DQMC Simulation of the Hubbard Model

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Overview

1. The Physics

   quadratic Hamiltonians, Hubbard model, Hubbard-Stratonovich transformation

2. The Simulation

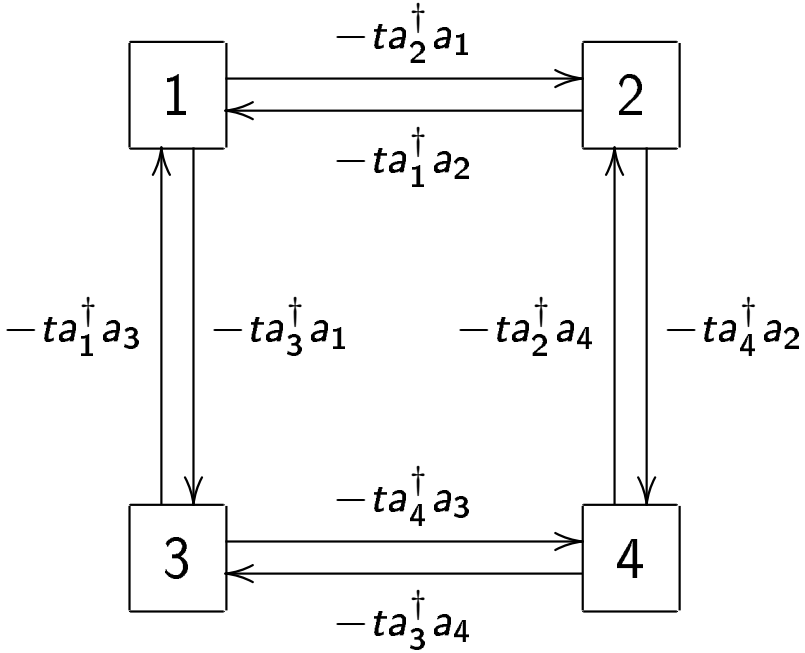
   Markov chain Monte Carlo

3. The System

   Python, NumPy, cProfile, weave, EC2, StarCluster

Hopping Hamiltonian

- Lattice of single-electron states, hopping terms connecting them.



$$\Longrightarrow \qquad \hat{H} = -t \sum_{\langle ij \rangle} a_i^\dagger a_j$$

Hopping Hamiltonian – Quadratic in Operators

- Adding chemical potential & spin multiplicity,

$$\hat{H} = -t \sum_{\langle ij \rangle} a^\dagger_{i\sigma} a_{j\sigma} - \mu_{i\sigma} \sum_i a^\dagger_{i\sigma} a_{i\sigma}$$

$$= \begin{pmatrix} a^\dagger_{1\sigma} & a^\dagger_{2\sigma} & \cdots \end{pmatrix} \begin{pmatrix} h_{11} & h_{12} & \cdots \\ h_{21} & h_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_{1\sigma} \\ a_{2\sigma} \\ \vdots \end{pmatrix}.$$

- Quadratic $\Rightarrow$ Exactly solvable!

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

Other rules for Green's functions $\left\langle a^\dagger_{i\sigma} a_{j\sigma} \right\rangle = \frac{\mathrm{tr}\left[a^\dagger_{i\sigma} a_{j\sigma} e^{-\beta \hat{H}}\right]}{\mathrm{tr}\left[e^{-\beta \hat{H}}\right]}$.

Adding Interactions

- Not too suprising that system is solvable $\leftarrow$ no interactions.
- Simplest possible interaction is on-site repulsion (fixed cost to doubly-occupied site):

$$\hat{H}_{int} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

...and here's the problem...

$$= U \sum_i a^\dagger_{i\uparrow} a_{i\uparrow} a^\dagger_{i\downarrow} a_{i\downarrow}.$$

- No longer have a quadratic Hamiltonian.

Adding Interactions – Discrete H-S Transformation

- For convenience:

$$\hat{H}_{int}: \qquad U\sum_i n_{i\uparrow}n_{i\downarrow} \quad \rightarrow \quad U\sum_i \left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)$$

- Here's a trick:

$$e^{-\beta U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = C\sum_{s_i} e^{-\beta(\lambda s_i n_{i\uparrow}-\lambda s_i n_{i\downarrow})}$$

$$e^{-\beta\hat{H}_{int}} = C^N\sum_{\{s_i\}} e^{-\beta\sum_i(\lambda s_i n_{i\uparrow}-\lambda s_i n_{i\downarrow})}$$

$$Z = \mathrm{tr}\left[e^{-\beta\hat{H}_{int}}\right] = C^N\sum_{\{s_i\}} \mathrm{tr}\left[e^{-\beta\sum_i(\lambda s_i n_{i\uparrow}-\lambda s_i n_{i\downarrow})}\right]$$

- Sum quadratic-Hamiltonian Z's over values of external field!

Adding Interactions – How does H-S really work?

- $\uparrow$ electrons and $\downarrow$ electrons are only connected through "randomly fluctuating" field... how does this create a repulsive interaction?
- Hubbard-Stratonovich transformation is closely related to mean-field methods.

Adding Interactions – Trotter Product

- "Not so fast..."

$$e^{-\beta(\hat{H}_0+\hat{H}_{int})} \neq e^{-\beta\hat{H}_0}\, e^{-\beta\hat{H}_{int}}.$$

- Happy resolution – the Trotter product formula!

$$e^{-\beta(\hat{H}_0+\hat{H}_{int})} = \lim_{\Delta\tau\to 0}\left(e^{-\Delta\tau\hat{H}_0}\, e^{-\Delta\tau\hat{H}_{int}}\right)^{\beta/\Delta\tau}.$$

  (Our trace-taking techniques survive the breakup.)

- H-S variables s_i are now $s_{i,\tau}$; a field in space(i)time.

Adding Interactions – Making Measurements

- Summing over all possible $\{s_{i,\tau}\}$ can give any measurement. For instance, the partition function:

$$
\begin{aligned}
Z &\approx \mathrm{tr}\left[\left(e^{-\Delta\tau\hat{H}_0}e^{-\Delta\tau\hat{H}_{int}}\right)^{\beta/\Delta\tau}\right] \\
&= \sum_{\{s_{i,l}\}} \mathrm{tr}\left[e^{-\Delta\tau\hat{H}_0}e^{-\Delta\tau\hat{H}_{HS}(\{s_{i,L}\})}\ldots e^{-\Delta\tau\hat{H}_0}e^{-\Delta\tau\hat{H}_{HS}(\{s_{i,1}\})}\right] \\
&= \sum_{\{s_{i,l}\}} \det \underbrace{\left[I + e^{-\Delta\tau h_0}e^{-\Delta\tau h_{HS}(\{s_{i,L}\})}\ldots e^{-\Delta\tau h_0}e^{-\Delta\tau h_{HS}(\{s_{i,1}\})}\right]}_{M(\{s_{i,l}\})}.
\end{aligned}
$$

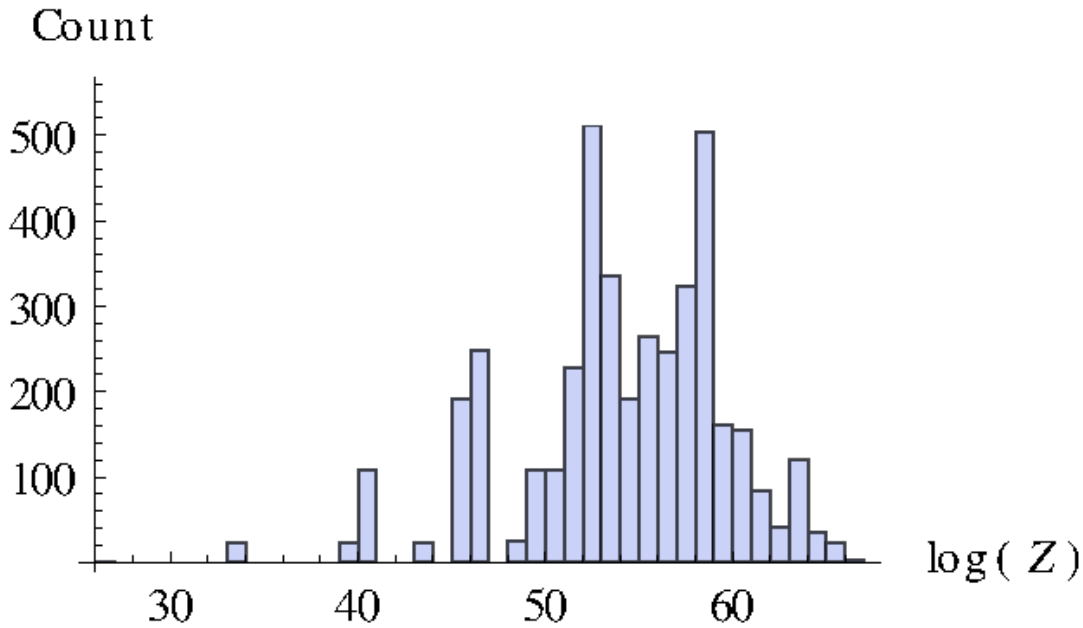
- Or correlation functions:

$$
\left\langle a^\dagger_{i\sigma}a_{j\sigma}\right\rangle_{\{s_{i,l}\}} = (I - M(\{s_{i,l}\})^{-1})_{ij}
$$

$$
\left\langle a^\dagger_{i\sigma}a_{j\sigma}\right\rangle = \sum_{\{s_{i,l}\}} \underbrace{\frac{\det\left[M(\{s_{i,l}\})\right]}{Z}}_{p(\{s_{i,l}\})} (I - M(\{s_{i,l}\})^{-1})_{ij}.
$$

Markov Chain Monte Carlo – Why?

- But $\sum_{\{s_{i,l}\}}$ is only a conceptual possibility
  - 6×6 grid, with *a single time-step*? 68,719,476,736 terms
  - (Each term involves a large matrix $\times$, $(\cdot)^{-1}$, $\det[\cdot]$)
- Random sampling?
  - Spend too much time in unlikely places:

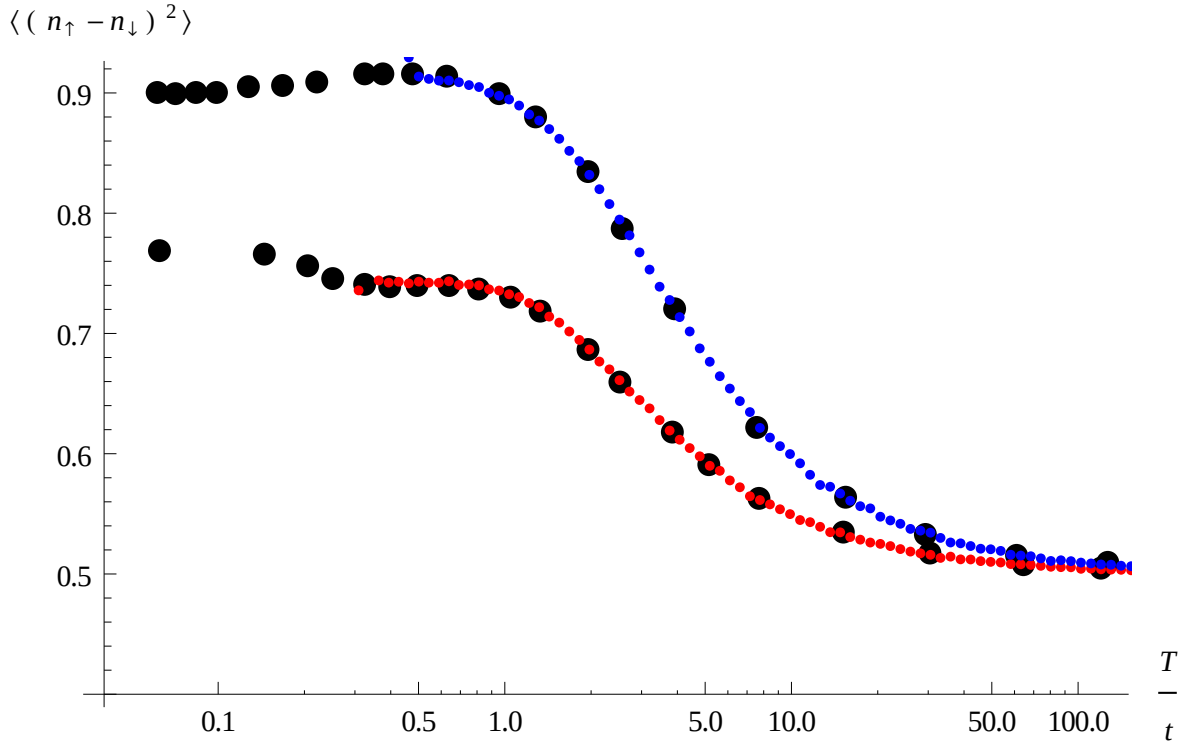


  - (And term computation is still slow)
- Solution: Markov chain Monte Carlo

Markov Chain Monte Carlo

- General idea: Construct a Markov chain with a desired probability distribution as its stationary distribution.
  - Our case – $\{s_{i,l}\}$ will take a random walk, by flipping spins with appropriately chosen rates
  - It will then sample the full distribution accurately
  - Only requires knowing ratios of probabilities: very easy!
- Efficient execution comes from keeping track of Green's-function matrices during random walk
  - test potential flips VERY quickly
  - update Green's functions in response to a spin-flip using the Sherman-Morrison formula
  - "wrap" Green's functions from each (i)time-step to the next

Results



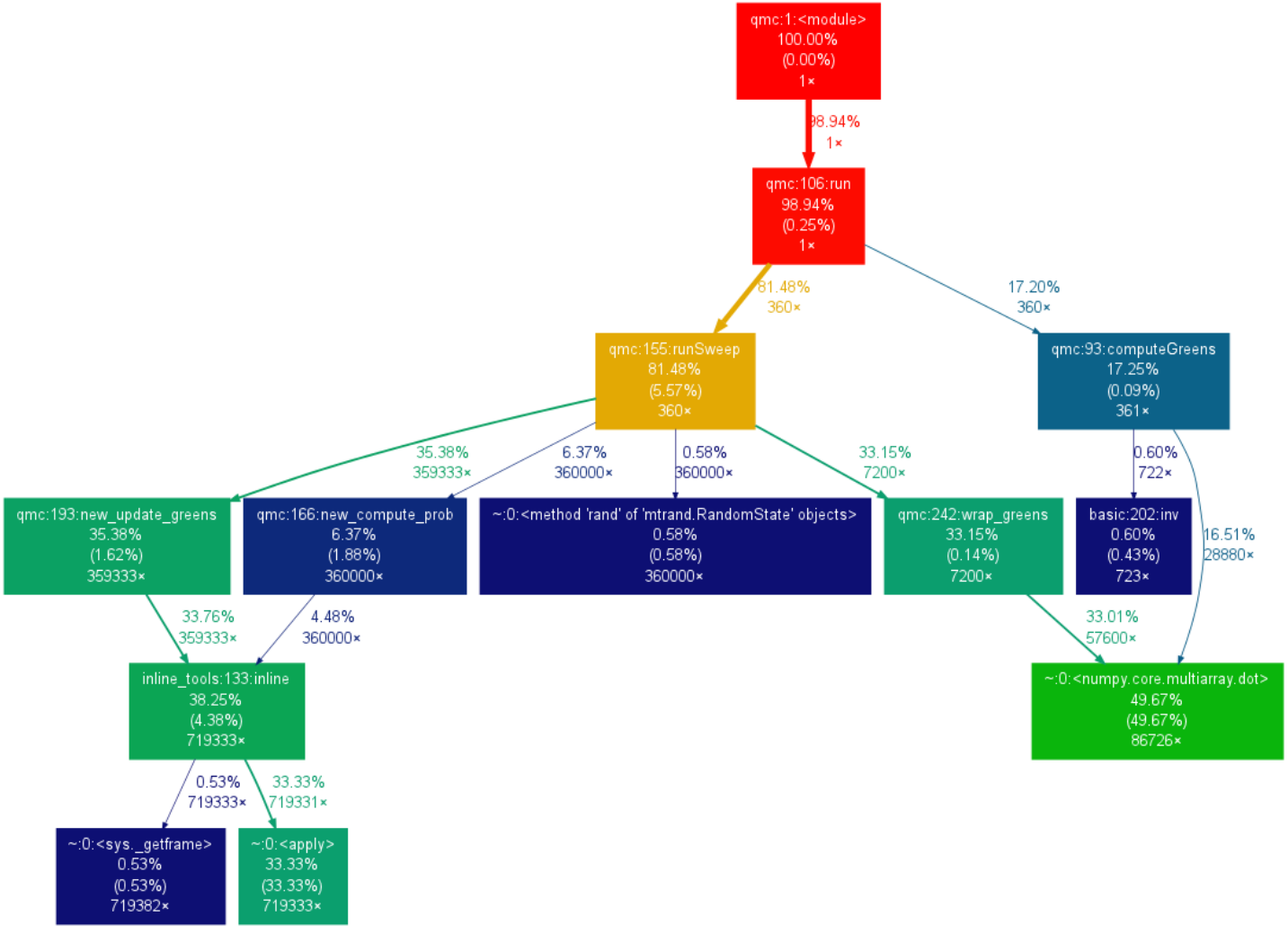
Shown: My results for $U = 4$ and $U = 8$; vs. **Scalettar**
(6×6 grid at half-filling)

The Python Environment

- **Python:** Modern language with expressive syntax, object-oriented/functional features, and ample libraries.
- **NumPy:** Adds fast numerical arrays to Python.
- **SciPy:** Large library of math algorithms based on NumPy.

- Why? I like Python. Wanted to see if it was up to the task.

Speeding Up Code: cProfile + gprof2dot, line_profiler



"Premature optimization is the root of all evil." – Donald Knuth

Speeding Up Code: weave

- Put C++ code in Python:

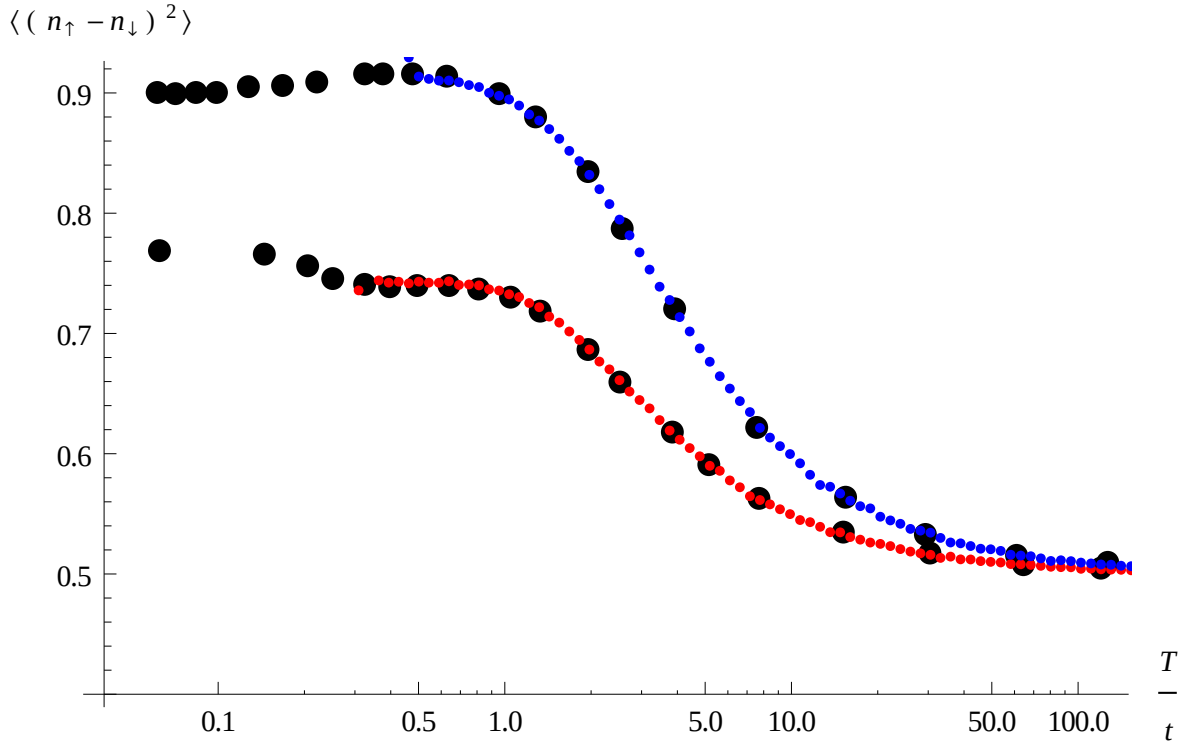
```
def update_G(self, G, new_G, i, Delta_coeff, det_ratio):
    coeff = float(Delta_coeff/det_ratio)
    N = self.N
    code = """
           for (int r = 0; r < N; r++) {
             for (int c = 0; c < N; c++) {
               new_G(r,c) = G(r,c) + G(r, i)*(G(i, c) - (c==i?1:0))*coeff;
             }
           }
           """
    weave.inline(code, ['G', 'N', 'i', 'coeff', 'new_G'],
                 type_converters=weave.converters.blitz,
                 compiler='gcc')
```

- Speed up bottlenecks without losing clarity/usability/development-speed of Python.

Commodity Clusters: Amazon EC2 & StarCluster

- Amazon EC2 offers virtual machines.
  - $0.08/core-hour, on-demand
- StarCluster configures everything.
  - shared filesystem (NFS), queueing system (SGE), etc.
- Almost certainly not competitive with academic resources[1], but a fascinating resource.
  - Note: SDSC charges $0.15/core-hour, with a $2500 minimum.
- In 5min computation, with 64 cores...

Results



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Problems & Future Directions

- Low temperature! Instabilities arise everywhere.
  - Dealt with so far: adaptive recomputation of Green's functions
  - Many more to go (fancy multiplication)
- Scaling
  - Can the system handle larger lattices? More complex models?
- Physics
  - Extend system to explore the universe.