Numerical Calculation for Bose-Hubbard Model

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MODEL INTRODUCTION

Hamiltonian

The Bose-Hubbard model (BHM) gives a description of the physics of interacting spinless Bosons on a lattice[1].

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i. \tag{1.1}$$

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Hopping Term — Superfluid

Bosons move between neighboring sites with amplitude t. The operator $\hat{b}_i^\dagger$ creates a particle at site i, while $\hat{b}_j$ removes one at site j.

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Bosons on the same site repel with strength U. The term $\hat{n}_i(\hat{n}_i - 1)$ penalizes multiple occupancy, where $\hat{n}_i$ counts particles at site i.

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Chemical Potential Term

Controls the average particle number via external field μ. For $\mu = 5$, the system will keep a fixed density of the mean particle number.

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SSE EXPANSION FOR BHM

Kernel Formula

Applying the Taylor expansion to the partition function

$$Z = \sum_{m=0}^{\infty} \frac{\beta^m}{m!} \sum_{\{i_1,\ldots,i_m\}} \sum_{\{b_1,\ldots,b_m\}} \prod_{k=1}^{m} \langle i_k | -H_{b_k} | i_{k+1} \rangle . \tag{2.1}$$

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Expasion Usage Example Taking the order $m = 3$ in 1D-4site model with the parameters

Parameters	t	U	μ	β	N	$\{b_1, b_2, b_3\}$
Values	1	2	5	4	4	$\{[(t, (1, 2)), (U, 3), (\mu, 4)]\}$
Notations	/	/	/	/	Total number of particles in the 4-site	Jumping, repulsion, chemical potential operators

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The state sequences become

1. $|i_1\rangle = |2, 1, 1, 0\rangle$.
2. $|i_2\rangle = |1, 2, 1, 0\rangle$.
3. $|i_3\rangle = |1, 2, 1, 0\rangle$.
4. $|i_4\rangle = |2, 1, 1, 0\rangle = |i_1\rangle$.

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NUMERICAL CALCULATION ANALYSIS: 3 SCHEMES

Scheme A: Heat Bath Update

Basic Principle

Weight-Proportional Sampling: Transition probabilities equal normalized weights $\pi_j = w_j / \sum w_k$.

No rejection step, i.e., always accept according to weights.

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Transition Matrix Structure

For 4 scattering processes (bounce, straight, jump, turn)

$$T_A = \begin{bmatrix} \pi_1 & \pi_2 & \pi_3 & \pi_4 \\ \pi_2 & \pi_1 & \pi_4 & \pi_3 \\ \pi_3 & \pi_4 & \pi_1 & \pi_2 \\ \pi_4 & \pi_3 & \pi_2 & \pi_1 \end{bmatrix}, \quad T_{A_{ii}} = \pi_i.$$

The diagonal term $T_{ii} = \pi_i$ allows state stagnation, then causes high autocorrelation.

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The diagonal term $T_{ii} = \pi_i$ allows state stagnation, then causes high autocorrelation.

Simple but inefficient due to frequent bounce moves.

Scheme B: Minimal Bounce Solution

Basic Principle

Linear Programming Optimization: Minimize total bounce probability $\mathrm{Tr}(T_B) = \sum_i T_{B_{ii}}$ subject to

- Normalization: $\sum_j T_{B_{ij}} = 1$.
- Detailed balance: $w_i T_{B_{ij}} = w_j T_{B_{ji}}$.

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Example Matrix

For weights $[0.2, 0.4, 0.3, 0.1]$

$$T_B = \begin{bmatrix} 0.1 & 0.5 & 0.3 & 0.1 \\ 0.5 & 0.1 & 0.1 & 0.3 \\ 0.3 & 0.1 & 0.1 & 0.5 \\ 0.1 & 0.3 & 0.5 & 0.1 \end{bmatrix}.$$

The diagonal term reduced: $T_{B_{11}} = 0.1$, in comparison to $\pi_1 = 0.2$ in Scheme A.

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Reduces wasted bounce moves via constrained optimization.

Scheme C: Locally Optimal Algorithm

Basic Principle

Peskun's theorem + Metropolization: Diagonal elements set to zero for all but the largest weight state

$$T_{C_{ii}} = 0 \quad (i \neq \max).$$

Prohibits lingering in low-weight states; Minimizes autocorrelation.

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Transition Matrix ($\pi_1 \leq \pi_2 \leq \pi_3 \leq \pi_4$)

$$T_C = \begin{bmatrix} 0 & \frac{\pi_2}{1-\pi_1} & \frac{\pi_3}{1-\pi_1} & \frac{\pi_4}{1-\pi_1} \\ \frac{\pi_1}{1-\pi_2} & 0 & \frac{\pi_3}{1-\pi_2} & \frac{\pi_4}{1-\pi_2} \\ \frac{\pi_1}{1-\pi_3} & \frac{\pi_2}{1-\pi_3} & 0 & \frac{\pi_4}{1-\pi_3} \\ \frac{\pi_1}{1-\pi_4'} & \frac{\pi_2}{1-\pi_4'} & \frac{\pi_3}{1-\pi_4'} & \pi_4' \end{bmatrix}.$$

Only $T_{C_{44}} \neq 0$; All other diagonals are zero.

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Optimal for balanced weights; Derived from Peskun's ordering theorem.

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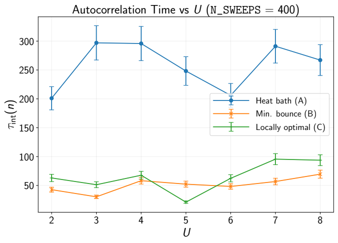
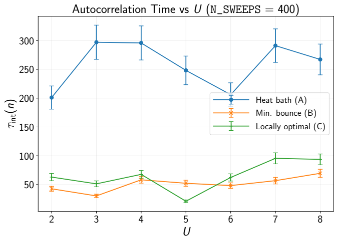
SIMULATION RESULTS

Simulations under different sweep numbers



(a) 400 Sweeps

Simulations under different sweep numbers



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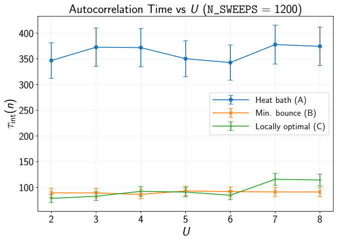

(b) 1200 Sweeps

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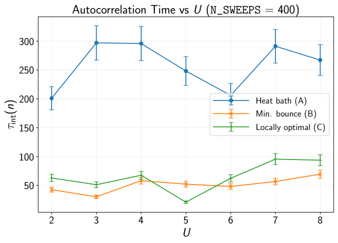

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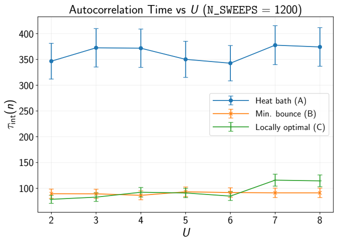

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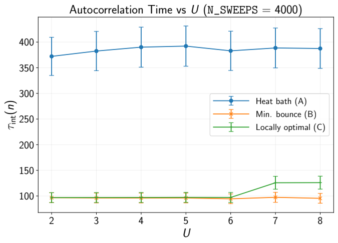

(c) 4000 Sweeps

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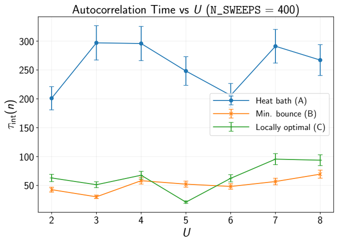

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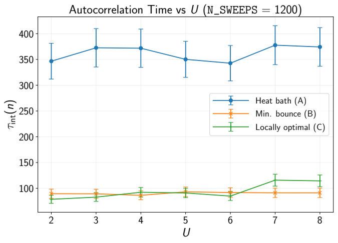

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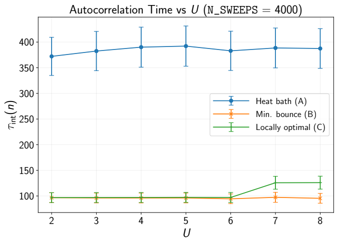

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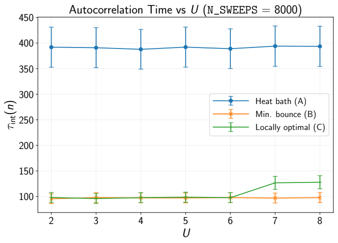
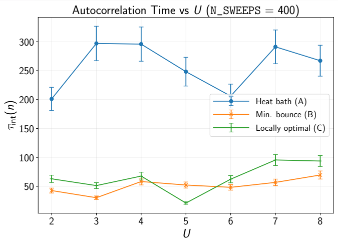


(d) 8000 Sweeps

Simulations under different sweep numbers



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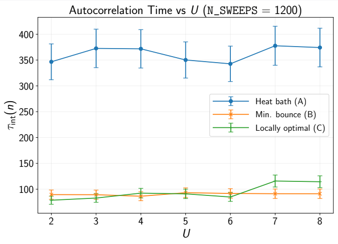

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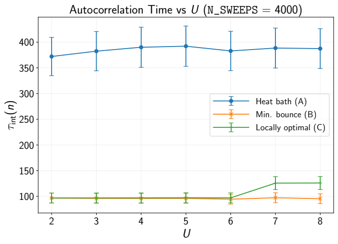

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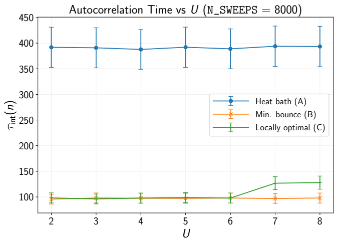

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As U increases, the diagonal weights in the SSE configuration space become dominant. Scheme C shows a slight increase in τ in comparison to B.

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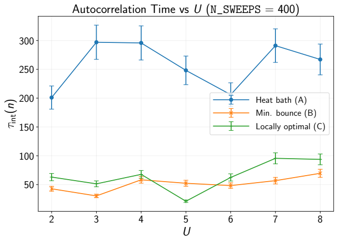

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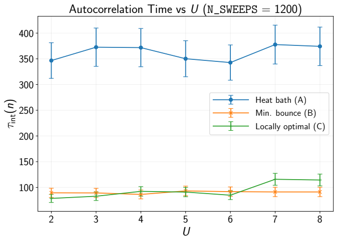

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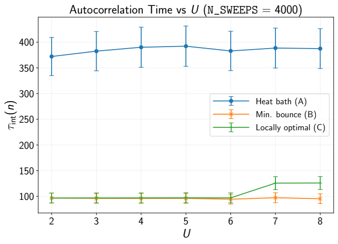

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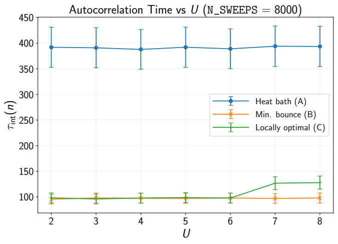

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Table. Comparasion under different U

Phases	Superfluid	Transition	Near-Mote
U	$U < 3$	$3 \leq U \leq 6$	$U \to 9$
(A)	$20 \sim 30$	$30 \sim 45$	$45 \sim 50$
(B)	$8 \sim 10$	$10 \sim 20$	$15 \sim 20$
(C)	$7 \sim 9$	$9 \sim 18$	$18 \sim 25$

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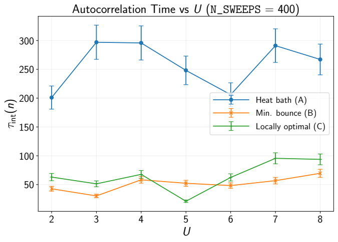

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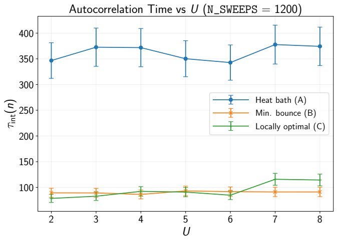

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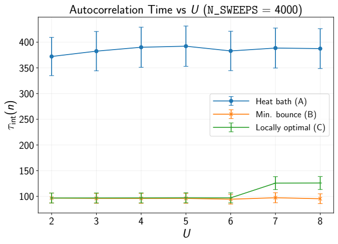

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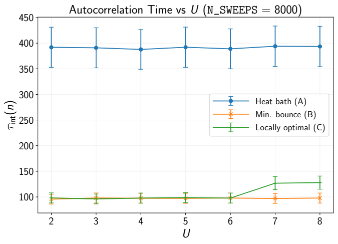

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A fixed random seed is loaded to ensure the fixed result for every time running.

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CONCLUSION

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Low U (weight balance) selects local optima (C), high U (diagonal weight dominance) selects minimum bounce (B).

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Core Design Principle

For efficient algorithms, the condition “Diagonal elements of non-maximum weight states returning to zero” is necessary (both B and C satisfy this), and the remaining degrees of freedom need to be adapted to the weight distribution.

SIMULATION METHOD

Configuration & Process

Key Parameters

- **Lattice**: 1D chain, $L = 64$, $t = 1$, $\mu = 5$.
- **Thermodynamics**: $\beta = L = 64$ (low-T), $U \in [0, 6]$.
- **Algorithm**: A: 16 loops $\times 4$; B/C: 4 loops.
- **Statistics**: 4000 independent chains, each with 1 million steps.
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Method: SSE + Directed Loop

Stochastic Series Expansion maps quantum problem to $(d+1)$D classical graph

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle .$$

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Procedure

1. **Burn-in**: Discard first 10% of samples.
2. **Worm updates**: Collect density series $\{n^{(t)}\}$.
3. **Autocorrelation**
$$\tau_{\mathrm{int}}(n) = \frac{1}{2} + \sum_{t=1}^{\infty} \frac{\langle n^{(i+t)} n^{(i)} \rangle - \langle n^{(i)} \rangle^2}{\langle n^{(i)2} \rangle - \langle n^{(i)} \rangle^2} .$$
4. **Average**: Mean over 4000 chains, plot U vs $\tau_{\mathrm{int}}(n)$.

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PYTHON IMPLEMENTATION

Class Initialization and State Representation

The class stores the lattice size L, inverse temperature β, and model parameters. The state is represented by an array of occupation numbers **n**.

```
def __init__(self, L, beta, U, mu, t = 1, method = 'A'):
    self.L = L
    self.beta = beta
    self.U = U
    self.mu = mu
    self.t = t
    self.method = method  # 'A', 'B', 'C'
```

Initialize state: occupation numbers on each site.

```
    self.n = np.zeros(L, dtype = int)
```

Starting density roughly μ/U to reach equilibrium faster.

```
    initial_dens = max(1, int(mu/U + .5)) if U > 0 else 1
    self.n[:] = initial_dens
```

Energy shift: Ensures diagonal weights in SSE remain positive. Calculated based on maximum expected local density.

```
    self.E_shift = .5 * U * 10 * 9 + 20
```

Calculating Vertex Weights

In SSE, the probability of choosing an operator depends on its "weight". Diagonal weights are related to the local energy, while off-diagonal weights are related to the hopping amplitude t.

```python
def get_vertex_weight(self, n1, n2, op_type):
  E1 = .5 * self.U * n1 * (n1 - 1) - self.mu * n1
  E2 = .5 * self.U * n2 * (n2 - 1) - self.mu * n2
  H_diag_val = .5 * (E1 + E2)
```

Branches for the Diagonal operator (1) and Off-diagonal: hopping (2).

```python
  if op_type == 1:
    return max(0, self.E_shift - H_diag_val)
  elif op_type == 2:
    return self.t
  return 0
```

Transition Matrix Schemes I

The core of the "Optimal Monte Carlo" paper is the design of the transition matrix T_{ij}. According to Peskun's theorem, to minimize the autocorrelation time, one should minimize the diagonal elements T_{ii} (the "bounce" or "stagnation" probability).

```python
def solve_greedy_min_bounce(self, weights):
w0, w1, w2 = weights
sw = w0 + w1 + w2
pi = np.array(weights) / sw
p_out = np.zeros(3)
```

- Scheme A: Heat Bath The core of the "Optimal Monte Carlo" paper is the design of the transition matrix T_{ij}. According to Peskun's theorem, to minimize the autocorrelation time, one should minimize the diagonal elements T_{ii} (the "bounce" or "stagnation" probability).
- Scheme B and C: Optimization via Peskun's Theorem Scheme B (Minimal Bounce) and Scheme C (Locally Optimal) aim to set $T_{ii} = 0$ whenever possible. The code implements this using a "greedy" approach or Metropolized Gibbs sampling.

Transition Matrix Schemes II

Metropolized Gibbs strategy: In [2], Using

$$T_{ij}^{MG} = \begin{bmatrix} 0 & \frac{\pi_2}{1-\pi_1} & \frac{\pi_3}{1-\pi_1} & \cdots & \frac{\pi_n}{1-\pi_1} \\ \frac{\pi_1}{1-\pi_1} & 1-\ldots & \frac{\pi_3}{1-\pi_2} & \cdots & \frac{\pi_n}{1-\pi_2} \\ \frac{\pi_1}{1-\pi_1} & \frac{\pi_2}{1-\pi_2} & 1-\ldots & \cdots & \frac{\pi_n}{1-\pi_3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\pi_1}{1-\pi_1} & \frac{\pi_2}{1-\pi_2} & \frac{\pi_3}{1-\pi_3} & \cdots & 1-\ldots \end{bmatrix} = \min\left(\frac{\pi_j}{1-\pi_i}, \frac{\pi_j}{1-\pi_j}\right).$$

```python
for i in [1, 2]:
    term1 = pi[i] / (1 - pi[0]) if (1 - pi[0]) > 1e-9 else 0
    term2 = pi[i] / (1 - pi[i]) if (1 - pi[i]) > 1e-9 else 1
    p_out[i] = min(term1, term2)
current_sum = p_out[1] + p_out[2]
if current_sum > 1:
    p_out[1] /= current_sum
    p_out[2] /= current_sum
    p_out[0] = 0
else:
    p_out[0] = 1 - current_sum
return p_out
```

The Simulation Loop

The run method performs the actual Markov Chain sweeps. Each site is updated based on the calculated transition probabilities.

```python
def run(self, n_sweeps):
  densities = []
  for _ in range(n_sweeps):
    for i in range(self.L):
      n_curr = self.n[i]
      w0 = self.get_vertex_weight(n_curr, n_curr, 1)
      w_plus = self.get_vertex_weight(n_curr, n_curr + 1, 2)
      w_minus = self.get_vertex_weight(n_curr, n_curr - 1, 2) if n_curr > 0
```

```python
      probs = self.solve_scattering([w0, w_plus, w_minus], self.method)
```

Sample the next state.

```python
      r = np.random.rand()
      if r < probs[0]:
        pass # Stay
      elif r < probs[0] + probs[1]:
        self.n[i] += 1
      else:
        self.n[i] -= 1
```

Record average density as the observable.

```python
    densities.append(np.mean(self.n))
  return densities
```

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Thanks for Listening! Any Questions?