Determinant quantum Monte Carlo algorithm for simulating Hubbard models

in collaboration with
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Quantum ensemble averages

Goal: compute canonical ensemble averages

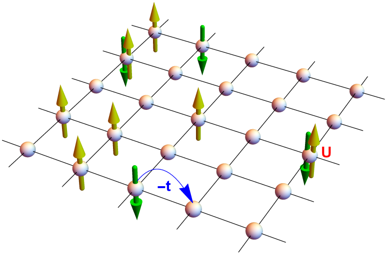
$$\langle \hat{A} \rangle = Z^{-1} \operatorname{tr}\left[\hat{A}\, e^{-\beta H}\right], \quad Z = \operatorname{tr}\left[e^{-\beta H}\right]$$

for a Hubbard-type Hamiltonian

$$H = K + V$$

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

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



t kinetic hopping amplitude
μ chemical potential
U el-el interaction strength

Traces in quantum Fock-space

For a Hamiltonian of *quadratic* form

$$H = \sum_{i,j} h_{ij}\, c_i^\dagger c_j$$

the following exact identity holds:

$$\mathrm{tr}\left[\mathrm{e}^{-\beta H}\right] \;=\; \det\left[\mathbb{1} + \mathrm{e}^{-\beta h}\right]$$

full quantum Fock-space ↗ ↖ single-particle space

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Simple to check for a single "orbital": $\mathrm{H} = \epsilon\, c^\dagger c$,

$$\mathrm{tr}\left[\mathrm{e}^{-\beta H}\right] = \langle 0|\mathrm{e}^{-\beta\epsilon c^\dagger c}|0\rangle + \langle 1|\mathrm{e}^{-\beta\epsilon c^\dagger c}|1\rangle = 1 + \mathrm{e}^{-\beta\epsilon}.$$

In the general case, consider a basis in which h is diagonal.

Blankenbecler et al. PRD 24, 2278 (1981)

Hubbard-Stratonovich transformation

However, Hubbard interaction term contains four-fermion operators . . .

May the 4th be with you!

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$\rightsquigarrow$ discrete Hubbard-Stratonovich transformation
(using that $n_{i\sigma} \in \{0, 1\}$, after Trotter splitting $\beta = \Delta\tau L$)

$$\mathrm{e}^{-\Delta\tau U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})} = \mathrm{e}^{-\Delta\tau U/4} \, \frac{1}{2} \sum_{s=\pm 1} \mathrm{e}^{-\Delta\tau s \lambda (n_{i\uparrow} - n_{i\downarrow})}$$

four-fermion ops.
($n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$)

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four-fermion ops. ($n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$) ↗

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λ determined by $\cosh(\Delta\tau\lambda) = e^{\Delta\tau U/2}$

White, Scalapino et al. PRB 40, 506 (1989)

From quantum ensemble averages to classical Monte Carlo

Applying Trotter splitting ($\beta = \Delta\tau L$) and the Hubbard-Stratonovich transformation eventually leads to

$$Z = \mathrm{tr}\left[\mathrm{e}^{-\beta H}\right] = \sum_{\{s_{i\ell}=\pm 1\}} \det\left[M^{\uparrow}(s)\right] \det\left[M^{\downarrow}(s)\right]$$

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with

$$M^{\sigma}(s) = \mathbb{1} + B^{\sigma}_{L-1}(s)\, B^{\sigma}_{L-2}(s) \cdots B^{\sigma}_{0}(s),$$

where

$$B^{\sigma}_{\ell}(s) = \mathrm{e}^{\mp \Delta\tau \lambda v(s_{\cdot\ell})}\, \mathrm{e}^{-\Delta\tau k}, \quad \ell = 0, 1, \ldots, L-1,$$

k is the kinetic single-particle matrix and

$$v(s_{\cdot\ell}) = \begin{pmatrix} s_{1\ell} & 0 & 0 & \ldots \\ 0 & s_{2\ell} & 0 & \ldots \\ 0 & 0 & s_{3\ell} & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

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From quantum ensemble averages to classical Monte Carlo

Idea: interpret as probability density

$$Z^{-1} \det\left[M^{\uparrow}(s)\right] \det\left[M^{\downarrow}(s)\right]$$

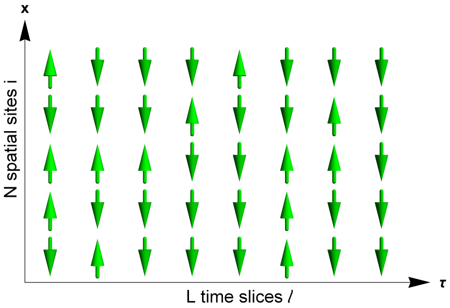

Figure: $\uparrow$: $s_{i\ell} = 1$, $\downarrow$: $s_{i\ell} = -1$

$\rightsquigarrow$ sample over Hubbard-Stratonovich field configurations $s_{i\ell}$ using classical Monte-Carlo

Imaginary time Green's function

Matsubara Green's function (with $\tau, \tau' \in [0, \beta]$):

$$G^{\sigma}(\tau, \tau')_{ij} = \langle \mathcal{T} c_{i\sigma}(\tau) c^{\dagger}_{j\sigma}(\tau') \rangle.$$

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For discretized version in the field s and $\tau = \tau'$, can derive that

$$G^\sigma(\ell, s) = \left[\mathbb{1} + B^\sigma_{\ell-1}(s) \cdots B^\sigma_0(s)\, B^\sigma_{L-1}(s) \cdots B^\sigma_\ell(s) \right]^{-1}$$

with $\tau = \Delta\tau\ell$ and

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$$R^{\sigma} = \frac{\det[M^{\sigma}(s')]}{\det[M^{\sigma}(s)]} = 1 + (1 - G^{\sigma}(\ell, s)_{ii}) \left(\mathrm{e}^{\pm 2\Delta\tau\lambda s_{i\ell}} - 1\right)$$

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- To avoid gradual loss of precision, still have to recompute Green's function from scratch after several steps (expensive)

White, Scalapino et al. PRB 40, 506 (1989)

Fermion sign problem

Algorithm relies on probability density

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To circumvent, factor into $\mathrm{sign}(s) \times$ absolute value, and pull sign towards observable:

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However, for low temperatures, $\langle\mathrm{sign}(s)\rangle$ becomes small, need many more Monte-Carlo samples to reliably estimate $\langle\hat{A}\rangle$.

Implementation

Many additional "tricks of the trade" to stabilize and speed up algorithm, for example

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Many additional "tricks of the trade" to stabilize and speed up algorithm, for example

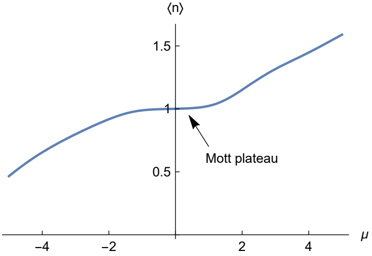
- Explicitly keep track of *determinants* of Green's functions, otherwise numerical loss of precision when computing them based on matrix entries
- Long chain of matrix multiplications in

$$G^{\sigma}(\ell, s) = \left[\mathbb{1} + B^{\sigma}_{\ell-1}(s) \cdots B^{\sigma}_{0}(s)\, B^{\sigma}_{L-1}(s) \cdots B^{\sigma}_{\ell}(s)\right]^{-1}$$

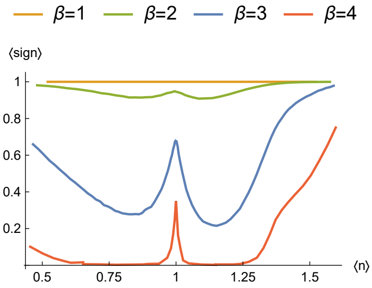
can lead to extremely large condition numbers; alleviate by sequential QR-decompositions with column pivoting

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

Example: occupancy and sign



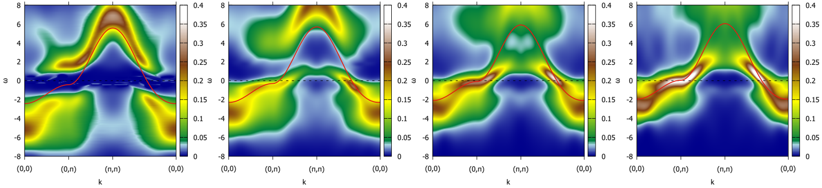
Average occupancy in dependence of chemical potential μ



Temperature dependence of sign

Parameters: 8×8 lattice, $t = 1$, $t' = -0.3$, $U = 8$, $\Delta\tau = 0.1$

Example: spectral function



$\langle n \rangle = 1$ $\langle n \rangle = 0.95$ $\langle n \rangle = 0.85$ $\langle n \rangle = 0.75$

Figure: Doping dependence of the spectral function $A(\mathbf{k}, \omega)$ along high symmetry cuts through the Brillouin zone

Parameters: 8×8 lattice, $t = 1$, $t' = -0.25$, $U = 8$, $\beta = 3$, $\Delta\tau = 0.1$

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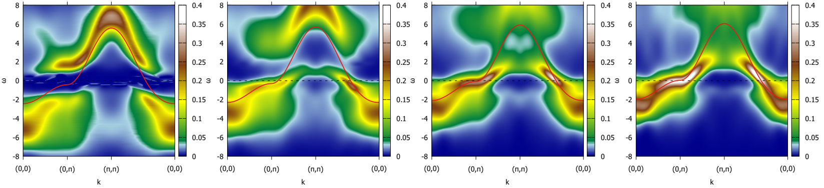

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Using maximum entropy analytic continuation to "real" frequencies ω,

$$G(\mathbf{k}, \tau) = \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\tau\omega}}{1 + \mathrm{e}^{-\beta\omega}} A(\mathbf{k}, \omega) \, \mathrm{d}\omega.$$

Jarrell and Gubernatis, Phys. Rep. 269, 133–195 (1996)

Summary

Main ingredients:

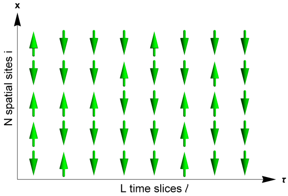
- From quantum Fock to single-particle space

$$\mathrm{tr}\left[e^{-\beta H}\right] = \det\left[\mathbb{1} + e^{-\beta h}\right]$$

- Introduce auxiliary Hubbard-Stratonovich field $s_{i\ell}$ to obtain quadratic form for U-term
- Efficient Metropolis sampling of

$$Z^{-1} \det\left[M^{\uparrow}(s)\right] \det\left[M^{\downarrow}(s)\right]$$

using Green's function



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Trotter splitting

Introduce an imaginary-time step $\Delta\tau$ such that $\beta = \Delta\tau L$. Trotter splitting $\rightsquigarrow$

$$Z = \mathrm{tr}\left[\mathrm{e}^{-\Delta\tau L H}\right] \simeq \left(\mathrm{tr}\left[\mathrm{e}^{-\Delta\tau V}\,\mathrm{e}^{-\Delta\tau K}\right]\right)^{L}$$

Imaginary time flow

Remark: the product

$$B_{L-1}(s)\, B_{L-2}(s) \cdots B_0(s)$$

with

$$B_\ell(s) = \mathrm{e}^{-\Delta\tau \lambda v(s_{\cdot \ell})}\, \mathrm{e}^{-\Delta\tau k}$$

is a discrete approximation of the imaginary time flow

$$U(\tau, \tau') = \mathcal{T} \exp\left[-\int_{\tau'}^{\tau} \mathrm{d}\hat{\tau}\, H(\hat{\tau}) \right]$$

in the field s, where $\mathcal{T}$ is the imaginary-time ordering operator.

Blankenbecler et al. PRD 24, 2278 (1981)