Advances of Numerical Methods for Hubbard Quantum Monte Carlo Simulations

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Outline

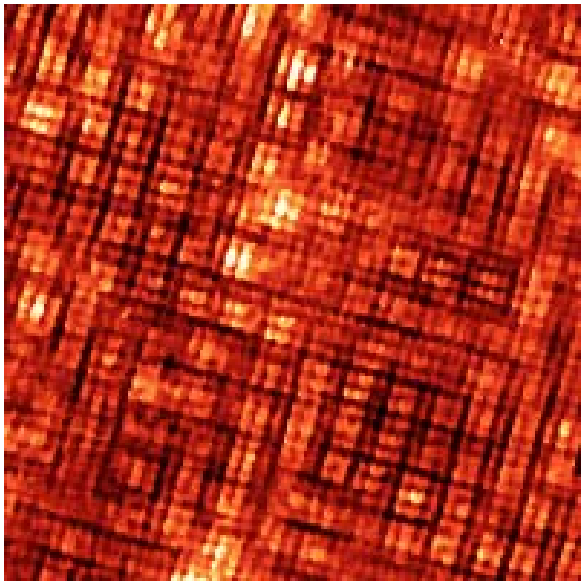
1. Hubbard model and quantum monte carlo simulation: an outline
2. Hubbard matrix analysis
3. Self-adapting direct linear solvers
4. Preconditioned iterative linear solvers

Hubbard Model and Quantum Monte Carlo Simulation

an outline

Computational Material Science

- The study of models of strongly interacting electrons: understand properties of solid-state materials, such as magnetism, metal-insulator transition, high temperature superconductivity.
- Conductance map of a 'checkerboard' electronic crystal state in lightly hole-doped $Ca_{2-x}Na_xCuO_22Cl_2$ obtained using scanning tunneling microscopy. This figure shows a clear pattern of modulations of the conductance at length scales four times the lattice constant and also complex internal structure at the atomic scale.



[T. Hanaguri *et al*, Nature 430, 1001 (2004)]

Hubbard Model

The Hamiltonian

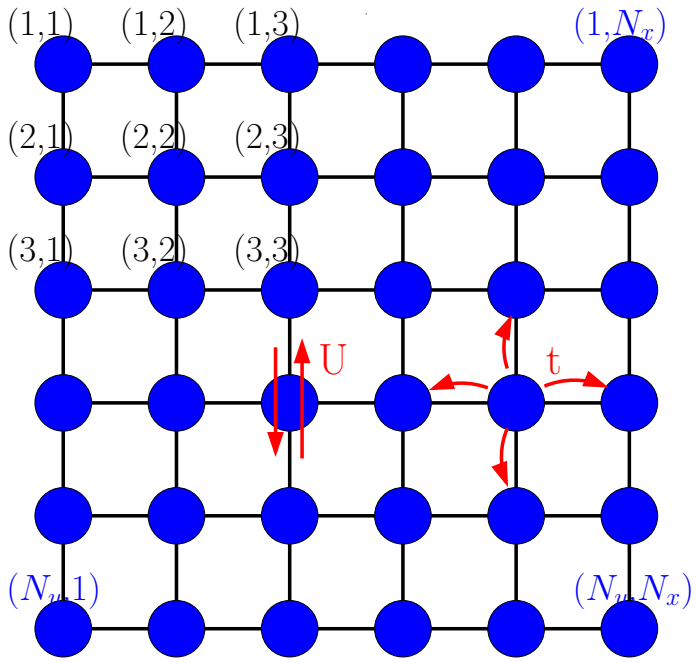
$$\begin{aligned}\mathcal{H} &= \mathcal{H}_K + \mathcal{H}_V + \mathcal{H}_\mu \\ &= -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) + \cdots\end{aligned}$$

- i and j label the spatial sites of the lattice

  $\langle i, j\rangle$: a pair of nearest-neighbor sites
- $\sigma = \uparrow\downarrow$: the spin direction of electrons
- $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (destroys) an electron of spin σ on site i
- t: hopping parameter (kinetic energy)
- $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$: count the number of electrons of spin σ on site i.
- $U n_{i\uparrow} n_{i\downarrow}$: energy cost U if the site i has two electrons on it (local repulsion) (potential energy)
- $\mathcal{H}_\mu$: chemical potential

Simple lattice and special cases

Rectangle lattice:



Special cases:

- no hopping: $t = 0$
- no interaction: $U = 0$

Physical Observable $\mathcal{E}$

The expected value of a physical observable $\mathcal{E}$, such as density-density correlation, spin-spin correlation, the magnetic susceptibility, is given by

$$\langle \mathcal{E} \rangle = \mathrm{Tr}\left(\mathcal{E}\mathcal{P}\right),$$

where $\mathcal{P}$ is the probability (Boltzmann) distribution

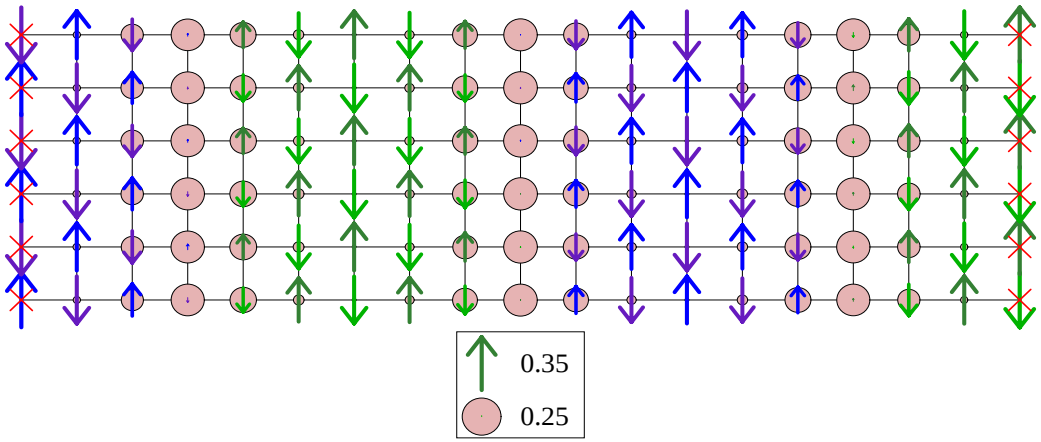
$$\mathcal{P} = \frac{1}{Z} e^{-\beta \mathcal{H}}$$

and $\mathcal{Z}$ is the partition function

$$\mathcal{Z} = \mathrm{tr}(e^{-\beta \mathcal{H}}),$$

and $\beta = 1/(k_B T) = 1/(\text{Boltzmann constant} \times \text{temperature})$.

Physical Observables



The complex stripe structure arising from removing electrons from the filling of one electron per site in the Hubbard model. The arrows and their sizes indicate the magnetic moments present on the sites, while the circles indicate the density of holes. The holes form (vertical) stripes separated by regions with strong antiferromagnetic correlations. [S.R. White *etal.*, Phys. Rev. Lett. 80, 1272(1998)].

“Discrete” approximation of Boltzmann distribution $\mathcal{P}$

$$\mathcal{P} \approx P(h) = \frac{1}{Z_h} \det M_+(h) \det M_-(h).$$

where

$$Z_h = \mathrm{tr}_h \det M_+(h) \det M_-(h).$$

and

$$M_\sigma(h) = I + B_{L,\sigma}(h_L) B_{L-1,\sigma}(h_{L-1}) \cdots B_{1,\sigma}(h_1)$$

and

$$B_{\ell,\sigma}(h_\ell) = e^{t\tau K} e^{\sigma V_\ell(h_\ell)}, \quad \sigma = \pm.$$

DQMC

1. Choose an initial configuration $h^{(0)}$.
2. MC loop
   (a) Try the new configuration h' by single spin-flip sampling: $h'_{\ell,i} = -h_{\ell,i}$.
   (b) Generate one random number $r \sim$Uniform$[0, 1]$ and update

$$h^{(n+1)} = \begin{cases} h', & \text{if } r \leq \min\left\{1, \frac{\det(M_+(h')M_-(h'))}{\det(M_+(h)M_-(h))}\right\} \\ h^{(n)}, & \text{otherwise.} \end{cases}$$

   (c) Go the next site and repeat updating,
3. Physical measurements are obtained from the elements of the Greens function $G_\sigma(h) = (M_\sigma(h))^{-1}$.

“Continuous” approximation of $\mathcal{P}$

$$\mathcal{P} \approx P(x) = \frac{1}{Z_x} e^{-S_B(x)} \det M_+(x) \det M_-(x)$$

where

$$\begin{aligned} Z_x &= \int [\delta x] e^{-S_B(x)} \det M_+(x) \det M_-(x). \\ M_\sigma(x) &= I + B_{L,\sigma}(x_L) B_{L-1,\sigma}(x_{L-1}) \cdots B_{1,\sigma}(x_1) \\ S_B(x) &= \tau \sum_{\ell,i} x_{\ell,i}^2 \end{aligned}$$

Two identities

Identity #1: Let

$$M = \begin{bmatrix} I & & & & B_1 \\ -B_2 & I & & & \\ & -B_3 & I & & \\ & & \ddots & \ddots & \\ & & & -B_L & I \end{bmatrix},$$

then

$$\det(M) = \det(I + B_L B_{L-1} \cdots B_1).$$

Identity #2: If A is symmetric and positive definite, then

$$\int e^{-v^T A^{-1} v} dv = (\sqrt{\pi})^{\dim(v)} \det(A^{\frac{1}{2}}),$$

HMQC = MD + MC

Introducing auxiliary variables, Φ_σ and p

$$P(x, p, \Phi_\sigma) = \frac{1}{Z_H} e^{-H(x,p,\Phi_\sigma)}$$

where

$$Z_H = \int [\delta x \delta p \delta \Phi_\sigma] e^{-H(x,p,\Phi_\sigma)}$$

where

$$H(x, p, \Phi_\sigma) == p^T p + \underbrace{S_B(x) + \sum_\sigma \Phi_\sigma^T (M_\sigma^T M_\sigma)^{-1} \Phi_\sigma}_{V(x,\Phi_\sigma)}$$

... MD + MC = HQMC

HMQC

1. Initialization ...
2. MC loop
   (a) MD step ...
   - generate $p^{(0)}$
   - initial step $p_{i,l}^{(\frac{1}{2})} = p_{i,l}^{(0)} - \frac{\partial V(x^{(0)})}{\partial x_{i,l}^{(1)}}\Delta t$
   - run MD steps:
   $$\begin{aligned} x_{i,l}^{(1)} - x_{i,l}^{(0)} &= 2p_{i,l}^{(\frac{1}{2})}\Delta t, \\ p_{i,l}^{(1)} - p_{i,l}^{(\frac{1}{2})} &= -\frac{\partial V(x^{(1)})}{\partial x_{i,l}^{(1)}}\Delta t \end{aligned}$$

   (b) Move $x^{(0)}$ to a new configuration $x^{(1)}$, compute $e^{-H(x^{(1)},p,\Phi_\sigma)}$
   Using Metropolis algorithm to decide whether we accept the configuration $x^{(1)}$: If $x^{(1)}$ is accepted, then $x^{(0)} = x^{(1)}$.

   (c) Goto step (a).
3. Measurement step for physical observables

Hubbard Matrix Analysis

Hubbard matrix

The kernel of the determinant and hybrid QMC (Quantum Monte Carlo) simulations is the computations (determinant, inversion ...) of the matrices

$$M = \begin{pmatrix} I & & & & B_1 \\ -B_2 & I & & & \\ & -B_3 & I & & \\ & & \ddots & \ddots & \\ & & & -B_L & I \end{pmatrix}$$

- $B_\ell = e^{t\tau K} e^{V_\ell}$,
- (i,j) element of K: $k_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are nearest neighbors,} \\ 0 & \text{otherwise.} \end{cases}$
- $V_\ell = \text{diag}(\nu h_{\ell i})$,
  $\nu = \cosh^{-1}(2U\tau) = \sqrt{U\tau} + \cdots$,
  $h_{\ell i}$: Hubbard-Stratonovich (random) variables

Multi-scaling

- Length-scales: N, L
  - $N = N_x \times N_y$, lattice size. $N = 8 \times 8, \ldots, 32 \times 32, \ldots, 64 \times 64$
  - L: the number of divisions of β, the inverse temperature, $L = \frac{\beta}{\tau} = 8, 16, \ldots, 160$
- Energy scales: t, U, β
  - t: hopping of electrons between two different atoms (kinetic energy). $t = 1, 2, \ldots$
  - U: strength of the interactions between the electrons (potential energy). $U = 0, 1, 2, \ldots, 6$
  - β: inverse temperature $\beta = 1, 2, \ldots, 10$
- Length and energy scale connection: $\tau = \frac{\beta}{L}$

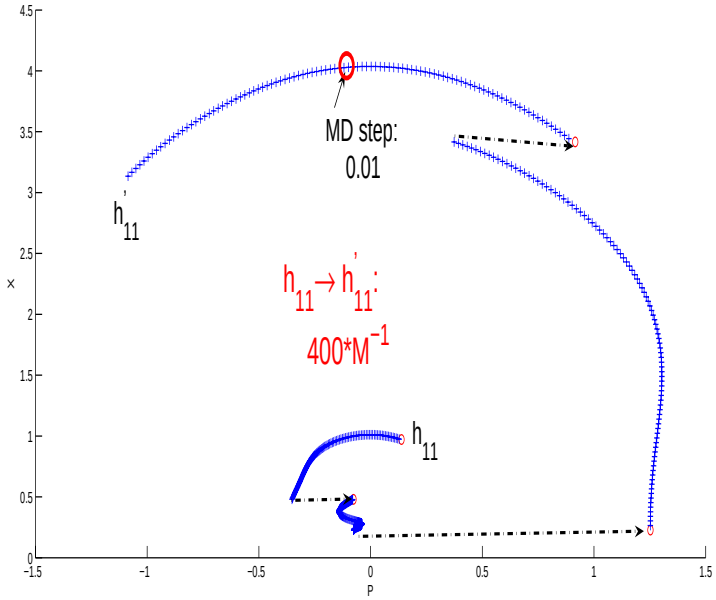
In more complex situations other energy scales also enter, such as the frequency of ionic vibrations (phonons) and the strength of the coupling of electrons to those vibrations

Computational challenges

- Dimension of M

$$\begin{aligned} N_x \times N_y \times L &= \ldots, 8 \times 8 \times 60, \ldots, 64 \times 64 \times 160, ... \\ &= \ldots, 3840, \ldots, 655360, ... \end{aligned}$$

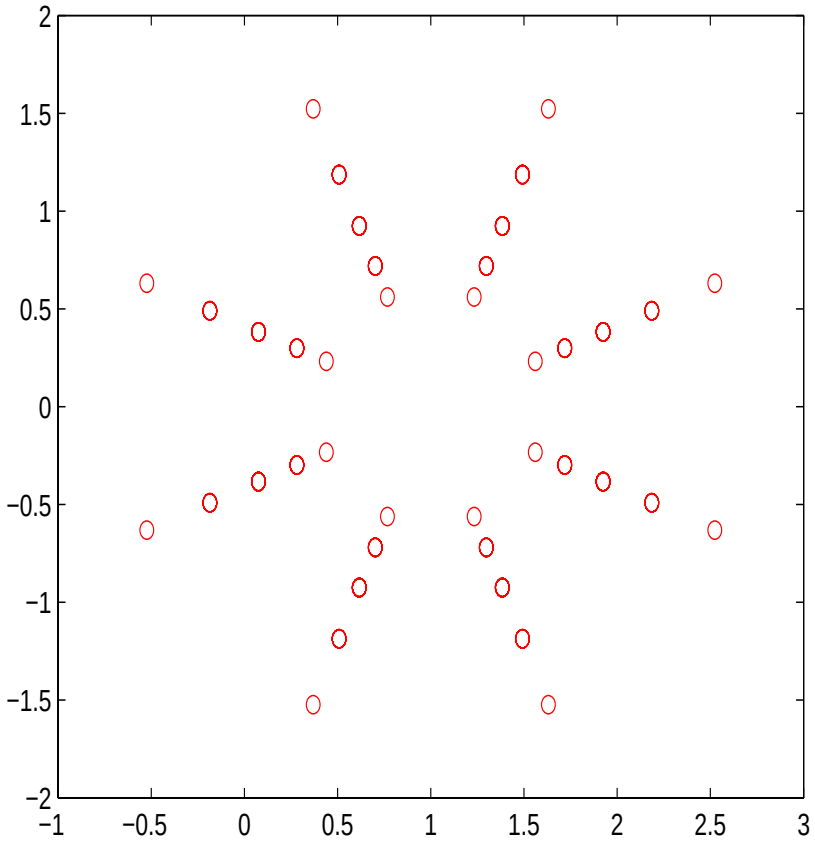
- The matrix computation problems, such as $\det(M)$ and $(M^T M)^{-1} b$, need to be solved about $100,000$ times in a full QMC simulation.
- A typical MD trajectory in HQMC



Hubbard matrix analysis – eigenvalue distribution

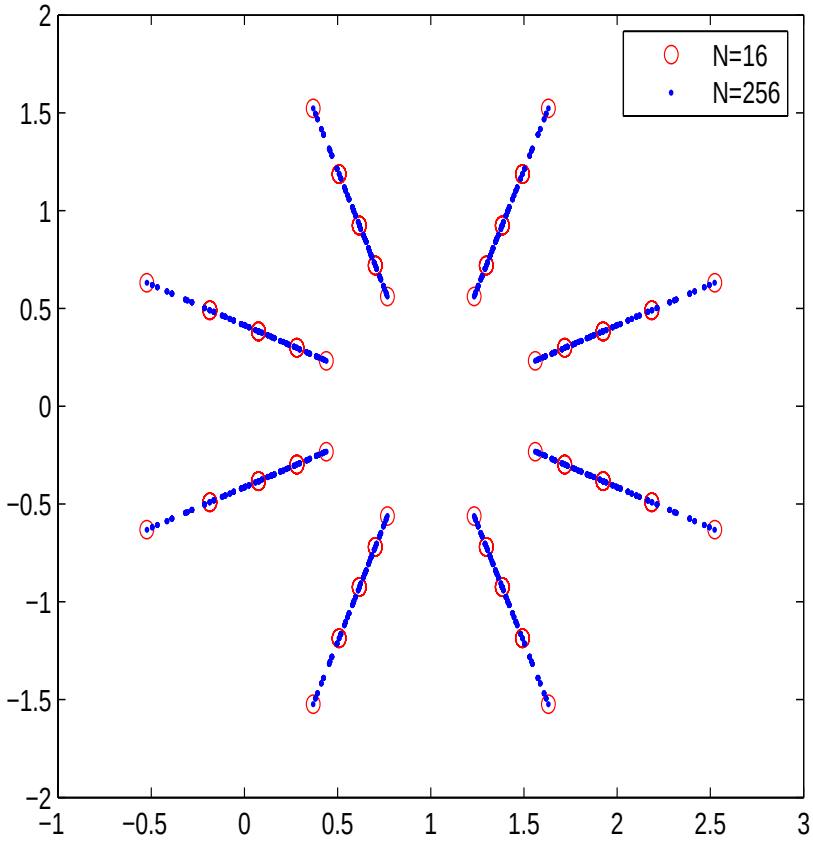
$$\lambda(M) = 1 - \lambda(B_L \cdots B_2 B_1)^{\frac{1}{L}} e^{\mathrm{i}\frac{(2\ell+1)\pi}{L}}, \quad 0 \leq \ell \leq L-1$$

[Frobenius ’12, Romanovsky ’43, Varga ’62]



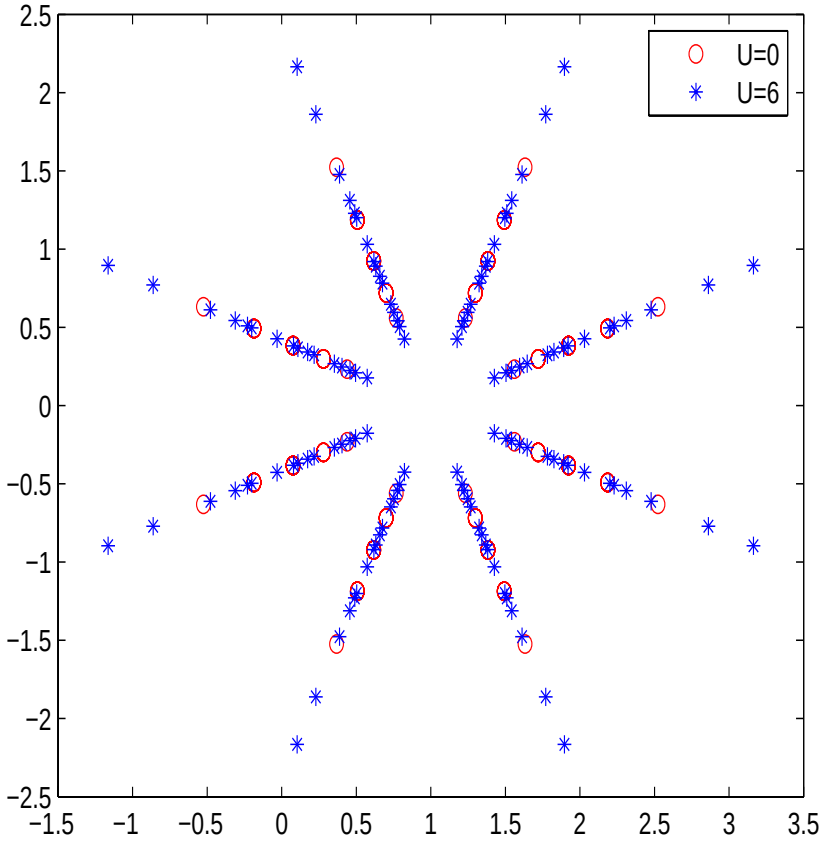
Hubbard matrix analysis – eigenvalue distribution

Lattice sizes $N = 4 \times 4 \rightarrow 16 \times 16$:



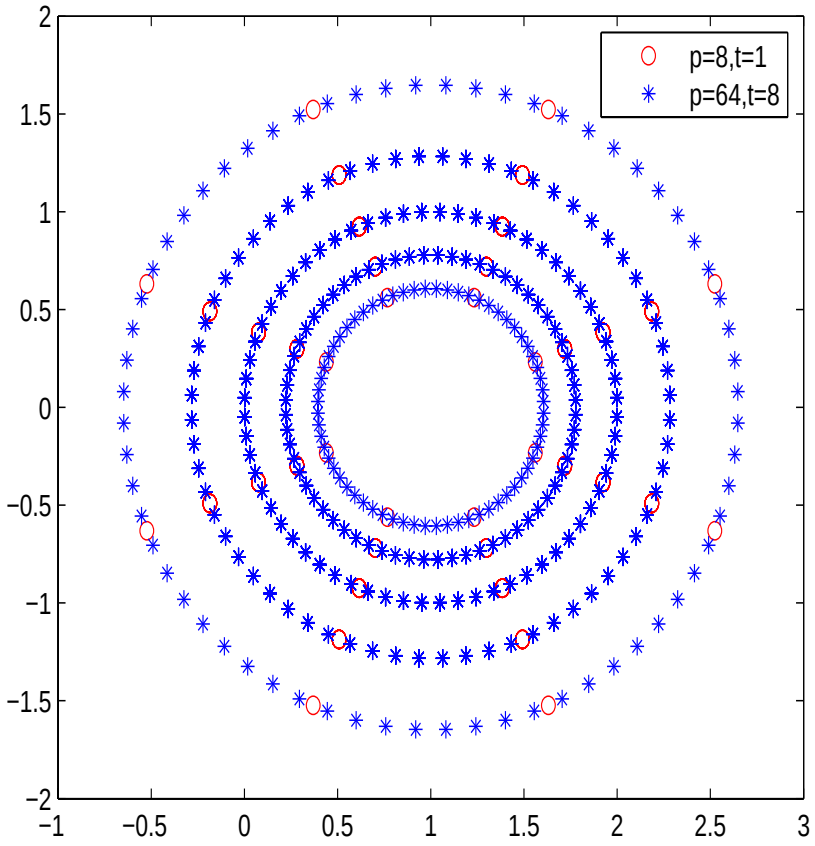
Hubbard matrix analysis – eigenvalue distribution

Potential energy scale $U = 0, 6$:



Hubbard matrix analysis – eigenvalue distribution

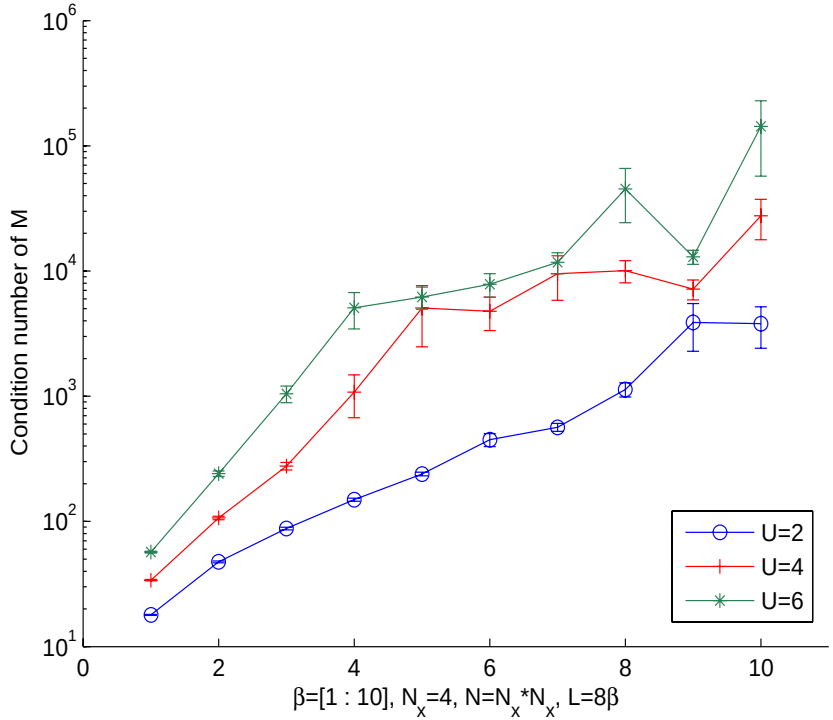
$(L, t) = (8, 1), (64, 8)$



Hubbard matrix analysis – condition number

Condition number $\kappa(M) = \|M\| \, \|M^{-1}\|$:

- If $U = 0$, $\kappa(M) \leq \dfrac{1 + e^{4t\tau}}{\sin \frac{\pi}{L}} \approx \mathcal{O}(L)$.
- If $U \neq 0$,



- Open problem: a rigorous bound of $\kappa(M)$

Hubbard matrix analysis – condition number

A structure-preserving factor-of-k reduction of the matrix M:

$$M^{(k)} = \begin{bmatrix} I & & & & B_1^{(k)} \\ -B_2^{(k)} & I & & & \\ & -B_3^{(k)} & I & & \\ & & \ddots & \ddots & \\ & & & -B_{L_k}^{(k)} & I \end{bmatrix}.$$

where $L_k = \lceil \frac{L}{k} \rceil$ and

$$\begin{aligned} B_1^{(k)} &= B_k B_{k-1} \cdots B_2 B_1 \\ B_2^{(k)} &= B_{2k} B_{2k-1} \cdots B_{k+2} B_{k+1} \\ &\vdots \\ B_{L_k}^{(k)} &= B_L B_{L-1} \cdots B_{(L_k-1)k+1}. \end{aligned}$$

Hubbard matrix analysis – condition number

Four results:

1. $\|B_\ell^{(k)}\| \leq e^{(4t\tau+\nu)k}$.
2. $\|M^{(k)}\| \leq c\, e^{(4t\tau+\nu)k}$
3. $(M^{(k)})^{-1}$ is a "submatrix" of $(M)^{-1}$.
4. $\|(M^{(k)})^{-1}\| \leq \|M^{-1}\|$.

Hubbard matrix analysis – condition number

U = 0:

1. $k = L$, i.e, the matrix M is reduced to a single block

$$M^{(L)} = I + B_L \cdots B_2 B_1 = I + B^L = I + (e^{t\tau K})^L = I + e^{t\beta K}.$$

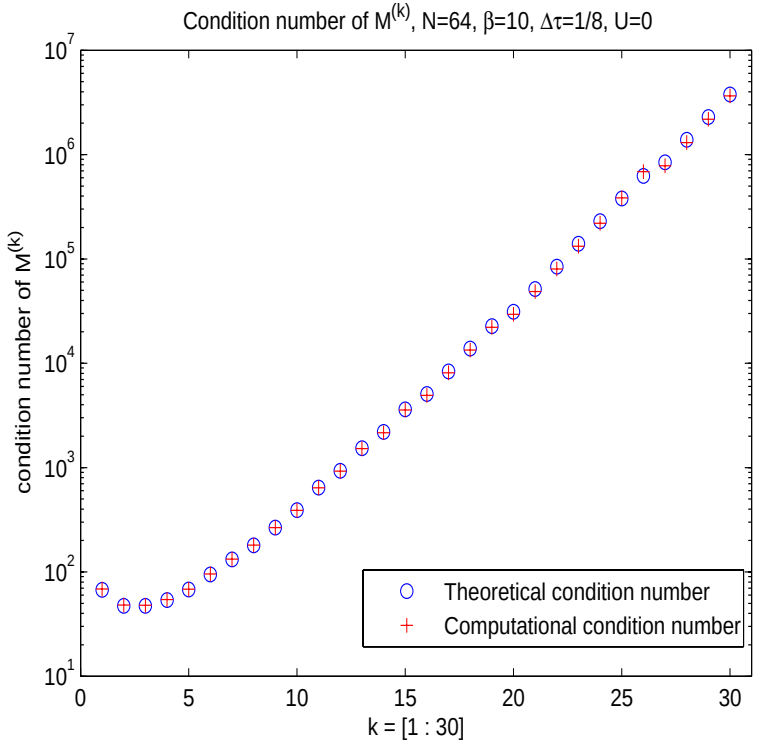
Then the condition number of $M^{(L)}$ is given by the eigendecomposition of the matrix K:

$$\kappa(M^{(L)}) = \frac{1 + e^{4t\beta}}{1 + e^{-4t\beta}}.$$

$M^{(L)}$ is extremely ill-conditioned when β is large.

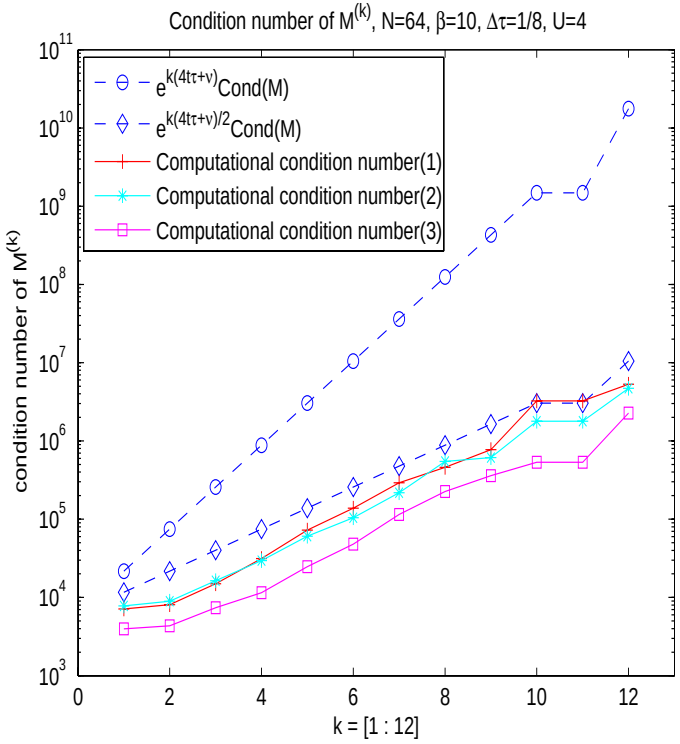
2. $L_k = \frac{L}{k}$ (an integer),

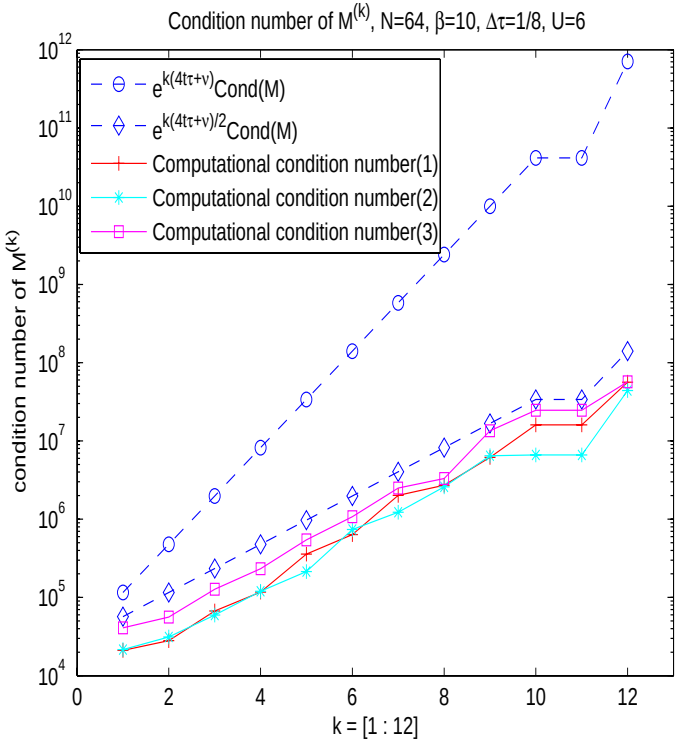
$$\kappa\big(M^{(k)}\big) \leq \frac{1 + e^{4t\tau k}}{\sin \frac{\pi}{L_k}}.$$



Hubbard matrix analysis – condition number

$$\underline{\mathbf{U \neq 0}:} \quad \kappa(M^{(k)}) = \|M^{(k)}\|\|(M^{(k)})^{-1}\|$$
$$\leq \|M^{(k)}\|\|M^{-1}\| \leq \frac{\|M^{(k)}\|}{\|M\|} \cdot \kappa(M) \leq ce^{k(4t\tau+\nu)}\kappa(M).$$





In practice, $\kappa(M^{(k)})$ is bounded by $e^{\frac{k}{2}(4t\tau+\nu)}\kappa(M)$.