Determinant Quantum Monte Carlo: An overview

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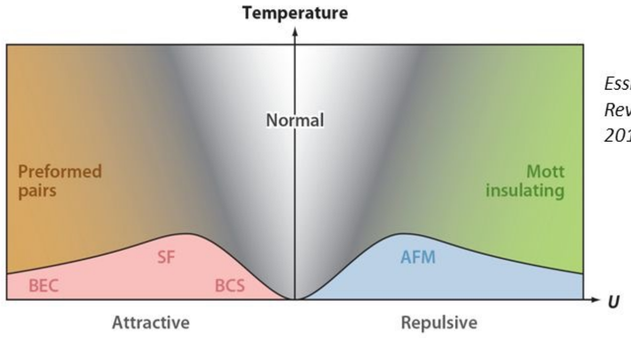
Determinant Quantum Monte Carlo

The Fermi Hubbard model is described by the hamiltonian:

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

Fermi-Hubbard model

Schematic phase diagram for the Fermi Hubbard model



- half-filling
- simple cubic lattice
- 3D

Esslinger, Annual Rev. of Cond. Mat. 2010

Experiments:
R. Jordens et al., Nature (2008)
U. Schneider et al., Science (2008).

Open questions:
- d-wave superfluid phase?
- Itinerant ferromagnetism?

- Not solvable analytically.
- Solved numerically using DMFT, QMC.
- Solution through Determinant Quantum Monte Carlo – DQMC.
- Leads to "fermionic sign problem"
- Sign problem attributed to anti commutative algebra of fermionic operators

DQMC and the sign problem - Overview

- Quantum phase transitions in n dimension can be converted into a classical phase transition in (n+1) dimension by adding imaginary time dimension.
- Write out the partition function as : $$Z = Tr(e^{-\beta H}) = \sum_n \langle n|e^{-\beta H}|n\rangle$$
- Trotter Suzuki decomposition: $$e^{\Delta\tau(T+V)} = e^{\Delta\tau T}e^{\Delta\tau V} + O(\Delta\tau^2)$$
- Divide the path integral into M time steps, and introduce a complete set of Grassmann states-

$$Z = \prod_{l=0}^{M} \int (d\bar{\psi}_l \psi_l) e^{-\Delta\tau \sum_{l=0}^{M} [(\frac{\bar{\psi}_l - \bar{\psi}_{l+1}}{\Delta\tau})\psi_l + H[\bar{\psi}_{l+1}, \psi_l]]}$$

- Express the Hamiltonian in bilinear form. This can be evaluated explicitly, using properties of Grassmann integrals, in terms of the matrix element $H_{l+1,l}$

DQMC and the sign problem - Overview

- The Quartic interaction term is decoupled using the identity $U\sum_i n_{i,\uparrow}n_{i\downarrow} = \frac{-U}{2}\sum_i (n_{i,\uparrow} - n_{i,\downarrow})^2 + \frac{U}{2}\sum_i (n_{i,\uparrow} + n_{i,\downarrow})$
- Rewrite the partition function, using the Trotter decomposition, $Z = Tr\prod_l e^{-\Delta\tau K}e^{-\Delta\tau V_l}$
- Identity (follows from Grassmann integration), whenever the matrices K and V are in the bilinear form.

$$Tr\prod_l e^{-\Delta\tau K}e^{-\Delta\tau V_l} = Det(I + \prod_l e^{-\Delta\tau K}e^{-\Delta\tau V_l})$$

- Convert the V_l into bilinear form by using the above identity and coupling it to an auxiliary field. This is the Hubbard Stratonovich transformation. In traditional scheme of things, this auxiliary field points along the direction of quantization of the local spins. - Auxiliary field DQMC.

DQMC and the sign problem - Overview

- Two choices of the auxiliary field -

$$m_{i,l} = \pm 1 \longrightarrow \text{Ising DQMC}$$

$$m_{i,l} \in [-1, 1] \longrightarrow \text{Hybrid DQMC}$$

- Ising DQMC – $$e^{-\Delta\tau V_l} = \sum_{m_{i,l}} e^{-\Delta\tau \sum_i ((\frac{U}{2}-\mu)(n_{i,\uparrow}+n_{i,\downarrow})+\frac{\lambda}{\Delta\tau}m_{i,l}(n_{i,\uparrow}-n_{i,\downarrow}))} \quad , cosh\lambda = e^{\Delta\tau/2}$$

- Hybrid DQMC – $$e^{-\Delta\tau V_l} = (\Delta\tau e^{-\frac{U\Delta\tau}{2}})^{1/2} \int \prod_i dm_{i,l} e^{-\Delta\tau \sum_i (m_{i,l}^2 + (2U)^{1/2} m_{i,l}(n_{i,\uparrow}-n_{i,\downarrow}))}$$

- In both schemes, the hamiltonian seperates into up and down spins, so we can write the partition function as:

$$Z = (A)^{LM} Tr_{m_{i,l}} \prod_\sigma Det(I + \prod_{l=1}^{M} B_\sigma^l(m_{i,l}))$$

- Propagator between time slices l,l+1

$$B_\sigma^l(m_{i,l}) = exp(-\Delta\tau K) exp(-\sigma\lambda Diag(m_{1,l}, m_{2,l} \ldots\ldots m_{L,l}))$$

- Probability of a configuration -

$$P(m) = \frac{\alpha}{Z} \prod Det(I + \prod B_\sigma^l(m_{i,l}))$$

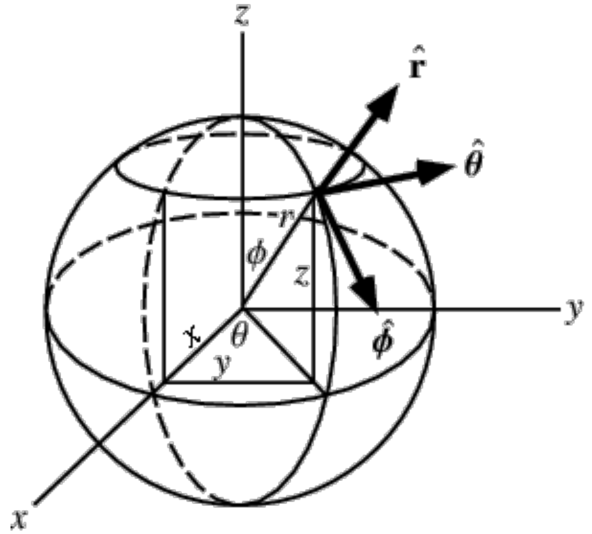
DQMC with O(3) spins

- The probabilities P(m) can be positive or negative! - so called sign problem
- Simulation of Ising DQMC by Hastings Metropolis – Generate a configuration {m'} from {m}

- Acceptance ratio = min(1,|P({m'})|/|P({m})|).

- Green's function is calculated from $$G^\sigma = [I + \prod_l B^l_\sigma(m_{i,l})]^{-1}$$

- Is there a way to get around the sign problem? Consider auxiliary fields to lie on a Bloch sphere now, instead of an Ising variable. This is an O(3) field now.



DQMC with O(3) spins

- We will start with the identity $U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i,\downarrow} = -\frac{2U}{3}\sum_i \hat{\vec{S}}_i \cdot \hat{\vec{S}}_i + \frac{U}{2}\sum_i (n_{i,\uparrow} + n_{i,\downarrow})$

- The interaction can now be decoupled as

$$e^{-U\Delta\tau\sum_i n_{i\uparrow}n_{i\downarrow}} = e^{-U\Delta\tau\sum_i(-\frac{2}{3}\vec{S}_i\cdot\vec{S}_i+\frac{1}{2}(n_{i\uparrow}+n_{i\downarrow}))}$$

- This will be our starting point. We will once again use the identity,

$$Tr\prod_l e^{-\Delta\tau K}e^{-\Delta\tau V_l} = Det(I+\prod_l e^{-\Delta\tau K}e^{-\Delta\tau V_l})$$

- Here, we will use Hubbard Stratonovich with an auxiliary O(3) field to transform the term S_i S_i

- There exists a positive constant C, λ, such that the following identity holds

$$e^{\frac{2U\Delta\tau}{3}\vec{S}\cdot\vec{S}} = C\int d\phi\sin\theta d\theta e^{\lambda\Delta\tau\vec{m}\cdot\vec{S}}$$

DQMC with O(3) spins

- The above identity can be verified by action on basis states, $|\psi\rangle = |0\rangle, |\uparrow\downarrow\rangle, |\uparrow\rangle, |\downarrow\rangle$

$$e^{\frac{2U\Delta\tau}{3}\vec{S}\cdot\vec{S}}|0\rangle = |0\rangle$$

$$e^{\frac{2U\Delta\tau}{3}\vec{S}\cdot\vec{S}}|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle$$

$$e^{\frac{2U\Delta\tau}{3}\vec{S}\cdot\vec{S}}|\uparrow\rangle = e^{\frac{U\Delta\tau}{2}}|\uparrow\rangle$$

$$e^{\frac{2U\Delta\tau}{3}\vec{S}\cdot\vec{S}}|\downarrow\rangle = e^{\frac{U\Delta\tau}{2}}|\downarrow\rangle$$

$$e^{\lambda\Delta\tau\frac{\sin\theta}{2}e^{-i\phi}S^+}e^{\lambda\Delta\tau\frac{sin\theta}{2}e^{i\phi}S^-}e^{\lambda\Delta\tau\cos\theta S^z}|0\rangle = |0\rangle$$

$$e^{\lambda\Delta\tau\frac{\sin\theta}{2}e^{-i\phi}S^+}e^{\lambda\Delta\tau\frac{sin\theta}{2}e^{i\phi}S^-}e^{\lambda\Delta\tau\cos\theta S^z}|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle$$

$$e^{\lambda\Delta\tau\frac{\sin\theta}{2}e^{-i\phi}S^+}e^{\lambda\Delta\tau\frac{sin\theta}{2}e^{i\phi}S^-}e^{\lambda\Delta\tau\cos\theta S^z}|\uparrow\rangle = e^{\lambda\Delta\tau\frac{\cos\theta}{2}}(|\uparrow\rangle + \lambda\Delta\tau\frac{\sin\theta}{2}e^{i\phi}|\downarrow\rangle)$$

$$e^{\lambda\Delta\tau\frac{\sin\theta}{2}e^{-i\phi}S^+}e^{\lambda\Delta\tau\frac{sin\theta}{2}e^{i\phi}S^-}e^{\lambda\Delta\tau\cos\theta S^z}|\downarrow\rangle = e^{-\lambda\Delta\tau\frac{\cos\theta}{2}}(|\downarrow\rangle + \lambda\Delta\tau\frac{\sin\theta}{2}e^{-i\phi}|\uparrow\rangle$$

$$C = \frac{1}{4\pi}, \quad \frac{1}{\lambda\Delta\tau/2}\cosh\frac{\lambda\Delta\tau}{2} = e^{\frac{U\Delta\tau}{2}}$$

DQMC with O(3) spins

- The partition function becomes,

$$Z_h = (\frac{1}{4\pi})^{NM} \int \prod_{i,m} d\vec{h}_{i,m} Det[I + \prod_{m=M}^{0} B_m(\{\vec{h}\})] \quad , \quad \frac{1}{\lambda\Delta\tau/2}\cosh\frac{\lambda\Delta\tau}{2} = e^{\frac{U\Delta\tau}{2}}$$

- The propagators are defined as –

$$B_m(\vec{h}) = e^{-\Delta\tau H^{(2)}} e^{-\Delta\tau H_m^{(4)}}$$

$$e^{-\Delta\tau H^{(2)}} = e^{-\Delta\tau[t\sum_{ij}(c_i^\dagger c_j + hc) - (\mu - \frac{U}{2})\sum_i(n_{i\uparrow}+n_{i\downarrow})]}$$

Quadratic piece

$$e^{-\Delta\tau H_m^{(4)}} = e^{-\lambda\Delta\tau\sum_i \vec{S}\cdot\vec{h}_{i,m}}$$

Quartic piece

- Ising DQMC

$$Z_h = (C_1)^{NM} Tr_{\vec{h}=\pm 1} Det[I + \prod_{m=M}^{0} B_{m,\sigma}(h_m)] \qquad \cosh\lambda\Delta\tau = e^{\frac{U\Delta\tau}{2}}$$

DQMC with O(3) spins

- The partition function is therefore

$$Z = (\frac{U\Delta\tau}{\pi})^{3NM/2}(e^{-\Delta\tau U})^{NM}\int\prod_{i,l} d\phi_{i,l}sin\theta_{i,l}d\theta_{i,l}P(m_{i,l})$$

- The matrices K and $V_l(m)$ are defined as

$$H_l = \psi^\dagger(K+V_l)\psi,\ \ \psi = (c_{1,\uparrow}, c_{1,\downarrow}, c_{2,\uparrow}, ...c_{N,\downarrow})$$

$$K = \begin{bmatrix} -(\mu-\frac{U}{2}) & 0 & -t & 0 & 0 & \dots & -t & 0 \\ 0 & -(\mu-\frac{U}{2}) & 0 & -t & 0 & \dots & 0 & -t \\ -t & 0 & -(\mu-\frac{U}{2}) & 0 & -t & \dots & \dots & \vdots \\ 0 & -t & 0 & -(\mu-\frac{U}{2}) & 0 & -t & \dots & \vdots \\ 0 & 0 & -t & 0 & -(\mu-\frac{U}{2}) & 0 & \dots & \vdots \\ 0 & 0 & 0 & -t & 0 & -(\mu-\frac{U}{2}) & & 0 \\ -t & 0 & 0 & 0 & -t & 0\ \ddots & 0 & \\ 0 & -t & 0 & 0 & 0 & 0 & 0 & -(\mu-\frac{U}{2}) \end{bmatrix}_{2N\times 2N} \longrightarrow$$

Kinetic term

$$V_l(m) = Diag(\vec{m_{1,l}}\cdot\vec{\sigma}, \vec{m_{2,l}}\cdot\vec{\sigma}, \vec{m_{3,l}}\cdot\vec{\sigma}..\vec{m_{N,l}}\cdot\vec{\sigma}) \longrightarrow$$

Interaction term

$$\vec{m_{N,l}}\cdot\vec{\sigma} = cos\phi_{N,l}sin\theta_{N.l}\sigma_x + sin\phi_{N,l}sin\theta_{N.l}\sigma_y + cos\theta_{N,l}\sigma_x$$