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Selected Topics in Computational Quantum Physics

量子物理计算方法选讲

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Quantum Monte Carlo

- classical Monte Carlo

    importance sampling, Markov chain, detailed balance, Metropolis method

- quantum Monte Carlo for spin and bosonic systems

    world line QMC, continuous time limit, Stochastic Series Expansion (SSE)

- quantum Monte Carlo for fermonic systems

    determinant QMC, Majorana QMC

selected review articles:
J. E. Hirsch, Phys. Rev. B 31, 4403 (1985).
R. R. dos Santos, arXiv:cond-mat/0303551.
Z.-X. Li and H. Yao, Annual Review of Condensed Matter Physics 10, 337 (2019).

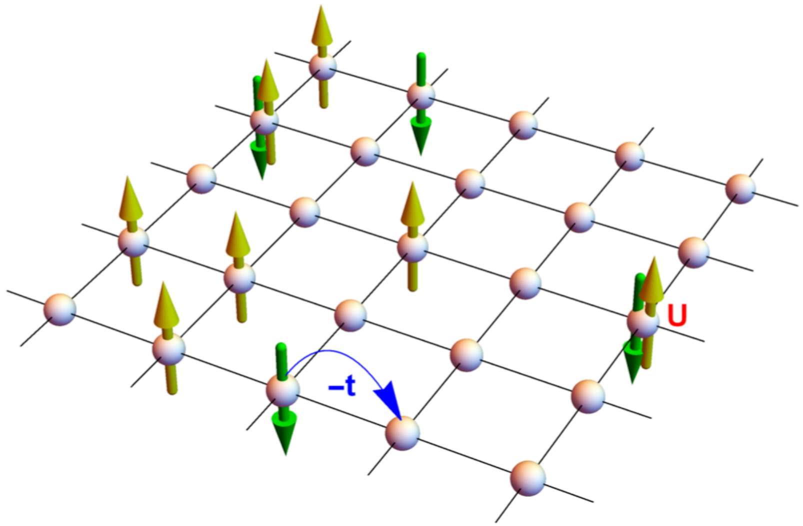
Hubbard model

- the Hamiltonian of the Hubbard model is

$$H = K + V$$

$$K = -t \sum_{\langle i,j \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) - \mu \sum_{i} \left(n_{i\uparrow} + n_{i\downarrow} - 1 \right)$$

$$V = U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right)$$



- particle-hole symmetry

the particle-hole transformation is $c_{i\sigma} \to (-1)^{i} d^{\dagger}_{i\sigma}, c^{\dagger}_{i\sigma} \to (-1)^{i} d_{i\sigma}$

in 2D, $i = (i_1, i_2), (-1)^{i} \to (-1)^{i_1 + i_2}$

for a pair of next neighbor $\langle i, j \rangle$ $(-1)^{i+j} = -1$

the hopping term and interaction term stay invariant, but $\mu \to -\mu$

$$K \to -t \sum_{\langle i,j \rangle \sigma} \left((-1)^{i} d_{i\sigma} (-1)^{j} d^{\dagger}_{j\sigma} + (-1)^{j} d_{j\sigma} (-1)^{i} d^{\dagger}_{i\sigma} \right) - \mu \sum_{i} \left(d_{i\uparrow} d^{\dagger}_{i\uparrow} + d_{i\downarrow} d^{\dagger}_{i\downarrow} - 1 \right)$$

$$= -t \sum_{\langle i,j \rangle \sigma} \left(d^{\dagger}_{i\sigma} d_{j\sigma} + d^{\dagger}_{j\sigma} d_{i\sigma} \right) + \mu \sum_{i} \left(\bar{n}_{i\uparrow} + \bar{n}_{i\downarrow} - 1 \right)$$

$$V \to U \sum_{i} \left(d_{i\uparrow} d^{\dagger}_{i\uparrow} - \frac{1}{2} \right) \left(d_{i\downarrow} d^{\dagger}_{i\downarrow} - \frac{1}{2} \right) = U \sum_{i} \left(\bar{n}_{i\uparrow} - \frac{1}{2} \right) \left(\bar{n}_{i\downarrow} - \frac{1}{2} \right)$$

Multidimensional Gaussian integration

- the equations involved in determinant QMC bear many similarities with multidimensional Gaussian integrals

- one dimensional Gaussian integral $\int_{-\infty}^{+\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}$

  many dimensional Gaussian integral

$$Z = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} dx_1 dx_2 \cdots dx_N e^{-\vec{x} A \vec{x}^T} = \frac{\pi^{N/2}}{\sqrt{\det A}}$$

- when the integrand includes factors of x_i

$$\langle x_i x_j \rangle = Z^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_N \; x_i x_j \; e^{-\vec{x} A \vec{x}^T} = \frac{1}{2} [A^{-1}]_{ij}$$

  further factors of x_i in the integrand generate expressions which are similar in form to Wick’s theorem

$$\begin{aligned} \langle x_i x_j x_k x_l \rangle &= Z^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_N x_i x_j x_k x_l e^{-\vec{x} A \vec{x}^T} \\ &= \frac{1}{4} ([A^{-1}]_{ij} [A^{-1}]_{kl} + [A^{-1}]_{ik} [A^{-1}]_{jl} + [A^{-1}]_{il} [A^{-1}]_{jk}) \end{aligned}$$

Trace in quantum Fock space

- in analogy with multidimensional Gaussian integration, we can do such traces if they are over quadratic forms of fermion operators

- suppose

$$H = \begin{pmatrix} c_{1\sigma}^\dagger & c_{2\sigma}^\dagger & . & . \end{pmatrix} \begin{pmatrix} h_{11} & h_{12} & . & . \\ h_{21} & h_{22} & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ . \\ . \end{pmatrix}$$

h is an $N \times N$ matrix

the identity is

$$Z = \mathrm{Tr} e^{-\beta H} = \det\left[\mathbb{I} + e^{-\beta h}\right]$$

full quantum Fock space

4^N dimensional

single particle space

$2N$ dimensional

- for a single fermion degree of freedom, $H = \epsilon c^\dagger c$

$$Z = \langle 0|e^{-\beta\epsilon c^\dagger c}|0\rangle + \langle 1|e^{-\beta\epsilon c^\dagger c}|1\rangle = 1 + e^{-\beta\epsilon}$$

for more than one fermion degree of freedom, it can be verified by going to the basis where h is diagonal

Details (1): taking the fermion trace

- we want to show that the Fock traces over bilinear fermion operators can be taken explicitly and give a one-particle determinant

$$\mathrm{Tr}\left(e^{\sum_{ij} A_{ij} c_i^\dagger c_j}\right) = \det\left[\mathbb{I} + e^A\right]$$

- the trace should be independent of the choice of basis

  we start by changing to a basis where the operator *D* is diagonal by performing a transformation

$$c_k = \sum_i \langle k \,|i\rangle \, c_i, \, c_k^\dagger = \sum_i \langle i \,|k\rangle \, c_i^\dagger$$

  so that in that basis *D* takes the form

$$D = \sum_k d_k c_k^\dagger c_k$$

- the trace over the fermion degrees of freedom then reads

$$\mathrm{Tr}\left(e^D\right) = \sum_{\{n_k\}} \langle \{n_k\}| \prod_k e^{d_k c_k^\dagger c_k} \,|\{n_k\}\rangle = \prod_k \sum_{n_k=0,1} e^{d_k n_k} = \prod_k \left(1 + e^{d_k}\right) = \det\left(\mathbb{I} + e^D\right)$$

Trace in quantum Fock space

- if one has a set of quadratic forms $l = 1, 2, \ldots, L$

$$H(l) = \begin{pmatrix} c^\dagger_{1\sigma} & c^\dagger_{2\sigma} & . & . \end{pmatrix} \begin{pmatrix} h(l)_{11} & h(l)_{12} & . & . \\ h(l)_{21} & h(l)_{22} & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ . \\ . \end{pmatrix}$$

there is a more general identity

$$Z = \mathrm{Tr}\left[e^{-\Delta\tau H(1)} e^{-\Delta\tau H(2)} \ldots e^{-\Delta\tau H(L)}\right] = \det\left[\mathbb{I} + e^{-\Delta\tau h(1)} e^{-\Delta\tau h(2)} \ldots e^{-\Delta\tau h(L)}\right]$$

- it is also true that

$$\begin{aligned} g^\sigma_{ij} = \left\langle c_{i\sigma} c^\dagger_{j\sigma} \right\rangle &= Z^{-1}\mathrm{Tr}\left[c_{i\sigma} c^\dagger_{j\sigma} e^{-\Delta\tau H(1)} e^{-\Delta\tau H(2)} \ldots e^{-\Delta\tau H(L)}\right] \\ &= \left[\mathbb{I} + e^{-\Delta\tau h(1)} e^{-\Delta\tau h(2)} \ldots e^{-\Delta\tau h(L)}\right]^{-1}_{ij} \end{aligned}$$

the fermion Green's function is just an appropriate matrix element of the inverse of the $N \times N$ matrix whose determinant gives the partition function

Details (2): equal-time Green's function

- we consider the single-particle Green's function in the diagonal representation

$$\left\langle c_i c_j^\dagger \right\rangle = \frac{\mathrm{Tr} c_i c_j^\dagger \prod_k e^{d_k c_k^\dagger c_k}}{\prod_k e^{d_k c_k^\dagger c_k}} = \sum_{k'} \langle i \, | k' \rangle \langle k' \, | j \rangle \, \frac{\mathrm{Tr} c_{k'} c_{k'}^\dagger \prod_k e^{d_k c_k^\dagger c_k}}{\prod_k (1+e^{d_k})}$$

- writing the trace explicitly

$$\begin{aligned}\mathrm{Tr} c_{k'} c_{k'}^\dagger \prod_k e^{d_k c_k^\dagger c_k} &= \sum_{\{n_k\}} \langle \{n_k\} | \, c_{k'} c_{k'}^\dagger \prod_k e^{d_k c_k^\dagger c_k} \, | \{n_k\} \rangle \\ &= \sum_{\{n_k\}} (1 - n_{k'}) \, e^{d_{k'} n_{k'}} \prod_{k \neq k'} e^{d_k n_k} = \prod_{k \neq k'} \sum_{n_k = 0,1} e^{d_k n_k}\end{aligned}$$

only states with $n_{k'} = 0$ contribute to the sum

- the Green's function becomes

$$\left\langle c_i c_j^\dagger \right\rangle = \sum_{k'} \langle i \, | k' \rangle \langle k' \, | j \rangle \, \frac{\prod_{k \neq k'} (1+e^{d_k})}{\prod_k (1+e^{d_k})} = \sum_{k'} \frac{\langle i \, | k' \rangle \langle k' \, | j \rangle}{1+e^{d_{k'}}} = \left(\frac{1}{\mathbb{I} + e^D} \right)_{ij} = \left(\mathbb{I} + e^D \right)^{-1}_{ij}$$

Hubbard-Stratonovich transformation

- the above formulae describe how to perform traces over quadratic forms of fermion degrees of freedom

  however, the Hubbard Hamiltonian has an interaction term which is quartic in the fermion operators

- for the repulsive case, the discrete Hubbard-Stratonovich transformation is

$$e^{-U\Delta\tau\left(n_\uparrow-\frac{1}{2}\right)\left(n_\downarrow-\frac{1}{2}\right)} = \omega \sum_{s=\pm 1} e^{s\lambda(n_\uparrow - n_\downarrow)}$$

with ω and λ to be found

for $(n_\uparrow, n_\downarrow) = (0,0)$ and $(1,1)$, $e^{-\frac{1}{4}U\Delta\tau} = 2\omega$

for $(n_\uparrow, n_\downarrow) = (0,1)$ and $(1,0)$, $e^{+\frac{1}{4}U\Delta\tau} = \omega\left(e^{+\lambda} + e^{-\lambda}\right) = 2\omega\cosh\lambda$

therefore, $\omega = \frac{1}{2}e^{-\frac{1}{4}U\Delta\tau}, \cosh\lambda = e^{\frac{1}{2}U\Delta\tau}$

$$e^{\boxed{-U\Delta\tau\left(n_\uparrow-\frac{1}{2}\right)\left(n_\downarrow-\frac{1}{2}\right)}} = \frac{1}{2}e^{-\frac{1}{4}U\Delta\tau}\sum_{s=\pm 1} e^{s\lambda(n_\uparrow - n_\downarrow)} = \frac{1}{2}e^{-\frac{1}{4}U\Delta\tau}\sum_{s=\pm 1}\prod_{\sigma=\uparrow,\downarrow} e^{\boxed{\sigma s\lambda n_\sigma}}$$

four-fermion operator

two-fermion operator

Hubbard-Stratonovich transformation

- for the attractive case, writing $U = -|U|$, $e^{|U|\Delta\tau\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right)} = \omega \sum_{s=\pm 1} e^{s\lambda(n_\uparrow + n_\downarrow - 1)}$

  for $(n_\uparrow, n_\downarrow) = (0,1)$ and $(1,0)$, $e^{-\frac{1}{4}|U|\Delta\tau} = 2\omega$

  for $(n_\uparrow, n_\downarrow) = (0,0)$ and $(1,1)$, $e^{+\frac{1}{4}|U|\Delta\tau} = \omega\left(e^{+\lambda} + e^{-\lambda}\right) = 2\omega\cosh\lambda$

  therefore, $\omega = \frac{1}{2}e^{-\frac{1}{4}|U|\Delta\tau}, \cosh\lambda = e^{\frac{1}{2}|U|\Delta\tau}$

$$e^{\boxed{|U|\Delta\tau\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right)}} = \frac{1}{2}e^{-\frac{1}{4}|U|\Delta\tau} \sum_{s=\pm 1} e^{s\lambda(n_\uparrow + n_\downarrow - 1)} = \frac{1}{2}e^{-\frac{1}{4}|U|\Delta\tau} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{\boxed{s\lambda\left(n_\sigma - \frac{1}{2}\right)}}$$

four-fermion operator

two-fermion operator

Formalism of determinant QMC

- in solving the Hubbard model we want to evaluate expressions like

$$\langle A\rangle = Z^{-1}\mathrm{Tr}\left[Ae^{-\beta H}\right], Z = \mathrm{Tr}e^{-\beta H}$$

  we divide $\beta = L\Delta\tau$ and employ the Trotter-Suzuki decomposition

$$Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\left[e^{-\Delta\tau K}\, e^{-\Delta\tau V}\, e^{-\Delta\tau K}\, e^{-\Delta\tau V} \ldots\right]$$

Formalism of determinant QMC

- for each factor of the L terms $e^{-\Delta\tau V}$ we introduce N Hubbard-Stratonovich field, one for each of the spatial sites

  the Hubbard-Stratonovich field $s(i, l)$ has two indices, space i and imaginary-time l

$$Z = \mathrm{Tr} \prod_{l=1}^{L} e^{-\Delta\tau \sum_\sigma H_{\mathrm{hop},\sigma}} e^{-\Delta\tau\left[-\mu \sum_i \left(\sum_\sigma n_{i\sigma} - 1\right)\right]} \prod_i \left[\frac{1}{2} e^{-\frac{1}{4}U\Delta\tau} \sum_{s(i,l)} e^{\sum_\sigma \sigma s(i,l)\lambda n_{i\sigma}}\right]$$

$$= \left(\frac{1}{2} e^{-\frac{1}{4}U\Delta\tau} e^{-\Delta\tau\mu}\right)^{LN} \sum_{s(i,l)} \mathrm{Tr} \prod_\sigma \left[\prod_{l=1}^{L} e^{-\Delta\tau H_{\mathrm{hop},\sigma}} e^{\sum_i (\Delta\tau\mu + \sigma s(i,l)\lambda) n_{i\sigma}}\right]$$

$$= c^{LN} \sum_{s(i,l)} \mathrm{Tr} \prod_\sigma \left[\prod_{l=1}^{L} B_l^\sigma\right] = c^{LN} \sum_{s(i,l)} \prod_\sigma \mathrm{Tr}\left[B_L^\sigma B_{L-1}^\sigma \cdots B_1^\sigma\right]$$

$$\boxed{= c^{LN} \sum_{s(i,l)} \prod_\sigma \det\left(\mathbb{I} + B_L^\sigma B_{L-1}^\sigma \cdots B_1^\sigma\right) = c^{LN} \sum_{s(i,l)} \det M^\uparrow \det M^\downarrow}$$

- here

$$\boxed{B_l^\sigma = e^{-\Delta\tau \sum_{ij} c_{i\sigma}^\dagger K_{ij} c_{j\sigma}} e^{\sum_i c_{i\sigma}^\dagger V_{il}^\sigma c_{i\sigma}}}$$

$$K_{ij} = \begin{cases} -t & \langle i, j\rangle \text{ nearest neighbours} \\ 0 & \text{others} \end{cases} \qquad \boxed{V_{il}^\sigma = \Delta\tau\mu + \sigma s(i,l)\lambda}$$

Formalism of determinant QMC

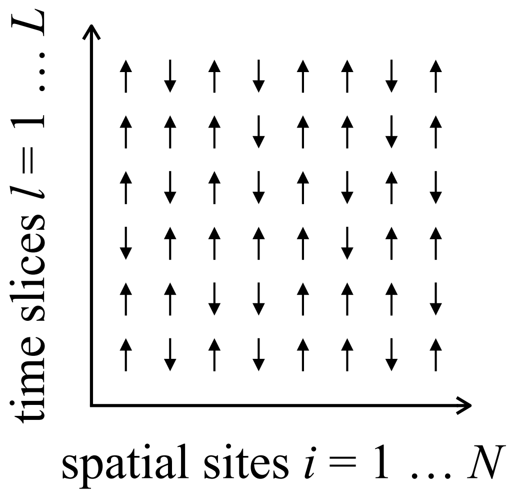
- for example, in 1D

$$B_l^\sigma = e^{-\Delta\tau \sum_{ij} c_{i\sigma}^\dagger K_{ij} c_{j\sigma}} e^{\sum_i c_{i\sigma}^\dagger V_{il}^\sigma c_{i\sigma}} \qquad V_{il}^\sigma = \Delta\tau\mu + \sigma s(i,l)\lambda$$

K, V, and M are $N \times N$ matrices

$$K = \begin{pmatrix} 0 & -t & 0 & \cdots & -t \\ -t & 0 & -t & \cdots & \cdots \\ 0 & -t & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -t \\ -t & 0 & \cdots & -t & 0 \end{pmatrix} \qquad V_l^\sigma = \begin{pmatrix} V_{1l}^\sigma & 0 & \cdots & \cdots & 0 \\ 0 & V_{1l}^\sigma & 0 & \cdots & \cdots \\ \vdots & 0 & \ddots & \ddots & \cdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & \vdots & \cdots & 0 & V_{Nl}^\sigma \end{pmatrix}$$

- we then sample over Hubbard-Stratonovich field configurations $s(i, l)$ using classical Monte Carlo



- the probability density is

$$\frac{1}{Z} \det M^\uparrow \det M^\downarrow$$

Determinant QMC algorithm

(1) initialize all the Hubbard-Stratonovich fields $s(i,l)$

(2) compute the matrices M^σ(s) and their determinants

(3) change one or more of the Hubbard-Stratonovich fields, and compute the new matrices M^σ(s') and their determinants

(4) throw a random number $0 < r < 1$ and accept the new configuration with probability

$$\min\left\{1, \frac{\det M^{\uparrow}(s')}{\det M^{\uparrow}(s)} \frac{\det M^{\downarrow}(s')}{\det M^{\downarrow}(s)}\right\}$$

the usual Metropolis algorithm

(5) repeat (1)-(4), measurements of the Greens function g_{ij} are obtained by accumulating $(M^{-1})_{ij}$

other observables like magnetic susceptibility by appropriate products of matrix elements of M^{-1}

Details (3): simplified ratio

- the ratio between the determinant products of two spin configurations *s* and *s'* is

$$R = R^{\uparrow} R^{\downarrow} = \frac{\det M^{\uparrow}(s')}{\det M^{\uparrow}(s)} \frac{\det M^{\downarrow}(s')}{\det M^{\downarrow}(s)}$$

- the most simple transition between two Markov configurations involves flipping at most one spin at a time $s(i,l) \to -s(i,l)$

- the change of the matrix element in V_{il}^{σ} is $\delta V_{il}^{\sigma} = -2\sigma s(i,l)\lambda$

  accordingly, the matrix B_l^{σ} is also changed $B_l^{\sigma} \to B_l^{\sigma} \Delta_{il}^{\sigma}$

  the elements of the matrix Δ_{il}^{σ} are

$$[\Delta_{il}^{\sigma}]_{jk} = \begin{cases} 0 & \text{if } j \neq k \\ 1 & \text{if } j = k \neq i \\ e^{-2\sigma s(i,l)\lambda} & \text{if } j = k = i \end{cases}$$

- the ratio R^{σ} can then be written in a simple form

$$R^{\sigma} = \frac{\det\left(\mathbb{I} + B_L^{\sigma} \cdots B_l^{\sigma} \Delta_{il}^{\sigma} B_{l-1}^{\sigma} \cdots B_1^{\sigma}\right)}{\det\left(\mathbb{I} + B_L^{\sigma} \cdots B_1^{\sigma}\right)} = \frac{\det\left[\mathbb{I} + \left(B_{l-1}^{\sigma} \cdots B_1^{\sigma}\right)\left(B_L^{\sigma} \cdots B_l^{\sigma}\right)\Delta_{il}^{\sigma}\right]}{\det\left[\mathbb{I} + \left(B_{l-1}^{\sigma} \cdots B_1^{\sigma}\right)\left(B_L^{\sigma} \cdots B_l^{\sigma}\right)\right]}$$

$$= \frac{\det\left[\mathbb{I} + F^{\sigma}(l)\Delta_{il}^{\sigma}\right]}{\det\left[\mathbb{I} + F^{\sigma}(l)\right]} = \det\left[\left(\mathbb{I} + F^{\sigma}(l)\Delta_{il}^{\sigma}\right) g^{\sigma}(l)\right] \qquad g^{\sigma}(l) = [\mathbb{I} + F^{\sigma}(l)]^{-1}$$

Details (3): simplified ratio

- since

$$g^\sigma(l) = [\mathbb{I} + F^\sigma(l)]^{-1}$$

$$\Rightarrow F^\sigma(l)\, g^\sigma(l) = \frac{F^\sigma(l)}{\mathbb{I} + F^\sigma(l)} = \mathbb{I} - \frac{1}{\mathbb{I} + F^\sigma(l)} = \mathbb{I} - g^\sigma(l)$$

the ratio becomes

$$R^\sigma = \det\left[g^\sigma(l) + F^\sigma(l)\, g^\sigma(l)\, \Delta^\sigma_{il}\right] = \det\left[g^\sigma(l) + (\mathbb{I} - g^\sigma(l))\, \Delta^\sigma_{il}\right] = \det\left[\mathbb{I} + (\mathbb{I} - g^\sigma(l))\,(\Delta^\sigma_{il} - \mathbb{I})\right]$$

- since $\Delta^\sigma_{il} - \mathbb{I}$ is a matrix such that all elements are zero except for the i^{th} position in the diagonal

$$\Delta^\sigma_{il} - \mathbb{I} = \begin{pmatrix} 0 & & & & \\ & \ddots & & & \\ & & e^{-2\sigma s(i,l)\lambda} - 1 & & \\ & & & \ddots & \\ & & & & 0 \end{pmatrix}$$

R^σ is given in terms of the Green's function

$$\boxed{R^\sigma = 1 + \left[1 - (g^\sigma(l))_{ii}\right]\left(e^{-2\sigma s(i,l)\lambda} - 1\right)}$$

so that one actually does not need to calculate determinants

Details (4): update Green's function

- if the new configuration is accepted, the whole Green's function for the current time slice must be updated
- since

$$R^\sigma = \frac{\det M^\sigma(s')}{\det M^\sigma(s)} = \det\left[\mathbb{I} + \left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)\right]$$

$$g'^\sigma(l) = \left[M^\sigma(s')\right]^{-1}, g^\sigma(l) = \left[M^\sigma(s)\right]^{-1}$$

we have

$$\frac{g^\sigma(l)}{g'^\sigma(l)} = \mathbb{I} + \left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)$$

so that

$$\boxed{g'^\sigma(l)} = \frac{g^\sigma(l)}{\mathbb{I} + \left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)}$$

$$= \frac{g^\sigma(l) + g^\sigma(l)\left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right) - g^\sigma(l)\left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)}{\mathbb{I} + \left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)}$$

$$= g^\sigma(l) - \frac{g^\sigma(l)\left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)}{\mathbb{I} + \left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)} = g^\sigma(l) - \frac{g^\sigma(l)\left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)}{1 + \left[1 - \left(g^\sigma(l)\right)_{ii}\right]\left(e^{-2\sigma s(i,l)\lambda} - 1\right)}$$

$$\boxed{= g^\sigma(l) - g^\sigma(l)\left(\mathbb{I} - g^\sigma(l)\right)\left(\Delta_{il}^\sigma - \mathbb{I}\right)/R^\sigma}$$

- we evaluate the new equal-time Green's function through the above relation

Details (4): update Green's function

- the Green's function for the $(l+1)^{\text{th}}$ time slice can be calculated either from

$$g^{\sigma}(l) = \left(\mathbb{I} + B_{l-1}^{\sigma} \cdots B_{1}^{\sigma} B_{L}^{\sigma} \cdots B_{l}^{\sigma}\right)^{-1}$$

or iteratively from the Green's function for the l^{th} time slice

- by comparing

$$g^{\sigma}(l) = \left[\mathbb{I} + \left(B_{l-1}^{\sigma} \cdots B_{1}^{\sigma}\right)\left(B_{L}^{\sigma} \cdots B_{l+1}^{\sigma} B_{l}^{\sigma}\right)\right]^{-1}$$

$$g^{\sigma}(l+1) = \left[\mathbb{I} + \left(B_{l}^{\sigma} B_{l-1}^{\sigma} \cdots B_{1}^{\sigma}\right)\left(B_{L}^{\sigma} \cdots B_{l+1}^{\sigma}\right)\right]^{-1}$$

we calculate

$$B_{l}^{\sigma}\left[g^{\sigma}(l)\right]^{-1}\left(B_{l}^{\sigma}\right)^{-1} = B_{l}^{\sigma}\left[\mathbb{I} + \left(B_{l-1}^{\sigma} \cdots B_{1}^{\sigma}\right)\left(B_{L}^{\sigma} \cdots B_{l+1}^{\sigma} B_{l}^{\sigma}\right)\right]\left(B_{l}^{\sigma}\right)^{-1}$$

$$= \mathbb{I} + \left(B_{l}^{\sigma} B_{l-1}^{\sigma} \cdots B_{1}^{\sigma}\right)\left(B_{L}^{\sigma} \cdots B_{l+1}^{\sigma}\right) = \left[g^{\sigma}(l+1)\right]^{-1}$$

$$\Rightarrow \boxed{g^{\sigma}(l+1) = B_{l}^{\sigma} g^{\sigma}(l)\left(B_{l}^{\sigma}\right)^{-1}}$$

which can be used to compute the Green's function in the subsequent time slice

- to avoid the gradual loss of precision, we still have to recompute Green's function from $g^{\sigma}(l) = \left(\mathbb{I} + B_{l-1}^{\sigma} \cdots B_{1}^{\sigma} B_{L}^{\sigma} \cdots B_{l}^{\sigma}\right)^{-1}$ after several steps

Details (5): matrix multiplications

- we are concerned with numerically solving the following linear system of equations involving a long chain of matrix multiplication

$$(\mathbb{I} + B_L \cdots B_2 B_1)\, x = b$$

- the linear system is often very ill-conditioned

  naturally one could attempt to improve its conditioning by certain equivalent transformations

- we compute the Singular Value Decomposition (SVD) of B_1

$$B_1 = U_1 S_1 V_1$$

then we compute $$B_2 U_1 S_1 = U_2 S_2 V_2$$

similarly $$B_l U_{l-1} S_{l-1} = U_l S_l V_l$$

- finally the linear system is transformed into

$$[\mathbb{I} + U_L S_L \, (V_L \cdots V_1)]\, x = b$$

Bai et al., Linear Algebra Appl. 435, 659-673 (2011).

Details (5): matrix multiplications

- for ill-conditioned system, the diagonal entries of S_L have wide range of magnitudes

  while (V_L … V_1) being orthogonal is perfectly well-conditioned

- we define two $L \times L$ diagonal matrices

$$(S_b)_{ii} = \begin{cases} (S_L)_{ii} & \text{if } (S_L)_{ii} > 1 \\ 1 & \text{if } (S_L)_{ii} \leq 1 \end{cases}, (S_s)_{ii} = \begin{cases} 1 & \text{if } (S_L)_{ii} > 1 \\ (S_L)_{ii} & \text{if } (S_L)_{ii} \leq 1 \end{cases}$$

  then
$$S_L = S_b S_s$$
  S_b^{-1} and S_s are among the same range of magnitudes

- now the linear system becomes

$$S_b^{-1} U_L^\dagger \left[\mathbb{I} + U_L S_b S_s \left(V_L \cdots V_1\right)\right] x = S_b^{-1} U_L^\dagger b$$

$$\left[S_b^{-1} U_L^\dagger + S_s \left(V_L \cdots V_1\right)\right] x = S_b^{-1} U_L^\dagger b$$

  thus can be solved as

$$x = \left[S_b^{-1} U_L^\dagger + S_s \left(V_L \cdots V_1\right)\right]^{-1} \left[S_b^{-1} U_L^\dagger b\right]$$

Implementation

Algorithm 1 Naive sweep through the space-time lattice

Require: $\mathbf{K}, \lambda, N, L$

procedure SWEEP($\{s_{1,1}, \dots, s_{N,1}, \dots, s_{1,L}, \dots, s_{N,L}\}, \mathbf{g}^{\sigma}(1)$)

  for $l \leftarrow 1, L$ **do**

    for $i \leftarrow 1, N$ **do**

      $s \leftarrow s_{i,l}$

      $g \leftarrow [\mathbf{g}^{\sigma}(l)]_{i,i}$

      $R^{\sigma} \leftarrow 1 + (1-g)\left(\mathrm{e}^{-2\sigma\lambda s} - 1\right)$ ▷ σ meant as $\sigma = \{\uparrow, \downarrow\}$

      $Y \leftarrow \min\left(1, R^{\uparrow} R^{\downarrow}\right)$ ▷ Metropolis algorithm

      if RAND$(0,1) < Y$ **then**

        $s_{i,l} \leftarrow -s_{i,l}$

        $\mathbf{g}^{\sigma}(l) \leftarrow$ UPDATE$(g^{\sigma}(l), i, s)$

      end if

    end for

    $\mathbf{B}_l^{\sigma} \leftarrow e^{\mathbf{K}} e^{\Delta\tau\mu + \sigma\lambda\{s_{1,l}, \cdots, s_{N,l}\}}$

    $\mathbf{g}^{\sigma}(l+1) \leftarrow \mathbf{B}_l^{\sigma} \mathbf{g}^{\sigma}(l) \left(\mathbf{B}_l^{\sigma}\right)^{-1}$ ▷ Wrapping

  end for

end procedure

procedure UPDATE($g^{\sigma}(l), i, s$)

  for $j, k \leftarrow 1, N$ **do**

$$[g^{\sigma}(l)]_{j,k} \leftarrow [g^{\sigma}(l)]_{j,k} - \frac{[g^{\sigma}(l)]_{j,i}\left(\delta_{i,k} - [g^{\sigma}(l)]_{i,k}\right)}{\left(e^{-2\sigma\lambda s} - 1\right)^{-1} + (1-g)}$$

  end for

end procedure

Fermion sign problem

- the algorithm relies on the probability density $\frac{1}{Z} \det M^{\uparrow} \det M^{\downarrow}$

  this can become negative for certain cases

- repulsive Hubbard model $\det M^{\sigma} = \mathrm{Tr}\left(B_L^{\sigma} B_{L-1}^{\sigma} \cdots B_1^{\sigma}\right)$

$$B_l^{\uparrow} = e^{t\Delta\tau \sum_{\langle ij\rangle}\left(c_{i\uparrow}^{\dagger} c_{j\uparrow} + h.c.\right)} e^{\sum_i c_{i\uparrow}^{\dagger}[\Delta\tau\mu + s(i,l)\lambda] c_{i\uparrow}}$$

$$B_l^{\downarrow} = e^{t\Delta\tau \sum_{\langle ij\rangle}\left(c_{i\downarrow}^{\dagger} c_{j\downarrow} + h.c.\right)} e^{\sum_i c_{i\downarrow}^{\dagger}[\Delta\tau\mu - s(i,l)\lambda] c_{i\downarrow}}$$

- at half filling $\mu = 0$, we apply particle-hole transformations to spin-up electrons

$$B_l^{\uparrow} \to e^{t\Delta\tau \sum_{\langle ij\rangle}\left(d_{i\uparrow}^{\dagger} d_{j\uparrow} + d_{j,\uparrow}^{\dagger} d_{i,\uparrow}\right)} e^{\sum_i s(i,l)\lambda\left(1 - d_{i\uparrow}^{\dagger} d_{i\uparrow}\right)}$$

$$= e^{\sum_i s(i,l)\lambda}\left[e^{t\Delta\tau \sum_{\langle ij\rangle}\left(d_{i\uparrow}^{\dagger} d_{j\uparrow} + d_{j,\uparrow}^{\dagger} d_{i,\uparrow}\right)} e^{-\sum_i s(i,l)\lambda d_{i\uparrow}^{\dagger} d_{i\uparrow}}\right]$$

$$B_l^{\downarrow} = e^{t\Delta\tau \sum_{\langle ij\rangle}\left(c_{i\downarrow}^{\dagger} c_{j\downarrow} + c_{j,\downarrow}^{\dagger} c_{i,\downarrow}\right)} e^{-\sum_i s(i,l)\lambda c_{i\downarrow}^{\dagger} c_{i\downarrow}}$$

$$\boxed{\det M^{\uparrow}} = \mathrm{Tr}_{d_{\uparrow}}\left(B_L^{\uparrow} B_{L-1}^{\uparrow} \cdots B_1^{\uparrow}\right) = e^{\sum_{il} s(i,l)\lambda}\mathrm{Tr}_{c_{\downarrow}}\left(B_L^{\downarrow} B_{L-1}^{\downarrow} \cdots B_1^{\downarrow}\right) = \boxed{e^{\sum_{il} s(i,l)\lambda} \det M^{\downarrow}}$$

the probability density $\det M^{\uparrow}(s) \det M^{\downarrow}(s)/Z$ is positive definite, so that it can be used as a Boltzmann weight

Fermion sign problem

- for the attractive Hubbard model, the lack of σ-dependence in the discrete Hubbard-Stratonovich transformation leads to $M^{\uparrow}(s) = M^{\downarrow}(s)$

  the product of determinants is positive for all fillings $\rightarrow$ no sign problem

- for the repulsive Hubbard model away from half filling, the product of determinants does become negative for certain field configurations

  in order to circumvent this problem, we write

$$P(s) = \det M^{\uparrow}(s) \det M^{\downarrow}(s) = |P(s)| \operatorname{sign}(s)$$

  the average of A can be replaced by an average weighted by $P'(s) = |P(s)|$

$$\langle A \rangle_s = \frac{\sum_s P(s)\, A(s)}{\sum_s P(s)} = \frac{\sum_s |P(s)| \operatorname{sign}(s)\, A(s)}{\sum_s |P(s)| \operatorname{sign}(s)} = \frac{\left[\sum_s |P(s)| \operatorname{sign}(s)\, A(s)\right] / \left[\sum_s |P(s)|\right]}{\left[\sum_s |P(s)| \operatorname{sign}(s)\right] / \left[\sum_s |P(s)|\right]}$$

$$= \frac{\sum_s P'(s) \left[\operatorname{sign}(s)\, A(s)\right]}{\sum_s P'(s) \left[\operatorname{sign}(s)\right]} = \frac{\langle \operatorname{sign}(s)\, A(s) \rangle_{P'(s)}}{\langle \operatorname{sign}(s) \rangle_{P'(s)}}$$

- importance sampling is now performed with respect to $|P(s)|$

  the final result has to be divided by the average value of the sign $\langle \operatorname{sign}(s) \rangle_{P'(s)}$

  when ever this quantity is small, much longer runs are necessary to compensate the strong fluctuations in $\langle A \rangle_s$

Fermion sign problem

- behaviors of $\langle \text{sign}\,(s) \rangle$ as functions of band filling and temperature

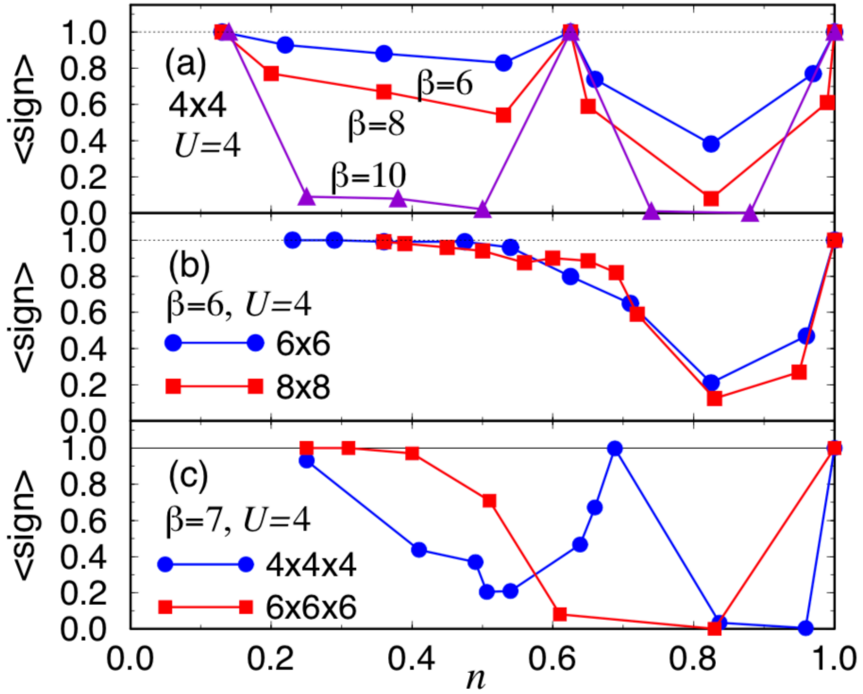


Figure 1. The average sign of the product of fermionic determinants as a function of band filling, for the Hubbard model with $U = 4$: (a) 4×4 square lattice, for inverse temperatures $\beta = 6$ (circles), 8 (squares), and 10 (triangles); adapted from Refs. [8] and [13]. (b) 6×6 (circles) and 8×8 (squares) square lattice, for fixed inverse temperature, $\beta = 6$; adapted from Ref. [13]. (c) $4 \times 4 \times 4$ (circles) and $6 \times 6 \times 6$ (squares) simple cubic lattice, for fixed inverse temperature, $\beta = 7$. Lines are guides to the eye in all cases.

[8] W. von der Linden, Phys. Rep. **220**, 53 (1992).

[13] S. R. White, D. J. Scalapino, R. L. Sugar, N. E. Bickers, and R. T. Scalettar, Phys. Rev. B **39**, 839 (1989).

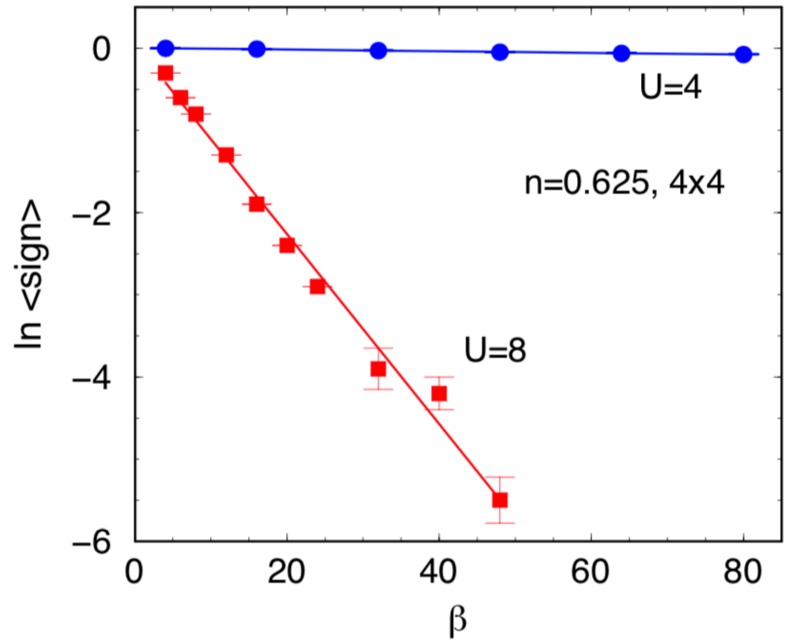


Figure 2. The logarithm of the average sign of the product of fermionic determinants as a function of inverse temperature, for the Hubbard model on a 4×4 square lattice with $n = 0.625$, and for different values of the Coulomb repulsion: $U = 4$ (circles) and 8 (squares). Lines are fits through the data points. Adapted from Ref. [40].

[40] E. Y. Loh, Jr. J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Phys. Rev. B **41**, 9301 (1990).

Results

- comparison with exact results

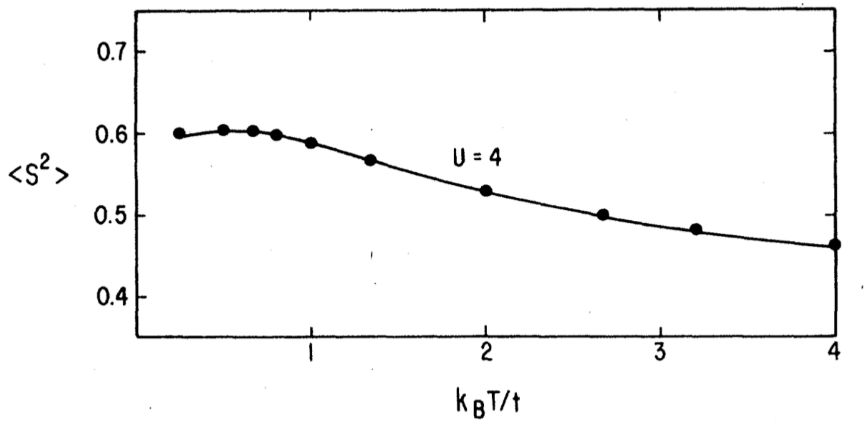


FIG. 4. Local moment versus temperature for a 6-site ring, $U=4$, with $\Delta\tau=0.125$. The solid line is the exact result of Shiba.

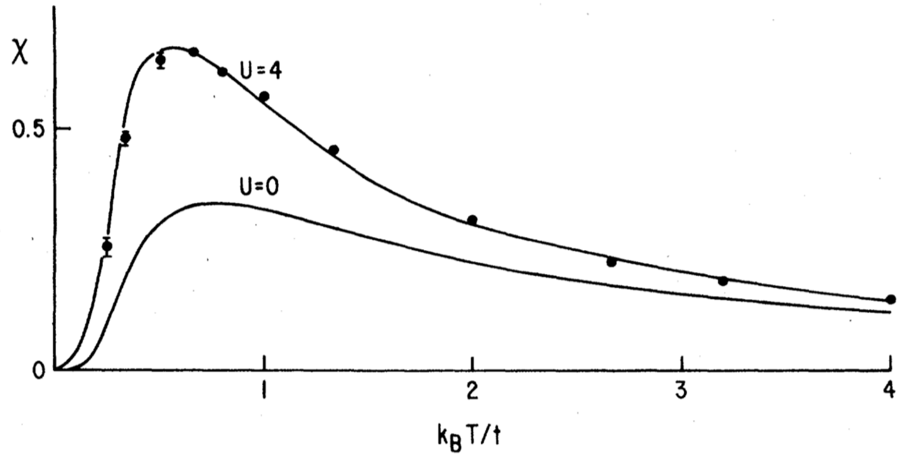


FIG. 5. Magnetic susceptibility versus temperature for a 6-site ring, $U=4$, with $\Delta\tau=0.125$. The solid line is the exact result of Shiba.

[7]H. Shiba and P. Pincus, Phys. Rev. B **5**, 1966 (1972); H. Shiba, Prog. Theor. Phys. **48**, 2171 (1972).

- results for the half filled band case

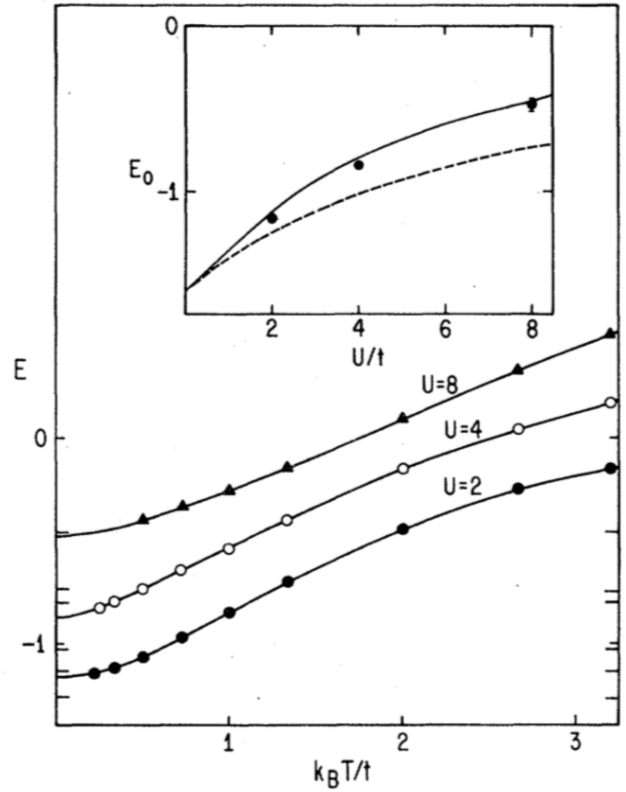


FIG. 9. Energy versus temperature for $U=2$, 4, and 8. The inset shows the extrapolated ground-state energy, compared with Hartree-Fock predictions (solid line) and the Langer-Mattis lower bound (dashed line).

J. E. Hirsch, Phys. Rev. B 31, 4403 (1985).
S. R. White et al., Phys. Rev. B 40, 506 (1989).

Results

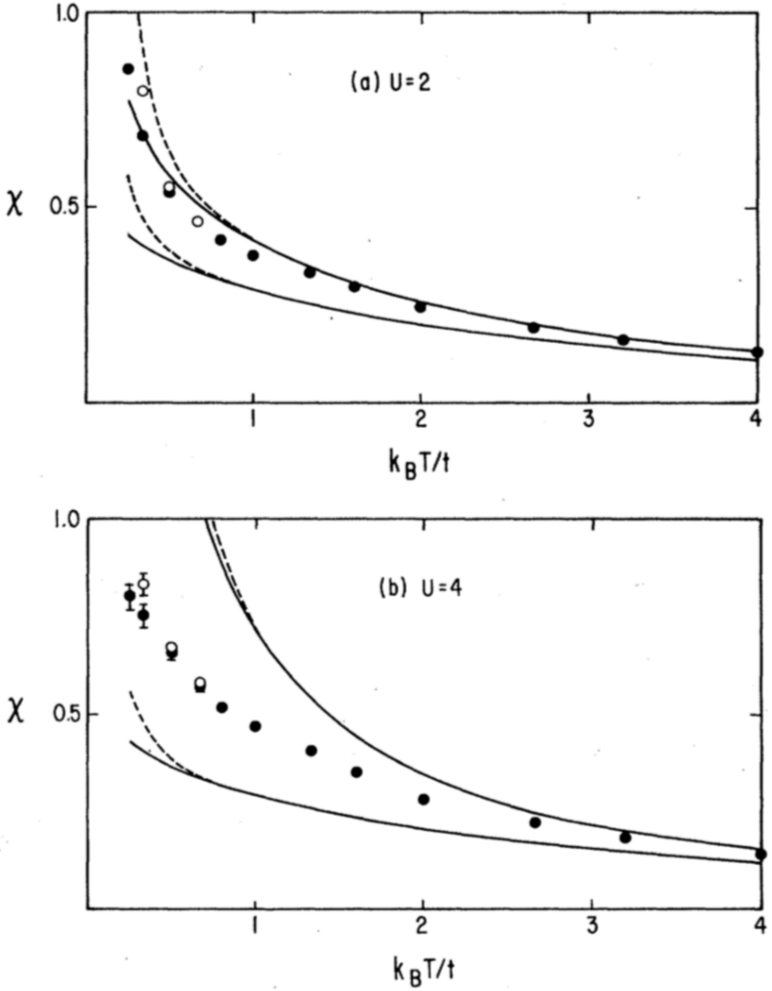


FIG. 7. Magnetic susceptibility versus temperature. The solid circles (open circles) are Monte Carlo results for a 6×6 (4×4) lattice. The lower solid line is the noninteracting result for an infinite lattice, the upper solid line the RPA prediction. The dashed line is the corresponding result for a 6×6 lattice, showing that finite-size effects start to appear around $T \sim 0.75$. For the interacting case, finite-size effects appear at a somewhat lower temperature.

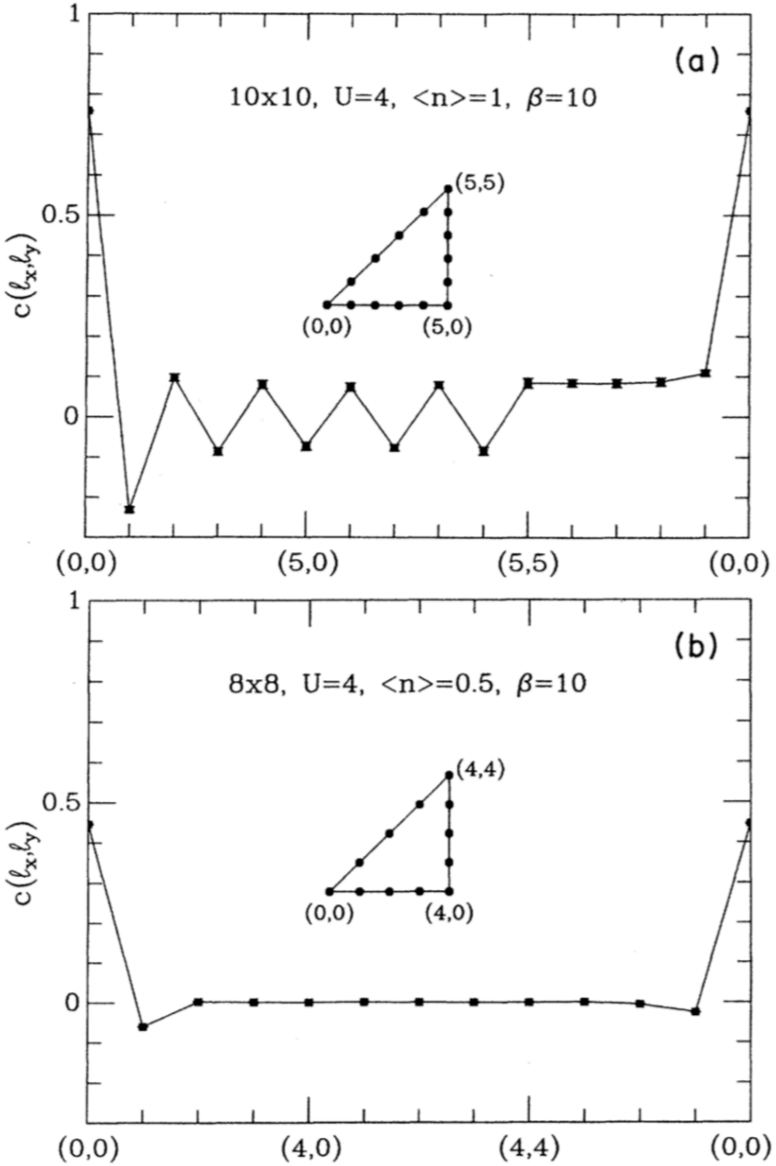


FIG. 1. Spin-spin correlation function $c(l_x, l_y)$. The horizontal axis traces out the triangular path showing in the center of the figure. Strong antiferromagnetic correlations are visible in (a), which is for a half-filled band, but are nearly absent in (b), which is at quarter-filling.

Results

- gaps and the spectral function for the Hubbard model at half filling

$$\Delta = \frac{1}{2}(\varepsilon_p + \varepsilon_h)$$

$$\varepsilon_{p,h} = - \lim_{\tau \to +\infty} \frac{\log\left(G^{p,h}(R=0,\tau)\right)}{\tau} = E(\mathcal{N}_p \pm 1) - E(\mathcal{N}_p)$$

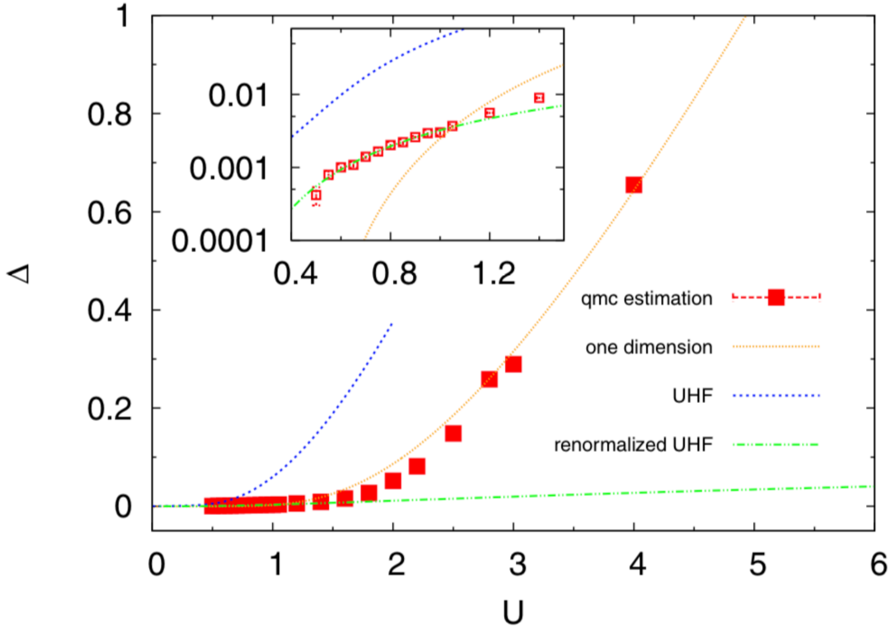


FIG. 9. Gap at half filling as a function of the interaction strength. Symbols are obtained from AFQMC calculations. Statistical error bars are shown but are smaller than symbol size. The (green) dashed line corresponds to a fit of the QMC data with a mean-field form allowing renormalized parameters. The (blue) dotted line is the actual mean-field result from unrestricted Hartree-Fock. The (orange) line at large U is the Bethe ansatz prediction for one dimension. The inset shows a zoom of the main graph at small U.

$$A(Q,\omega) = \begin{cases} \sum_n \left|\langle \Psi_n^{\mathcal{N}_p+1} | \hat{c}^\dagger_{Q,\sigma} | \Psi_0 \rangle\right|^2 \delta\left(\omega - \left(E_n^{\mathcal{N}_p+1} - E_0^{\mathcal{N}_p}\right)\right), & \omega > \mu \\ \sum_n \left|\langle \Psi_n^{\mathcal{N}_p-1} | \hat{c}_{Q,\sigma} | \Psi_0 \rangle\right|^2 \delta\left(\omega + \left(E_n^{\mathcal{N}_p-1} - E_0^{\mathcal{N}_p}\right)\right), & \omega < \mu \end{cases}$$

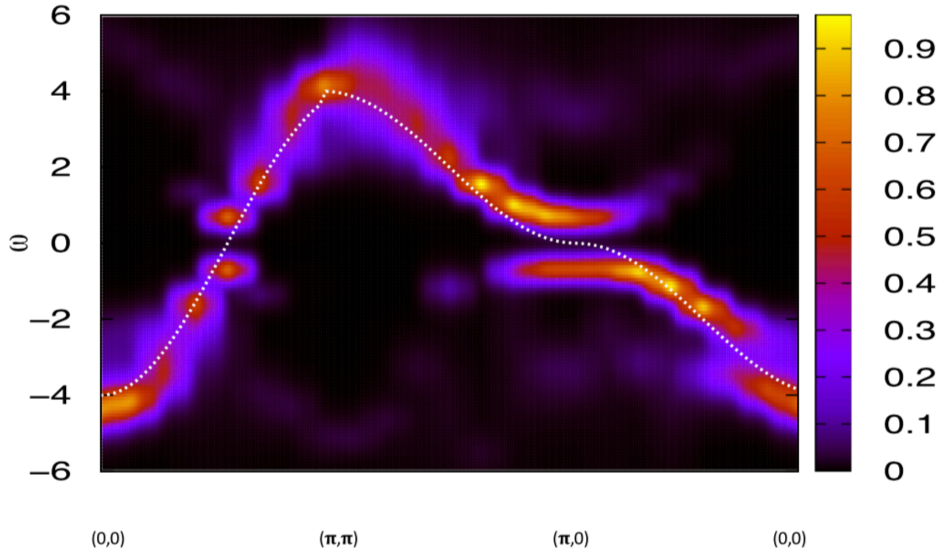


FIG. 10. Color plot of the spectral function $A(Q,\omega)$ as a function of momentum Q (horizontal axis) along the principal directions in the Brillouin zone and frequency ω (vertical axis). The spectral function has been obtained by performing an analytic continuation of the calculated imaginary time Green functions in momentum space. The system was a 16×16 lattice at $U/t = 4$. The dotted line is the noninteracting dispersion relation.

E. Vitali, H. Shi, M. Qin, and S. Zhang, Phys. Rev. B 94, 085140 (2016).

Fermion sign problem

- spinful Hubbard model, determinant QMC relies on the probability density
$$\frac{1}{Z}\det M^{\uparrow}\det M^{\downarrow}$$

- repulsive Hubbard model, at half filling $\mu = 0$

$$\det M^{\uparrow}(s) = e^{\sum_{il} s(i,l)\lambda}\det M^{\downarrow}(s)$$

the probability density $\det M^{\uparrow}(s)\det M^{\downarrow}(s)/Z$ is positive definite, so that it can be used as a Boltzmann weight

- repulsive Hubbard model away from half filling, the product of determinants does become negative for certain field configurations

- attractive Hubbard model, the lack of σ-dependence in the discrete Hubbard-Stratonovich transformation leads to $M^{\uparrow}(s) = M^{\downarrow}(s)$

  the product of determinants is positive for all fillings $\rightarrow$ no sign problem

Majorana QMC

- how about spinless fermion models?

$$H = H_0 + H_{\text{int}}, \qquad H_0 = -\sum_{ij}\left[t_{ij}c_i^\dagger c_j + h.c.\right], \qquad H_{\text{int}} = \sum_{ij} V_{ij}(n_i - 1/2)(n_j - 1/2)$$

- we consider the t-V_1-V_2 model on a bipartite lattice

  the partition function after Trotter decomposition is

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] \simeq \mathrm{Tr}\left[\prod_{n=1}^{N_\tau} e^{-H_0(n)\Delta\tau} e^{-H_{\text{int}}(n)\Delta\tau}\right]$$

- the Hamiltonian can be rewritten in terms of Majorana fermions $\{\gamma^i, \gamma^j\} = 2\delta_{i,j}$

  in Majorana representation, complex fermions operators are

$$c_i = \frac{1}{2}(\gamma_i^1 + i\gamma_i^2), \quad c_i^\dagger = \frac{1}{2}(\gamma_i^1 - i\gamma_i^2)$$

  which enable us to rewrite the Hamiltonian

$$H_0 = \sum_{\langle ij\rangle} \frac{it}{2}(\gamma_i^1\gamma_j^1 + \gamma_i^2\gamma_j^2),$$

$$H_{\text{int}} = -\frac{V_1}{4}\sum_{\langle ij\rangle}(i\gamma_i^1\gamma_j^1)(i\gamma_i^2\gamma_j^2) - \frac{V_2}{4}\sum_{\langle\langle ij\rangle\rangle}(i\gamma_i^1\gamma_j^1)(i\gamma_i^2\gamma_j^2)$$

Z.-X. Li, Y.-F. Jiang, and H. Yao, Phys. Rev. B 91, 241117 (2015).

Majorana QMC

- Hubbard-Stratonovich transformations for interactions are given by

$$e^{\frac{V_1\Delta\tau}{4}(i\gamma_i^1\gamma_j^1)(i\gamma_i^2\gamma_j^2)} = \frac{1}{2}\sum_{\sigma_{ij}=\pm1} e^{\frac{1}{2}\lambda_1\sigma_{ij}(i\gamma_i^1\gamma_j^1+i\gamma_i^2\gamma_j^2)-\frac{V_1\Delta\tau}{4}}$$

$$e^{\frac{V_2\Delta\tau}{4}(i\gamma_i^1\gamma_j^1)(i\gamma_i^2\gamma_j^2)} = \frac{1}{2}\sum_{\sigma_{ij}=\pm1} e^{\frac{1}{2}\lambda_2\sigma_{ij}(i\gamma_i^1\gamma_j^1-i\gamma_i^2\gamma_j^2)+\frac{V_2\Delta\tau}{4}}$$

here $V_1 > 0$, $V_2 < 0$

where λ_1 and λ_2 are constants determined through

$$\cosh\lambda_1 = e^{\frac{V_1\Delta\tau}{2}} \qquad \cosh\lambda_2 = e^{\frac{-V_2\Delta\tau}{2}}$$

- Boltzmann weight is a function of auxiliary field configurations in space-time

$$Z = \sum_{\{\sigma\}} W(\{\sigma\}) \qquad W(\{\sigma\}) = \mathrm{Tr}\left[\prod_{n=1}^{N_\tau} e^{\sum_{a=1}^{2}\frac{1}{4}\tilde{\gamma}^a h^a(n)\gamma^a}\right]$$

$$h_{ij}^a(n) = i\left[t\Delta\tau\delta_{\langle ij\rangle} + \lambda_1\sigma_{ij}(n)\delta_{\langle ij\rangle} \pm \lambda_2\sigma_{ij}(n)\delta_{\langle\langle ij\rangle\rangle}\right]$$

- because two components of Majorana fermions are decoupled

tracing out Majorana fermions can be done independently

$$W(\{\sigma\}) = W_1(\{\sigma\})W_2(\{\sigma\}) \qquad W_a(\{\sigma\}) = \left\{\det\left[\mathbb{I} + \prod_{n=1}^{N_\tau} e^{h^a(n)}\right]\right\}^{\frac{1}{2}}$$

Fermion sign free in Majorana QMC

- under the time-reversal transformation

  $\Theta = TK \qquad T: \gamma_i^1 \to (-1)^i \gamma_i^1 \qquad K$ is the complex conjugation

  the Hamiltonian $h^1(n)$ can be mapped to a Hamiltonian identical to $h^2(n)$

- on a bipartite lattice $(-1)^{i+j} = \begin{cases} -1 & \text{NN } \langle i,j\rangle \\ +1 & \text{NNN } \langle\langle i,j\rangle\rangle \end{cases}$

$$\begin{aligned}
\tilde{\gamma}^1 h^1(n)\gamma^1 &= i\tilde{\gamma}^1\left[t\Delta\tau\delta_{\langle ij\rangle} + \lambda_1\sigma_{ij}(n)\delta_{\langle ij\rangle} + \lambda_2\sigma_{ij}(n)\delta_{\langle\langle ij\rangle\rangle}\right]\gamma^1 \\
&\to -i\tilde{\gamma}^1\left[t\Delta\tau\delta_{\langle ij\rangle} + \lambda_1\sigma_{ij}(n)\delta_{\langle ij\rangle} - \lambda_2\sigma_{ij}(n)\delta_{\langle\langle ij\rangle\rangle}\right]\gamma^1 \\
\tilde{\gamma}^2 h^2(n)\gamma^2 &= i\tilde{\gamma}^2\left[t\Delta\tau\delta_{\langle ij\rangle} + \lambda_1\sigma_{ij}(n)\delta_{\langle ij\rangle} - \lambda_2\sigma_{ij}(n)\delta_{\langle\langle ij\rangle\rangle}\right]\gamma^2
\end{aligned}$$

- tracing out Majorana fermions, we obtain $W_1(\{\sigma\}) = W_2^*(\{\sigma\})$

  the Boltzmann weight $\boxed{W(\{\sigma\}) = W_1(\{\sigma\})W_2(\{\sigma\}) = W_1(\{\sigma\})W_1^*(\{\sigma\}) \geq 0}$

$$W(\{\sigma\}) = \left|\det\left[\mathbb{I} + \prod_{n=1}^{N_\tau} e^{h^a(n)}\right]\right|$$

- other fermion sign free models include $SU(N)$ fermonic models with odd N which are sign-free only in the Majorana QMC method

New progress

Flexible class of exact Hubbard-Stratonovich transformations

Seher Karakuzu, Benjamin Cohen-Stead, Cristian D. Batista, Steven Johnston, and Kipton Barros
Phys. Rev. E **107**, 055301 – Published 4 May 2023

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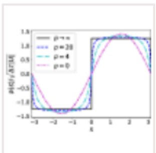
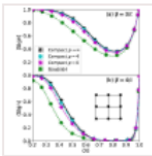
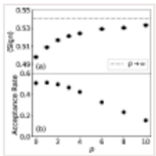
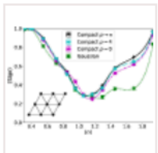
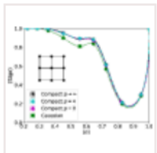
ABSTRACT

We consider a class of Hubbard-Stratonovich transformations suitable for treating Hubbard interactions in the context of quantum Monte Carlo simulations. A tunable parameter p allows us to continuously vary from a discrete Ising auxiliary field ($p = \infty$) to a compact auxiliary field that couples to electrons sinusoidally ($p = 0$). In tests on the single-band square and triangular Hubbard models, we find that the severity of the sign problem decreases systematically with increasing p. Selecting p finite, however, enables continuous sampling methods such as the Langevin or Hamiltonian Monte Carlo methods. We explore the tradeoffs between various simulation methods through numerical benchmarks.

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Development of computational quantum many-body physics

- Exact Diagonalization (ED)
- Numerical Renormalization Group (NRG)
- Density Matrix Renormalization Group (DMRG)
- Quantum Monte Carlo (QMC)
- Tensor Networks (TN)
- Machine Learning (ML)
- Density Functional Theory (DFT)
- Dynamical Mean Field Theory (DMFT)

Some suggestions and expectations

- be self-motivated

  focus on it and enjoy it

- be persistent

  do not stop until getting things done

- be bold but cautious

  create your own ideas, check results carefully

- be confidence

  if others can do it, I can too, maybe I can do better

Good Luck!