Institute of Physics, CAS

Self-Learning Determinantal Quantum Monte Carlo Method

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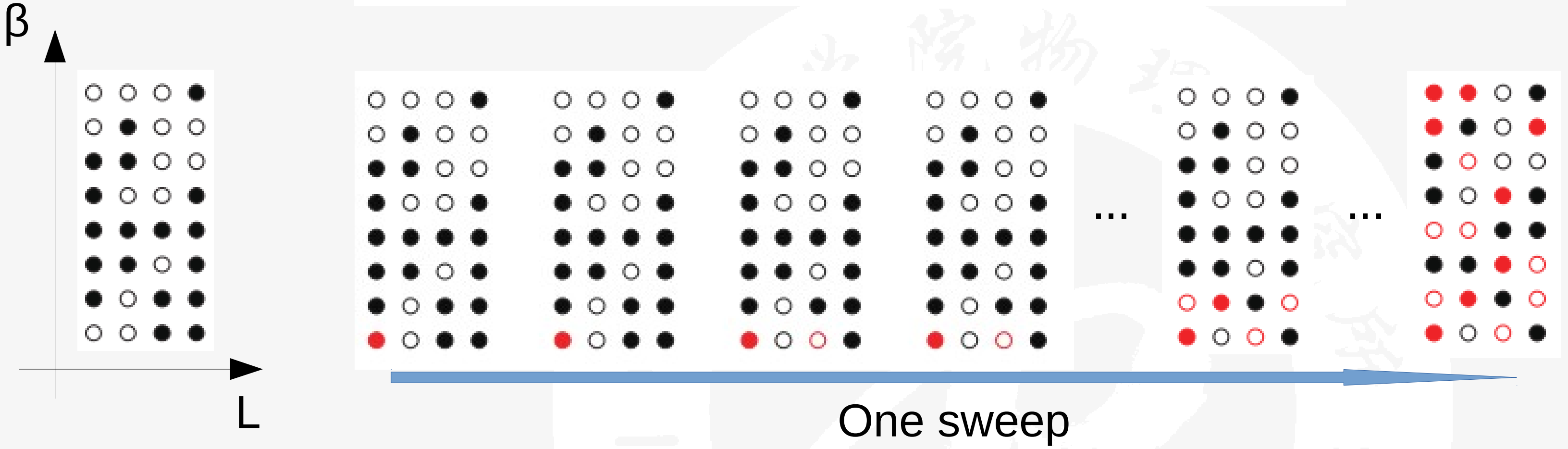
Conventional Determinantal Quantum Monte Carlo

$$Z = \sum_{\{C\}} \phi(C) \det\left(\mathbf{1} + \mathbf{B}(\beta, 0; C)\right)$$



one sweep contain βN local updates

one local update

- Cal. accept ratio: O(1)
- Update Green function: $O(N^2)$

$\boxed{\text{Complexity for one sweep: } \beta N^3}$

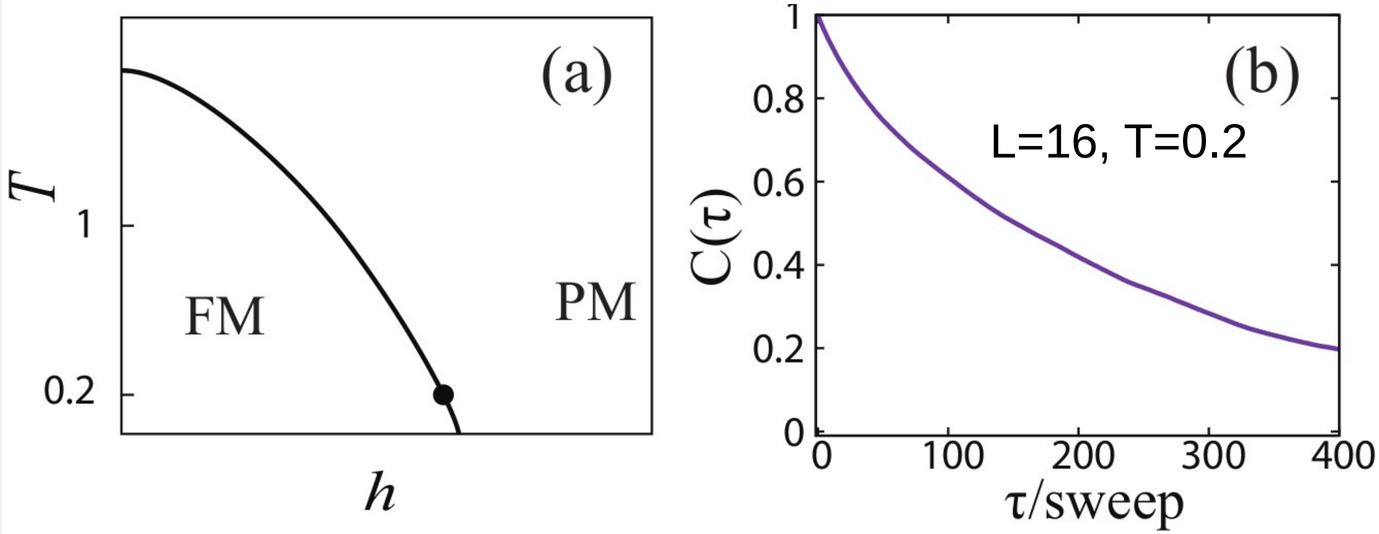
Conventional Determinantal Quantum Monte Carlo

$$H = H_f + H_{sf} + H_s,$$

$$H_f = -t \sum_{\langle ij \rangle \lambda\sigma} c^\dagger_{i\lambda\sigma} c_{j\lambda\sigma} + h.c. - \mu \sum_{i\lambda\sigma} n_{i\lambda\sigma}$$

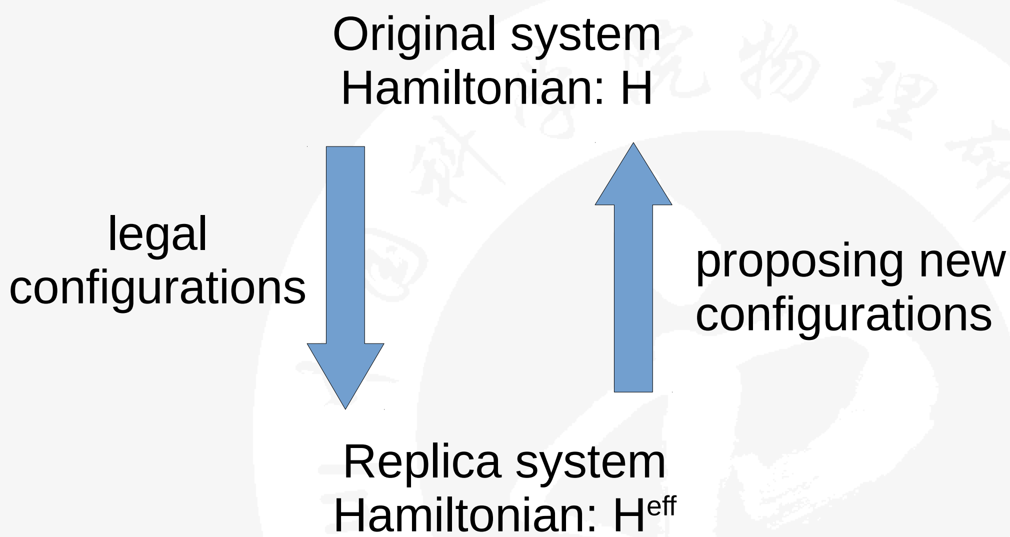
$$H_{sf} = -\xi \sum_i s^z_i (\sigma^z_{i1} - \sigma^z_{i2}),$$

$$H_s = -J \sum_{\langle ij \rangle} s^z_i s^z_j - h \sum_i s^x_i,$$

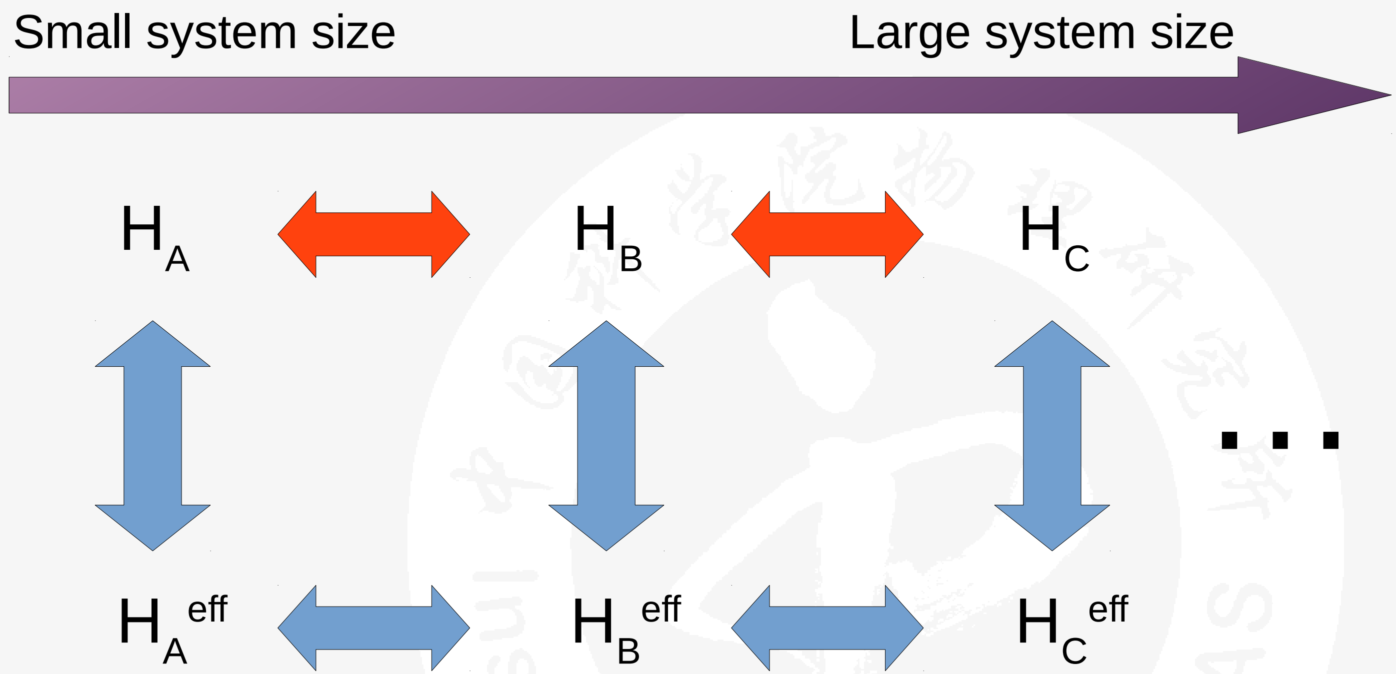


Complexity for getting an independent configuration: $\beta N^3 \tau_L$

Self-Learning Monte Carlo



Self-Learning Monte Carlo



Self-Learning Determinantal Quantum Monte Carlo

$$H^{\mathrm{eff}} = E_0 + \sum_{(i\tau);(j,\tau')} J_{i,\tau;j\tau'} s_{i,\tau} s_{j,\tau'} + \cdots$$

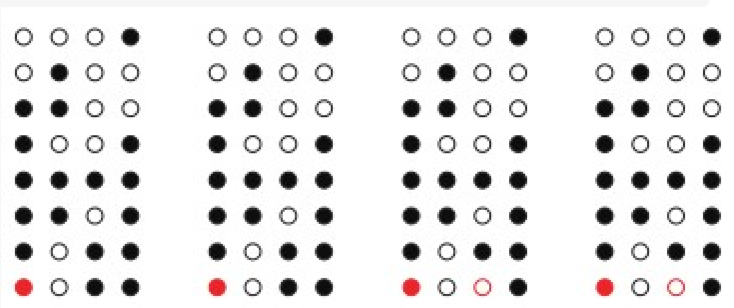
$$Z = \sum_{\{C\}} \phi(C) \det\left(\mathbf{1} + \mathbf{B}(\beta,0;C)\right)$$

Original system

Training Effective Hamiltonian

Generate some configurations

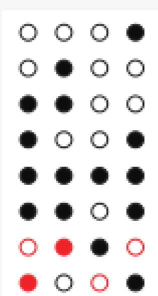
$$-\beta H^{\mathrm{eff}}[C] = \ln\left(\omega[C]\right)$$



Detail balance

$$A(C \to C') = \min\left\{1, \frac{\omega[C']}{\omega[C]} \frac{\exp\left(-\beta H^{\mathrm{eff}}[C]\right)}{\exp\left(-\beta H^{\mathrm{eff}}[C']\right)}\right\}$$

...



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… Repeat τ_L sweeps "cumulative update"

proposing new configurations

Self-Learning Determinantal Quantum Monte Carlo

Complexity

- Cumulative update: $\gamma \beta N \tau_L$
- Detail balance: N^3
- Sweep Green's function: βN^2

Complexity speed up $\mathcal{S} = o\left(\frac{N^2}{\gamma} + N\tau_L + \beta\tau_L\right)$

Self-Learning Determinantal Quantum Monte Carlo