangle = |\psi_1, \psi_2, \dots, \psi_M\rangle$$

$$\sum_k c_{k,i} |\chi_k\rangle \quad \text{basis}$$

$$|\Psi_0\rangle = \sum_\phi \Psi_\phi |\phi\rangle$$



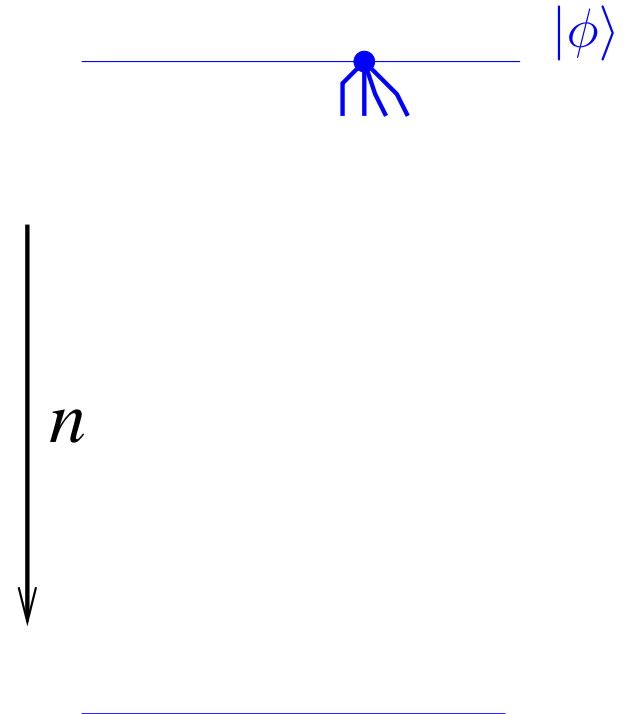
$$|\Psi_0\rangle \doteq \sum_{\text{MC}} |\phi\rangle$$

- The formalism is appealing — each random walker is a full Slater determinant
- Close formal relation to mean-field approaches. The QMC thus shares the same machinery as DFT or Hartree-Fock, using *any* one-particle basis
 - Second-quantization, antisymmetry automatically imposed
 - The single-particle problem (\hat{H}_1) is solved exactly, with no statistical error
 - Correlation effects are obtained by building stochastic ensembles of independent-particle solutions
- Core-electron problem: non-local pseudopotential can be implemented straightforwardly — *locality approximation* eliminated
- Convenient calculation of observables (including off-diagonal) and correlation functions, e.g., $\langle \phi' | c_i^\dagger c_j^\dagger c_k c_l | \phi \rangle$
- **But**

Sign problem for model Hamiltonians

Sign problem (if \hat{v} is real):

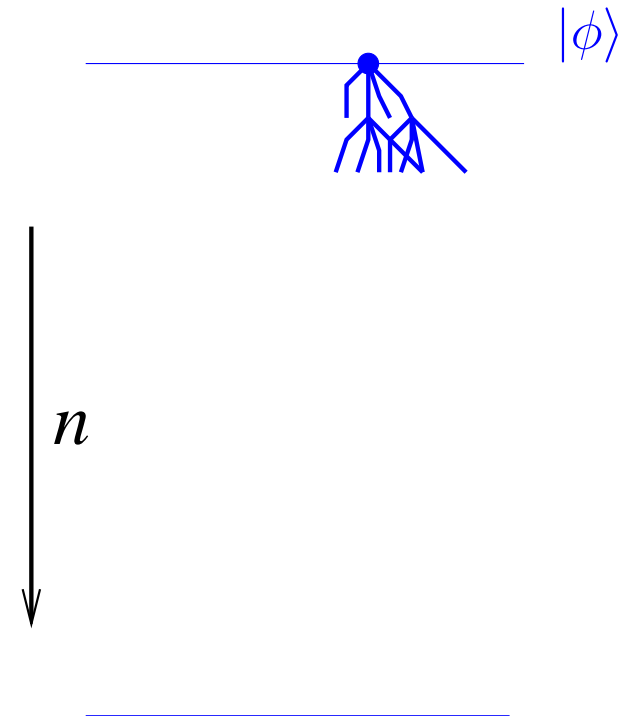
- $e^{-\tau\hat{H}}$ leads to paths in determinant space;
paths are “fractal”-like



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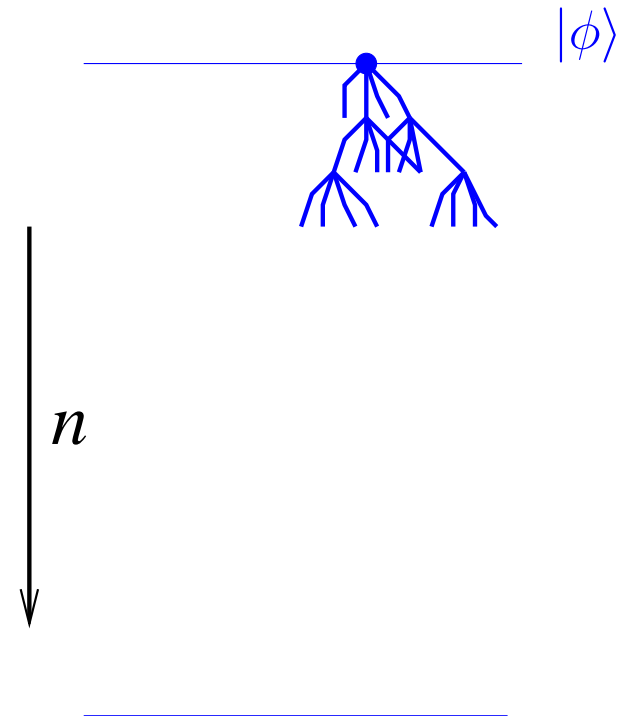
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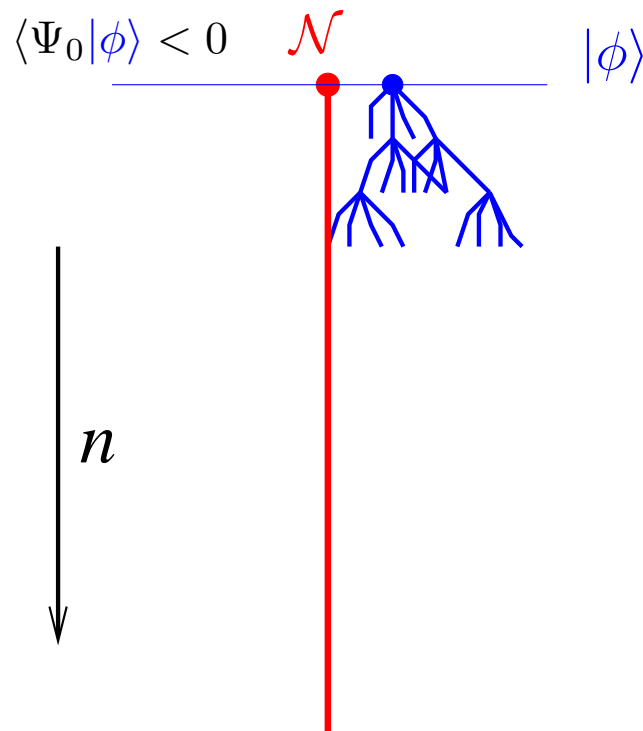
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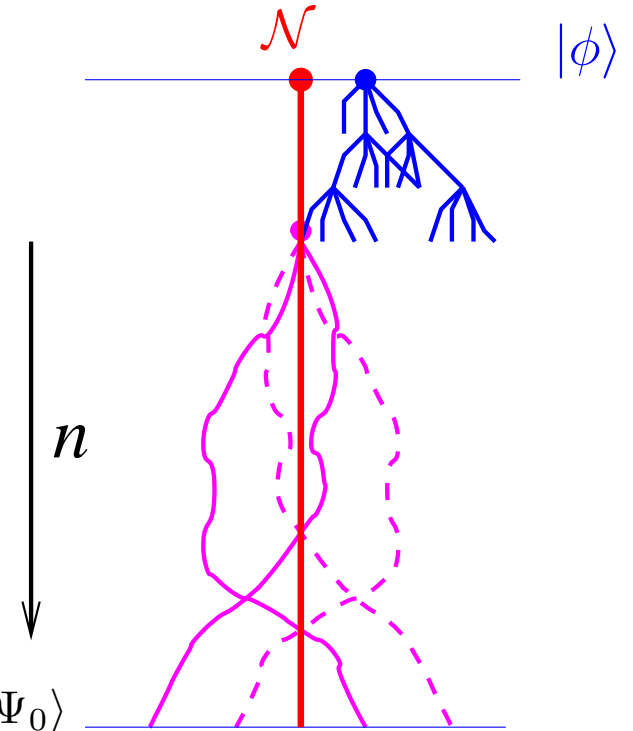
- $e^{-\tau\hat{H}}$ leads to **paths** in **determinant space**;
paths are “fractal”-like
- At $\tau \rightarrow 0$, **paths** are continuous
- Suppose the exact w.f. $|\Psi_0\rangle$ is known:
 - Define ‘**Node**’ \mathcal{N} : $\langle\Psi_0|\phi\rangle = 0$



Sign problem for model Hamiltonians

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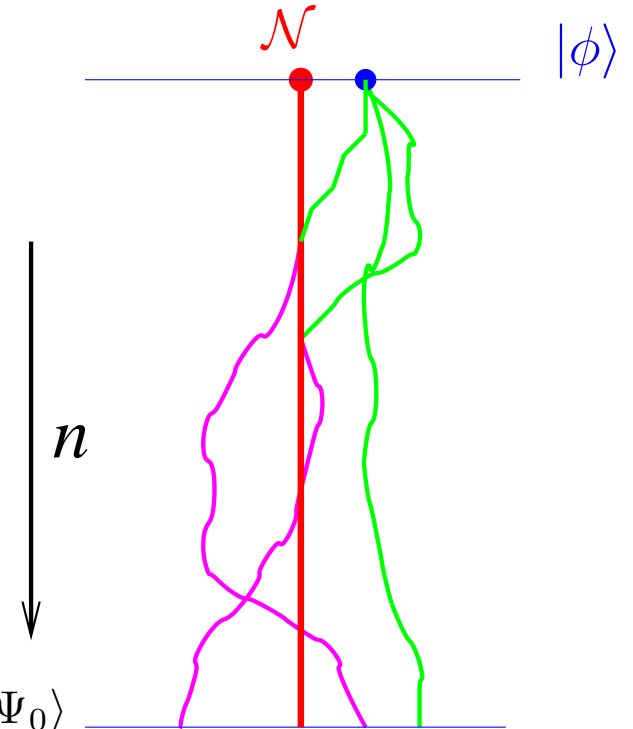
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- Suppose the exact w.f. $|\Psi_0\rangle$ is known:
 - Define ‘Node’ \mathcal{N} : $\langle\Psi_0|\phi\rangle = 0$
 - Consider a path that reaches \mathcal{N} for the first time
 - * $\langle\Psi_0|\phi\rangle = 0$
 - $\Rightarrow \langle\Psi_0|e^{-n\tau H}|\phi\rangle = 0$
 - \Rightarrow descendents of $|\phi\rangle$ collectively contribute 0 to $|\Psi_0\rangle$
 - * i.e., paths that reach \mathcal{N} become noise



Sign problem for model Hamiltonians

Sign problem (if \hat{v} is real):

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 - \Rightarrow descendants of $|\phi\rangle$ collectively contribute 0 to $|\Psi_0\rangle$
 - * i.e., paths that reach \mathcal{N} become noise
 - Only constrained paths contribute
- As n increases, MC Signal is exponentially small compared to noise (except for special cases e.g., 1/2-filled Hubbard where symmetry confines paths to one side)



Sign problem for model Hamiltonians — how to control it

The constrained path approximation: *Zhang, Carlson, Gubernatis, '97*

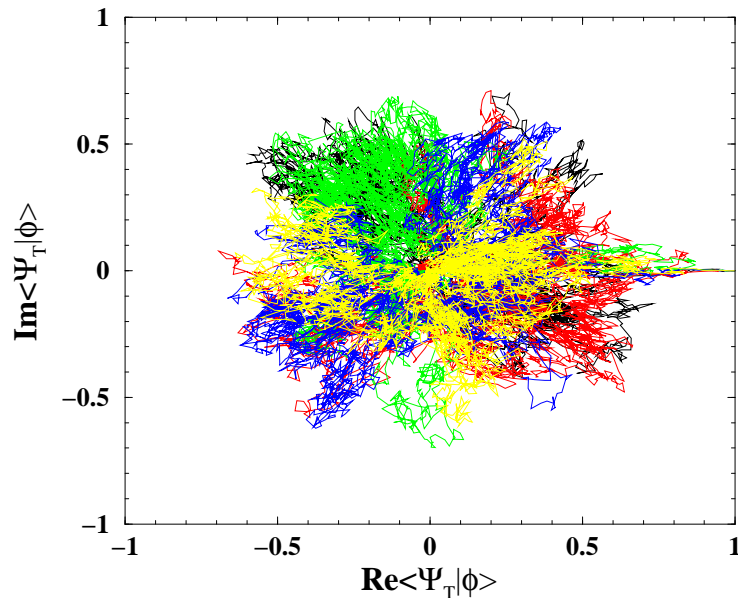
Paths that reach \mathcal{N} should be eliminated — require $\langle \Psi_T | \phi \rangle > 0$ for every $|\phi\rangle$,
with a trial wave function $|\Psi_T\rangle$

- Eliminates sign decay
- Becomes exact if $|\Psi_T\rangle$ is exact
- Is similar in spirit to fixed-node in DMC, but in different space — opportunities to do better ?

Phase problem for realistic Hamiltonians

Phase problem (if \hat{v} is complex):

“Rotational invariance” in Slater determinant space:



Problem!

Trajectories of 5 walkers (color) during the random walk, shown in the complex plane $\langle \Psi_T | \phi \rangle$.

- For all but a few special forms of interactions, this problem occurs, severely limiting the applicability of AF QMC.
- Straightforward generalization of constrained path approximation is not good.

New method: how to control the phase problem

Zhang and Krakauer, '03

(a) Phaseless formalism

- Seek MC representation of $|\Psi_0\rangle$ in the form: $|\Psi_0\rangle \doteq \sum_{\phi} \frac{|\phi\rangle}{\langle\Psi_T|\phi\rangle}$
i.e., the contribution of each $|\phi\rangle$ is independent of its phase (if $|\psi_T\rangle$ is exact)
- This is accomplished by an “importance-sampling” transformation to modify the propagator:

$$\int \langle\Psi_T|\phi'(\sigma)\rangle e^{-\frac{1}{2}\sigma^2} B(\sigma) d\sigma \frac{1}{\langle\Psi_T|\phi\rangle} = e^{-\tau\hat{H}_1} \int e^{-\sigma^2/2} e^{(\sigma-\bar{\sigma})\sqrt{\tau}\hat{v}} d\sigma e^{-\tau\text{Re}\{E_L(\phi)\}}$$

★ Force bias: $\bar{\sigma} \equiv -\frac{\langle\Psi_T|\sqrt{\tau}\hat{v}|\phi\rangle}{\langle\Psi_T|\phi\rangle}$ ← complex!

★ Local energy: $E_L(\phi) \equiv \frac{\langle\Psi_T|\hat{H}|\phi\rangle}{\langle\Psi_T|\phi\rangle}$

(b) Projection to break “rotational invariance”

- With (a), we can confine the RW to one overall phase (e.g., 0)
- This is accomplished by projecting the RW onto 1D: reducing the weight of a walker according to its phase change, e.g., by $\cos(\Delta\theta)$

New method for realistic Hamiltonians

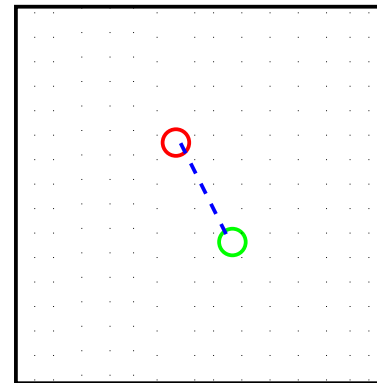
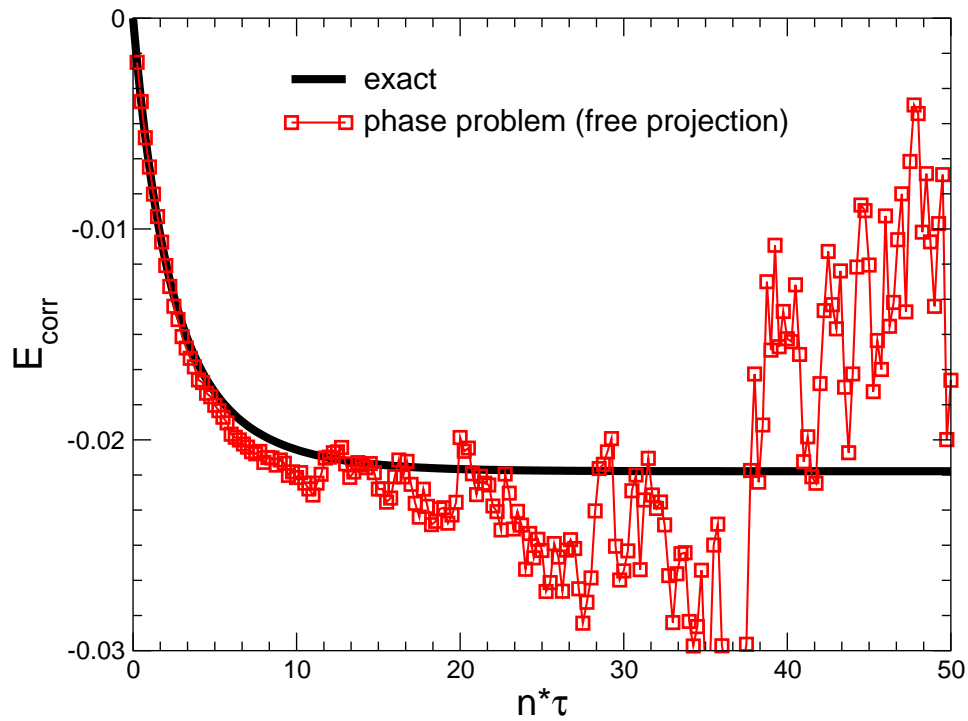
Comments

- **Approximate** — becomes exact if $|\Psi_T\rangle$ is exact
- No upper bound property — the mixed estimate of the ground-state energy is not variational.
- In “importance sampling” transformation in **(a)**, it is crucial to use $\langle\Psi_T|\phi\rangle$ (**complex**). Our conventional notion of probabilistic importance functions (**real positive**, or **modulus**) is not ‘forward-compatible’ with this, and leads to poor results.
- The “two-dimensionality” here seems unique, different from fixed-node or fixed-phase DMC, or Slater det. RW with a real \hat{v} . This makes step **(b)** necessary.
- The method reduces to the constrained path Monte Carlo method when \hat{v} is real.

New method for realistic Hamiltonians

Two-electron jellium:

- $r_s = 10$, $N = 19$ plane wave basis functions
- Correlation energy (in Ry) vs. projection time:



Periodic box (supercell)

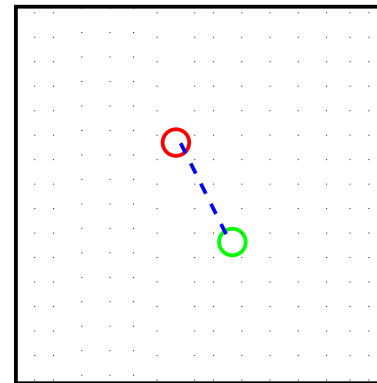
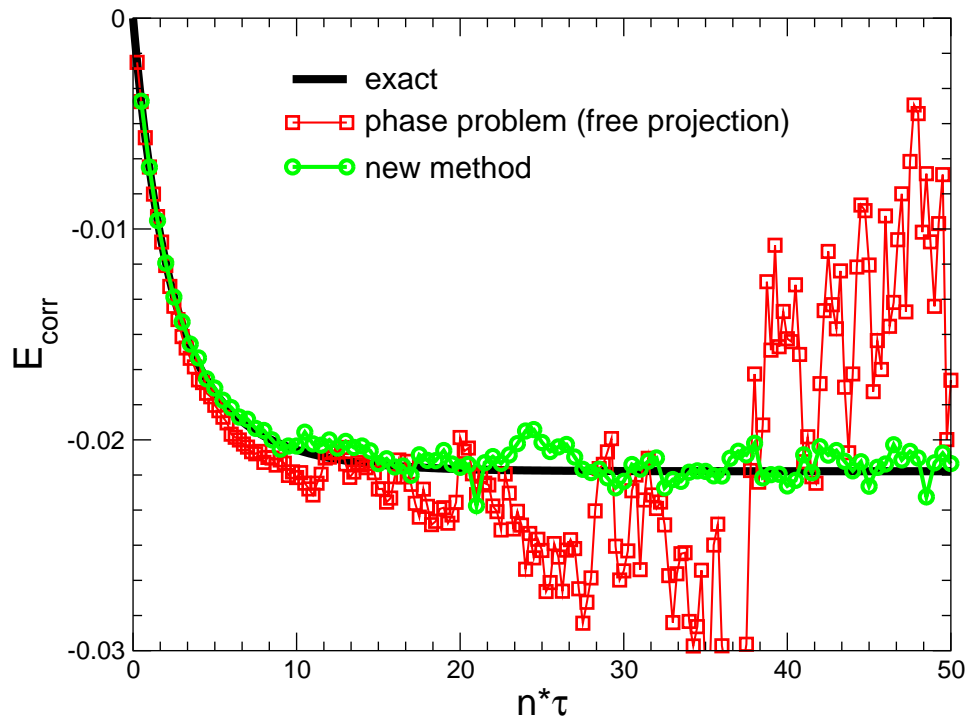
○ electron, spin \uparrow

○ electron, spin \downarrow

New method for realistic Hamiltonians

Two-electron jellium:

- $r_s = 10$, $N = 19$ plane wave basis functions
- Correlation energy (in Ry) vs. projection time:



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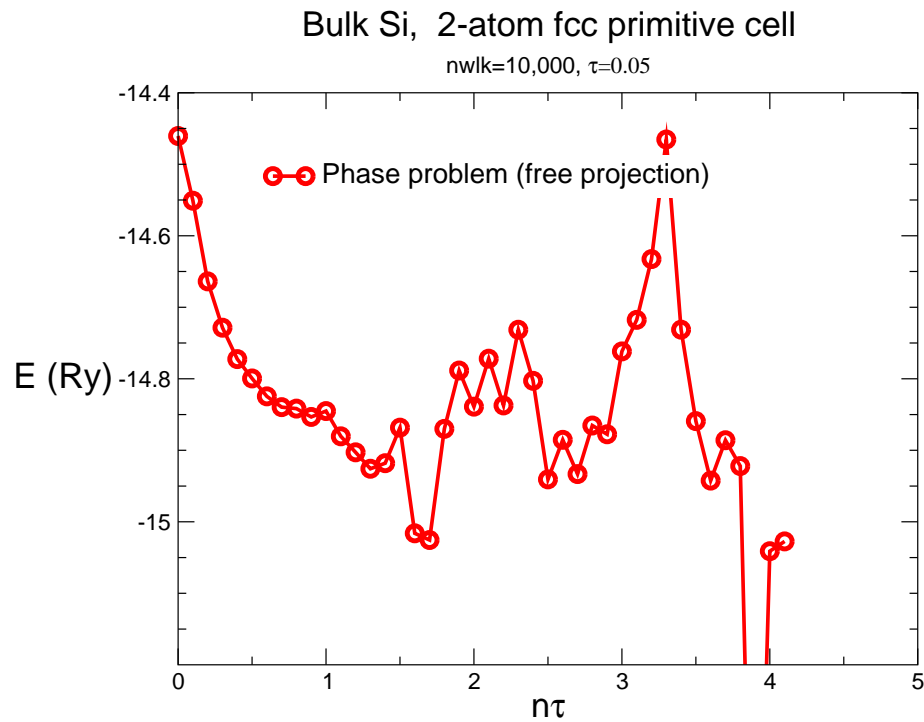
○ electron, spin \uparrow

○ electron, spin \downarrow

New method for realistic Hamiltonians

Two-atom Si fcc cell:

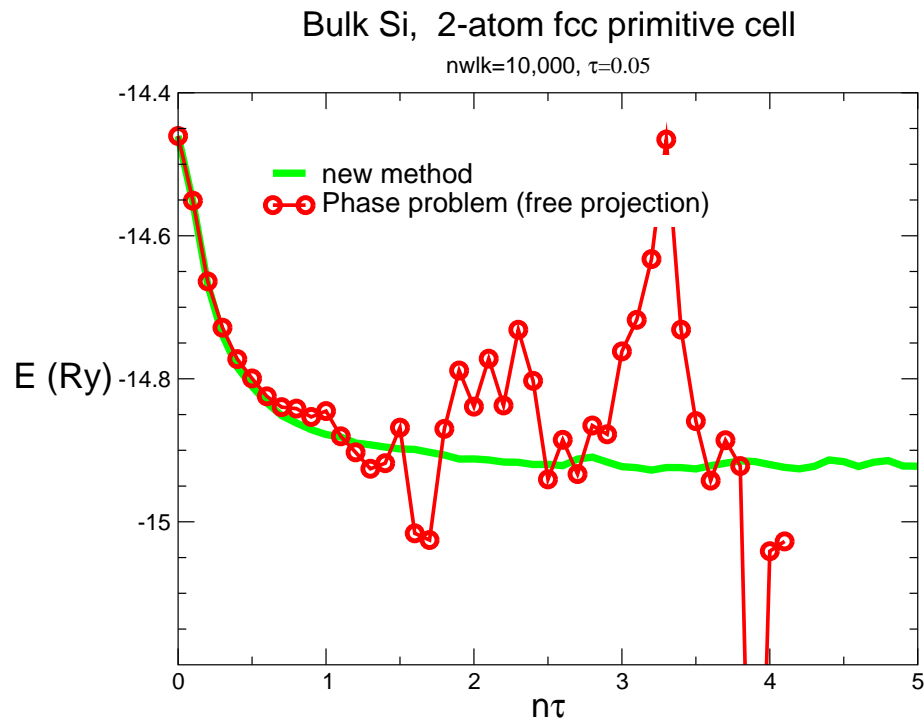
- 8 valence electrons
- Starting from LDA solution:



New method for realistic Hamiltonians

Two-atom Si fcc cell:

- 8 valence electrons
- Starting from LDA solution:



Finite- T method: preliminaries

Standard finite-T method *Blankenbecler, Scalapino, and Sugar, '81*

Partition function for Hamiltonian H is: ($\beta = 1/kT$)

$$\text{Tr}(e^{-\beta H}) = \text{Tr}(e^{-\tau H} e^{-\tau H} \dots e^{-\tau H})$$

Need:

$$e^{-\tau H} = \sum_{\mathbf{x}} B(\mathbf{x})$$

$$\langle O \rangle = \frac{\text{Tr}(O e^{-\beta H})}{\text{Tr}(e^{-\beta H})} = \frac{\sum_{\{\mathbf{x}_l\}} \text{Tr}(O B(\mathbf{x}_L) B(\mathbf{x}_{L-1}) \dots B(\mathbf{x}_1))}{\sum_{\{\mathbf{x}_l\}} \text{Tr}(B(\mathbf{x}_L) B(\mathbf{x}_{L-1}) \dots B(\mathbf{x}_1))}$$

Analytically evaluate trace: $\text{Tr}(e^{-\beta H}) = \sum_{\{\mathbf{x}_l\}} \det[I + B(\mathbf{x}_L) B(\mathbf{x}_{L-1}) \dots B(\mathbf{x}_1)]$

Sample fields $\{\mathbf{x}_l\}$ by Metropolis Monte Carlo to compute sum.

Sign Problem in standard finite-T AF QMC:

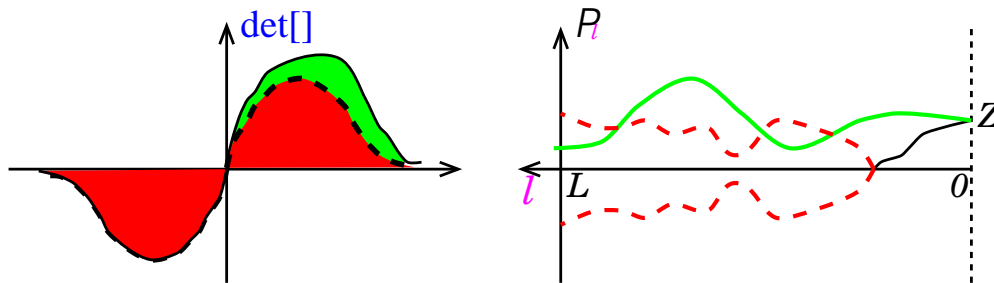
- As T lowers, average sign of $\det[] \rightarrow 0$ exponentially.
- We need to control the sign problem — focus on real auxiliary fields, i.e., real \hat{v}

Finite- T method: origin of the sign problem

Imagine introducing path integrals one time slice at a time: *Zhang, '99*

$$\begin{aligned}
 Z &= \text{Tr}(e^{-\tau H} e^{-\tau H} \dots e^{-\tau H} e^{-\tau H}) && P_0 \\
 &= \sum_{\{\mathbf{x}_1\}} \text{Tr}(e^{-\tau H} e^{-\tau H} \dots e^{-\tau H} B(\mathbf{x}_1)) && P_1(\{\mathbf{x}_1\}) \quad \leftarrow \text{integrand} \\
 &= \sum_{\{\mathbf{x}_1, \mathbf{x}_2\}} \text{Tr}(e^{-\tau H} e^{-\tau H} \dots B(\mathbf{x}_2) B(\mathbf{x}_1)) && P_2(\{\mathbf{x}_1, \mathbf{x}_2\}) \\
 &= \dots \\
 &= \sum_{\{\mathbf{x}_l\}} \det[I + B(\mathbf{x}_L) B(\mathbf{x}_{L-1}) \dots B(\mathbf{x}_1)] && P_L(\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_L\})
 \end{aligned}$$

Suppose we know $e^{-\tau H}$. Consider P_l :



- If $P_l = 0$, all future paths $\{\mathbf{x}_{l+1}, \mathbf{x}_{l+2}, \dots, \mathbf{x}_L\}$ collectively contribute 0 in Z .
- A complete path $\{\mathbf{x}_l\}$ contributes to Z **iff** $P_l > 0$ for all l .

Finite- T method: How to control the sign problem?

Constraint to control the sign problem

Require: $P_1(\{\mathbf{x}_1\}) > 0$; $P_2(\{\mathbf{x}_1, \mathbf{x}_2\}) > 0$; ...; $P_L(\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_L\}) > 0$.

- Constraint eliminates all noise paths ('dashed lines').
- In practice, we use **trial B_T** for $e^{-\tau H}$ — **approximate**.

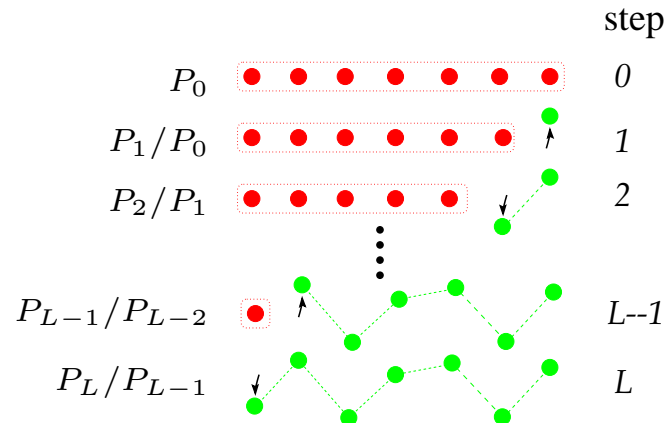
Monte Carlo sampling algorithm to incorporate constraint

If B_T is \sum (mean-field), then $\text{Tr} \rightarrow \det[\]$ in P_l .

Sampling — random walk of L steps:

Note:

$$P_L = \frac{P_L}{P_{L-1}} \frac{P_{L-1}}{P_{L-2}} \dots \frac{P_2}{P_1} \frac{P_1}{P_0} P_0$$

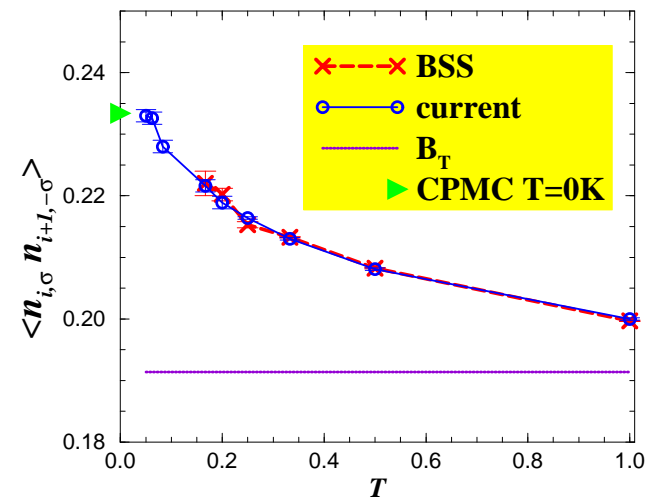
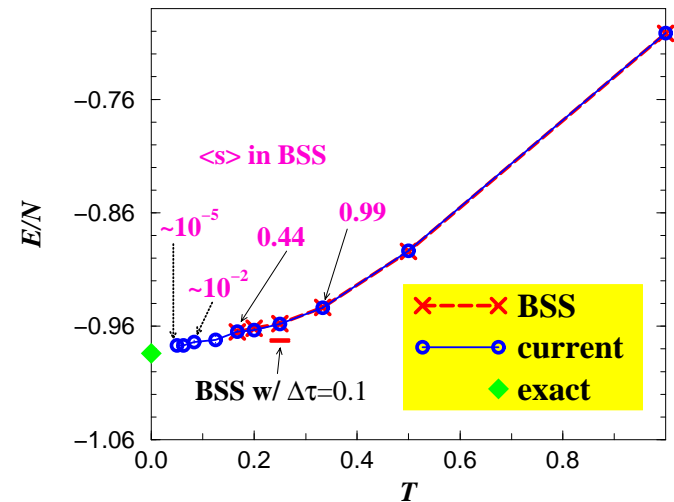


Test results

Benchmark results on 2-D Hubbard model for finite-T method

- Standard method limited to $\beta \sim 6$
- New method shown up to $\beta = 20$
- Excellent agreement:
 - high T : BSS
 - low T : $\rightarrow 0$ K exact
- B_T gives wrong physics
- Method still accurately predicts AF correlation

Benchmark on 4x4 with $U=4$ at $\langle n \rangle = 0.875$
sign problem severe



Test applications

Test applications of new phaseless Slater determinant RW method

- Plane-wave basis
- Kleinman-Bylander (KB) norm-conserving non-local pseudopotentials — straightforward to implement
- Same set-up as in a DFT calculation ($G, G' < E_{\text{cut}}$)
- Trial w.f. $|\psi_T\rangle$: single Slater determinant from LDA or HF
- Systems:
 - Si atom, dimer, and bulk (54 atom fcc supercell, 216 electrons)
 - Be, P, S atoms and dimers, TiO molecule
- **Collaborators:**
Henry Krakauer, Wissam Al-Saidi, Hendra Kwee, Milliga (Cherry) Suewattana

Test applications

Cohesive energy of bulk Si (eV):

	16-atom fcc	54-atom fcc	∞
LDA	3.836	4.836	5.086
QMC	3.79(4)	4.51(3)	4.59(3)
experiment			4.62(8)
DMC			4.63(2) [†]

[†] Leung *et.al.* 1999

- QMC results at ∞ are from 54-atom with finite-size corrections:
 - independent-particle correction (from LDA)
 - Coulomb correction from Kent *et.al.*, 1999
- Computational details:
 - $E_{\text{cut}} = 12.25\text{Ry}$; 5,209 plane waves
 - 216 electrons for 54-atom fcc supercell
 - KB pseudopotential (OPIUM); LDA done using ABINIT

Test applications

Binding energy of Be_2 (in eV) at expt bond length $4.63a_B$:

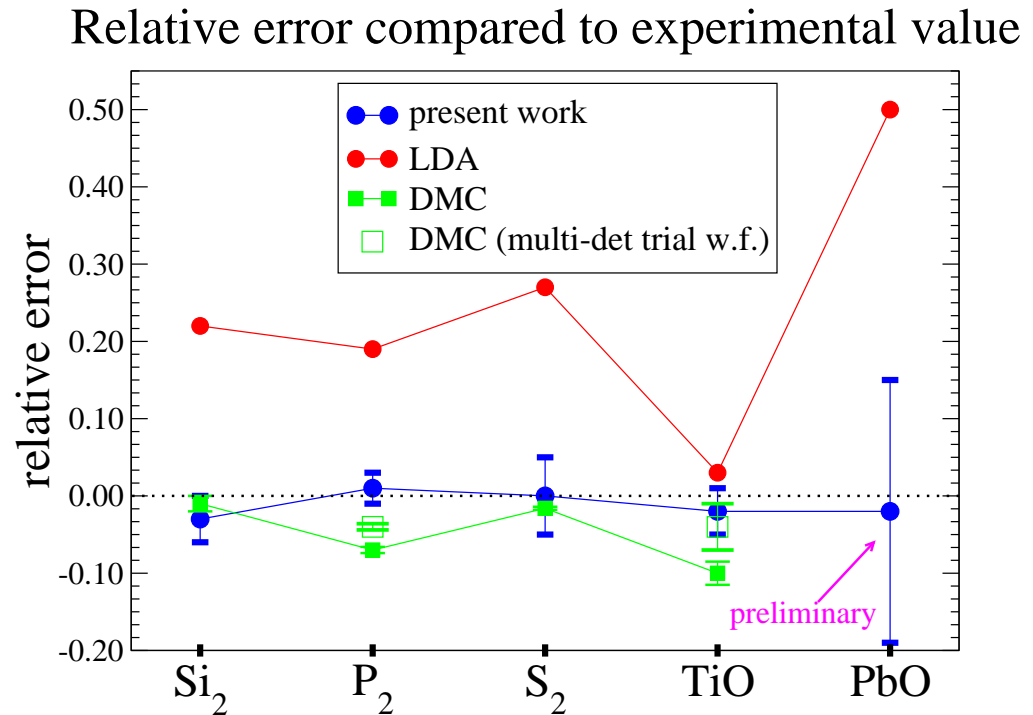
HF	unbound	
LDA	0.53	
present QMC	0.07(2)	LDA trial w.f.
experiment	0.11(1)	
DMC (psp)	0.05(3)	multi-determinant trial w.f. (Schautz et al, '98)
AF QMC (psp)	0.0(2)	phase problem (Baer et al '00)

- Difficult case because of near $2s$ and $2p$ degeneracy; full CI up to 1 billion det.'s !
- Standard DMC does not bind with optimized single Slater-determinant (\times Jastrow) trial wave functions

Test applications

Molecular binding energies:

- large supercells
- expt bond length
- s -, p -, and d -electrons
- P_2 :
 - Bad case for DMC (Grossman, '02)
 - Multi-det trial w.f.:
det's (66 for P; 269 for P_2)
× Jastrow
- S_2 :
 - Hartree-Fock w.f. (−40% error) gives same answer with present QMC method
- TiO: (preliminary)
 - Ti ($3s3p3d 4s$) included as valence electrons; $E_{\text{cut}} = 50\text{Ry}$; 11,197 plane waves
 - DMC results shown are with single- and multi-det HF trial w.f.'s (from Wagner and Mitas, Chem. Phys. Lett, '03)



What we have not covered

- Ground-state method for bosons (*Purwanto & Zhang, '04*)
 - Walker $|\phi\rangle$ is a permanent in which all bosons occupy identical orbitals, i.e., Φ is a matrix with 1 column
 - Permutation symmetry automatically imposed
 - Exact when \hat{v} is real (e.g., attractive interaction); has phase problem when \hat{v} is complex — can be controlled using the phaseless approach for fermions
 - Will be subject of the afternoon Lab (trapped boson atoms)
- The back-propagation approach for observables to correct for bias of mixed estimator — similar to forward walking in DMC, but you can calculate off-diagonal expectations (see References, *Zhang et. al. '97, Purwanto '04*)
- Twisted averaging boundary condition (*Ceperley*) — straightforward to implement for any \mathbf{k} -point.

Summary and outlook

- Introduction to QMC methods with auxiliary fields
- Constrained path Monte Carlo methods for “lattice models” of correlated systems — ground-state *and* finite-temperature
- A new QMC method for realistic materials
 - allows choice of any single-particle basis
 - reduces the reliance of QMC on trial w.f. (so far)
 - Potentially a general method for *ab initio* calculations of materials which systematically goes beyond mean-field (e.g., LDA) while using much of its existing machinery
- Further development — many opportunities for improvement, for example
 - different single-particle basis (PAW, Gaussian,)
 - different HS transformation
 - calculation of observables and correlation functions
- Applications — much to do, including to strongly correlated systems

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physics.wm.edu/~shiwei
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