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Joint DEMOCRITOS - ICTP School on

CONTINUUM QUANTUM MONTE CARLO METHODS

12 - 23 January 2004

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 catagories according to primary applications:

	Continuum	**Lattice**
Applications	• electronic structure • quantum chemistry • ^{3}He • few-body nuclei	• correlated electron models • nuclear shell model • quantum field theory
	GROUND-STATE:	
Algorithm	**Diffusion MC**	**auxiliary-field/projector QMC ← (1)**
Description	- random walks - 1st quantized form - in configuration space	- auxiliary-fields - 2nd quantized form
Sign problem	fixed-node approximation	constrained path MC ← **(2) + (3)**

Overview of QMC methods

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	Continuum	**Lattice**
Applications	• electronic structure • quantum chemistry • ^{3}He • few-body nuclei	• correlated electron models • nuclear shell model • quantum field theory
	FINITE-TEMPERATURE:	
Algorithm	**Path-Integral MC**	**QMC/BSS** ← **(1)**
Description	- Mapping to classical ring-polymer system.	- related to above - grand canonical ensemble
Sign problem	restricted path appr.	"new" finite-T method ← **(5)**

- Cross-fertilization: e.g., GFMC ⇒ lattice models (*Ceperley, Sorella, ...*)
- The reverse: auxiliary-field ⇒ continuum (realistic systems) has appealing features but had *phase problem* ← 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 $\hat{H}$,

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

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

Difference in methods:

different ways of realizing above process stochastically $\qquad$ 1/sqrt scaling of MC

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

Diffusion Monte Carlo (DMC)

Summary

- $\Psi_0(R) =< R|\Psi_0\rangle$ obtained by random walks in electronic configuration space
  $|R\rangle = |\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_M\rangle$
- 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

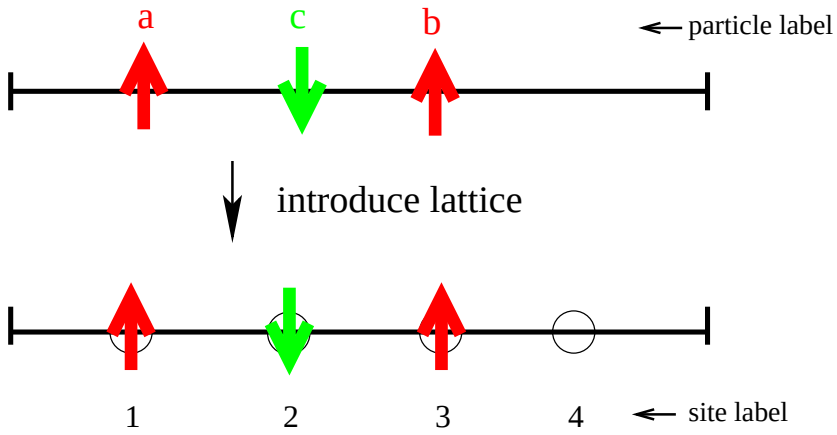
$$\hat{H} = \hat{H}_1 + \hat{H}_2 = \sum_{i,j} T_{ij} c_i^\dagger c_j + \sum_{i,j,k,l} V_{ijlk} c_i^\dagger c_j^\dagger c_k c_l$$

  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 $V(R) = a_s\delta(r_{\rm a} - r_{\rm c}) + a_s\delta(r_{\rm b} - r_{\rm c})$ (no s-wave bt. a & b)



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

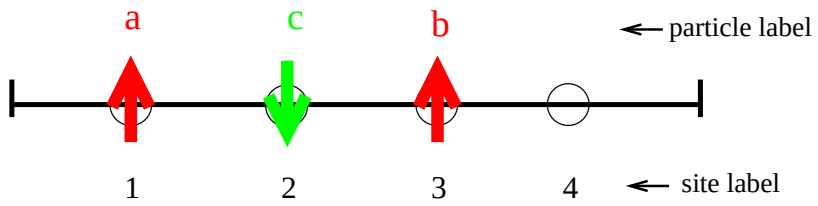
$$H = K + V = -t \sum_{\langle ij\rangle\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

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

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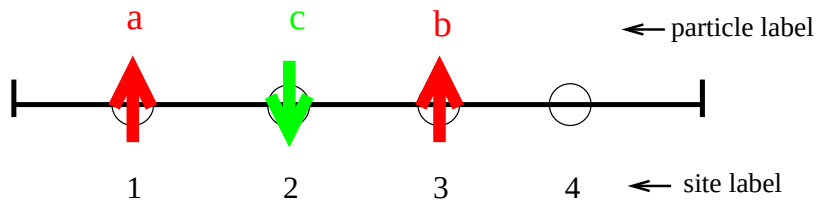


- What is the ground state when $U = 0$, *i.e., without interaction*?
  - Diagonalize single-particle Hamiltonian directly
  - Alternatively, use power method to obtain $|\Psi_0\rangle$

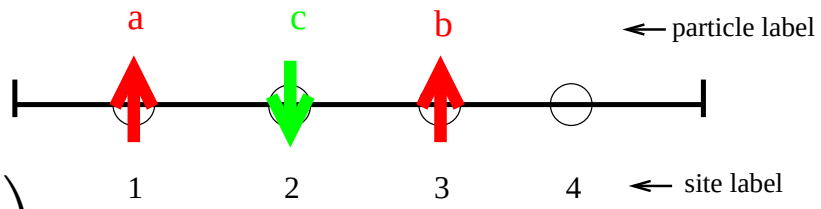
$$e^{-\tau H}: \quad \left(\begin{array}{c} 4 \times 4 \end{array} \right) \otimes \left(\begin{array}{c} 4 \times 4 \end{array} \right) \equiv B_K \quad \text{operate on any } |\Psi^{(0)}\rangle \text{ repeatedly} \quad \Rightarrow |\Psi_0\rangle$$

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:



$$|\phi\rangle: \quad \Phi = \begin{pmatrix} 0.37 & -0.60 \\ 0.60 & -0.37 \\ 0.60 & 0.37 \\ 0.37 & 0.60 \end{pmatrix} \otimes \begin{pmatrix} 0.37 \\ 0.60 \\ 0.60 \\ 0.37 \end{pmatrix} \quad \leftarrow \text{matrix rep.}$$

- 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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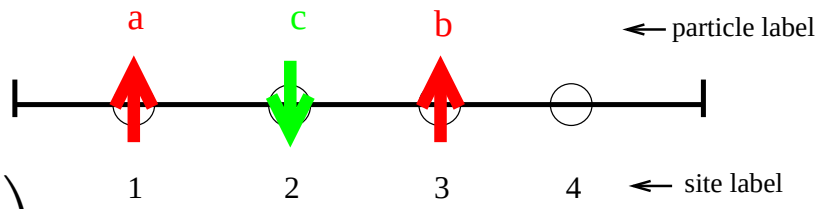

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A: Simple matrix manipulations (See Lab exercises)

A toy problem

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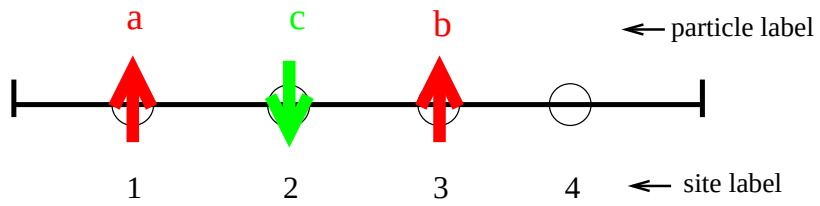

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$$e^{-\tau H}: \qquad \left(\begin{array}{c} 4 \times 4 \end{array} \right) \otimes \left(\begin{array}{c} 4 \times 4 \end{array} \right) \equiv B_K \quad \text{operate on any } |\Psi^{(0)}\rangle \text{ repeatedly} \quad \Rightarrow |\Psi_0\rangle$$

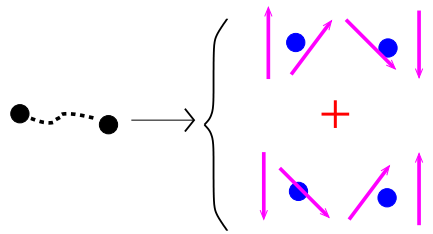
- What is the ground state, now $U \neq 0$, *i.e., with interaction*?
  - Diagonalizing many-body H involves a matrix whose size grows rapidly with N and $M_\uparrow$ or $M_\downarrow$ (Lanczos method)
  - Can we still write $e^{-\tau H}$ in one-body form?
    Yes — **Hubbard-Stratonivich transformation**

AF QMC — introduction

Hubbard-Stratonivich transformation

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

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



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

- Illustration of HS transformation — Hubbard-like interaction:

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

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

Or trick by Hirsch:

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} = e^{-\tau U (n_{i\uparrow} + n_{i\downarrow})/2} \cdot \sum\nolimits_{x=\pm 1} \frac{1}{2}\; e^{\gamma\, x\, (n_{i\uparrow} - n_{i\downarrow})} \qquad \cosh\gamma = e^{\tau U/2}$$

AF QMC — introduction

Back to toy problem

Hubbard-Stratonivich transformation

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} = \text{factor} \times \sum\nolimits_{x=\pm 1} \frac{1}{2}\; e^{\gamma\, x\, n_{i\uparrow}}\; e^{-\gamma\, x\, n_{i\downarrow}} \qquad \cosh\gamma = e^{\tau U/2}$$

$$e^{-\tau H} = \int d\mathbf{x}\; p(\mathbf{x}) \left(\begin{array}{cccc} e^{\gamma x_1} & 0 & 0 & 0 \\ 0 & e^{\gamma x_2} & 0 & 0 \\ 0 & 0 & e^{\gamma x_3} & 0 \\ 0 & 0 & 0 & e^{\gamma x_4} \end{array} \right) \cdot B_{K,\uparrow}$$

$$\otimes \left(\begin{array}{cccc} e^{-\gamma x_1} & 0 & 0 & 0 \\ 0 & e^{-\gamma x_2} & 0 & 0 \\ 0 & 0 & e^{-\gamma x_3} & 0 \\ 0 & 0 & 0 & e^{-\gamma x_4} \end{array} \right) \cdot B_{K,\downarrow}$$

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

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

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

$U \neq 0$ 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*

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

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

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

Choose $|\Psi^{(0)}\rangle$ as a Slater determinant $\boxed{B(\mathbf{x})|\phi\rangle = |\phi'\rangle}$

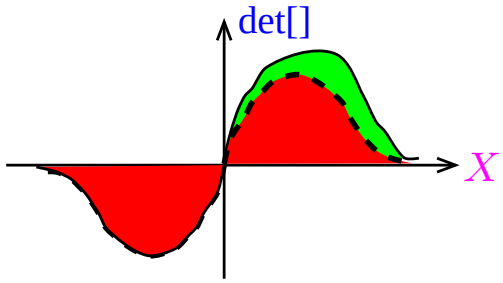
Many-dim integral can be done by Monte Carlo: $\dfrac{\int O_{\mathrm{Gr}}(X) p(X) \det[X] dX}{\int p(X) \det[X] dX}$ $\qquad X \equiv \{\mathbf{x}^{(l)}\}$

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[ ] $\to 0$ 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 $i = 1, 2, \cdots, N$
- 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., $\langle\phi|\phi'\rangle = \det(\Phi^{\mathrm{T}}\Phi')$; $\quad G_{ij} \equiv \frac{\langle\phi|c_i^\dagger c_j|\phi'\rangle}{\langle\phi|\phi'\rangle} = [\Phi'(\Phi^{\mathrm{T}}\Phi')^{-1}\Phi^{\mathrm{T}}]_{ij}$;
  any 2-body correlation $\leftarrow \{G_{ij}\}$

Random walks in Slater determinant space: preliminaries II

For example in electronic systems:

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

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

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

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

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

$$\underline{\rho(\mathbf{Q})} \nwarrow \sum_i c^\dagger_{\mathbf{G}_i + \mathbf{Q}} c_{\mathbf{G}_i}$$

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

Random walks in Slater determinant space

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

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

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

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:

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

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

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

$$|\Psi_0\rangle \doteq \textstyle\sum_\phi |\phi\rangle$$

Connection with Diffusion Monte Carlo

Many-dim. electronic configuration space: $R = \{ \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_M \}$

$$\hat{H} = \sum_i^M \frac{\hat{\mathbf{p}}_i^2}{2m} + \hat{V}$$

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

$$e^{-\tau \hat{\mathbf{p}}_i^2/2m} = \int e^{-\sigma^2/2} \; e^{i \hat{\mathbf{p}}_i \cdot (\gamma \, \sigma)} \; d\sigma \qquad \gamma = \sqrt{\tfrac{\tau}{m}}$$

$$e^{-\tau \hat{H}} = \int e^{-\vec{\sigma}^2/2} \; e^{i \hat{P} \cdot (\gamma \, \vec{\sigma})} \; d\vec{\sigma} \; \; e^{-\tau \hat{V}} \qquad \vec{\sigma}\text{: } 3M\text{-dim vector}$$

translation op.

Random walk realization of $\cdots$: basic idea (importance sampling can also be derived)

$$|\Psi^{(0)}\rangle \xrightarrow{e^{-\tau H}} |\Psi^{(1)}\rangle \; .... \; \rightarrow \; |\Psi_0\rangle$$

$$|R^{(0)}\rangle \xrightarrow[\text{sample } \vec{\sigma} \text{ from Gaussian;}]{\text{multiply weight by } e^{-\tau V(R^{(0)})}} |R^{(1)}\rangle \; \rightarrow \; |R\rangle \quad \text{diffusion + branching}$$

$$\text{translate } R^{(0)} \text{ by } (-\gamma \vec{\sigma})$$

$$\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{array}$$

New QMC method: Random walks in Slater determinant space

Standard DMC

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

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

$\Downarrow$

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

Slater determinant RW

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

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

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

$\Downarrow$

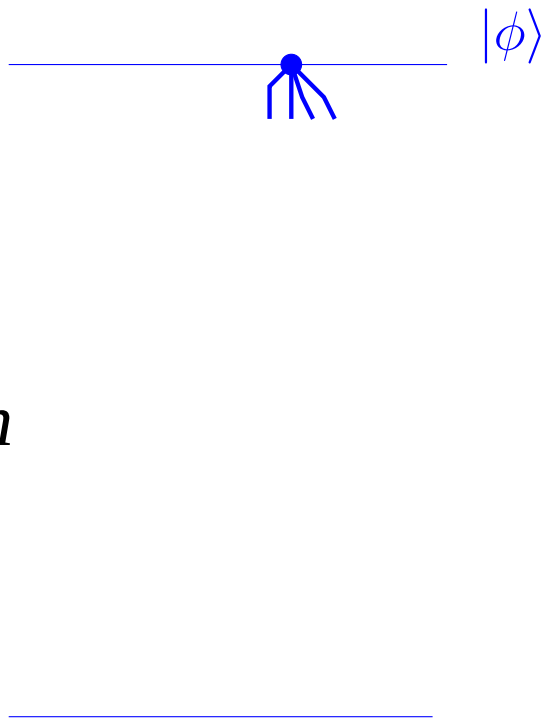
$|\Psi_0\rangle \doteq \sum_{\rm MC} |\phi\rangle$

- 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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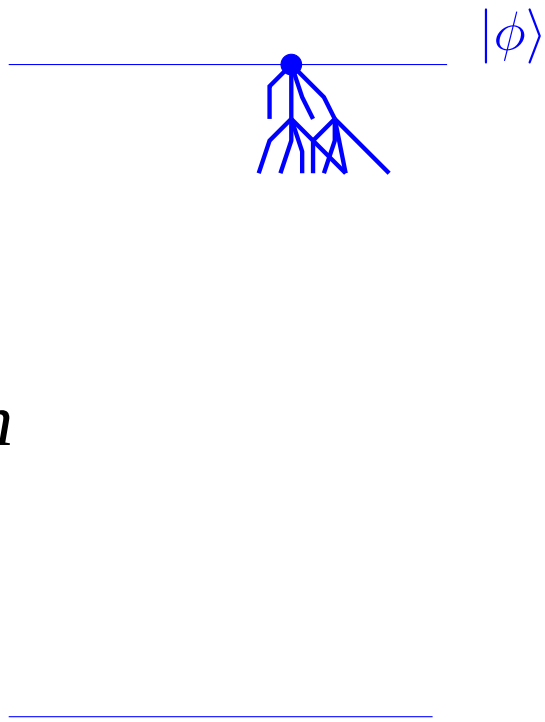

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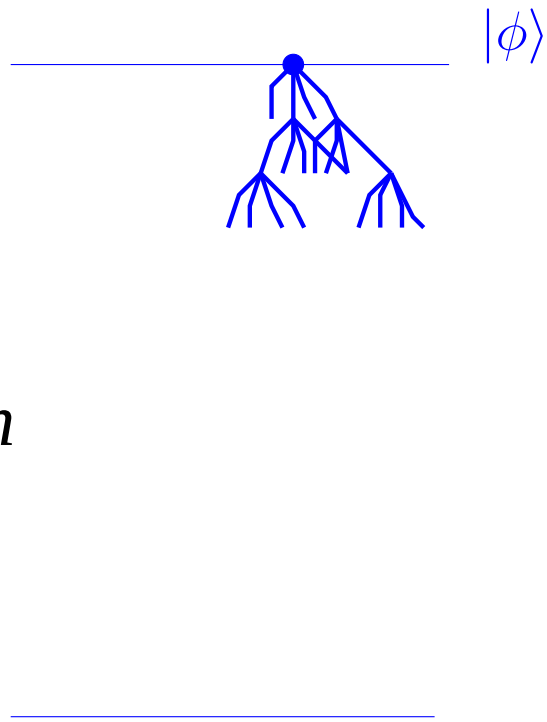
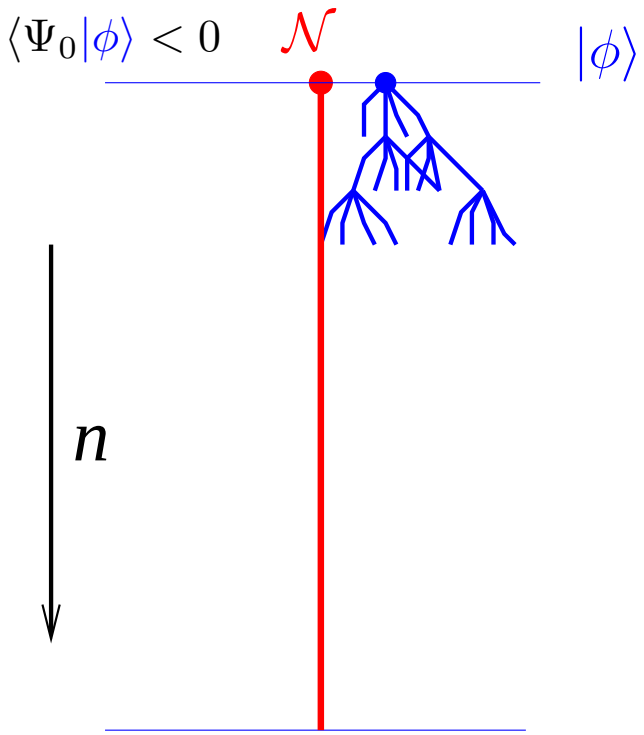


Sign problem for model Hamiltonians

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

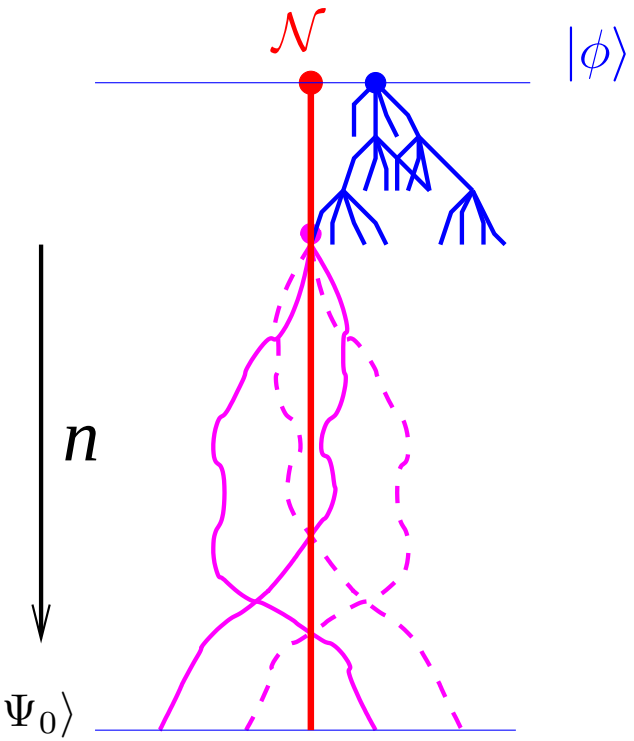
- $e^{-\tau \hat{H}}$ leads to paths in determinant space; paths are "fractal"-like
- At $\tau \to 0$, paths are continuous
- Suppose the exact w.f. $|\Psi_0\rangle$ is known:
  - Define 'Node' $\mathcal{N}$: $\langle \Psi_0 | \phi \rangle = 0$



Sign problem for model Hamiltonians

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

- $e^{-\tau \hat{H}}$ leads to paths in determinant space; paths are "fractal"-like
- At $\tau \to 0$, paths are continuous
- 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



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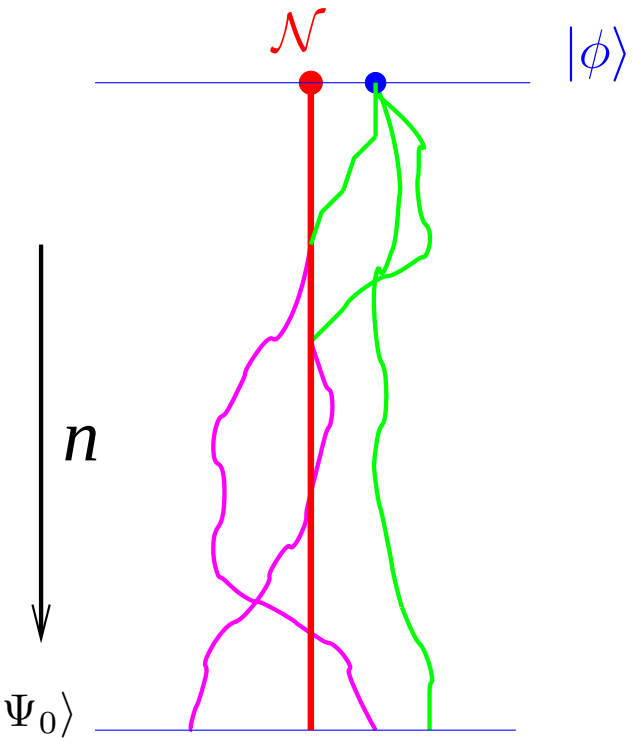
      $\Rightarrow$ descendents of $|\phi\rangle$ collectively contribute 0 to $|\Psi_0\rangle$
    - i.e., paths that reach $\mathcal{N}$ become noise
  - Only constrained paths contribute
- As n increases, MC Signal is exponentially small compared to noise (except for special cases e.g., 1/2-filled Hubbard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



Sign problem for model Hamiltonians — how to control it

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

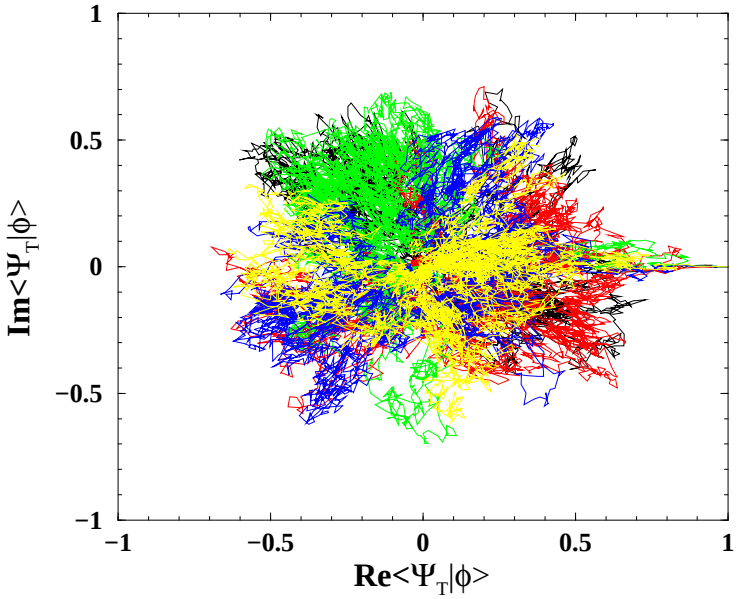
Paths that reach $\mathcal{N}$ should be eliminated — require $\langle \Psi_T | \phi \rangle > 0$ for every $|\phi\rangle$,
with a trial wave function $|\Psi_T\rangle$

- 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:

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

  ⋆ 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

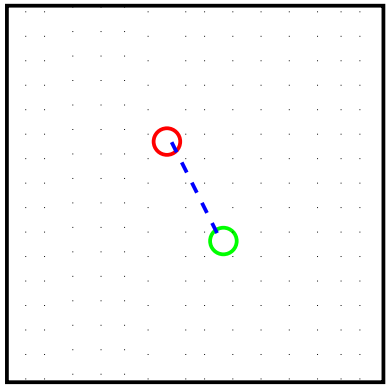
Comments

- 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:

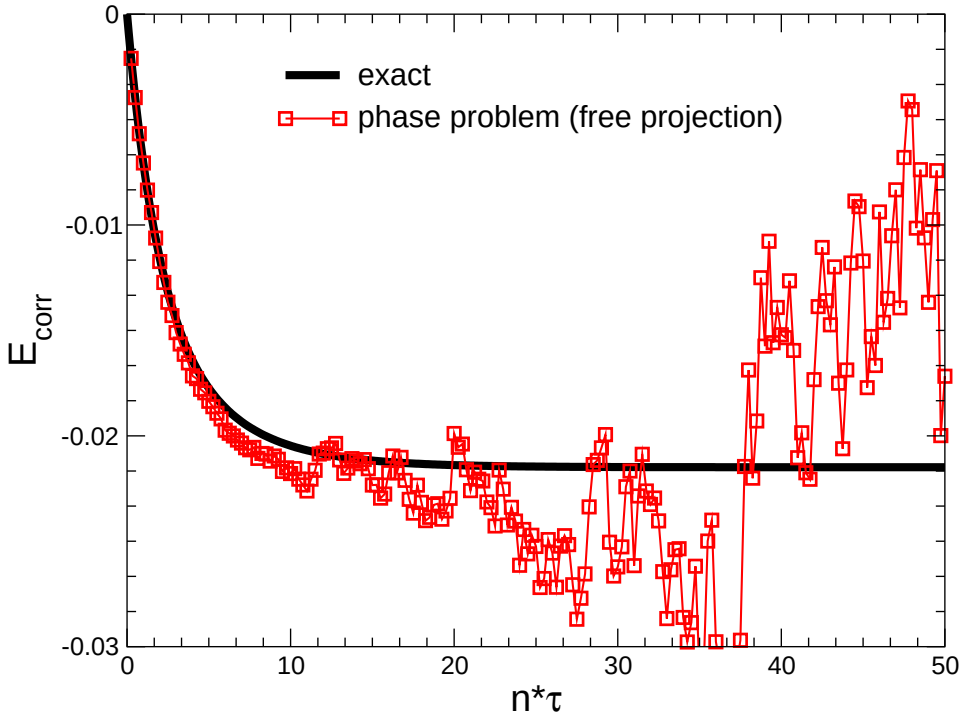
- $r_s = 10$, $N = 19$ plane wave basis functions
- Correlation energy (in Ry) vs. projection time:



Periodic box (supercell)

electron, spin ↑

electron, spin ↓



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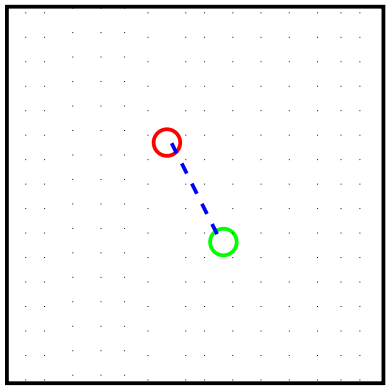

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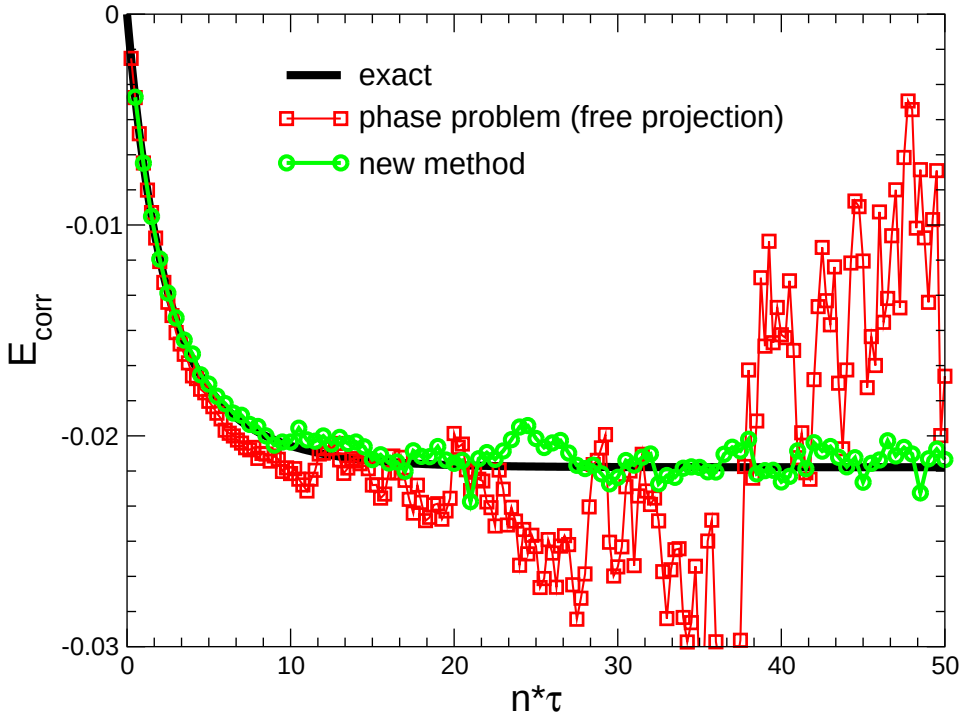
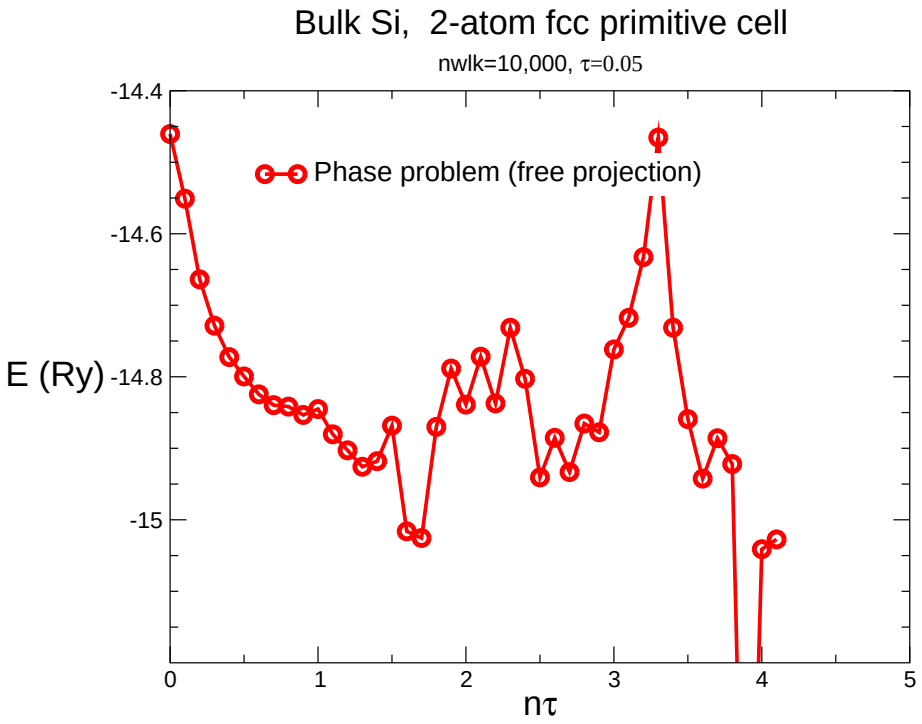


New method for realistic Hamiltonians

Two-atom Si fcc cell:

- 8 valence electrons
- Starting from LDA solution:



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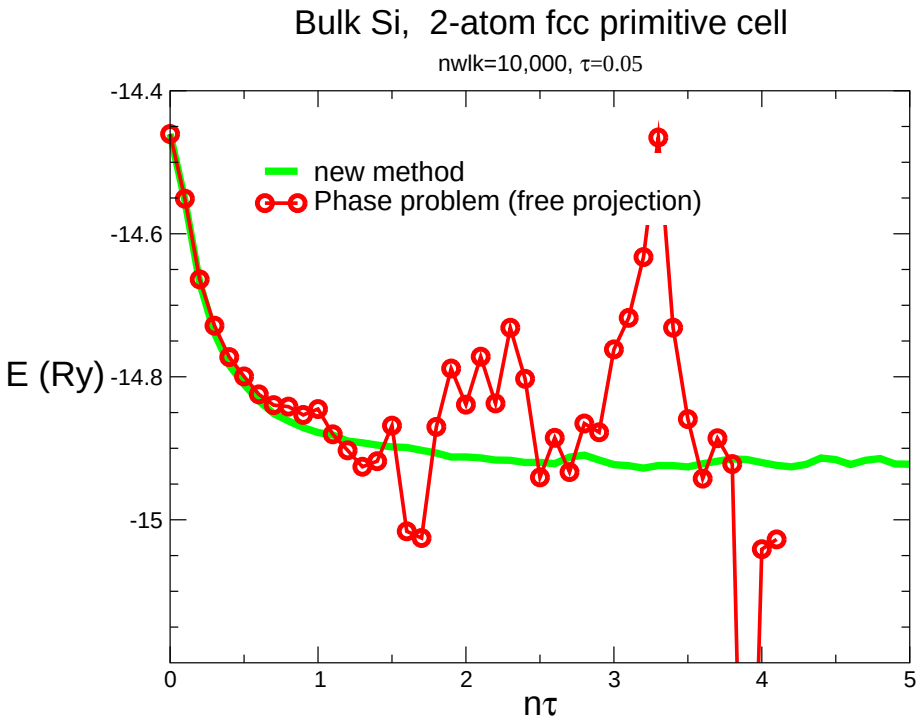


Finite-T method: preliminaries

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

Partition function for Hamiltonian H is: $(\beta = 1/k\,T)$

$$\mathrm{Tr}(e^{-\beta H}) = \mathrm{Tr}(\, e^{-\tau H}\, e^{-\tau H}\, \cdots\, e^{-\tau H}\,)$$

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

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

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

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

Sign Problem in standard finite-T AF QMC:

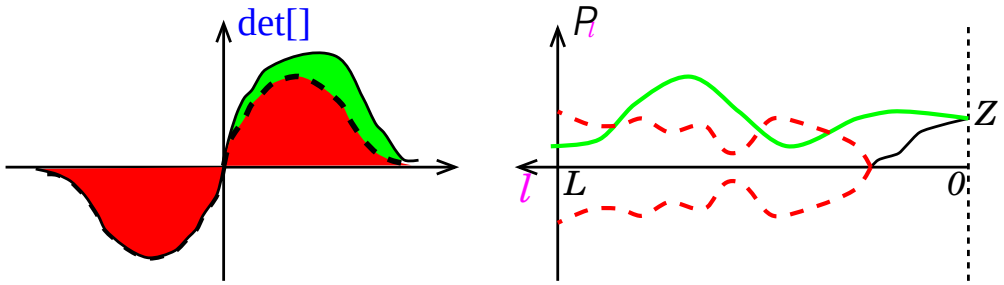
- As T lowers, average sign of $\det[\ ] \to 0$ exponentially.
- We need to control the sign problem — focus on real auxiliary fields, i.e., real $\hat{v}$

Finite-T method: origin of the sign problem

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

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

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



- If $P_l = 0$, all future paths $\{\mathbf{x}_{l+1}, \mathbf{x}_{l+2}, \cdots, \mathbf{x}_L\}$ 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: $P_1(\{\mathbf{x}_1\}) > 0$; $P_2(\{\mathbf{x}_1, \mathbf{x}_2\}) > 0$; ....; $P_L(\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_L\}) > 0$.

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

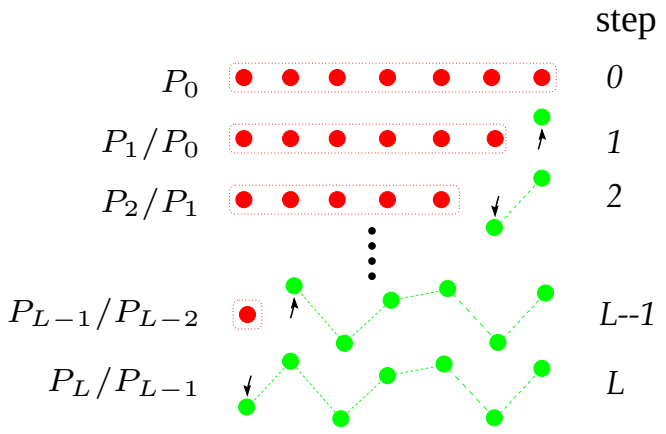
Monte Carlo sampling algorithm to incorporate constraint

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

Sampling — random walk of L steps:

Note:

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



Test results

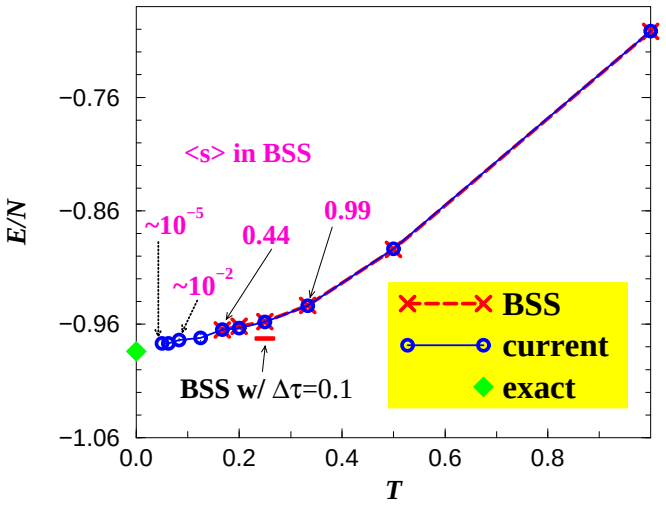
Benchmark results on 2-D Hubbard model for finite-T method

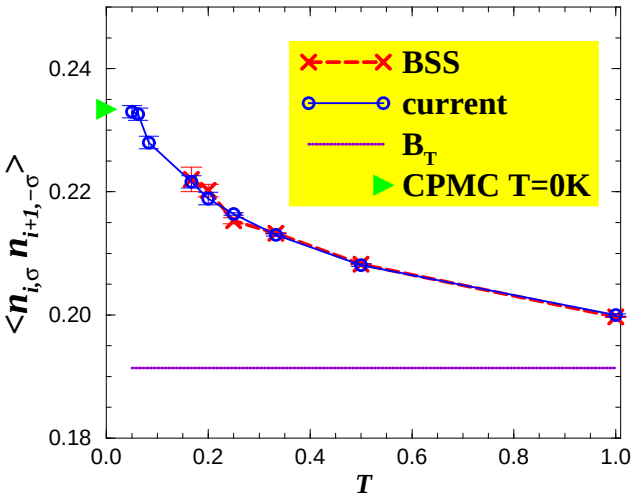
- Standard method limited to $\beta \sim 6$
- New method shown up to $\beta = 20$

- Excellent agreement:
  - high T: BSS
  - low T: $\rightarrow 0\,\mathrm{K}$ exact
- B_T gives wrong physics
- Method still accurately predicts AF correlation

Benchmark on 4x4 with U=4 at <n>=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 ($G, G' < E_{\rm cut}$)
- 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:
  - $E_{\text{cut}} = 12.25$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 $4.63 a_B$:

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 at al, '98)
AF QMC (psp)	0.0(2)	phase problem (Baer et al '00)

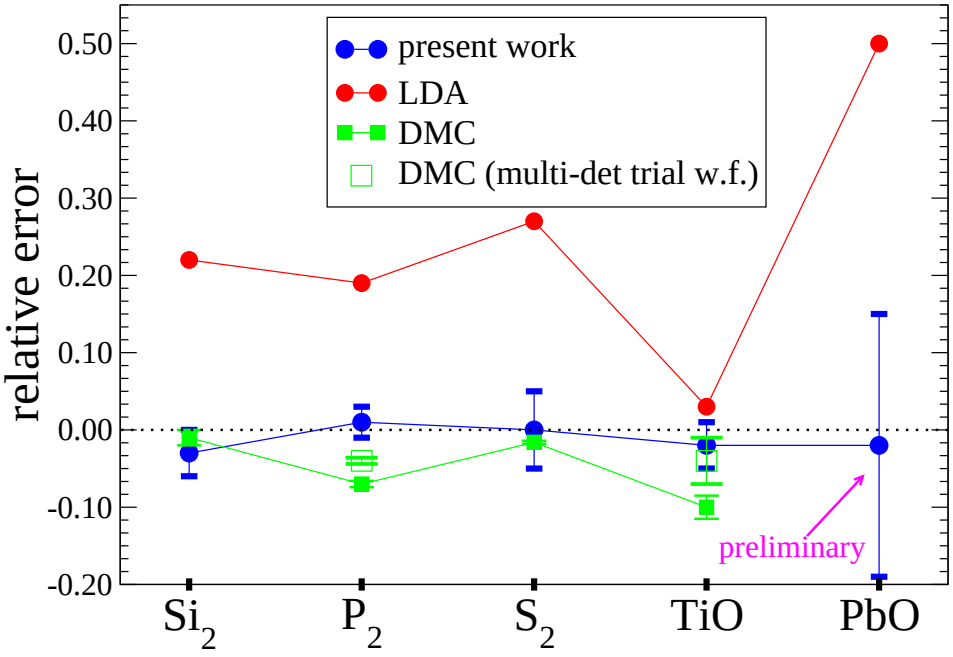
- Difficult case because of near $2s$ and $2p$ degeneracy; full CI up to 1 billion det.'s !
- Standard DMC does not bind with optimized single Slater-determinant ($\times$ Jastrow) trial wave functions

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) $\times$ Jastrow

Relative error compared to experimental value



- S_2:
  - Hartree-Fock w.f. (-40% error) gives same answer with present QMC method
- TiO: (preliminary)
  - Ti ($3s3p3d\,4s$) included as valence electrons; $E_{\rm cut} = 50$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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