Self-Learning quantum Monte Carlo method in interacting fermion systems

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Serials works on SLMC

IOP: Zi Hong Liu, Zi Yang Meng
MIT: Junwei Liu, Yang Qi, Huitao Shen, Yuki Nagai, Liang Fu
UM: Kai Sun

arXiv:1610.03137
arXiv:1611.09364
arXiv:1612.03804
arXiv:1705.06724
arXiv:1706.10004

Similar work from Li Huang, Yi-feng Yang, Lei Wang
arXiv:1610.02746
arXiv:1612.01871

The power of SLMC

- Reduce the time cost per sweep
  For 100×100×20 lattice
  DQMC ~ 150000 seconds/sweep
  SLMC ~ 500 seconds/sweep

- Reduce the auto-correlation time
  DQMC ~ may scale with system size at critical point
  SLMC ~ constants ideally, model dependent

Determinantal QMC (DQMC)

DQMC(BSS algorithm)

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Monte Carlo calculations of coupled boson-fermion systems. I

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We present a formalism for carrying out Monte Carlo calculations of field theories with both boson and fermion degrees of freedom. The basic approach is to integrate out the fermion degrees of freedom and obtain an effective action for the boson fields to which standard Monte Carlo techniques can be applied. We study the structure of the effective action for a wide class of theories. We develop a procedure for making rapid calculations of the variation in the effective action due to local changes in the boson fields, which is essential for practical numerical calculations.

DQMC(BSS algorithm)

$$S = S_B + \int d\tau \int d^d x \, \psi^\dagger(x,\tau) \hat{O} \psi(x,\tau) \qquad e^{-S_{\mathrm{eff}}} = e^{-S_B} \det \hat{O}$$

$$D = \det_{x,\tau}\left(\frac{\partial}{\partial \tau} + H\right) \qquad \sim(\beta N)^3$$

$$= \det_x \left[I + T \exp\left(- \int_0^\beta d\tau \, H(\tau) \right) \right] \qquad \sim \beta N^3$$

DQMC basics

Slater determinant and its properties

Occupation number representation

Ne particle states $\hat{c}_1^\dagger \hat{c}_2^\dagger \cdots \hat{c}_{N_e}^\dagger |0\rangle$

operator with form $\hat{u} \equiv e^{-\hat{\mathbf{c}}^\dagger \mathbf{A} \hat{\mathbf{c}}}$ $\hat{u}\hat{c}_1^\dagger \hat{c}_2^\dagger \cdots \hat{c}_{N_e}^\dagger |0\rangle = \prod_{i=1}^{N_e} \left(\hat{\mathbf{c}}^\dagger e^{-\mathbf{A}}\right)_i |0\rangle$

overlap of slater determinant

$$|\Psi\rangle = \prod_{i=1}^{N_e} \left(\hat{\mathbf{c}}^\dagger \mathbf{P}\right)_i |0\rangle \qquad |\tilde{\Psi}\rangle = \prod_{i=1}^{N_e} \left(\hat{\mathbf{c}}^\dagger \tilde{\mathbf{P}}\right)_i |0\rangle$$

$$\langle \Psi | \tilde{\Psi} \rangle = \det\left[\mathbf{P}^\dagger \tilde{\mathbf{P}}\right]$$

DQMC basics

Hubbard-Stratonovich transformation

deal with interaction term

A continuous form

$$\exp(\frac{1}{2}\hat{A}^2) = \sqrt{2\pi}\int d\phi \exp(-\frac{1}{2}\phi^2 - \phi\hat{A})$$

Other examples

$$\begin{aligned} e^{-\Delta\tau U(\hat{n}_\uparrow - 1/2)(\hat{n}_\downarrow - 1/2)} &= \frac{1}{2}e^{-\Delta\tau|U|/4}\sum_{s=\pm1} e^{\alpha s(\hat{n}_\uparrow - \hat{n}_\downarrow)}, \quad U > 0 \\ &= \frac{1}{2}e^{-\Delta\tau|U|/4}\sum_{s=\pm1} e^{\alpha s(\hat{n}_\uparrow + \hat{n}_\downarrow - 1)}, \quad U < 0 \end{aligned}$$

$$e^{\Delta\tau W\hat{A}^2} = \frac{1}{4}\sum_{l=\pm2,\pm1}\gamma(l)\exp\left(\sqrt{\Delta\tau W}\phi(l)\hat{A}\right) + o(\Delta\tau^4)$$

DQMC

Trotter decomposition

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] = \mathrm{Tr}\left[(e^{-\Delta_\tau \hat{H}_I} e^{-\Delta_\tau \hat{H}_0})^M\right] + \mathcal{O}(\Delta_\tau^2)$$

HS transformation

$$Z = \sum_{\mathcal{C}} \mathcal{W}^s_{\mathcal{C}} \mathrm{Tr}\left[\prod_{\tau=M}^{1} e^{\hat{\mathbf{c}}^\dagger \mathbf{V}(\mathcal{C}) \hat{\mathbf{c}}} e^{-\Delta_\tau \hat{\mathbf{c}}^\dagger \mathbf{T} \hat{\mathbf{c}}}\right] + \mathcal{O}(\Delta_\tau^2)$$

Trace out fermions

(trace over all Ne particle basis, $Ne=1,\ldots,N$)

$$Z = \sum_{\mathcal{C}} \mathcal{W}^s_{\mathcal{C}} \mathrm{Tr}\left[\hat{U}(\beta, 0)\right] \qquad \hat{U}(\tau_2, \tau_1) = \prod_{n=n_1+1}^{n_2} e^{\hat{\mathbf{c}}^\dagger \mathbf{V}(\mathcal{C}) \hat{\mathbf{c}}} e^{-\Delta_\tau \hat{\mathbf{c}}^\dagger \mathbf{T} \hat{\mathbf{c}}}$$

$$Z = \sum_{\mathcal{C}} \mathcal{W}^s_{\mathcal{C}} \det\left[\mathbf{1} + \mathbf{B}(\beta, 0)\right] \qquad \mathbf{B}(\tau_2, \tau_1) = \prod_{n=n_1+1}^{n_2} e^{\mathbf{V}(\mathcal{C})} e^{-\Delta_\tau \mathbf{T}}$$

DQMC

partition function

$$Z = \sum_{\mathcal{C}} \mathcal{W}^s_{\mathcal{C}} \det\left[\mathbf{1} + \mathbf{B}(\beta, 0)\right]$$

Importance sampling of configurations

$$\mathcal{P}_{\mathcal{C}} = \frac{\mathcal{W}^s_{\mathcal{C}} \det\left[\mathbf{1} + \mathbf{B}(\beta, 0)\right]}{\sum_{\mathcal{C}} \mathcal{W}^s_{\mathcal{C}} \det\left[\mathbf{1} + \mathbf{B}(\beta, 0)\right]}$$

$$\begin{aligned} \langle \hat{O} \rangle &= \sum_{\mathcal{C}} \mathcal{P}_{\mathcal{C}} \langle \hat{O} \rangle_{\mathcal{C}} \\ &\approx \frac{1}{N_{\text{sample}}} \sum_{i=1}^{N_{\text{sample}}} \langle \hat{O} \rangle_{\mathcal{C}_i} \end{aligned}$$

$$\langle \hat{O} \rangle_{\mathcal{C}} = \frac{\mathrm{Tr}\left[\hat{U}(\beta, \tau)\hat{O}\hat{U}(\tau, 0)\right]}{\mathrm{Tr}\left[\hat{U}(\beta, 0)\right]}$$

Application of DQMC

Coupled Fermion-boson lattice systems

- Interacting systems after HS transformation
  Hubbard like models
  Mott transition, chiral Ising and chiral Heisenberg transition, bosonic SPT etc.

- build-in coupled fermion-boson
  AFM in metal, SDW, nematic QCP, FM QCP,
  Z2 deconfined phase transtion

Issues of DQMC

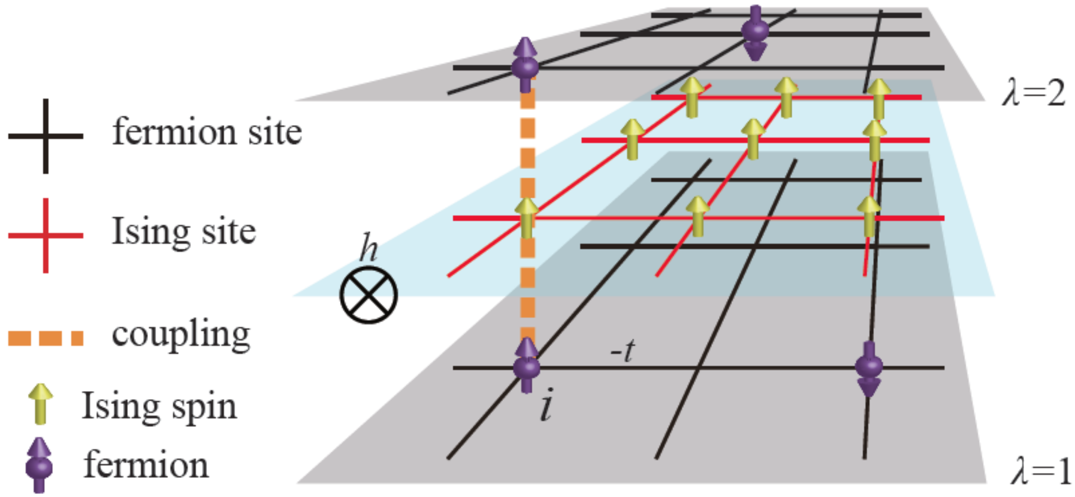
- **Local update is level 1 BLAS algorithm**

Size limited, L=20 is the typical size

- **(critical) slowing down in some models**

build-in coupled fermion-boson problem

Slowing down for some models in DQMC

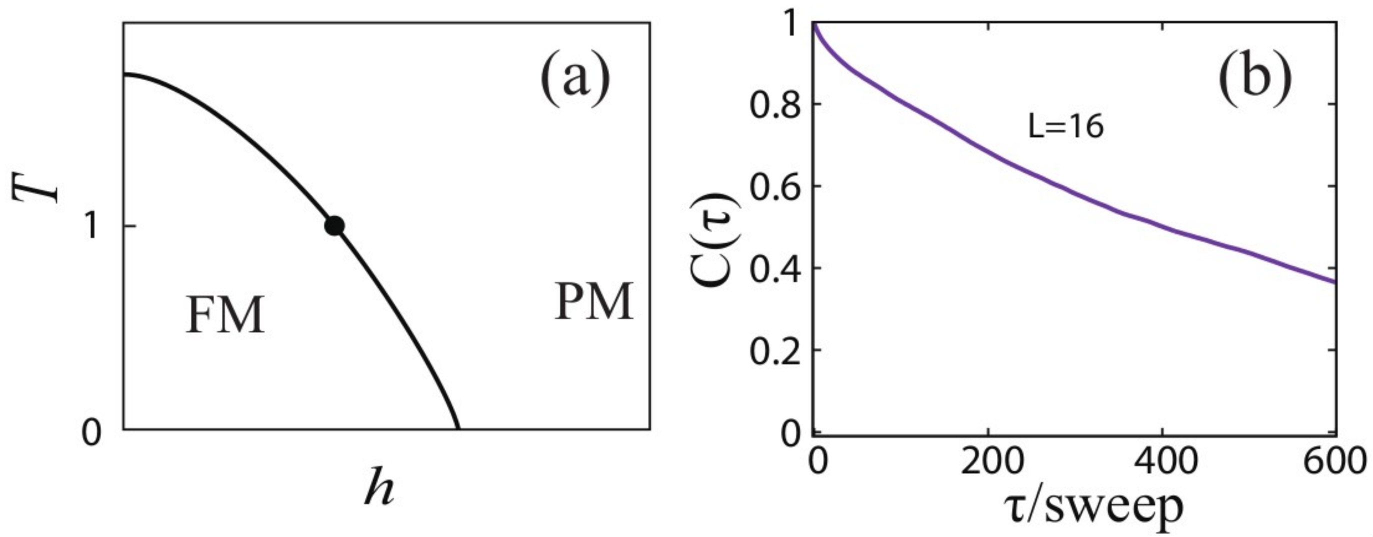


$$\hat{H} = \hat{H}_f + \hat{H}_s + \hat{H}_{sf}$$

$$\hat{H}_f = -t \sum_{\langle ij \rangle \lambda\sigma} \hat{c}^\dagger_{i\lambda\sigma} \hat{c}_{j\lambda\sigma} + h.c. - \mu \sum_{i\lambda\sigma} \hat{n}_{i\lambda\sigma}$$

$$\hat{H}_s = -J \sum_{\langle ij \rangle} \hat{s}^z_i \hat{s}^z_j - h \sum_i \hat{s}^x_i$$

$$\hat{H}_{sf} = -\xi \sum_i s^z_i (\hat{\sigma}^z_{i1} + \hat{\sigma}^z_{i2})$$

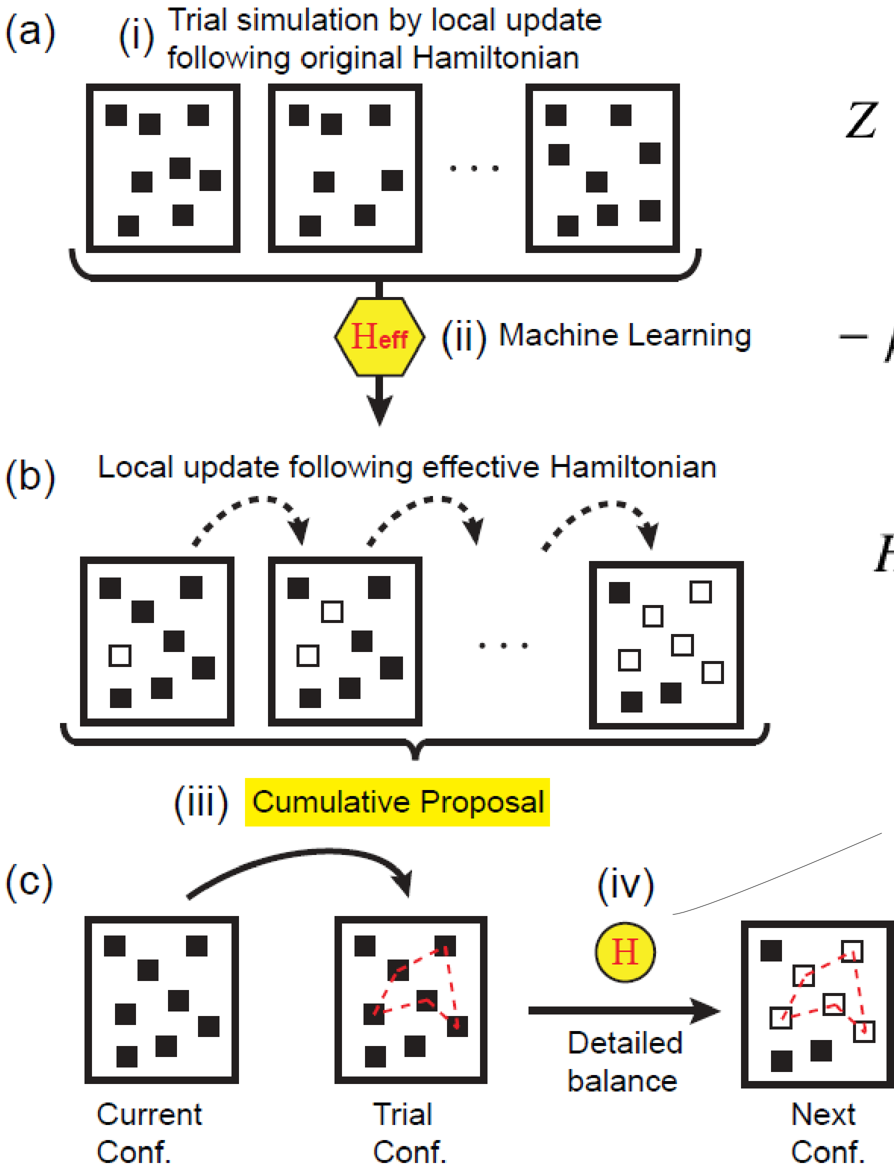


Complexity for getting an independent configuration: $\beta N^3 \tau_L$

Self-learning DQMC

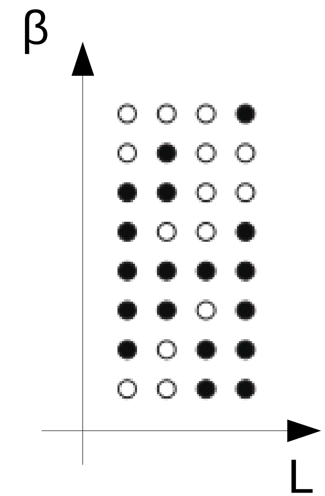
arXiv:1612.03804
arXiv:1706.10004

Self-Learning Monte Carlo



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

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



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

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

arXiv:1612.03804

Self-Learning Determinantal Quantum Monte Carlo

Complexity

- Cumulative update: $\gamma \beta N \tau_L$
- Detail balance: N^3

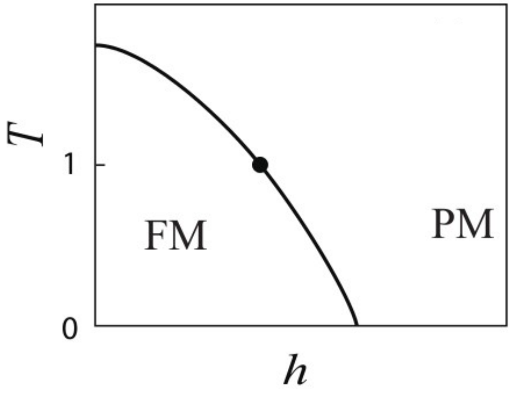
$$\begin{aligned} \omega_{\mathcal{C}} &= \phi(\mathcal{C}) \det\left(\mathbf{1} + \mathbf{B}(\beta,\tau)\mathbf{B}(\tau,0)\right) \\ &= \phi(\mathcal{C}) \det\left(\mathbf{G}(0,0)\right)^{-1} \end{aligned}$$

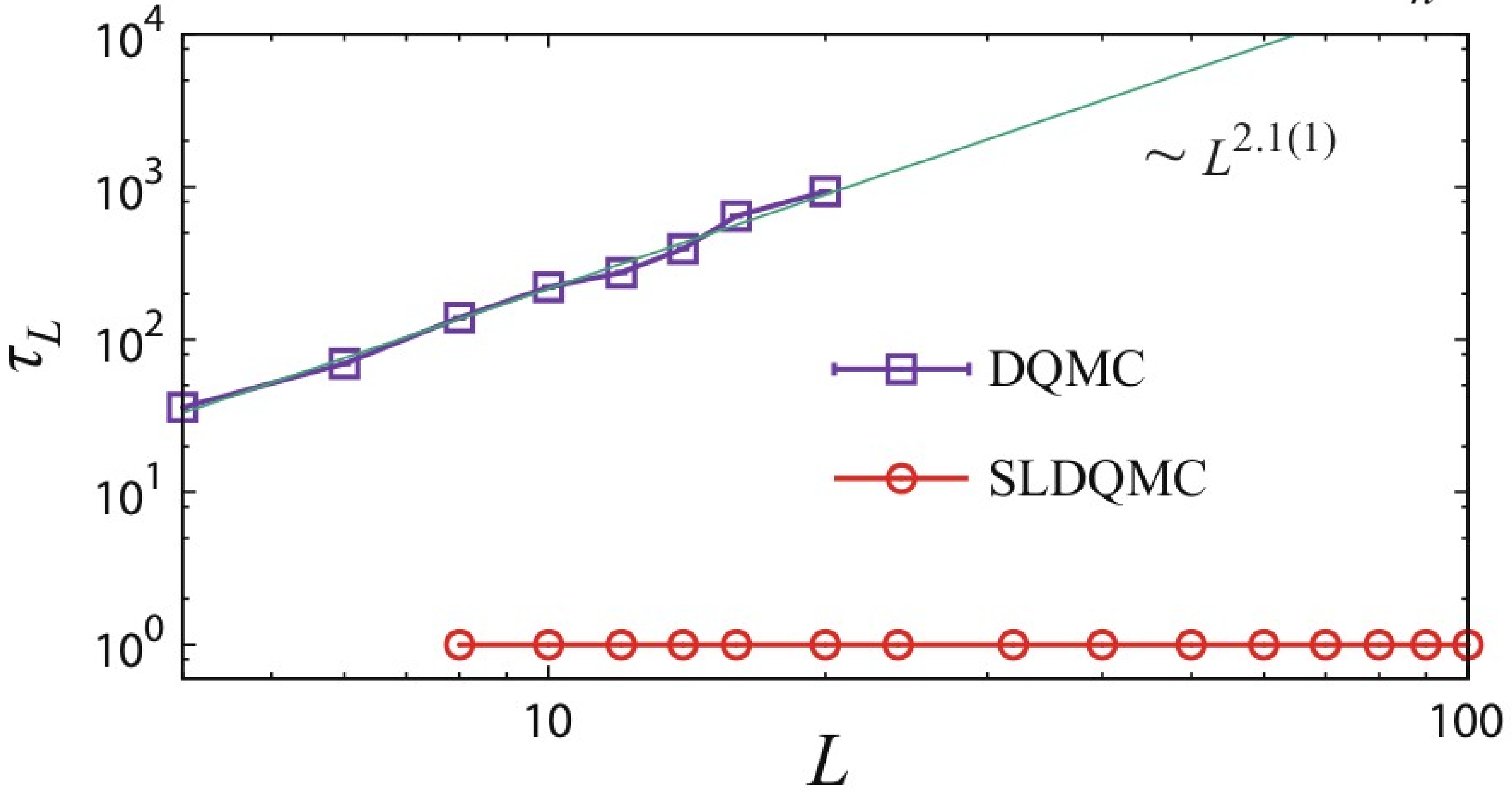
- Sweep Green's function: βN^2

$$\mathbf{G}(\tau+1,\tau+1) = \mathbf{B}(\tau+1,\tau)\mathbf{G}(\tau,\tau)\mathbf{B}^{-1}(\tau+1,\tau)$$

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

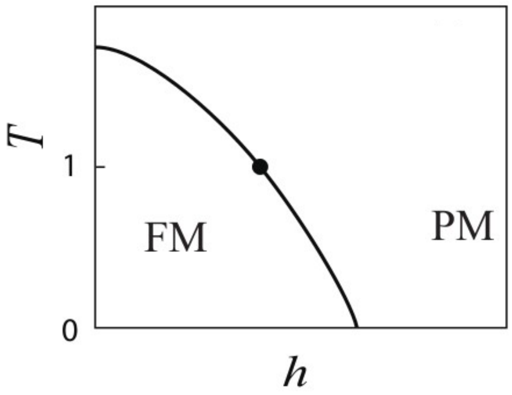
Autocorrelation time

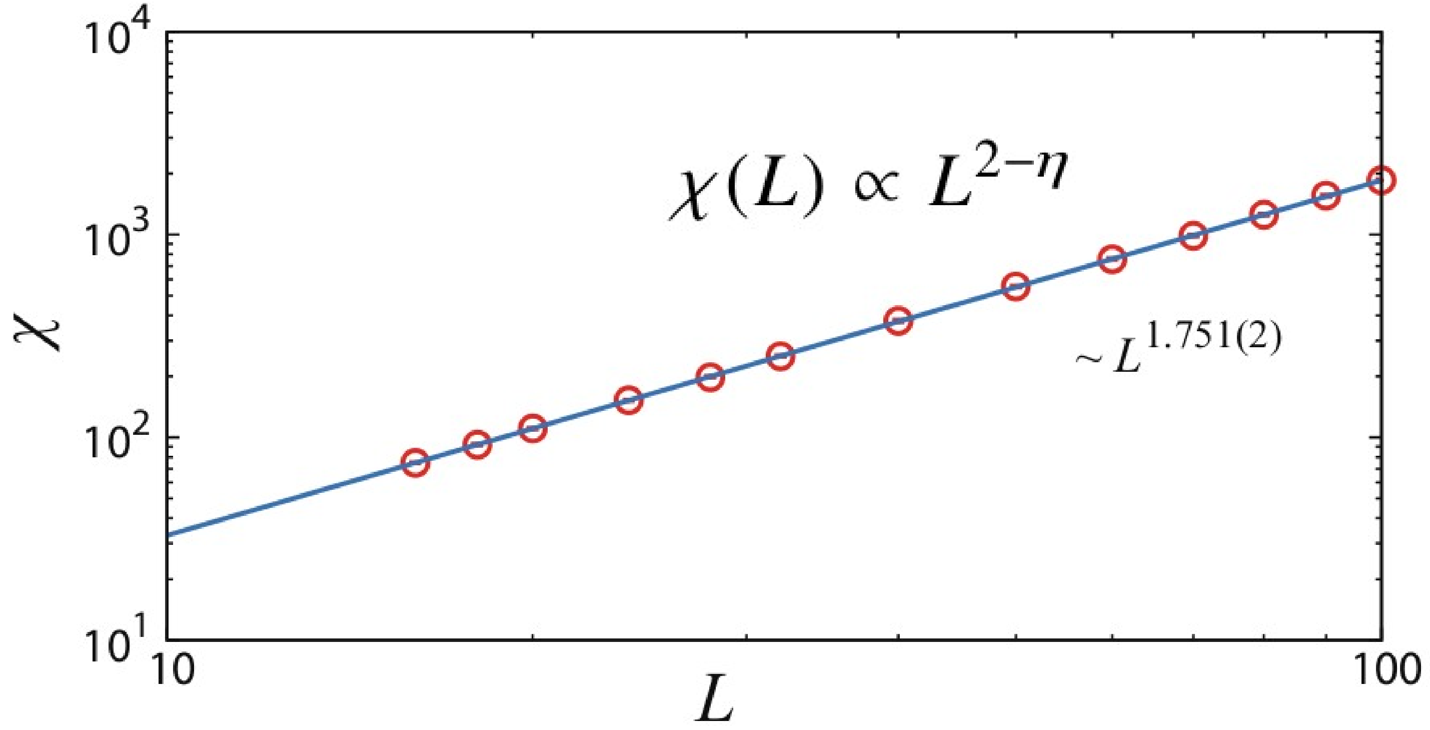




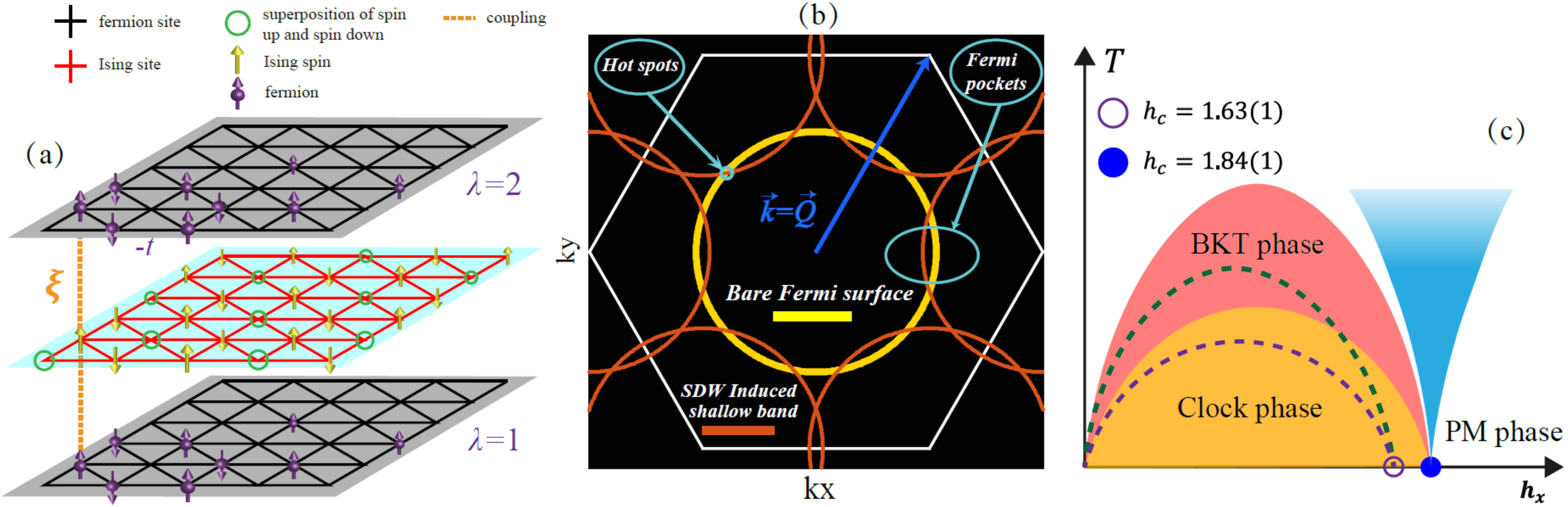
Self-Learning Determinantal Quantum Monte Carlo

$$\chi(L) = \frac{1}{L^2} \sum_{ij} \int_0^\beta d\tau \langle s^z_{i,\tau} s^z_{j,0} \rangle$$



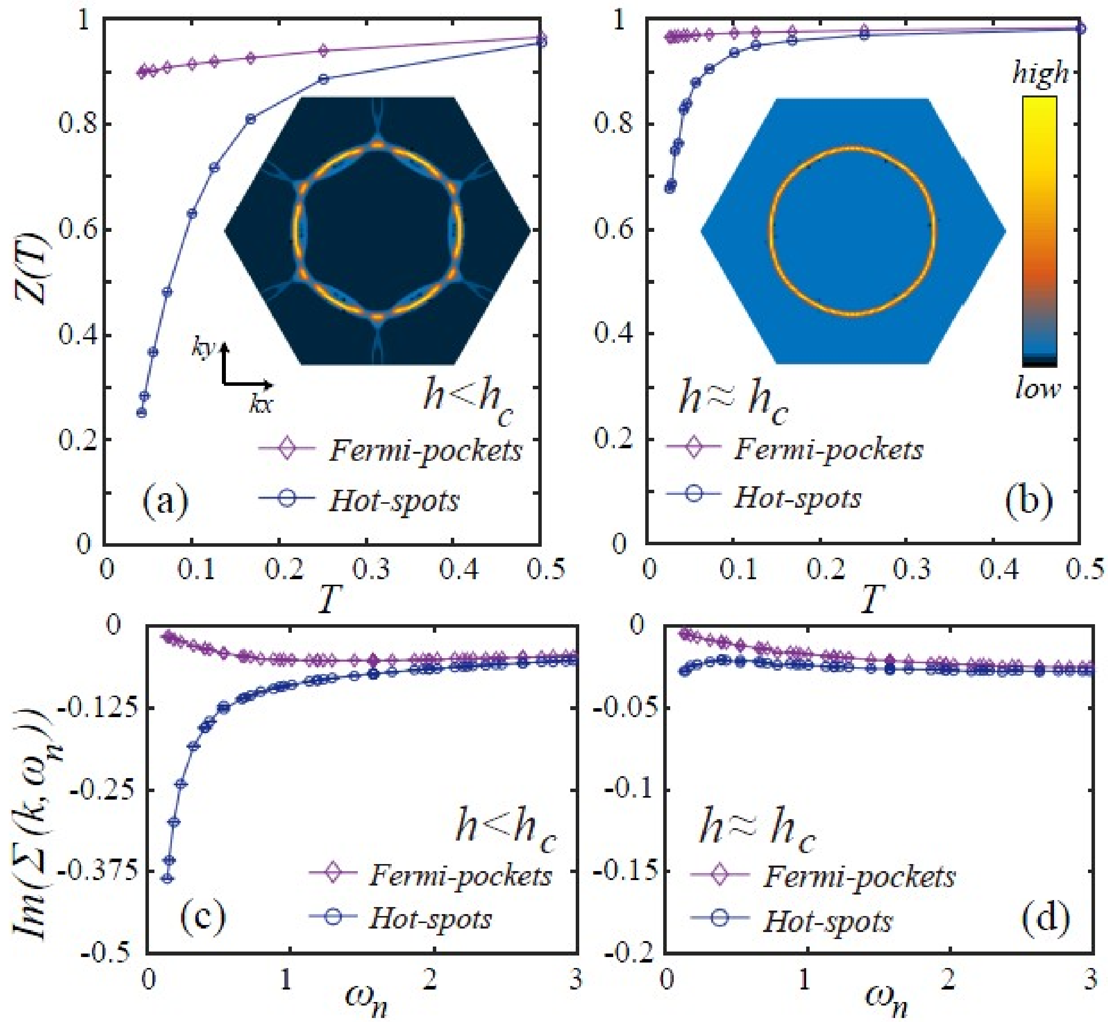


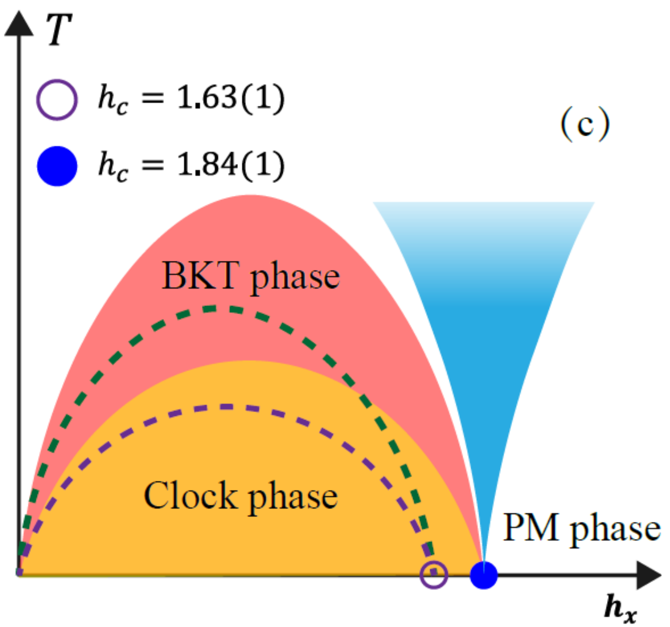
Itinerant quantum critical point with frustration



arXiv:1706.10004

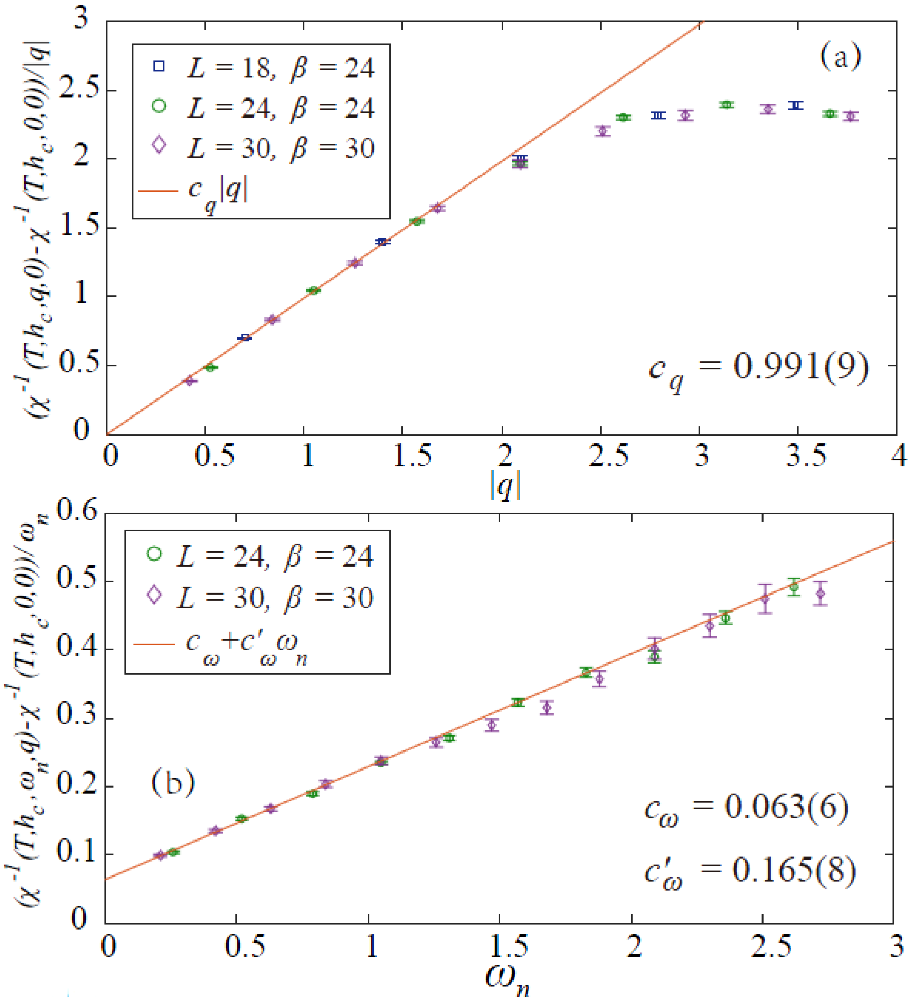
Itinerant quantum critical point with frustration

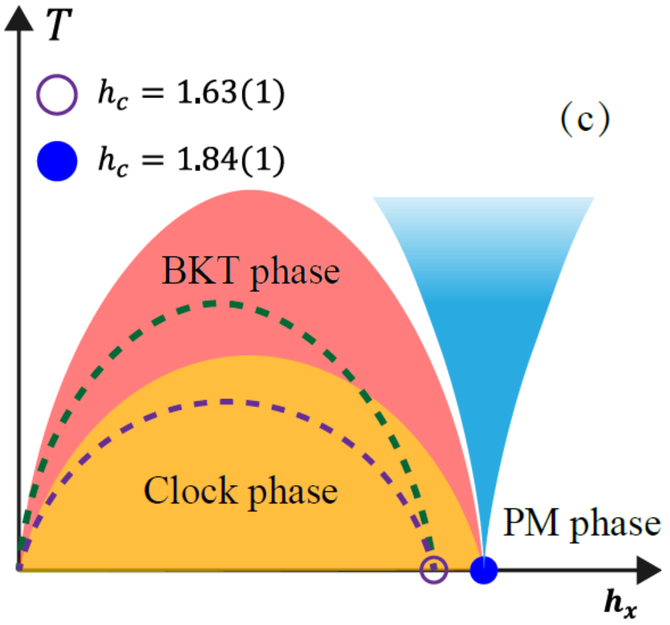




Non-fermi liquid behavior on hot spots

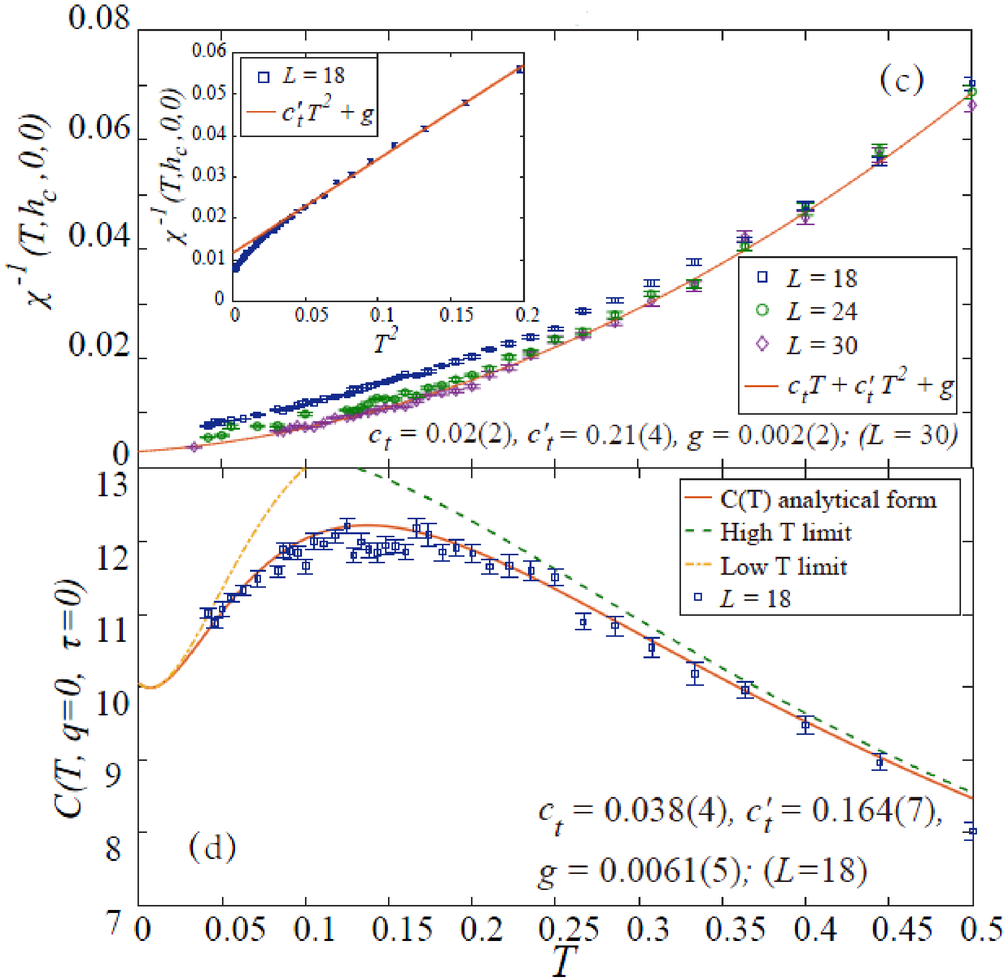
Itinerant quantum critical point with frustration



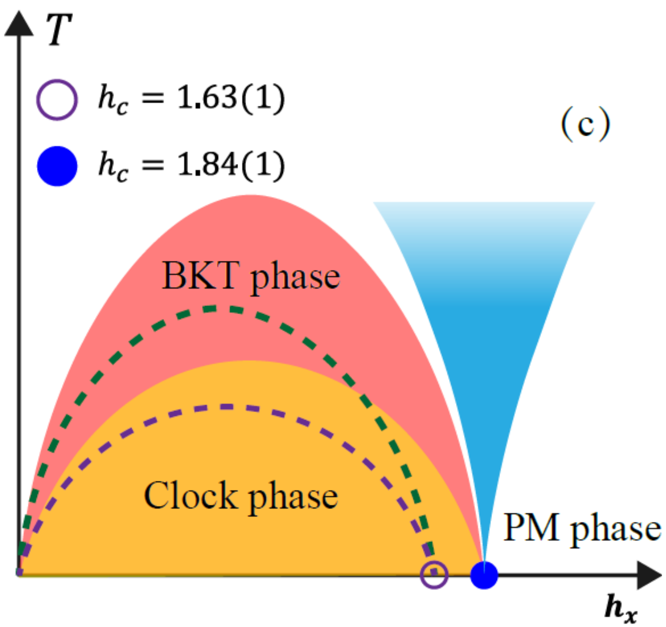


dynamical exponents z=2

Itinerant quantum critical point with frustration



L=30, beta=30
(30×30×600)

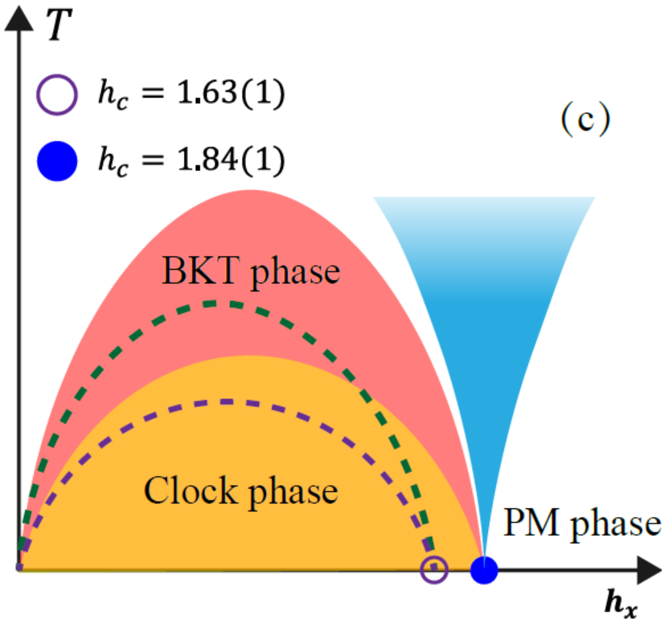


Linear T dependence in spin susceptibility

Itinerant quantum critical point with frustration

$$\chi(T,h,\mathbf{q},\omega_n) = \frac{1}{(c_t T + c_t' T^2) + c_h |h - h_c|^\gamma + c_q |\mathbf{q}|^2 + (c_\omega \omega + c_\omega' \omega^2)}$$

Hertz-Millis-Moriya theory on finite momentum QCP

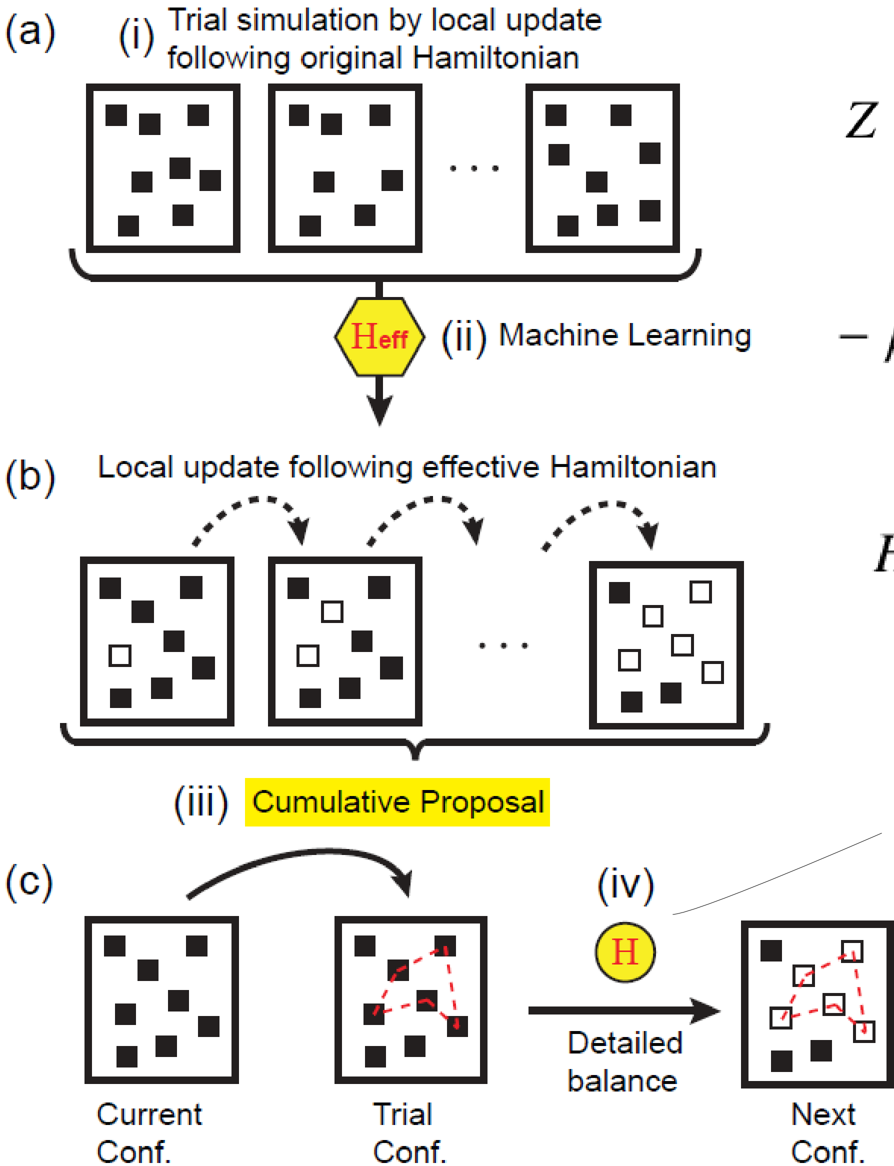


Summary and outlook

SLMC can be used to attack some hard problems

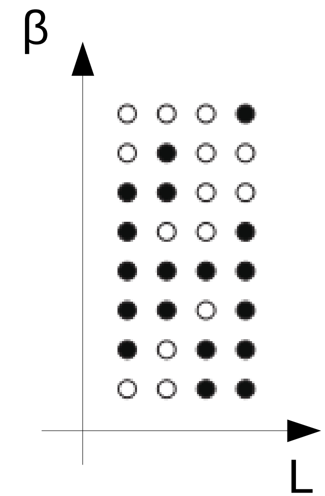
How general can it be is still a question

Self-Learning Monte Carlo



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

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



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

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

arXiv:1612.03804