Itinerant Quantum Critical Points and Self-learning Monte Carlo Method

Zi Yang Meng

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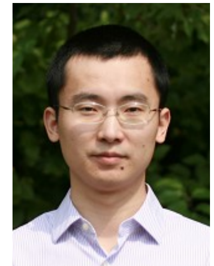
Itinerant Quantum Critical Points


Xiao Yan Xu

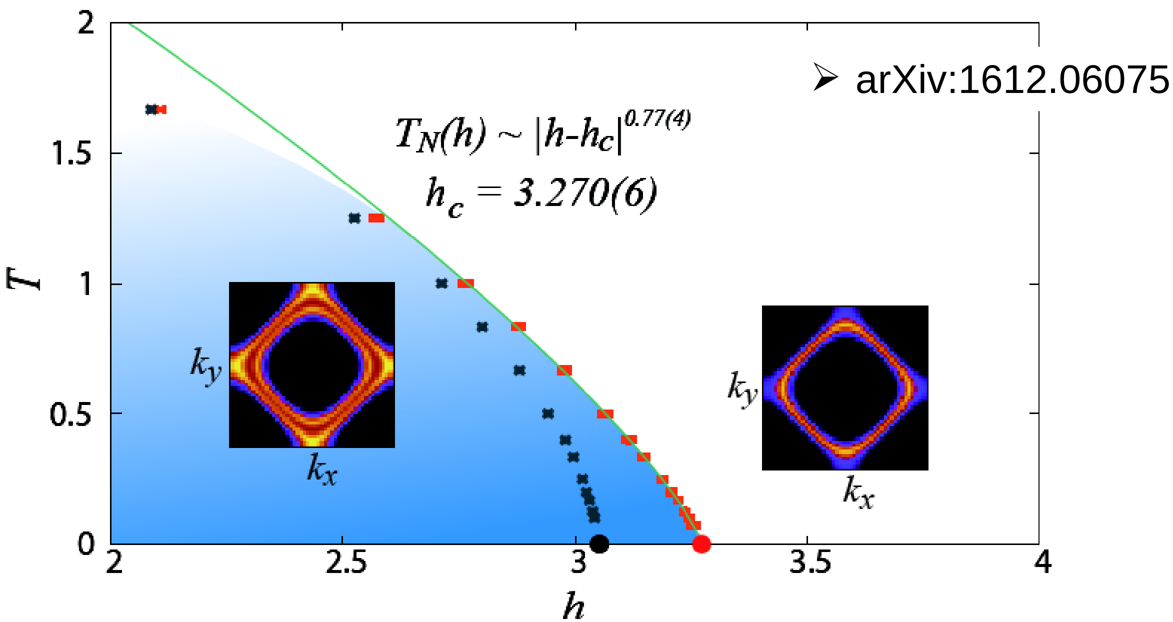

Yoni Schattner

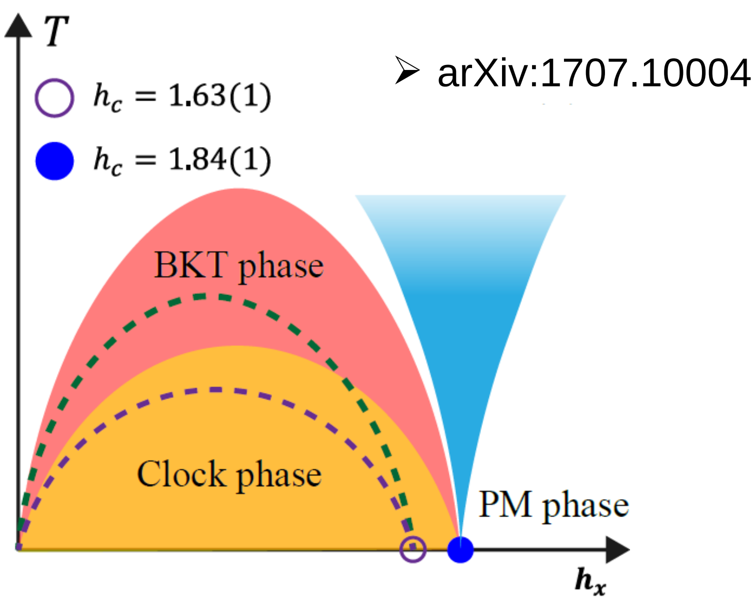

Erez Berg


Kai Sun


Zi Hong Liu

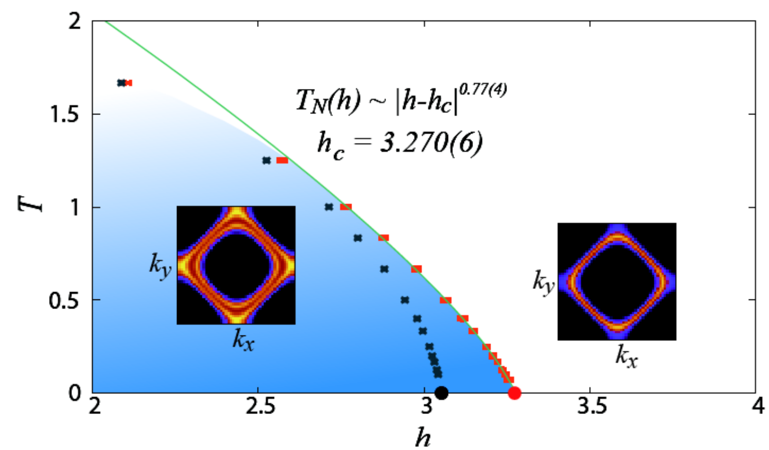

Yang Qi





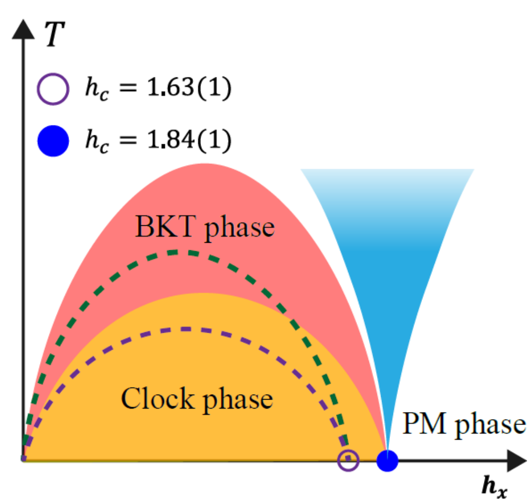
Content

- Fermi surface coupled to critical bosonic fluctuations



- Results
  - ➢ phase diagram
  - ➢ Non-Fermi liquid and itinerant FM/AFM-QCPs

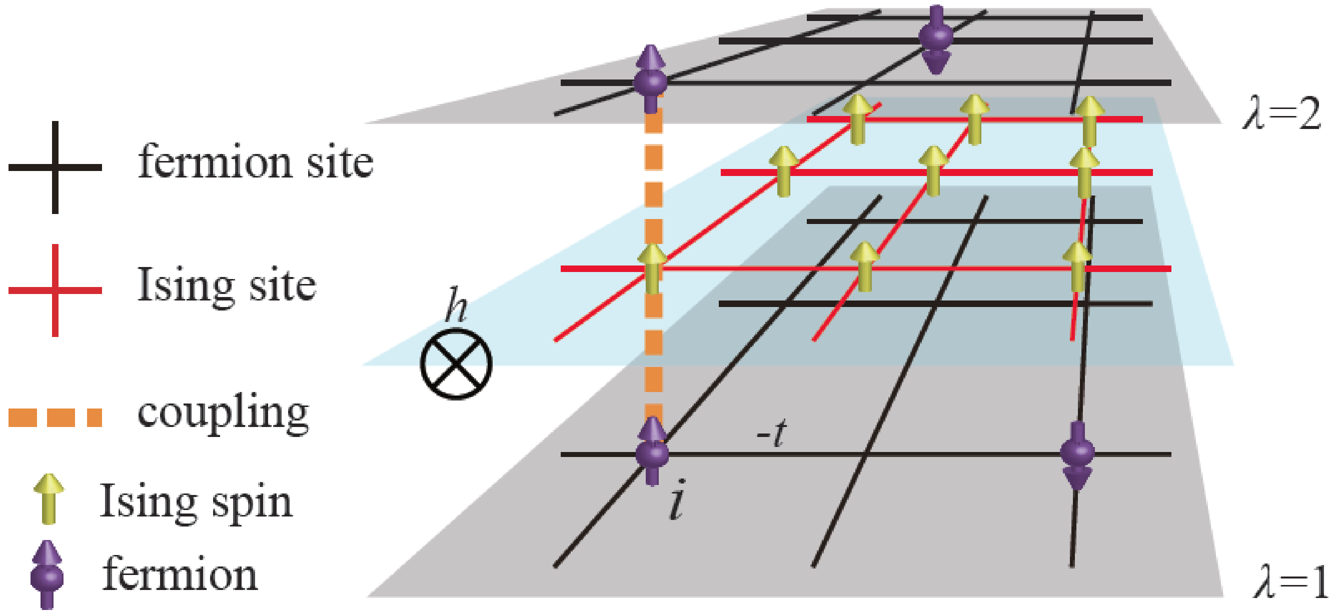
➢ arXiv:1612.06075



- Self-learning Monte Carlo method

➢ arXiv:1707.10004

Model

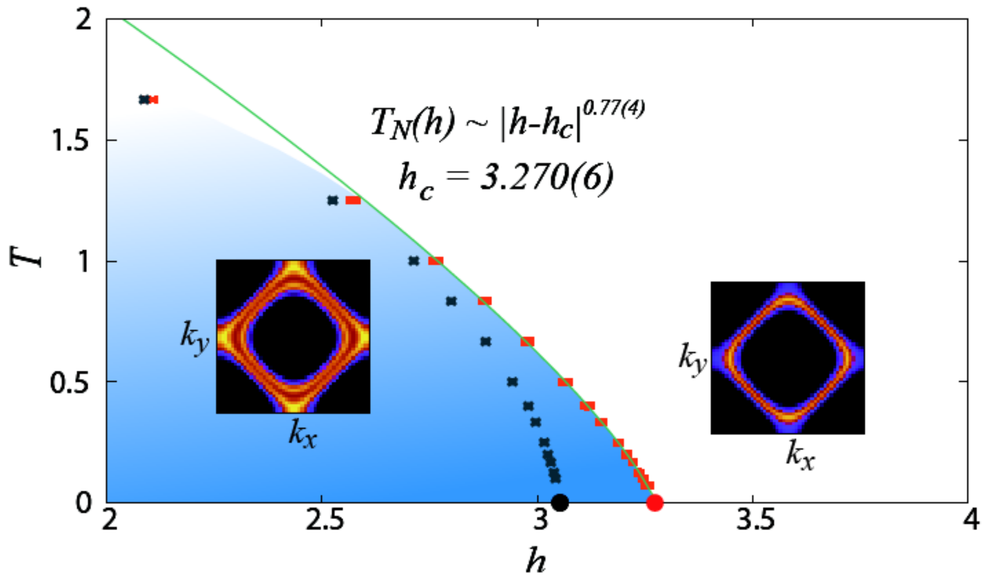


$$\hat{H} = \hat{H}_f + \hat{H}_s + \hat{H}_{sf}$$

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

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

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



Quantum Monte Carlo

$$Z = \mathbf{Tr}\left[e^{-\beta\hat{H}}\right]$$

$$= \sum_{s_{b_1}\cdots s_{b_N}=\pm 1} \mathbf{Tr}_F \left\langle s_{b_1}\cdots s_{b_N} \left| \left(e^{-\Delta\tau\hat{H}}\right)^M \right| s_{b_1}\cdots s_{b_N} \right\rangle$$

$$= \sum_{\vec{S}_1\cdots\vec{S}_M} \mathrm{Tr}_F \langle \vec{S}_1 | e^{-\Delta\tau\hat{H}} | \vec{S}_M \rangle \langle \vec{S}_M | e^{-\Delta\tau\hat{H}} | \vec{S}_{M-1} \rangle \cdots \langle \vec{S}_2 | e^{-\Delta\tau\hat{H}} | \vec{S}_1 \rangle$$

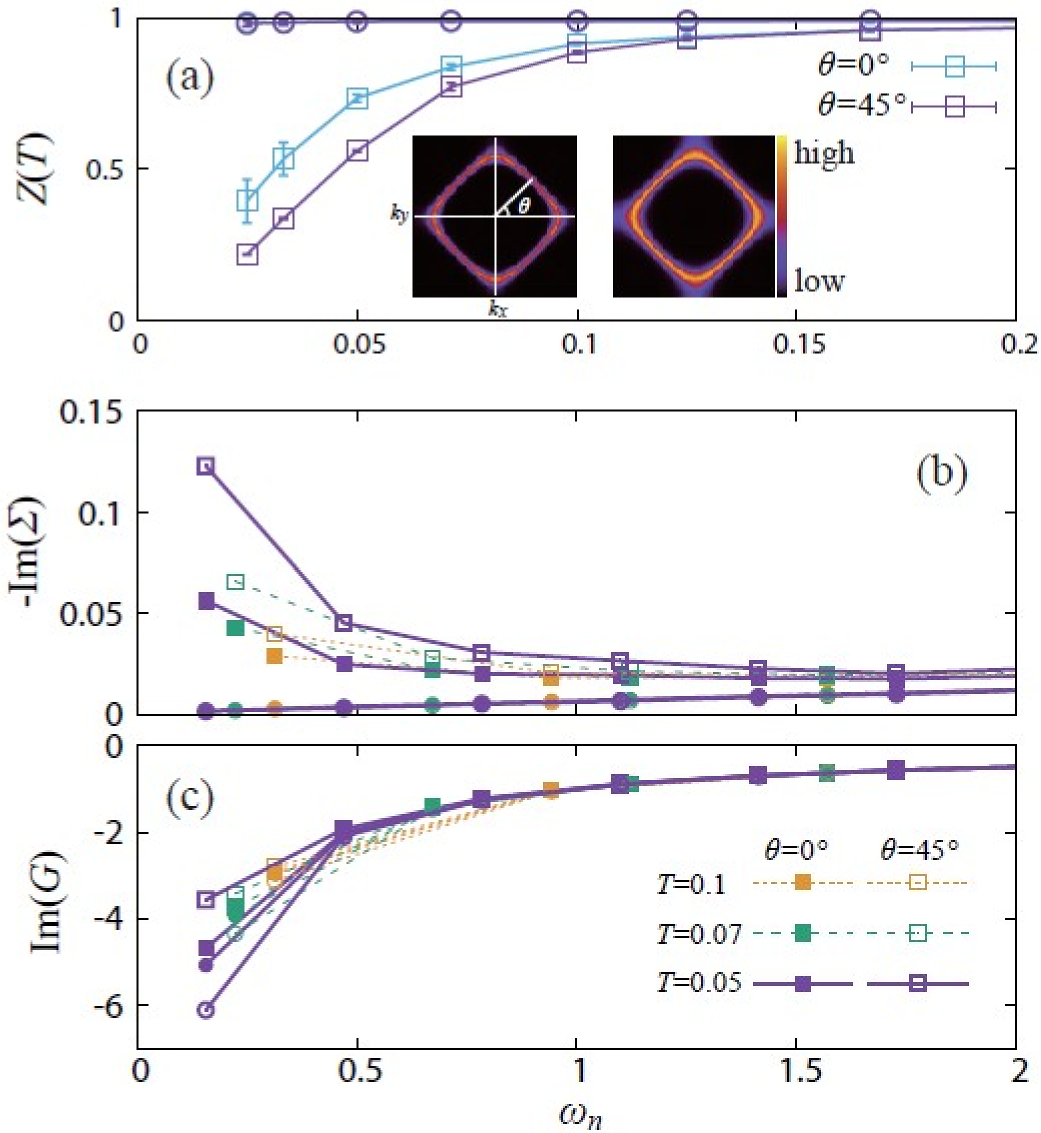
$$= \sum_{\mathcal{C}} \omega_{\mathcal{C}} \text{ with configuration } \mathcal{C} = \left\{\vec{S}_1, \cdots \vec{S}_M\right\}$$

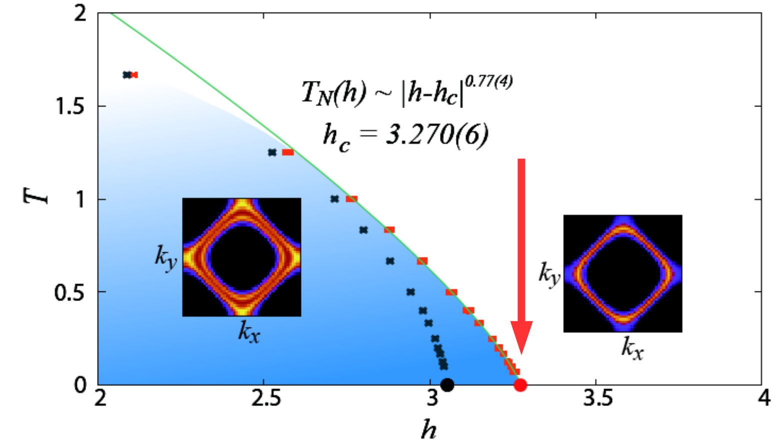
$$\omega_{\mathcal{C}} = \left(\prod_{\tau}\prod_{\langle i,j\rangle} e^{\Delta\tau J s_{i,\tau} s_{j,\tau}}\right)\left(\prod_{i}\prod_{\langle\tau,\tau'\rangle} \Lambda e^{\gamma s_{\tau,i} s_{\tau',i}}\right)\left|\prod_{\sigma} \det\left(\mathbf{1} + \mathbf{B}_M^{1\sigma}\cdots\mathbf{B}_1^{1\sigma}\right)\right|^2$$

- Self-learning Monte Carlo Method

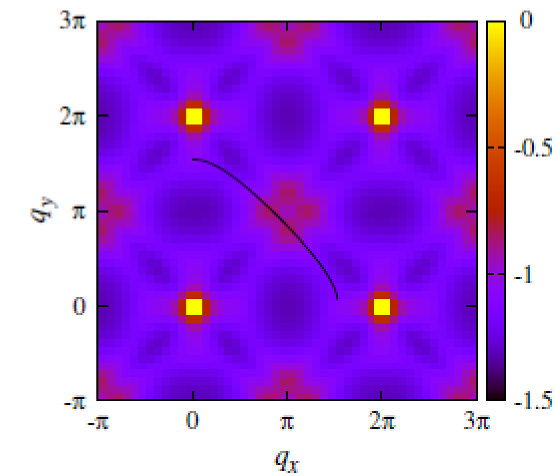
O(N) speedup, large lattice is possible

Non-Fermi liquid





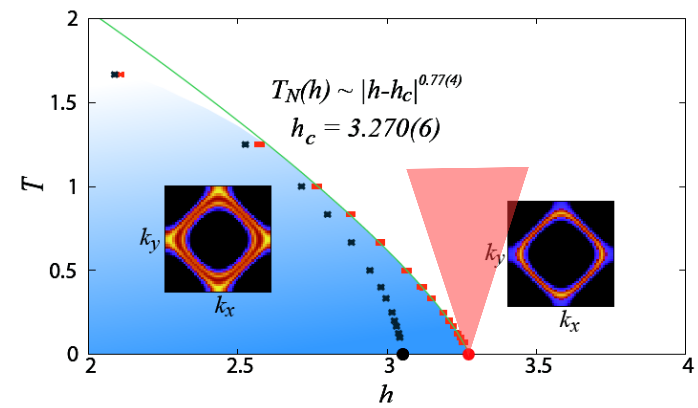
$$Z_{\mathbf{k}_F} \approx \frac{1}{1 - \frac{\mathrm{Im}\Sigma(\mathbf{k}_F, i\omega_0)}{\omega_0}}$$



FM-QCP

$$\chi(h,T,\mathbf{q},i\omega_n) = \frac{1}{L^2}\sum_{ij}\int_0^\beta d\tau e^{i\omega_n\tau - i\mathbf{q}\cdot\mathbf{r}_{ij}}\langle s_i(\tau)s_j(0)\rangle$$

$$= \frac{1}{c_t T^{a_t} + c_h|h-h_c|^\gamma + (c_q q^2 + c_\omega \omega^2)^{a_q/2} + \Delta(\mathbf{q},\omega_n)}$$



$a_t = 2$ $\quad \gamma = 1$ $\quad a_q = 2$ $\quad \Delta(\mathbf{q},\omega_n) = c_{HM}\frac{|\omega_n|}{\sqrt{\omega_n^2 + (v_f q)^2}}$

$$a_q = 2 - \eta$$

$$\nu = \gamma/a_q$$

$$\chi(h=h_c, T=0, \mathbf{q}, \omega_n=0)^{-1} = c_q q^2$$

$$\chi(h=h_c, T=0, \mathbf{q}=0, \omega_n)^{-1} = c_{HM} + c_\omega \omega_n^2$$

$\eta = 0$	$\nu = 0.5$	$\gamma = 1$	$z = 3$	Hertz-Millis-Moriya
$\eta = 0.04$	$\nu = 0.63$	$\gamma = 1.24$	$z = 1$	(2+1)d Ising model
$\eta = 0.15(3)$	$\nu = 0.64(3)$	$\gamma = 1.18(4)$		Our model

FM-QCP

$$\chi(h,T,\mathbf{q},i\omega_n) = \frac{1}{L^2}\sum_{ij}\int_0^{\beta} d\tau e^{i\omega_n\tau - i\mathbf{q}\cdot\mathbf{r}_{ij}}\langle s_i(\tau)s_j(0)\rangle$$

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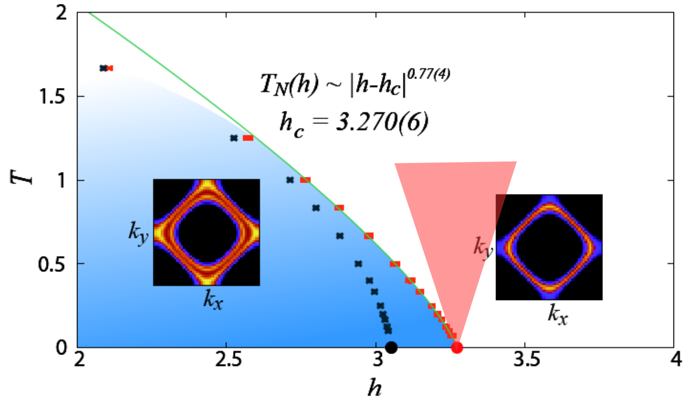
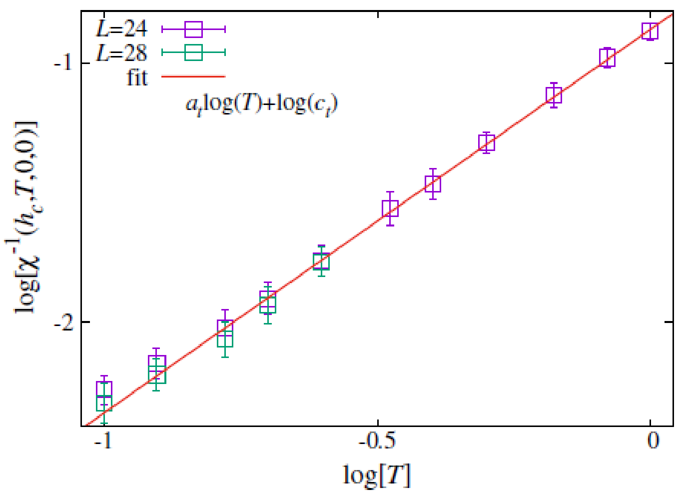
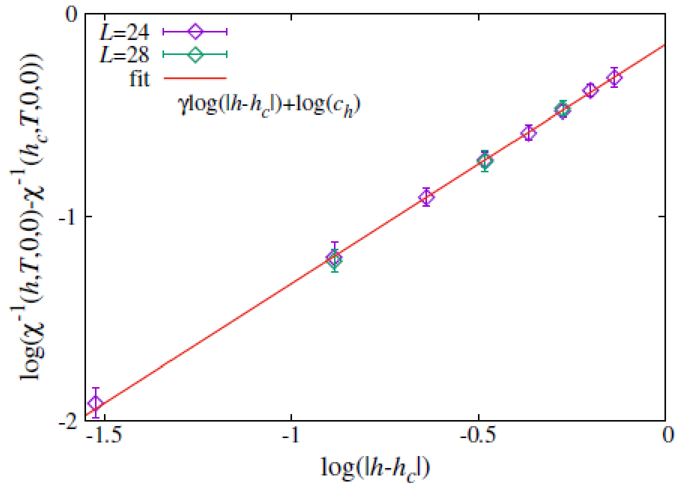


$$\chi(h_c,T,\mathbf{q}=0,\omega=0) = \frac{1}{c_t T^{a_t}}$$

$$\chi(h,T=0,\mathbf{q}=0,\omega=0) = \frac{1}{c_h|h-h_c|^{\gamma}}$$



$a_t = 1.48(4)$



$\gamma = 1.18(4)$

$\eta = 0$	$\nu = 0.5$	$\gamma = 1$	$z = 3$	Hertz-Millis-Moriya
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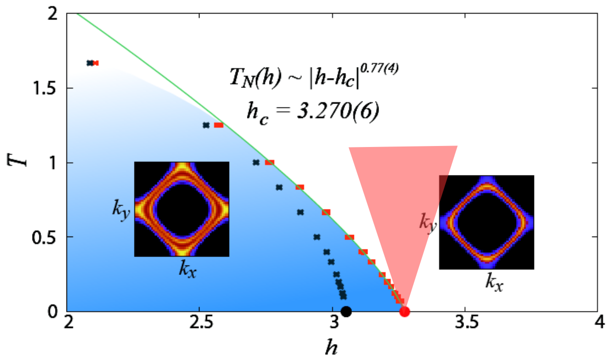
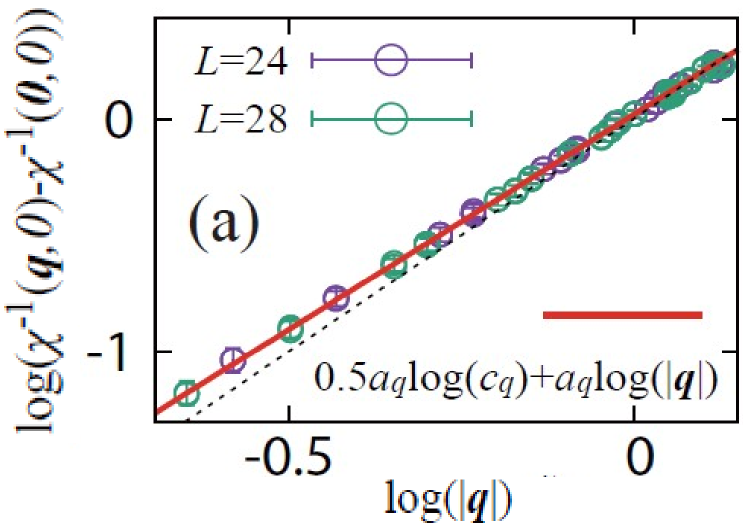


$$\chi(h=h_c,T=0,\mathbf{q},\omega=0)=\frac{1}{c_q^{a_q/2}|\mathbf{q}|^{a_q}}$$

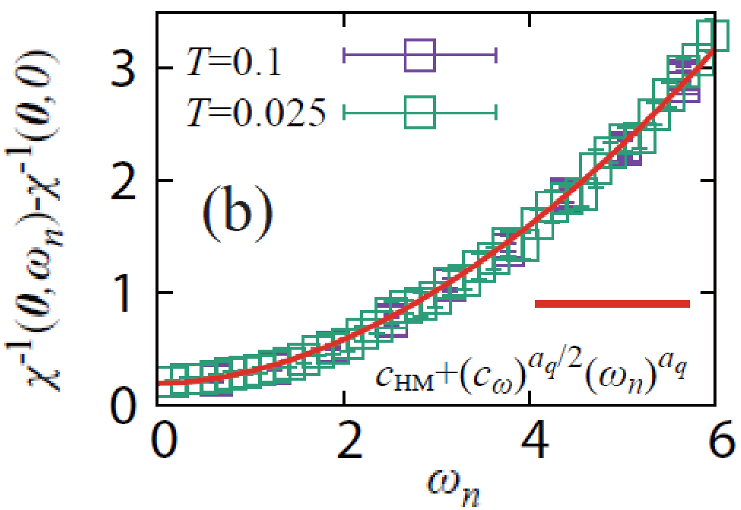
$$\chi(h=h_c,T=0,\mathbf{q}=0,\omega)=\frac{1}{c_\omega^{a_q/2}(\omega_n)^{a_q}+c_{HM}}$$



$$a_q = 2-\eta$$

$$a_q = 1.85(3)$$

$$\nu=\gamma/a_q$$



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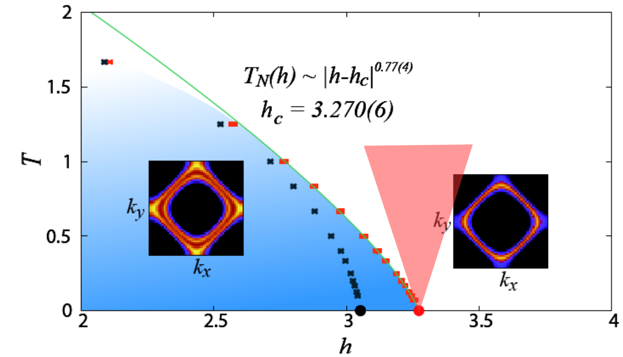

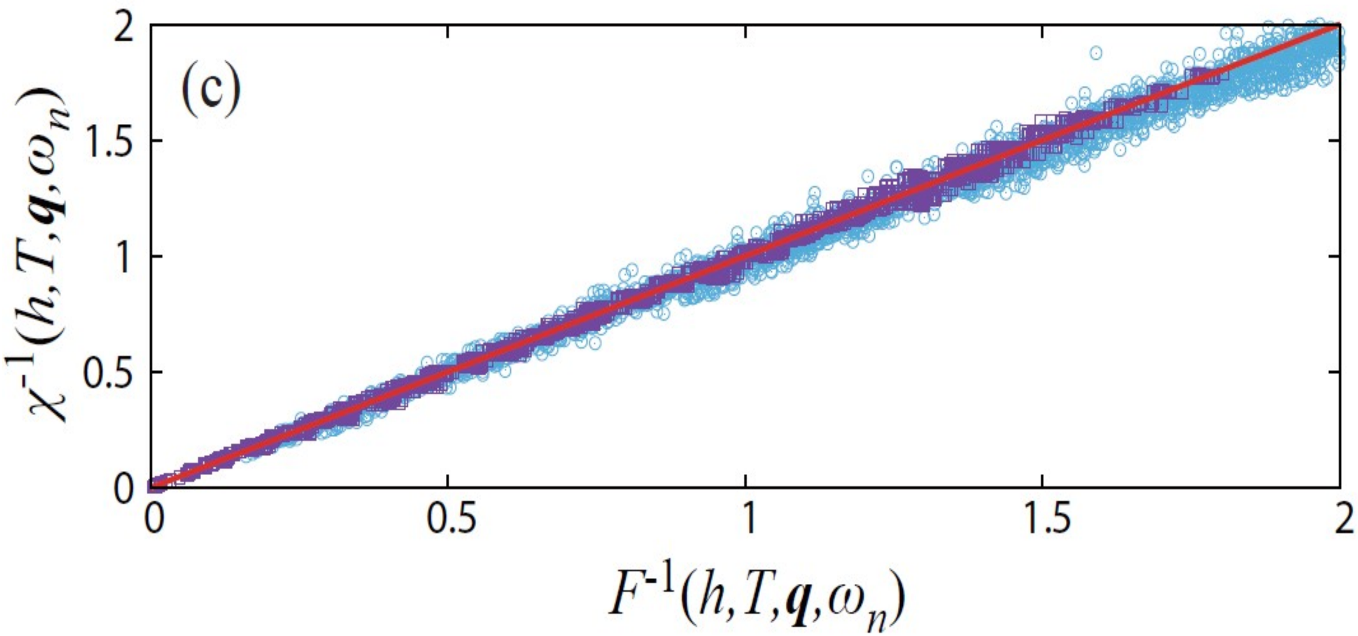

dark blue square:
3946 points in total

light blue circle:
6069 points in total

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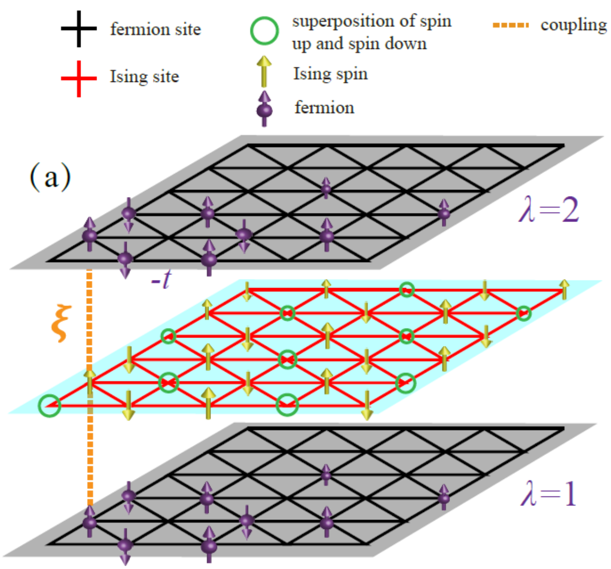
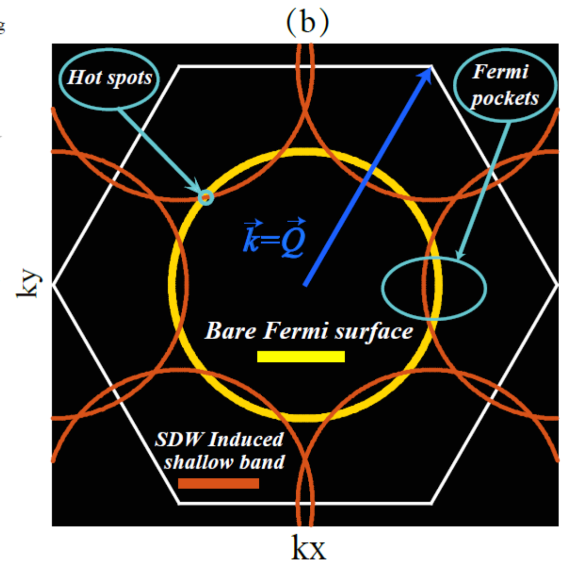
$\eta = 0.15(3)$	$\nu = 0.64(3)$	$\gamma = 1.18(4)$		Our model

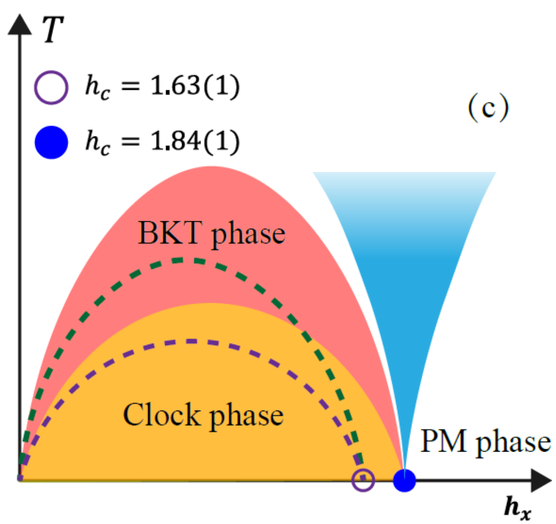
Triangle lattice

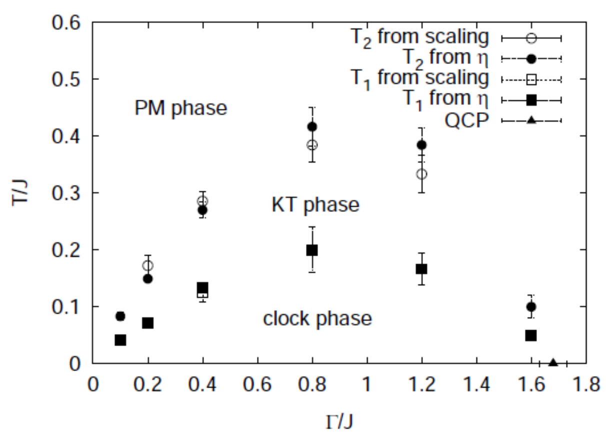
Zi Hong Liu



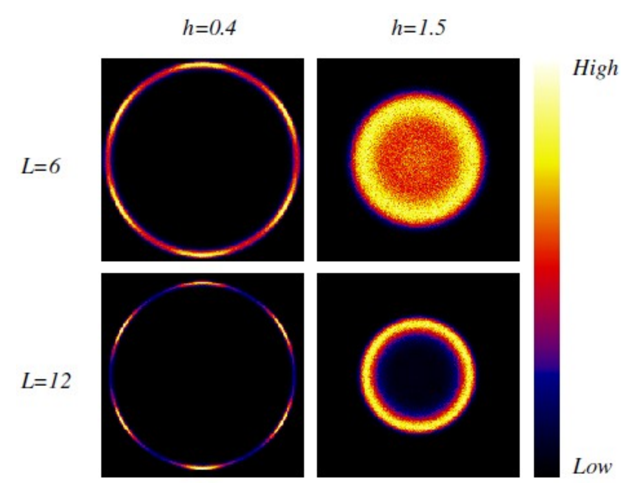


- arXiv:1707.10004





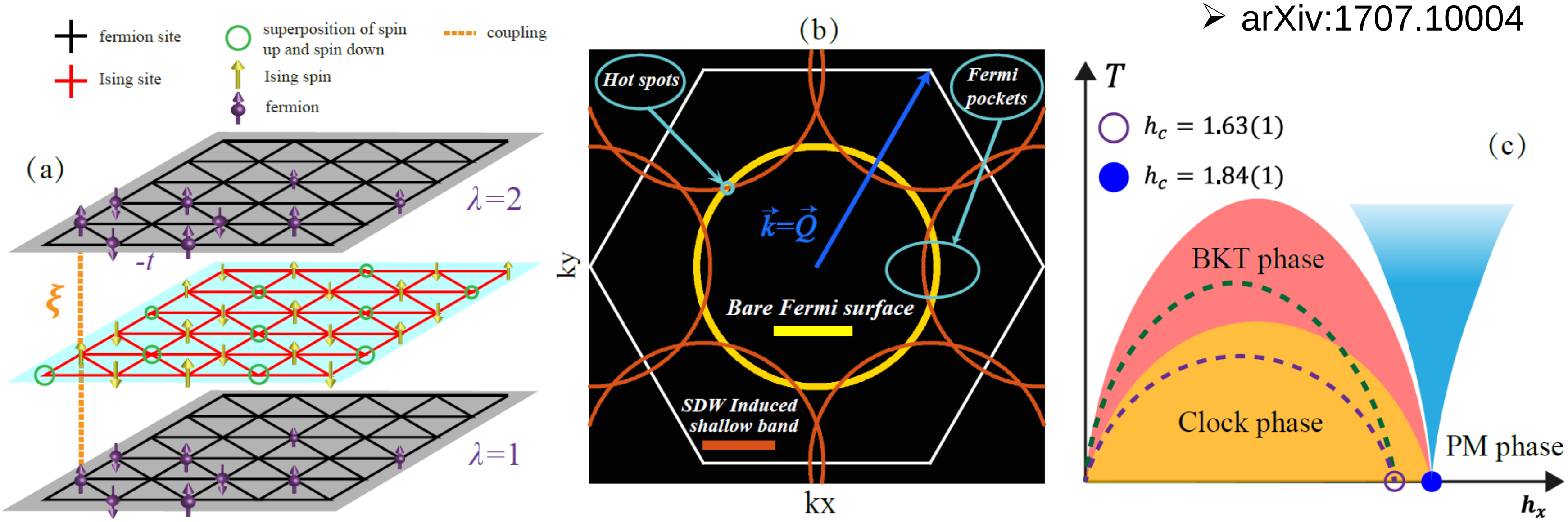
S. V. Isakov and R. Moessner, PRB 68, 104409 (2003)



Y.-C. Wang, Y. Qi, S. Chen, Z. Y. Meng, arXiv:1602.02839

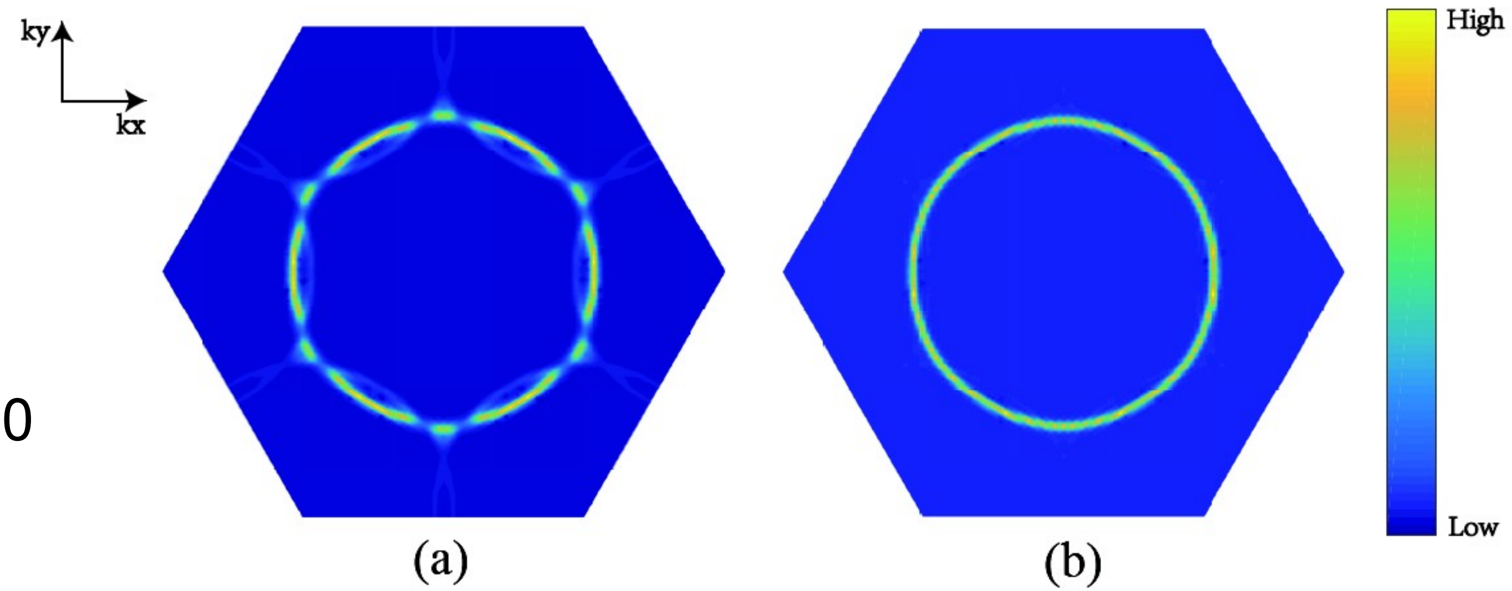
Triangle lattice

Zi Hong Liu

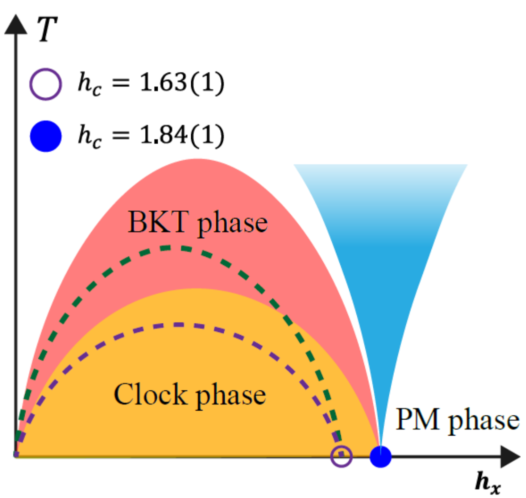


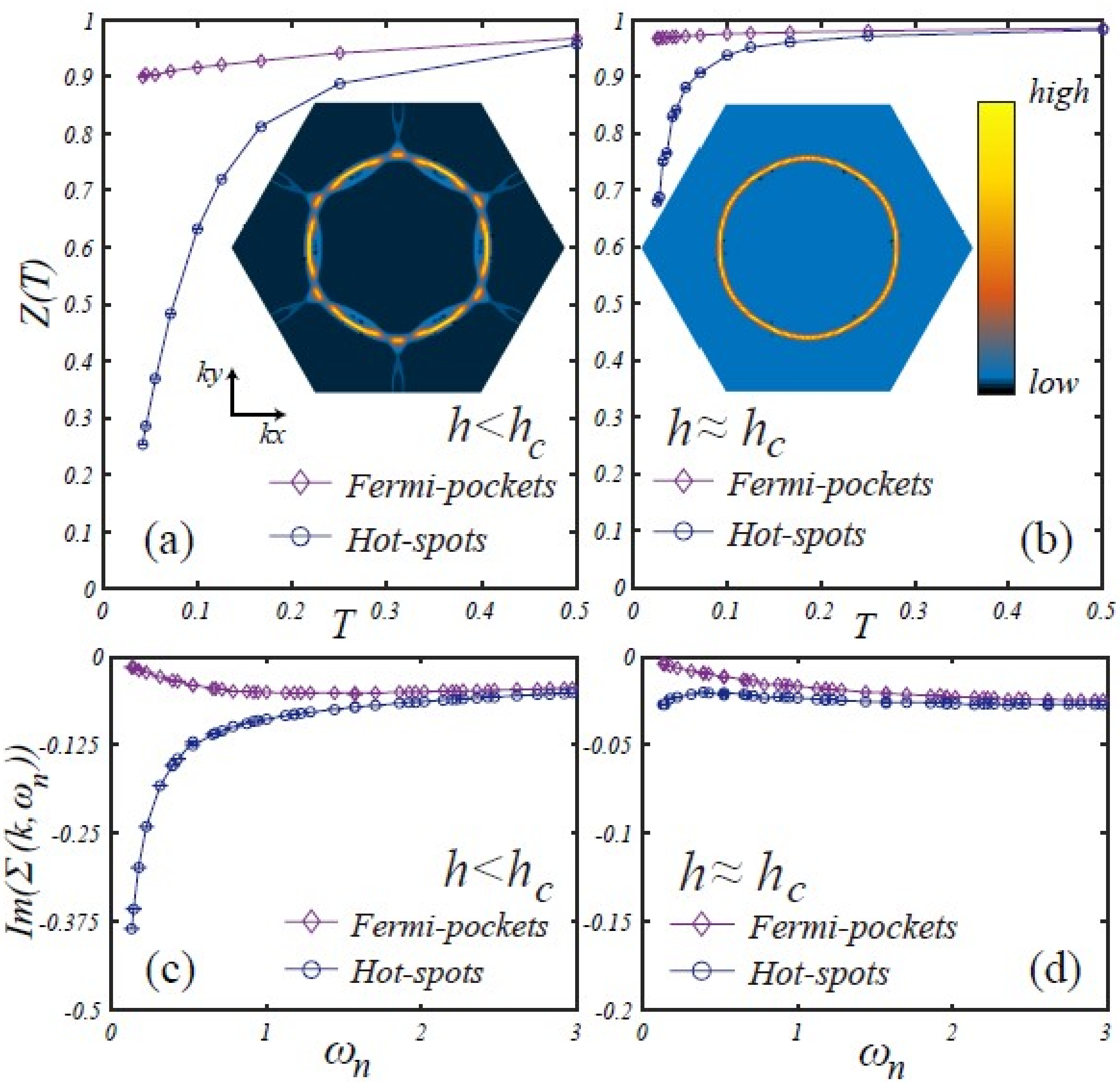
- arXiv:1707.10004

L=30, beta=30
(30x30x600)



Triangle lattice

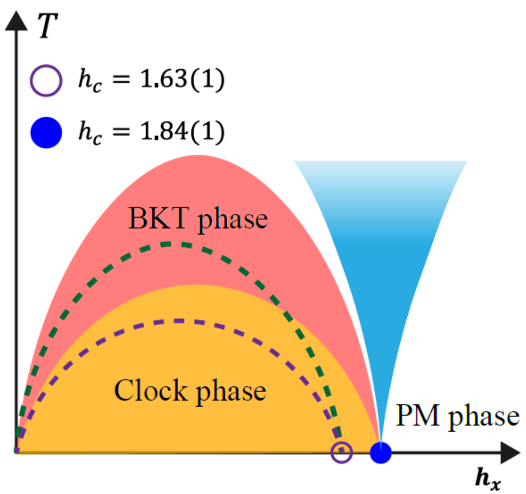


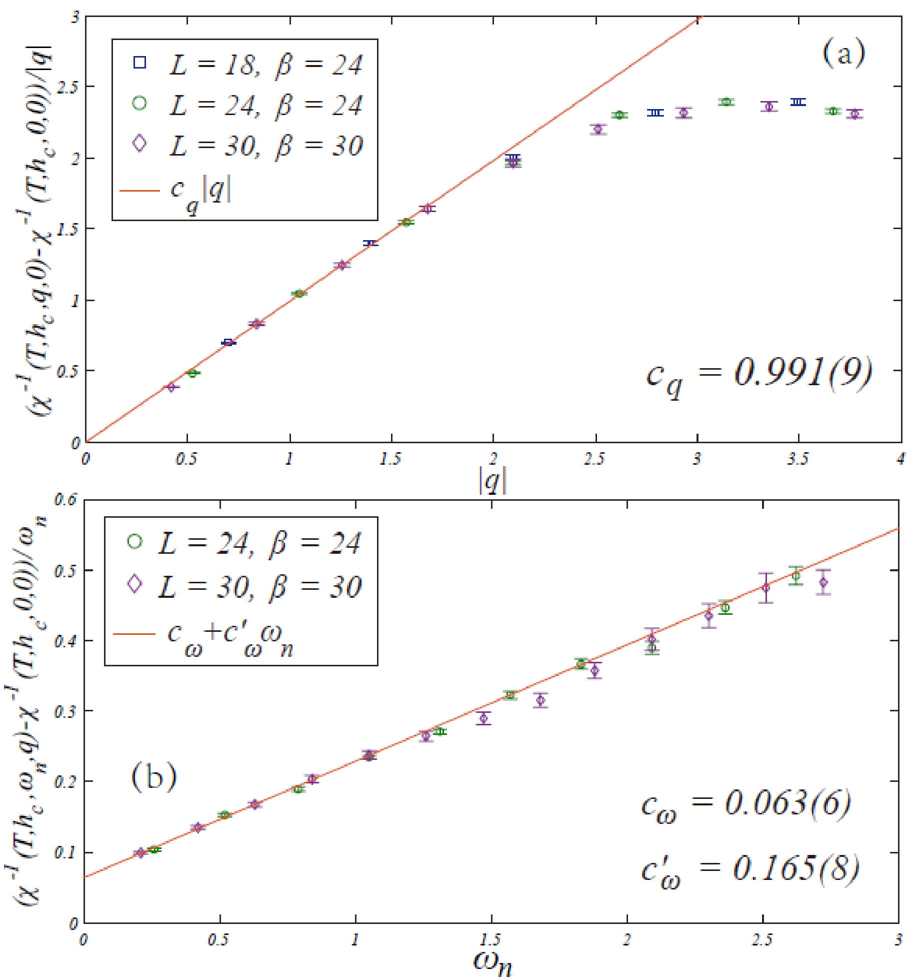


L=30, beta=30
(30x30x600)

AFM-QCP

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





L=30, beta=30
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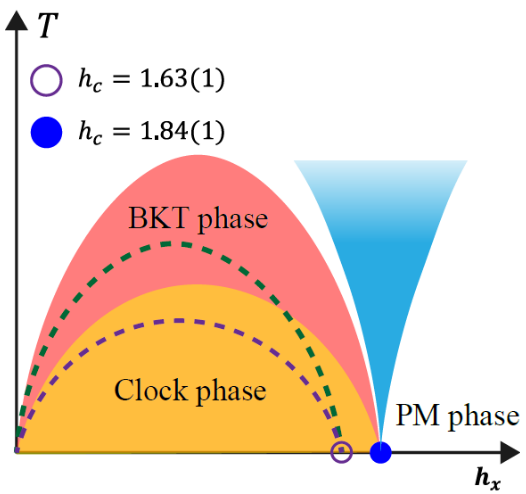
AFM-QCP

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



L=30, beta=30
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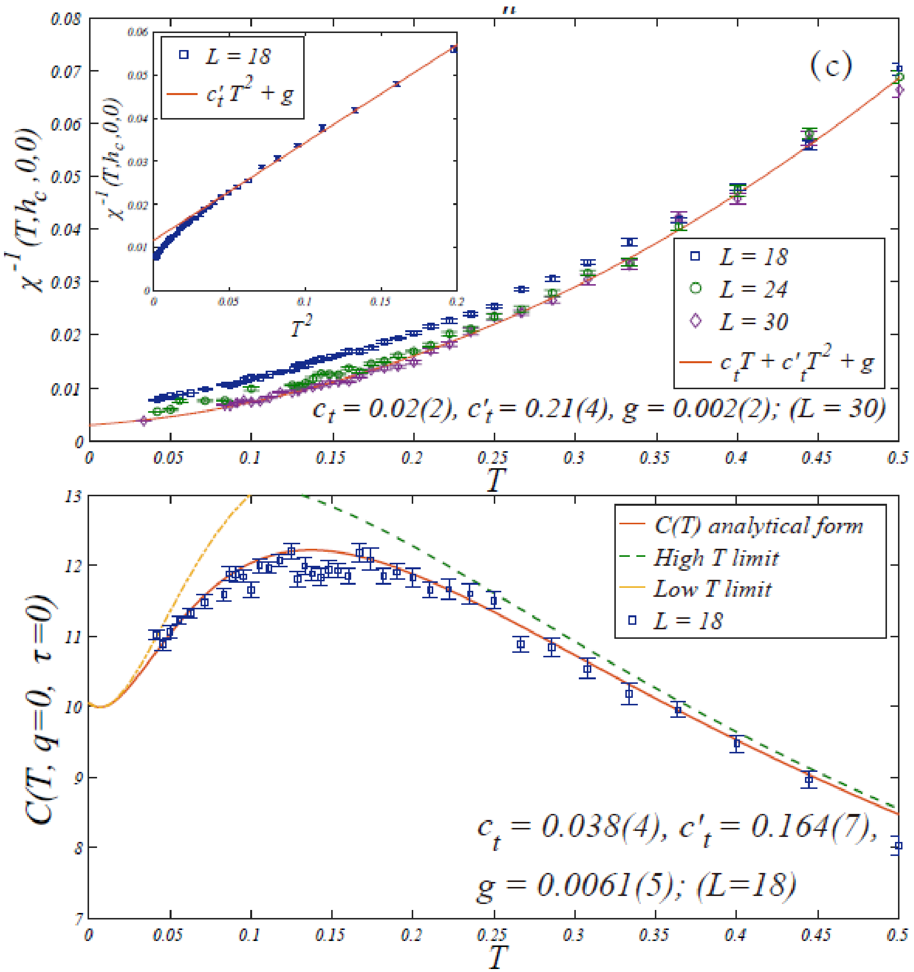
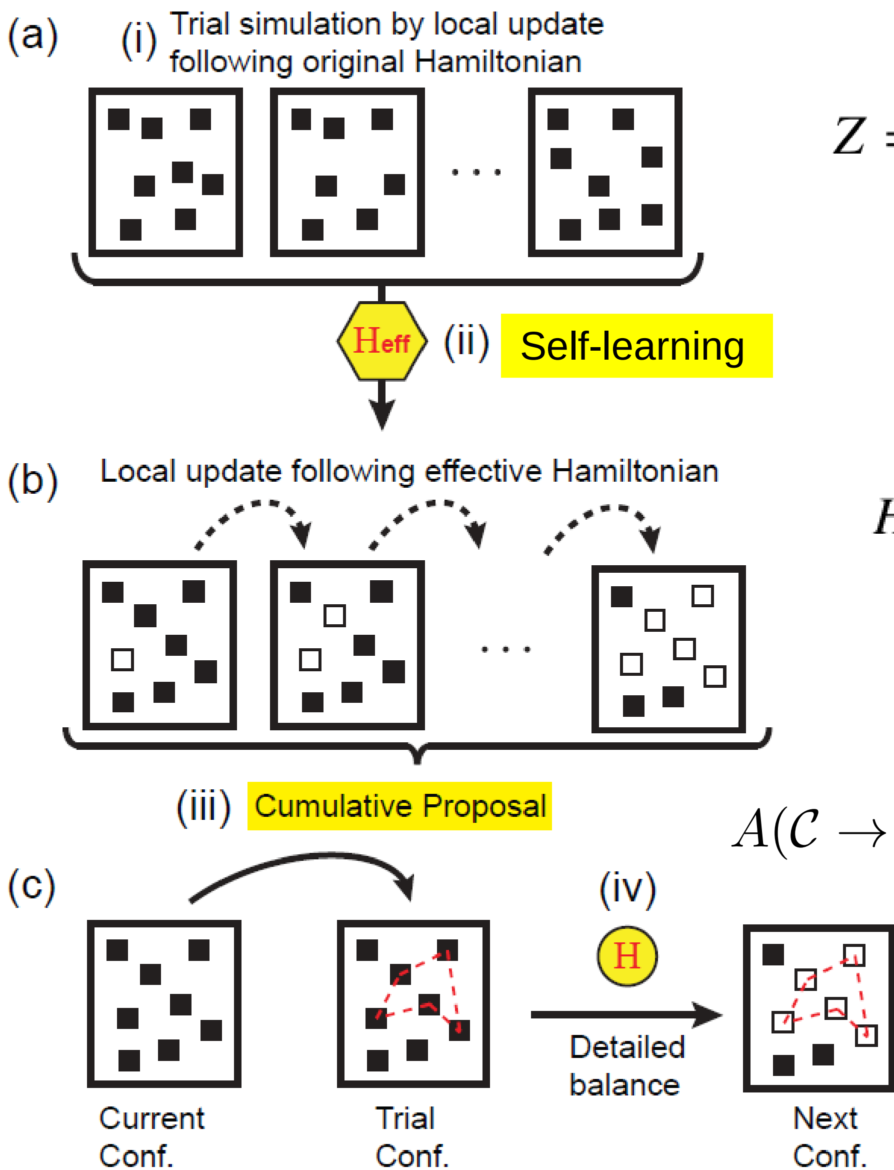


A Trio of Self-learning Monte Carlo Method

- Xiao Yan Xu, Zi Hong Liu, IOP, CAS
- Huitao Shen, Jiuwei Liu, Liang Fu, MIT
- Yang Qi, Fudan University

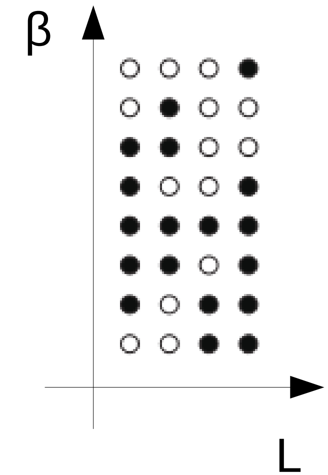
- Self-Learning Monte Carlo Method,
  PRB 95. 041101(R) (2017)
- Self-learning Monte Carlo method and cumulative update in fermion systems,
  PRB 95, 241104(R) (2017)
- Self-learning quantum Monte Carlo method in interacting fermion systems,
  PRB 96, 041119(R) (2017)

Self-learning Monte Carlo (SLMC)



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

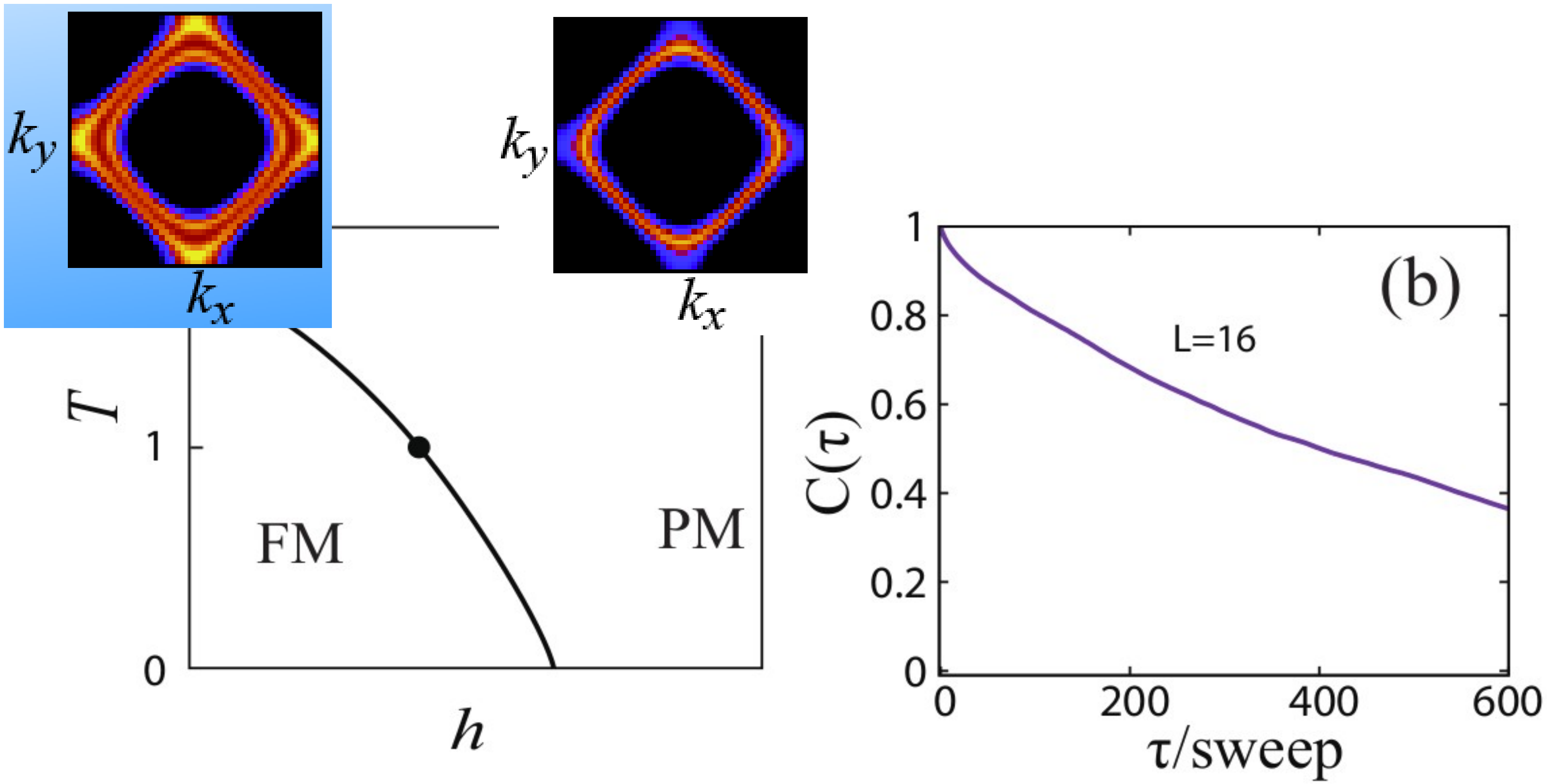
$$-\beta H^{\mathrm{eff}}[C] = \ln\left(\omega[C]\right)$$



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

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

Testing case



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

Testing case

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

Complexity for SLMC

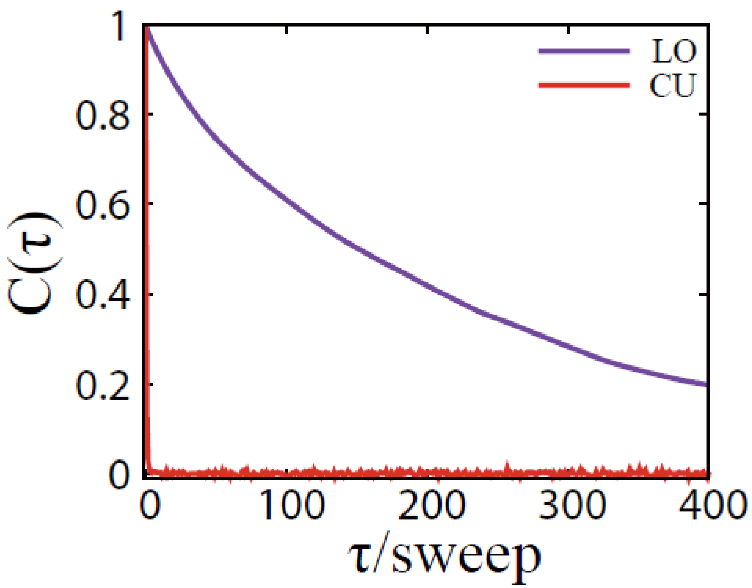
- Cumulative update: $\gamma \beta N \tau_L$
- Detail balance: N^3

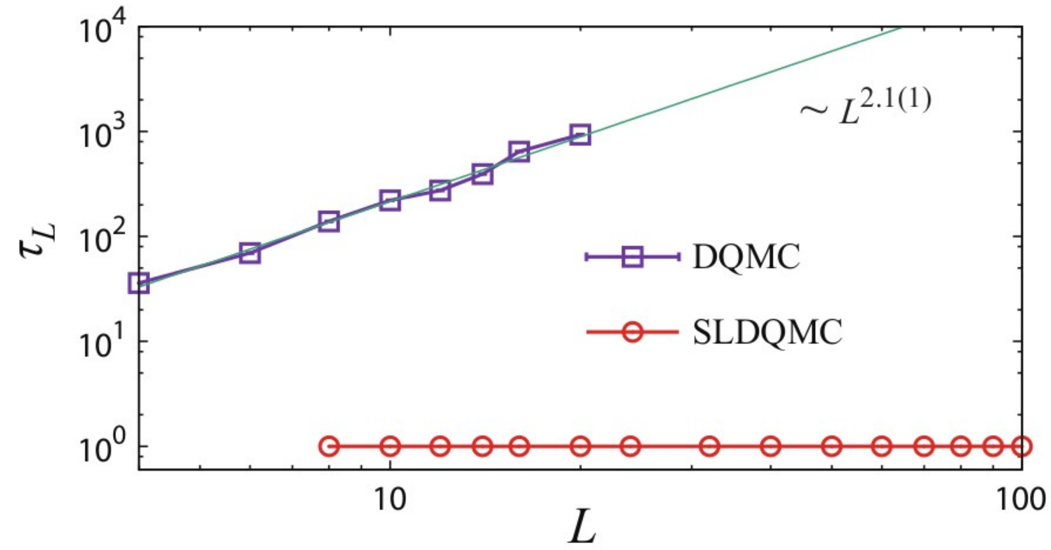
$$\begin{aligned} \omega_{\mathcal{C}} &= \phi(\mathcal{C}) \det \left(\mathbf{1} + \mathbf{B}(\beta,\tau)\mathbf{B}(\tau,0)\right) \\ &= \phi(\mathcal{C}) \det \left(\mathbf{G}(0,0)\right)^{-1} \end{aligned}$$

- Sweep Green's function: βN^2

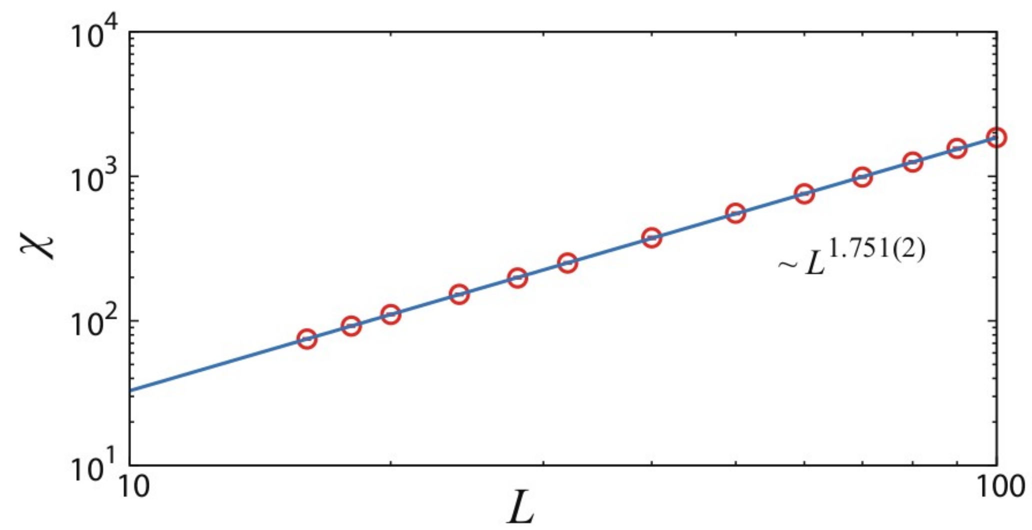
Complexity speed up $\mathcal{S} = \min(\frac{N^2}{\gamma}, \beta\tau_L, N\tau_L)$

Testing case





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



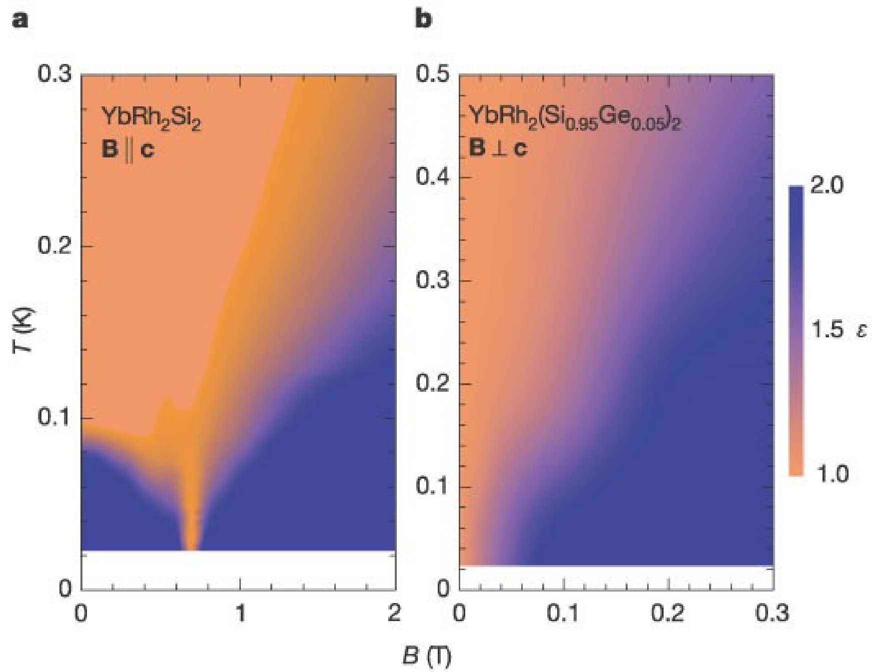
Outlook

- Possible directions:

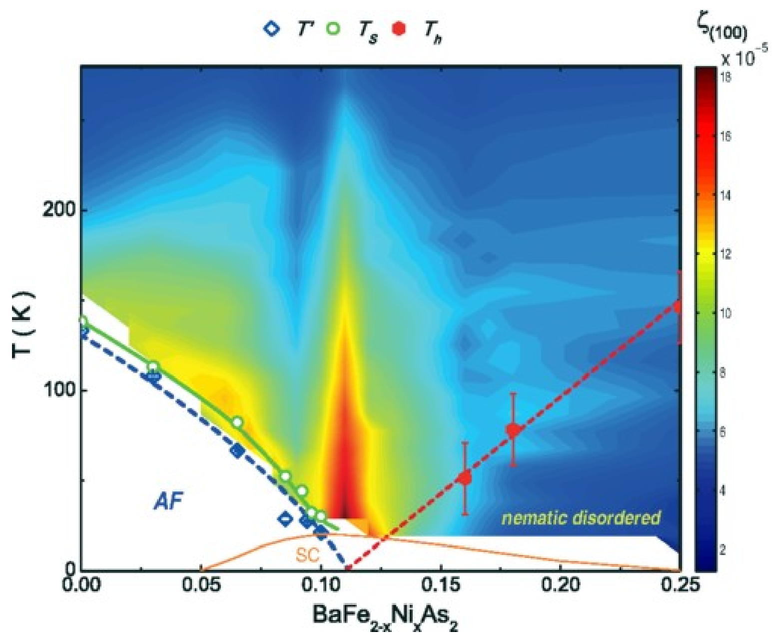
Other lattices, FM / AFM / Nematic fluctuations of itinerant electron systems

Non-Fermi liquid, fluctuation induced superconductivity

Beyond Hertz-Millis-Moriya mean-field theory, itinerant QCP



Nature 424, 524-527 (2003)



Phys. Rev. Lett. 117, 157002 (2016)