An Introduction to Quantum Monte Carlo for Strongly Correlated Electrons

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AICS Cafe (24/02/2012)
Outline

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   - methods

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   - formulation
   - Example: 2d Hubbard model

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   - formulation
   - Example: 1d extended Hubbard model coupled to lattice

4 Summary
# condensed matter physics

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the 20th century

Bloch’s theorem (1928)
→ Band theory

“free” electrons (weekly correlated)

Next generation

"strongly correlated"

target materials
• transition metal oxide
• rare earth compound
• molecular conductors etc...

High-Tc material

semiconductor
strongly-correlated electron systems

**basic science:**
- quantum many-body systems
- coupled degrees of freedom
  - charge, spin, orbital, lattice
- variety: phase transitions
  "More is different."
  P. W. Anderson (1967)
- challenging

**applied physics:**
- High-Tc superconductivity
- magnetism
- ferroelectricity
- multiferroic
- material design / phase control
High-Tc fever in 1986

- doped Mott insulators
electrons in lattice: tight-binding model

“site”: 
outermost orbital / HOMO

electron:
  • charge (-e) & spin (↑ or ↓)
  • Pauli exclusion principle

filling:
  \[ n = \frac{N_e}{N} \leq 2 \]

Ne: # of electrons
N : # of sites

“CuO2 plane”
electrons in lattice: band insulator

\[ n = \frac{N_e}{N} = 2 \]

Insulating state due to periodic potential
Background

det-QMC

SSE-QMC

Summary

Electrons in lattice: Mott insulator

\[ n = \frac{N_e}{N} = 1 \]

Insulating state due to Coulomb interactions
canonical model: Hubbard model

\[ \mathcal{H} = \mathcal{H}_t + \mathcal{H}_U \]

\[ \mathcal{H}_t = -t \sum_{\sigma=\uparrow,\downarrow} \sum_{<i,j>} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) \]
\[ \sim \text{kinetic energy} \]

\[ \mathcal{H}_U = U \sum_i n_{i\uparrow} n_{i\downarrow} \]
\[ \sim \text{Coulomb repulsion} \]

- “quantum”
\[ \mathcal{H}_t \mathcal{H}_U \neq \mathcal{H}_U \mathcal{H}_t \]

- “many-body”
\[ n_{i\uparrow} n_{i\downarrow} \neq n_{i\uparrow} \langle n_{i\downarrow} \rangle \]

parameters:
\[ U/t, n, T/t \]
numerical methods for strongly-correlated electrons

- **Exact Diagonalization (ED)**
  - “exact”
  - only for small cluster \((N \sim 40)\)

- **Density Matrix Renormalization Group (DMRG)**
  - large system \((N \sim 1000)\)
  - only for 1D

- **Quantum Monte Carlo (QMC)**
  - large system \((N \sim 1000)\)
  - \(d > 1\)
  - negative sign problem
**What is QMC?**

QMC = quantum-classical mapping + importance sampling

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**“quantum-classical mapping”**

classical: \[ \langle A \rangle = \frac{1}{Z} \sum_n A_n e^{-\beta E_n} \]

quantum: \[ \langle A \rangle = \frac{1}{Z} \sum_{\alpha} \langle \alpha | \hat{A} e^{-\beta \hat{H}} | \alpha \rangle \]

**Q:** How to integrate out without diagonalization?

**A:** map to \((d + 1)\) dim. classical system

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**“importance sampling”**

\[ \langle A \rangle = \frac{1}{Z} \sum_{\{c\}} A(\{c\}) W(\{c\}) \]

\[ Z = \sum_{\{c\}} W(\{c\}) \]

- configuration: \( \{c\} \sim 2^N \)
- general method for high dimensional integrals

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QMC for strongly correlated electrons  
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(roughly) 3 ways for quantum-classical mapping

1. world-line QMC (WL-QMC)
   - path-integral w/ checkerboard decomposition
   - electrons: only for 1d
   - spins: without frustration

2. Stochastic Series Expansion (SSE-QMC)
   - based on high-temperature series expansion
   - similar to WL-QMC

3. determinant QMC (det-QMC)
   - path-integral w/ Hubbard-Stratonovitch transformation
   - $d > 1$
organization

- determinant QMC
  - procedure:
    - Suzuki-Trotter decomposition
    - Hubbard-Stratonovich transformation → \( \{s_{il}\} \): auxiliary field
    - Integrating out fermions
    - MC sampling for \( \{s_{il}\} \)
  - example:
    - some results for 2d Hubbard model
Suzuki-Trotter decomposition

\[ Z = \text{Tr} \, e^{-\beta \mathcal{H}} \]
\[ = \text{Tr} \, e^{-L \Delta \tau (\mathcal{H}_t + \mathcal{H}_U)} \]
\[ \approx \text{Tr} \prod_{l=1}^{L} e^{-\Delta \tau \mathcal{H}_t} e^{-\Delta \tau \mathcal{H}_U} \]
\[ (\beta = L \Delta \tau) \]

- quantum-to-classical mapping
- \(d\)-dim. quantum system = \((d+1)\)-dim. classical system
discrete Hubbard-Stratonovich transformation

\[ e^{-\Delta \tau U(n_i^\uparrow - \frac{1}{2})(n_i^\downarrow - \frac{1}{2})} = \frac{1}{2} e^{-\Delta \tau U/4} \sum_{s_{ii}=\pm1} e^{-\lambda s_{ii}(n_i^\uparrow - n_i^\downarrow)} \]

\[ \{s_{ii}\}: \text{auxiliary field} \]

\[ \Rightarrow Z = \text{Tr}_{\{s_{ii}\}} \text{Tr}_F \prod_{l=1}^{L} D_{\uparrow l} D_{\downarrow l} \]

\[ \text{Tr}_{\{s_{ii}\}}: \text{trace over Ising spins } (2^{NL}) \]

\[ \text{Tr}_F: \text{trace over free fermions} \]
Trace out fermions

\[
\text{Tr}_F \prod_{l=1}^{L} D_{\uparrow l} D_{\downarrow l} = \det \mathcal{O}_{\uparrow} \det \mathcal{O}_{\downarrow}
\]

\[
\mathcal{O}_\sigma = \begin{pmatrix}
I & 0 & \ldots & 0 & B_{\sigma 1} \\
-B_{\sigma 2} & I & 0 & \ldots & 0 \\
0 & -B_{\sigma 3} & I & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \ldots & 0 & -B_{\sigma L} & I
\end{pmatrix}
\]

\[
B_{\sigma l} = e^{-K} e^{-V_{\sigma l}} : N \times N \text{ matrix}
\]

\[
\det \mathcal{O}_\sigma = \det M_\sigma
\]

\[
M_\sigma = I + B_{\sigma L} B_{\sigma L-1} \cdots B_{\sigma 1}
\]

\[
\Rightarrow Z = \text{Tr}\{s_{li}\} \det M_{\uparrow} \det M_{\downarrow}
\]
Physical observables: Green’s function

$$\langle \langle c_{i\sigma} c_{j\sigma}^\dagger \rangle \rangle = \frac{1}{Z} \text{Tr} \left( c_{i\sigma} c_{j\sigma}^\dagger e^{-\beta \mathcal{H}} \right)$$

$$= \frac{\text{Tr} \{ s_l \} \langle c_{i\sigma} c_{j\sigma}^\dagger \rangle \det M \uparrow \det M \downarrow}{\text{Tr} \{ s_l \} \det M \uparrow \det M \downarrow}$$

$$\langle c_{i\sigma} c_{j\sigma}^\dagger \rangle = \frac{\text{Tr}_F c_{i\sigma} c_{j\sigma}^\dagger \prod_{l=1}^{L} D_{\sigma l}}{\text{Tr}_F \prod_{l=1}^{L} D_{\sigma l}} = (M_{\sigma}^{-1})_{ij}$$

MC sampling for configuration of Ising spins:

$$\langle \langle c_{i\sigma} c_{j\sigma}^\dagger \rangle \rangle = \lim_{N_{\text{MC}} \to \infty} \frac{1}{N_{\text{MC}}} \sum_{\text{MC}} \langle c_{i\sigma} c_{j\sigma}^\dagger \rangle$$

with weight $W[\{ s_l \}] = \det M \uparrow \det M \downarrow$
**negative sign problem**

- In general, \( W \) is **not** positive definite.

\[
\langle \langle A \rangle \rangle = \frac{\sum_{\{s_{li}\}} \langle A \rangle W[\{s_{li}\}]}{\sum_{\{s_{li}\}} W[\{s_{li}\}]}
\]

- some exceptions:
  - w/ p-h symmetry & bipartite lattice

- exponentially hard (?)

- Murphy’s Law (?)

\[
\langle \text{sgn} W[\{s_{li}\}] \rangle = \frac{W[\{s_{li}\}]}{|W[\{s_{li}\}]|}
\]
**Effect of randomness on Mott insulator**

**Anderson-Hubbard model**

\[ H = -t \sum_{\langle j,k \rangle, \sigma} \left( c_{j\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \epsilon_i n_i \]

- Mott insulator: gapful, AF
- Anderson insulator: gapless, para

\[ \rightarrow \text{collapse of charge gap} \]

Hubbard model with staggered flux

\[ \mathcal{H} = \sum_{\langle j, k \rangle, \sigma} \left( c_{j\sigma}^\dagger t_{jk} c_{k\sigma} + c_{k\sigma}^\dagger t_{jk}^* c_{j\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ t_{jk} = t e^{i\theta_{jk}} \Rightarrow \phi = \sum_{\text{plaquette}} \theta_{jk} = \pm \pi \]

Suppression of AF due to flux

charge fluctuations in $k$-space

$$\kappa(k) = \left. \frac{dn(k)}{d\mu} \right|_{\mu=0}$$

N=16x16, $\sim$ 100 MCS/1hour  

Stochastic Series Expansion

- procedure:
  - high-temperature series-expansion
  - truncation at fixed $L \to \{S_L\}$: operator string
  - graphical representation
  - MC sampling for $\{S_L\}$

- example:
  - 1d extended Hubbard model coupled to lattice
Heisenberg model

\[ H = J \sum_{\langle i, j \rangle} \left\{ \Delta S_i^z S_j^z + \left( S_i^x S_j^x + S_i^y S_j^y \right) \right\} \]

\[ = J \sum_{\langle i, j \rangle} \left\{ \Delta S_i^z S_j^z + \frac{1}{2} \left( S_i^+ S_j^- + S_i^- S_j^+ \right) \right\} \]

base: \[ |\alpha\rangle = |\sigma_1 \sigma_2 \sigma_3 \cdots \sigma_N\rangle, \quad \sigma_i = \uparrow, \downarrow \]

\[ S_i^z | \uparrow_i \rangle = | \uparrow_i \rangle \]
\[ S_i^z | \downarrow_i \rangle = | \downarrow_i \rangle \]
\[ S_i^+ | \uparrow_i \rangle = 0 \]
\[ S_i^+ | \downarrow_i \rangle = | \uparrow_i \rangle \]
\[ S_i^- | \uparrow_i \rangle = | \downarrow_i \rangle \]
\[ S_i^- | \downarrow_i \rangle = 0 \]
(1): Write $H$ as a sum of bond operators

$$H = -\sum_{a=1}^{2} \sum_{b=1}^{M} H_{a,b}$$

- $a$: operator type (1=diagonal, 2=off-diagonal)
- $b$: bond index ($b$ connects $i(b)$ and $j(b)$)

$$H_{1,b} = C - \Delta S_{i(b)}^{z} S_{j(b)}^{z}, \quad C > \Delta/4 : \text{constant}$$

$$H_{2,b} = \frac{1}{2} \left( S_{i(b)}^{+} S_{j(b)}^{-} + S_{i(b)}^{-} S_{j(b)}^{+} \right)$$
(2): high-temperature series-expansion

\[ Z = \text{Tr} \left\{ e^{-\beta H} \right\} \]

\[ = \sum_\alpha \langle \alpha | e^{-\beta H} | \alpha \rangle \]

\[ = \sum_\alpha \sum_{n=0}^\infty \frac{\beta^n}{n!} \langle \alpha | H^n | \alpha \rangle \]

\[ = \sum_\alpha \sum_{n=0}^\infty \sum S_n \frac{\beta^n}{n!} \langle \alpha | H_{l_1} H_{l_2} H_{l_3} \cdots H_{l_n} | \alpha \rangle \]

\[ l_j : (a, b) \]

\[ S_n : [l_1, l_2, \cdots, l_n] \quad \text{(operator string)} \]
(3): truncate at $n = L$

$$Z \simeq \sum_{\alpha} \sum_{n=0}^{L} \sum_{S_n} \frac{\beta^n}{n!} \langle \alpha | \prod_{l} H_{l} | \alpha \rangle$$

∴ $\langle n \rangle = -\beta \langle H \rangle$ (finite lattice)
(4): insert unit operators

\[ Z = \sum_{\alpha} \sum_{S_L} \frac{\beta^n (L - n)!}{L!} \langle \alpha | \prod_{l_j=1}^{L} H_{l_j} | \alpha \rangle \]

\[ l_j : \quad 0 \text{ or } (a, b) \]

\[ H_0 = I \]
\begin{equation}
\langle A \rangle = \frac{1}{Z} \text{Tr} \left\{ A e^{-\beta H} \right\} = \frac{1}{Z} \langle \alpha | A e^{-\beta H} | \alpha \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{S_L} \frac{\beta^n (L - n)!}{L!} \langle \alpha | A \prod H_j | \alpha \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{S_L} \frac{\langle \alpha | A \prod H_j | \alpha \rangle}{\langle \alpha | \prod H_j | \alpha \rangle} \cdot \frac{\beta^n (L - n)!}{L!} \langle \alpha | \prod H_j | \alpha \rangle = \sum_{\alpha} \sum_{S_L} A(\alpha, S_L) W(\alpha, S_L) \frac{\sum_{\alpha} \sum_{S_L} W(\alpha, S_L)}{\sum_{\alpha} \sum_{S_L} W(\alpha, S_L)}
\end{equation}

importance sampling for configuration \((\alpha, S_L) \Rightarrow \text{MC}\)
graphical representation for vertices

\[ W(\alpha, S_L) = \frac{\beta^n (L - n)!}{L!} \langle \alpha(L) | H_L | \alpha(L - 1) \rangle \cdots \langle \alpha(2) | H_2 | \alpha(1) \rangle \cdot \langle \alpha(1) | H_1 | \alpha(0) \rangle \]

diagonal operator: \( H_{1,b} \)

off-diagonal operator: \( H_{2,b} \)
graphical representation for operator string

\[ W(\alpha, S_L) = \frac{\beta^n(L - n)!}{L!} \langle \alpha(L) | H_L | \alpha(L - 1) \rangle \cdots \langle \alpha(2) | H_2 | \alpha(1) \rangle \cdot \langle \alpha(1) | H_1 | \alpha(0) \rangle \]

Ex. 4-site case:

\[ \begin{align*}
N &= 4 \\
L &= 5 \\
|\alpha(0)\rangle &= |\downarrow\uparrow\uparrow\downarrow\rangle \\
S_L &= (H_{1,1}, H_{2,3}, H_{0,0}, H_{2,3}, H_{1,1})
\end{align*} \]

⇒ operator string: world-line (doubly linked list)
Molecular conductor: 1D $\pi$-electron system
Molecular conductor: “colorful” phase diagrams

similar one-electron band structures but variety of properties → interactions are important!
Molecular conductor: “colorful” phase diagrams

- “soft” → electron-lattice coupling, pressure
- low dimensinality → quantum/thermal fluctuations
- clean & material design → “model” material

charge order (CO): $U, V$

dimer-Mott (DM): $U, t_d$

CO+SP

DM+SP

SP: spin-Peierls

Molecular conductor: new phase diagram

\[ \hat{H} = \hat{H}_{\text{extHub}} + \hat{H}_{e-l} + \hat{H}_\perp \]

\[ \hat{H}_{\text{extHub}} = - \sum_{i,\sigma} t_i \left( c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} \right) + \sum_i U n_i^\uparrow n_i^\downarrow + \sum_i V n_i n_{i+1} \]

\[ \hat{H}_{e-l} = - \sum_{i,\sigma} t_i u_i \left( c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} \right) + \frac{K_P}{2} \sum_i u_i^2 + \frac{K_{P2}}{4} \sum_i u_i^4 \]

\[ \hat{H}_\perp = V_\perp \sum_{\langle j,k \rangle} n_j^\dagger n_j^k \]

- ¼-filled extended Hubbard model
- electron-lattice coupling
- inter-chain interaction

H. Seo et al., JPSJ 2007.
Molecular conductor: finite-\( T \) phase diagram

(a): \( \delta_d = 0, K_{P_2} = 0 \)

(b): \( \delta_d = 0, K_{P_2} = 0.75 \)

(c): \( \delta_d = 0.02, K_{P_2} = 0 \)

CO v.s. DM

CO+DM

\rightarrow \text{ferroelectoricity}

cf. TMTTF-salt

Molecular conductor: comparison with experiments

Summary

1. Determinant QMC
   - Procedure:
     - Trotter decomposition.
     - Hubbard-Stratonovich transformation $\rightarrow \{s_{il}\}$: auxiliary field
     - Integrating out fermions
     - MC sampling for $\{s_{il}\}$
   - Example: 2d Hubbard model

2. Stochastic Series Expansion
   - Procedure:
     - High-temperature series-expansion
     - Truncation at fixed $L \rightarrow \{S_L\}$: operator string
     - Graphical representation
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   - Example: 1d extended Hubbard model coupled to lattice