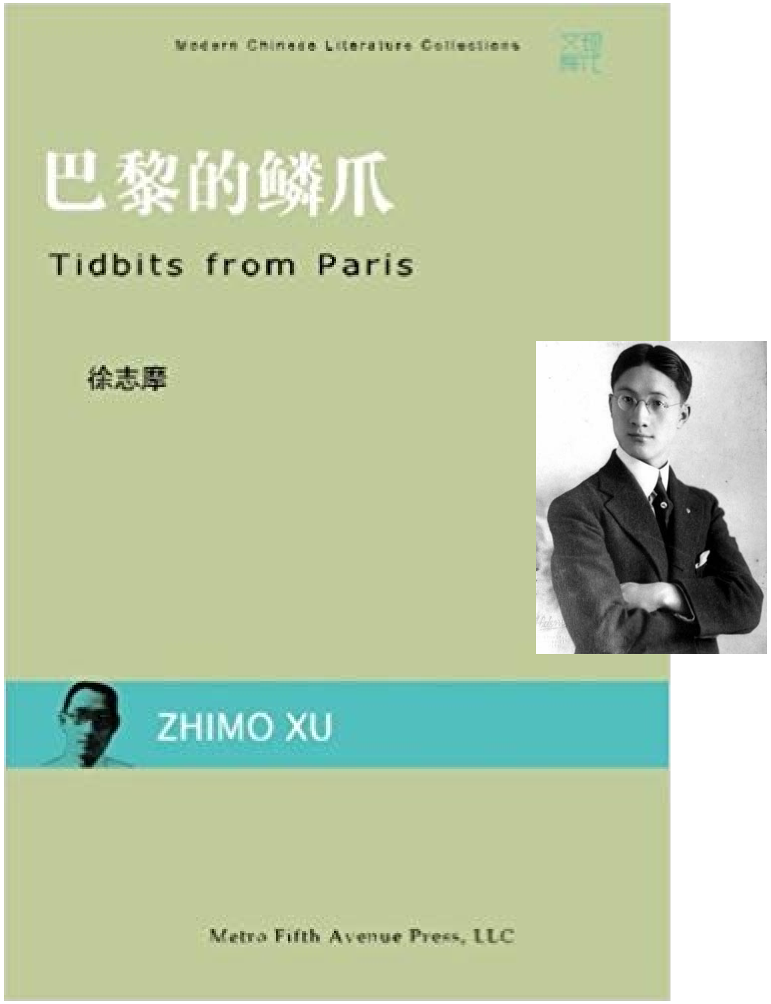
Introduction to fermionic quantum Monte Carlo Simulations

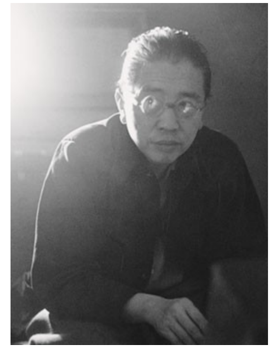
蒙特卡洛的鳞爪

Zi Yang Meng
孟　子　杨

Zhimo Xu (1897 – 1931) Poet, essayist



Chang Yu (1901 – 1966) Chinese-French painter



Fengmian Lin (1900 – 1991) Chinese painter

Monte Carlo

Casino de Monte-Carlo, Since 1858

清 · 同治二年

(Late Qing dynasty

2nd year of emperor Tongzhi)

Monte Carlo

- Widely used in statistical and quantum many-body physics
- Unbiased: statistical error $1/\sqrt{N}$

Calculation of Pi

https://en.wikipedia.org/wiki/Monte_Carlo_method#/media/File:Pi_30K.gif

- ➢ Optimization
- ➢ Numerical integration
- ➢ Generate probability distributions

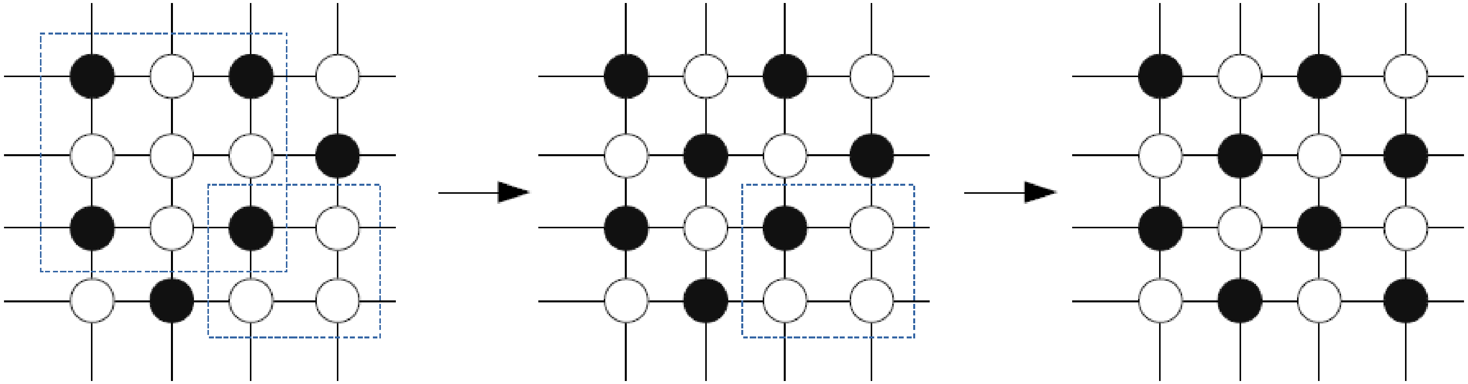
- Central limit theorem $((\frac{1}{N}\sum_{1}^{N} X_i) - \mu) \rightarrow \frac{1}{\sqrt{N}} N(0, \sigma^2)$

Monte Carlo – Ising Model

$$Z = \sum_{\mathcal{C}} e^{-\beta H[\mathcal{C}]} = \sum_{\mathcal{C}} W(\mathcal{C})$$

- Markov chain Monte Carlo is a way to do important sampling

$$\cdots \to \mathcal{C}_{i-1} \to \mathcal{C}_i \to \mathcal{C}_{i+1} \to \cdots$$



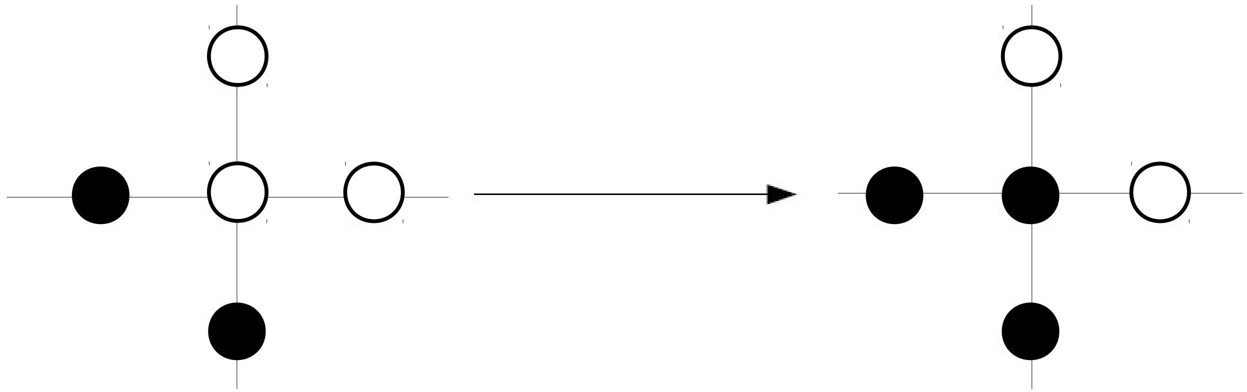
- Metropolis – Hastings

$$p(\mathcal{C} \to \mathcal{D}) = q(\mathcal{C} \to \mathcal{D})\alpha(\mathcal{C} \to \mathcal{D})$$

$$\frac{p(\mathcal{C} \to \mathcal{D})}{p(\mathcal{D} \to \mathcal{C})} = \frac{W(\mathcal{D})}{W(\mathcal{C})} \qquad \alpha(\mathcal{C} \to \mathcal{D}) = \min\{1, \frac{W(\mathcal{D})q(\mathcal{D} \to \mathcal{C})}{W(\mathcal{C})q(\mathcal{C} \to \mathcal{D})}\}$$

- N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953)
- W. H. Hastings, Biometrika **57**, 97 (1970)

Metropolis – Hastings: local



- Local update $q(\mathcal{C} \to \mathcal{D}) = q(\mathcal{D} \to \mathcal{C}) = \frac{1}{N}$
- Acceptance ratio $\alpha(\mathcal{C} \to \mathcal{D}) = \min\{1, \frac{W(\mathcal{D})}{W(\mathcal{C})}\}$

$$\frac{W(\mathcal{D})}{W(\mathcal{C})} = e^{-\beta(E(\mathcal{D})-E(\mathcal{C}))} = e^{-\beta([-1-1+1+1]-[1+1-1-1])} = 1$$

➢ N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953)

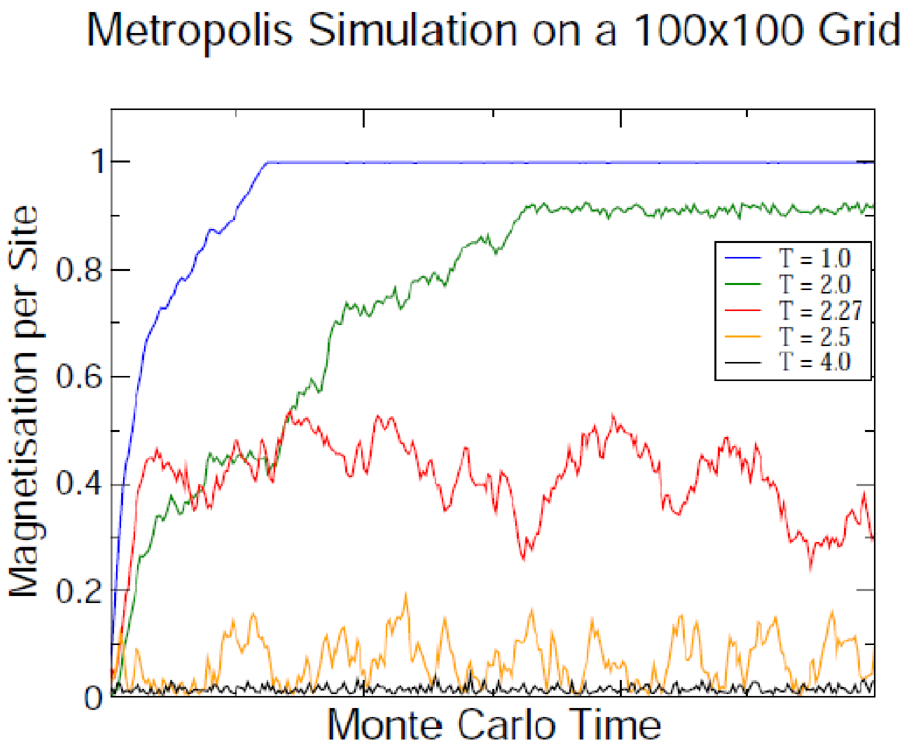
2D Ising simulation

https://mattbierbaum.github.io/ising.js/

Metropolis – Hastings: critical slowing down

- Dynamical relaxation time diverges at the critical point: critical system is slow to equilibrate.

- For 2D Ising model $\tau \propto L^z, z = 2.125$



Metropolis – Hastings: autocorrelation

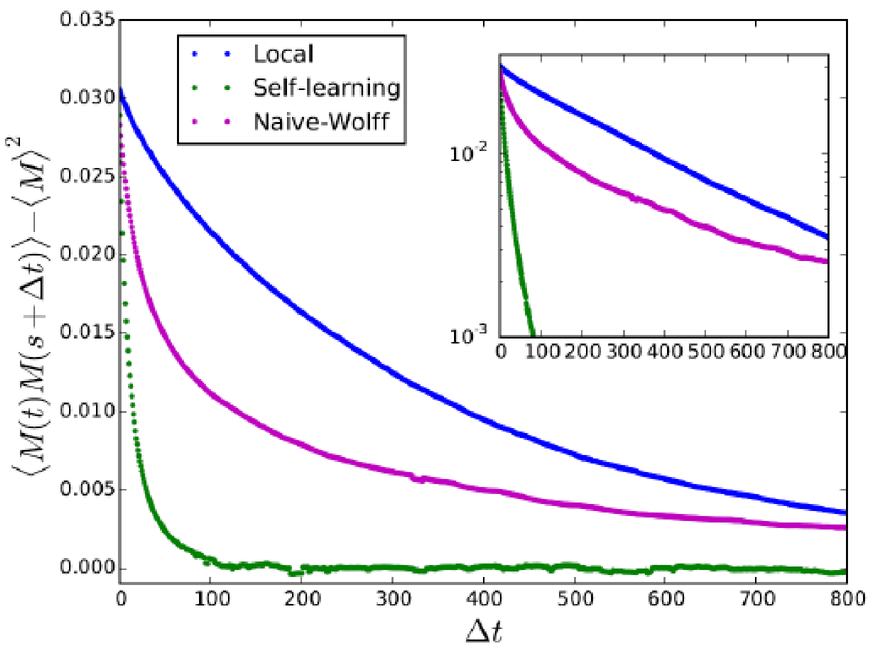
- Markov process, Monte Carlo time sequence

$$\cdots \to O(t-1) \to O(t) \to O(t+1) \to \cdots$$

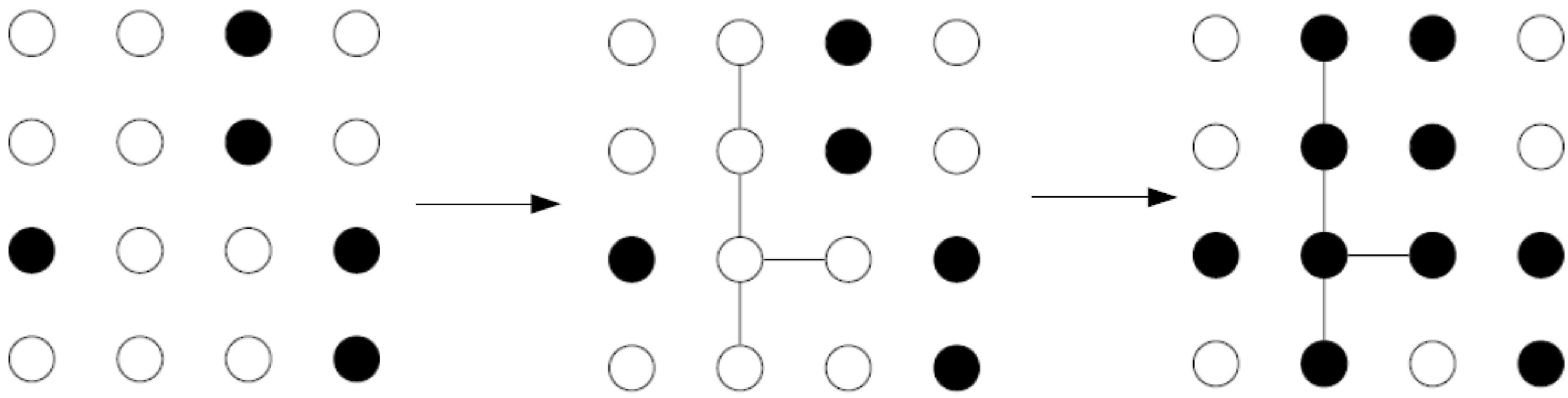
$$O(t) = O[\mathcal{C}(t)]$$

- Autocorrelation function

$$A_O(\Delta t) = \langle O(t) O(t+\Delta t) \rangle - \langle O(t) \rangle^2 \propto e^{-\Delta t/\tau}$$



Metropolis – Hastings: cluster



- A cluster is built from bonds
- Probability of activating a bond is cleverly designed

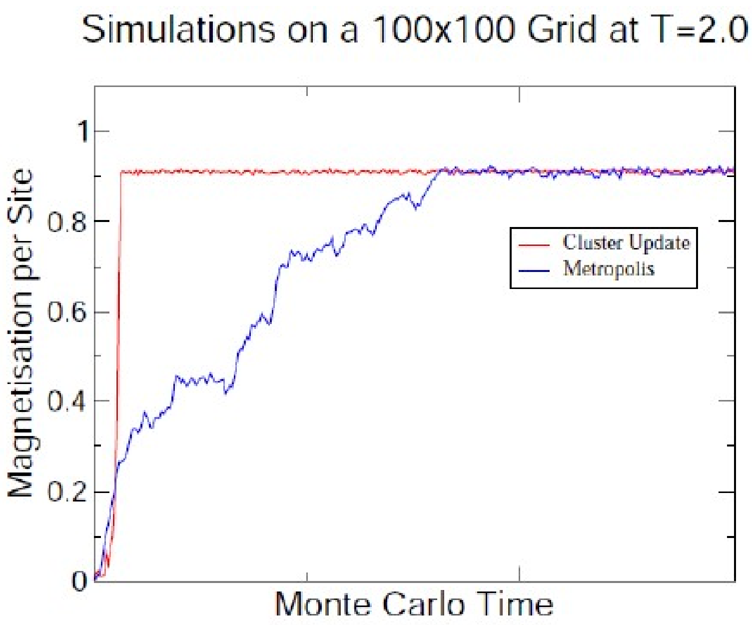
$$q(i \to j) = 1 - e^{\min\{0, -2\beta S_i S_j\}}$$

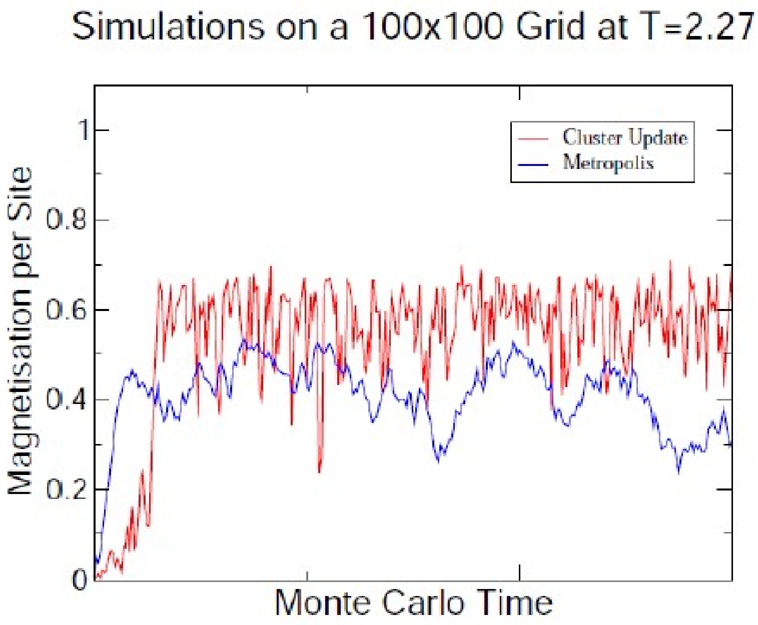
$$\frac{q(\mathcal{A} \to \mathcal{B})}{q(\mathcal{B} \to \mathcal{A})} = \prod_{\langle i,j \rangle, i \in c, j \notin c} \frac{1 - q(i \to j)_{\mathcal{A}}}{1 - q(i \to j)_{\mathcal{B}}} = \prod_{\langle i,j \rangle, i \in c, j \notin c} e^{-2\beta(S_i^{\mathcal{A}} S_j^{\mathcal{A}} - S_i^{\mathcal{B}} S_j^{\mathcal{B}})} = \frac{W(\mathcal{B})}{W(\mathcal{A})}$$

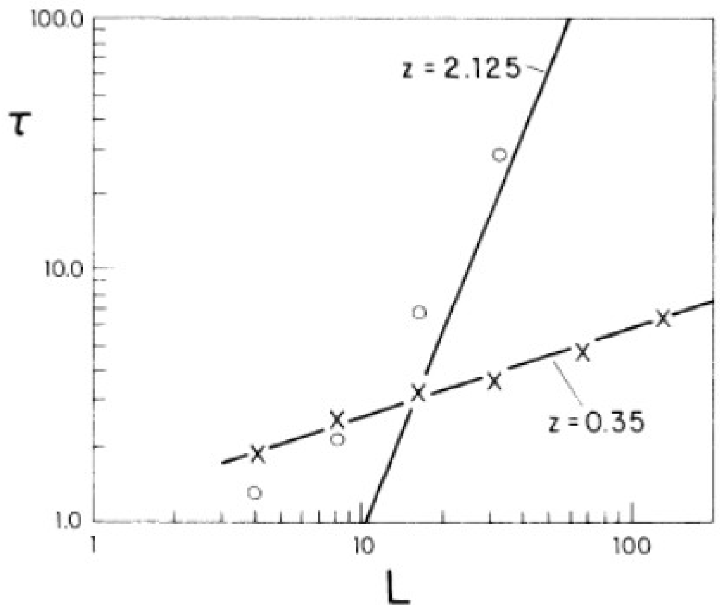
- an ideal acceptance ratio $\alpha(\mathcal{A} \to \mathcal{B}) = 1$

➢ U. Wolff, Phys. Rev. Lett. **62**, 361 (1989)

Metropolis – Hastings: cluster







- Swendsen and Wang, Phys. Rev. Lett. **58**, 86 (1987)

Metropolis – Hastings: Self-learning

爱上物理 改变世界

“认识你自己”——自学习蒙特卡洛三部曲

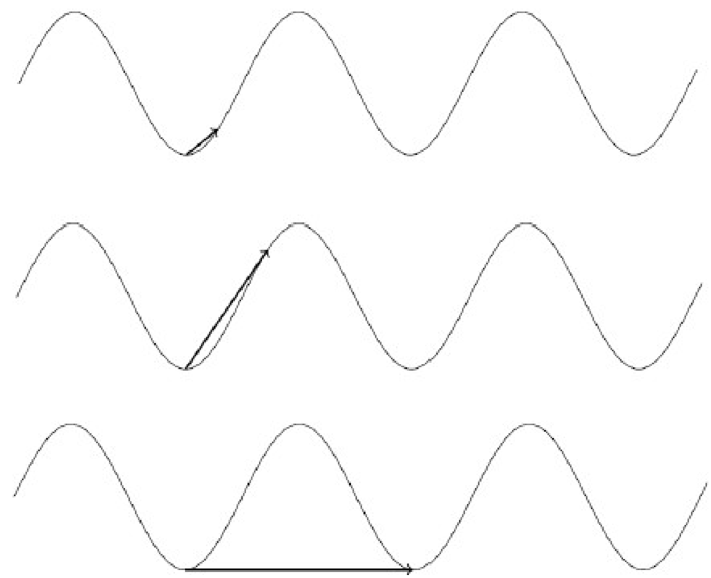
在这篇文章中，笔者只希望讲述我们最近发展的自学习蒙特卡洛方法三部曲，讲述我们如何通过自我观照、自我学习蒙特卡洛构型，设计出自学习蒙特卡洛方法，解决了凝聚态量子多体系统蒙特卡洛模拟中一些诸如临界慢化和接收概率低等瓶颈性的问题，推动领域的发展。

2016-12-22

"Know thyself"

(Greek: γνῶθι σεαυτόν)

Thales of Miletus (c. 62



"Know thyself" (Greek: γνῶθι σεαυτόν, gnothi seauton)

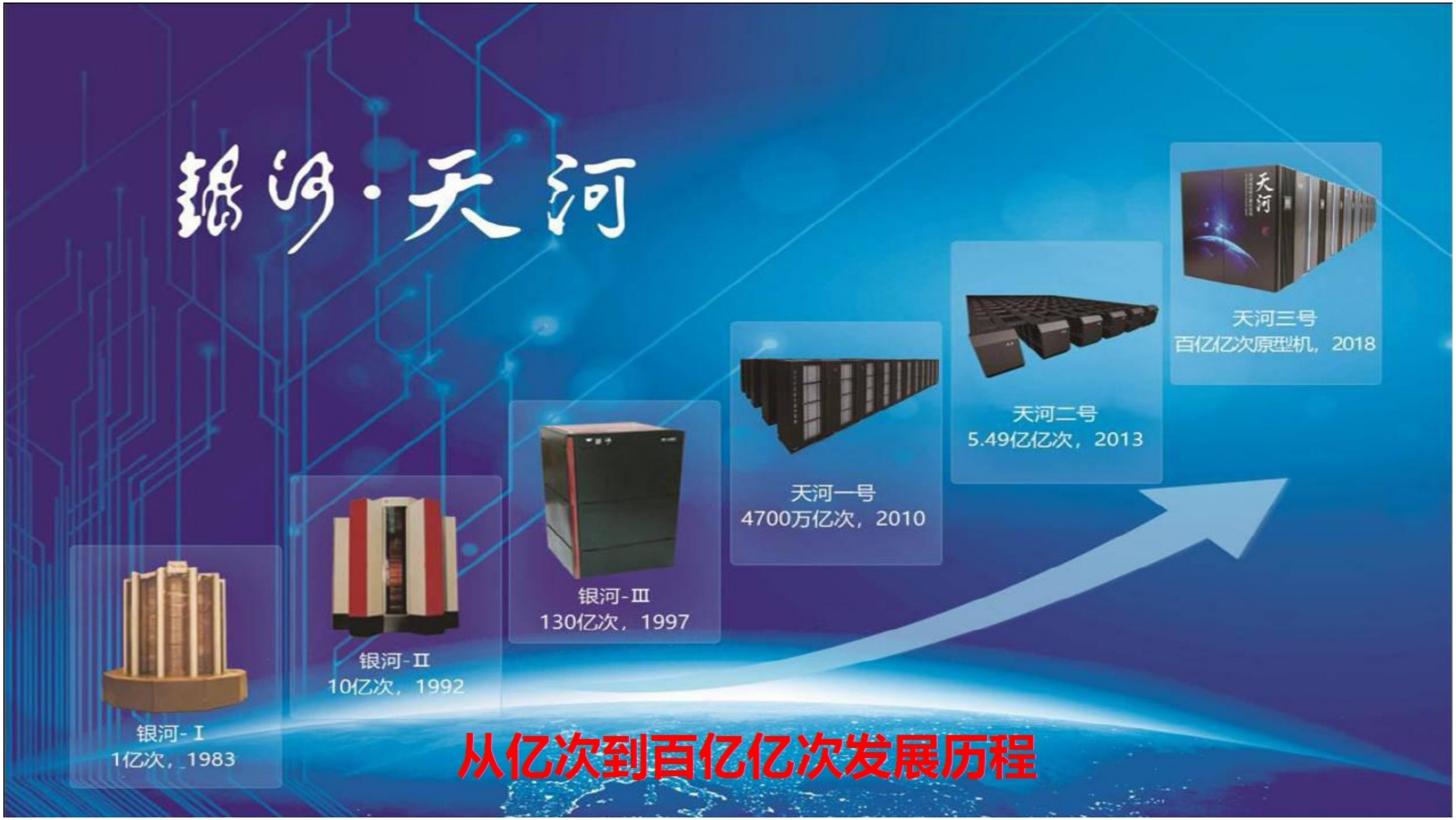
one of the Delphic maxims and was inscribed in the pronaos (forecourt) of the Temple of Apollo at Delphi

Xiao Yan Xu	IOP, HKUST, UCSD
Junwei Liu	IOP, MIT,HKUST
Qi Yang	MIT, Fudan
Liang Fu	MIT
Huitao Shen	MIT
Yuki Nagai	MIT, Japan Atomic Energy Agency, RIKEN

……

- PRB 95, 041101(R) (2017)
- PRB 95, 041101(R) (2017)
- PRB 96, 041119(R) (2017)
- PRL 122, 077601 (2019)

Computing facilities



1 GigaFLOPs: 10^9

5 PetaFLOPs: 10^15

50 PetaFLOPs: 10^15

1 ExaFLOPs: 10^18

NSCC 国家超级计算天津中心
National Supercomputer Center in Tianjin

国家超级计算广州中心
NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

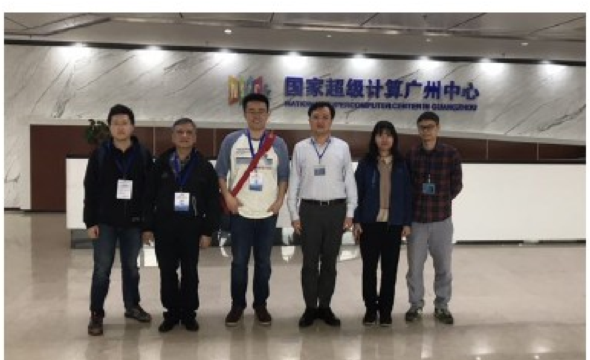
Computing facilities

国家超级计算天津中心
National Supercomputer Center in Tianjin

GigaFLOPS: 10^9
TeraFLOPS: 10^12
PetaFLOPS: 10^15
ExaFLOPS: 10^18

Tianhe-1: 5PetaFLOPS
K-computer: 10PetaFLOPS
Tianhe-2: 100PetaFLOPS
TaihuLight: 100PetaFLOPs
Tianhe-3: 1000PetaFLOPS

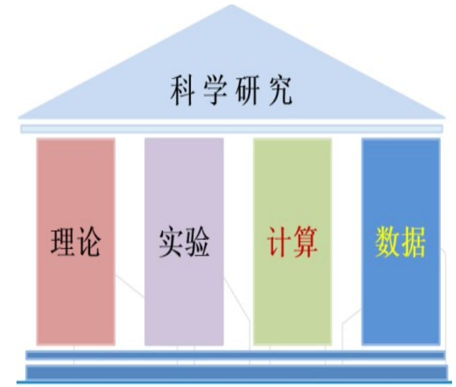
亿： 10^8
兆： 10^12
京： 10^16
垓： 10^20
…
恒河沙数： infty

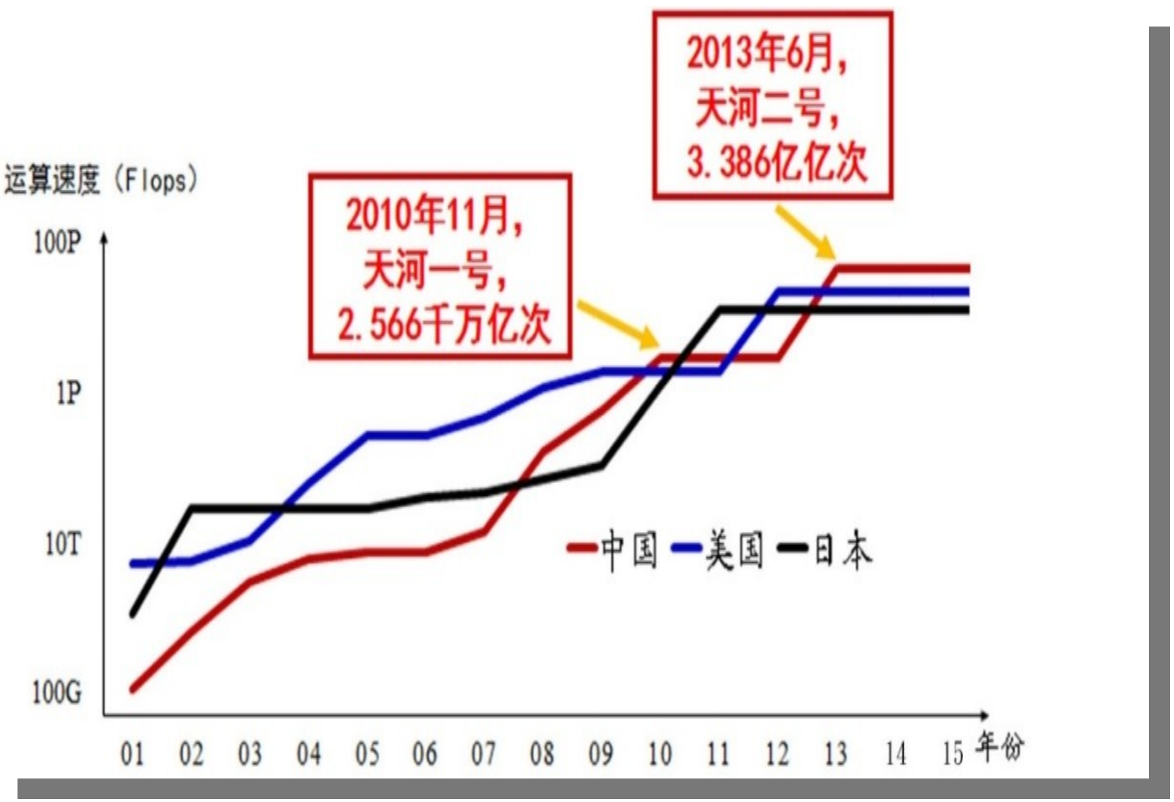


国家超级计算广州中心
NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

Computing facilities

- **超级计算机对科学发现、技术创新、产业革命的重要作用**
  - 高性能计算：是科学研究的三大手段之一
  - 大数据处理：正成为科学研究的第四范式
- **世界各国争相角逐超级计算机系统的主导地位**





世界超级计算机排行榜 Top500“ 六连冠”

2013.6~2016.6

国际共轭梯度 HPCG 排行榜“五连冠”

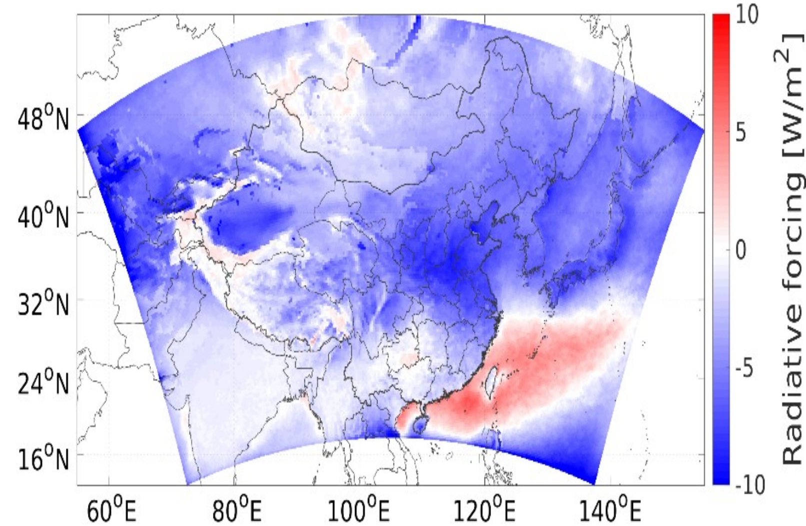
2014.6~2016.1

天河二号是 2017.11 全球唯一一台 TOP500 、 HPCG 两项权威排名均位列前三的系统，充分体现其平衡系统设计的优势

2、中心应用情况：大气海洋环境平台

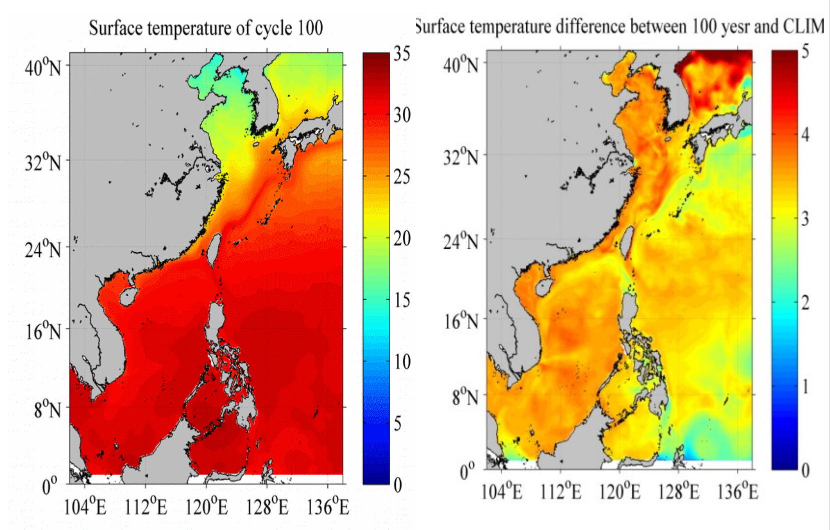
东亚区域气候模拟（香港应用）

- 建立了区域气候降尺度模拟系统
- 模拟并预测未来 50 年气候变化背景下东亚沙尘对区域气候的影响



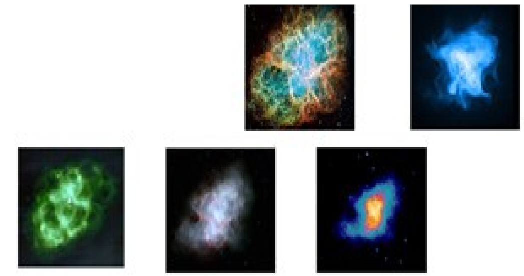
南海碳循环过程模拟（香港应用）

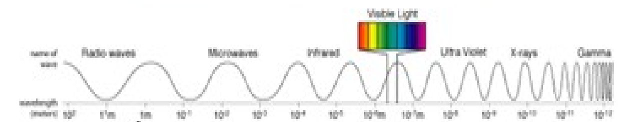
- 揭密南海三层逆向环流，及其相关的生态系统维持
- 通过物理 - 生物 - 化学三维耦合模拟系统分析南海碳循环
- 预测未来 100 年海水动力，生物生产力及海洋酸化趋势

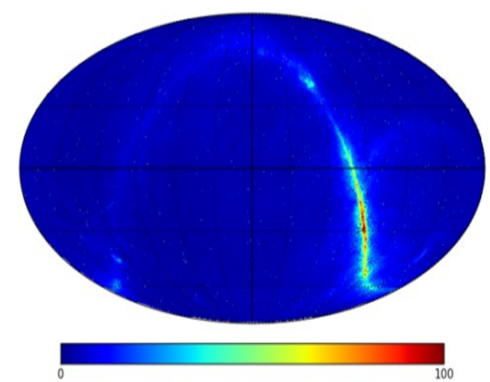


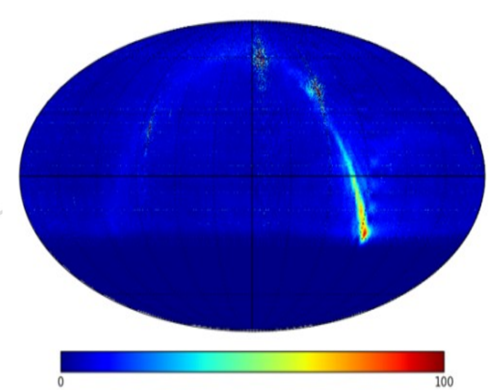
2、中心应用情况：天文地球物理平台

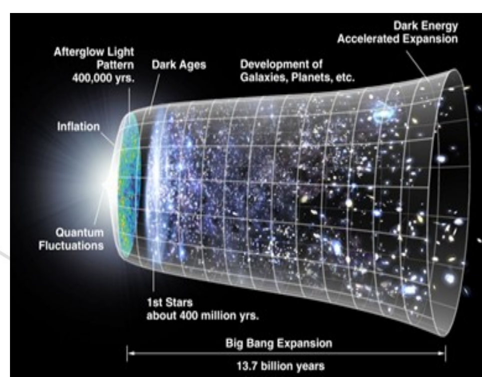
- **SKA（平方公里阵列射电望远镜）数据处理**
  – 国际首次部署、最大规模 SDP 数据处理框架、亚洲分中心
- **天籁计划和天琴计划的数据处理**
- **暗物质，暗能量，引力波研究**
- **高能物理、天体物理、星体研究，标准烛光测量**
- **地外生命寻找**



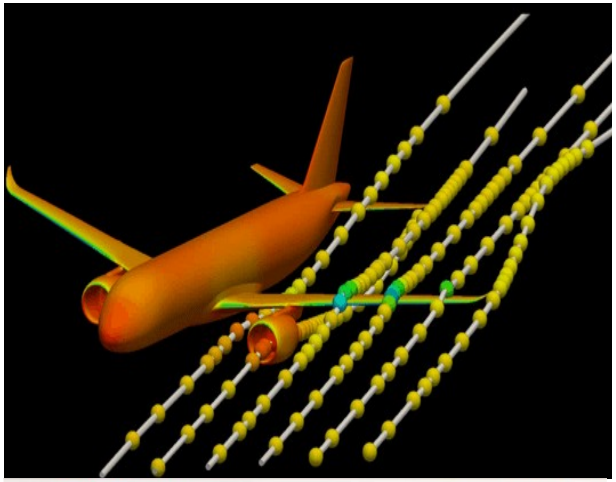








2、中心应用情况：大型工程与装备仿真平台



商飞全机气动参数优化设计

– 6 天完成过去 2 年的工作量

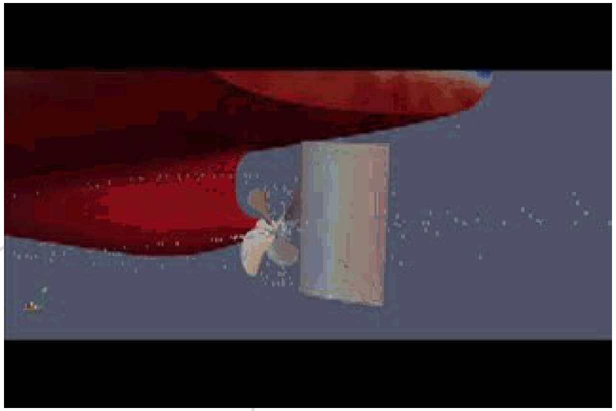
广汽集团车身侧面碰撞模拟

– 精度达到 85% 以上

广船国际船舶性能预估与设计

– 缩短设计周期，已完成 5 万吨油船、 7.5 万吨油船 、 8.2 万吨散货船、 11 万吨斜尾原油船航态性能预估与设计

– 精度超过 95% ，成本降低 9 成



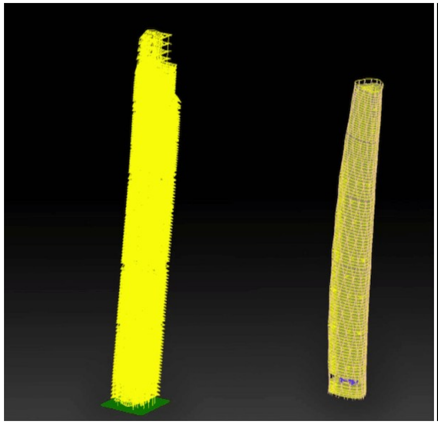
国产微电子元器件辅助设计

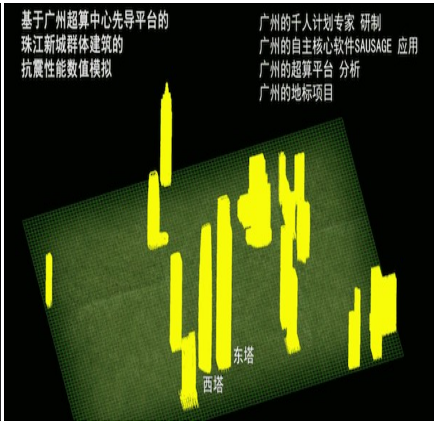
– 飞腾新一代处理器，电子器件，芯片设计

2、中心应用情况：大型工程与装备仿真平台

珠江新城高层群体抗震性能数值模拟

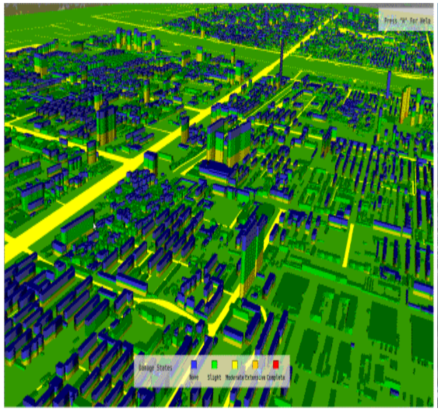
- **自主核心**软件 SAUSAGE；
- 与施工现场实际监测结果高度吻合
- 科学指导高楼结构施工，**防灾减灾**





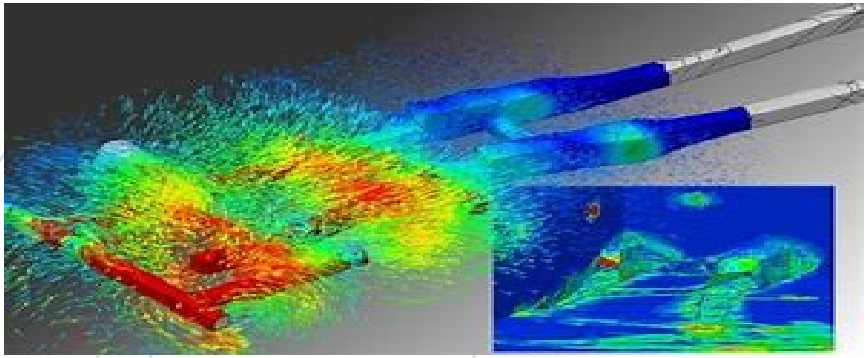
城市建筑群地震灾害模拟

- **百万数量级建筑群**弹塑性精细仿真时间缩短至 **10 分钟**以内
- 区域与城市地震灾害风险识别评估平台



岩土材料研究与应用

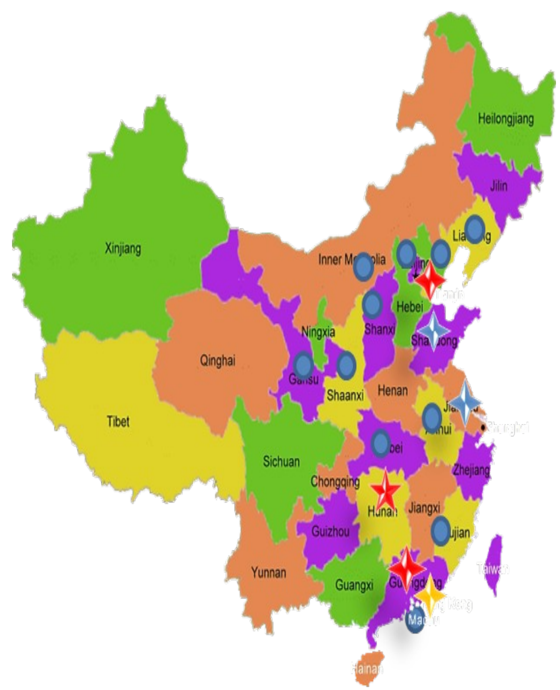
- 解决岩土材料随机场与有限元数值模拟的多尺度耦合问题，随机场与离散元的有效耦合难题
- 成果应用在**深圳地铁 8 号线**、**长沙地铁 4 号线**、**珠三角城际轨道**、**广州市金融城地下空间等大型工程项目中**



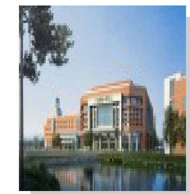
Computing facilities

银河天河系列超级计算机

国家级超算中心的分布

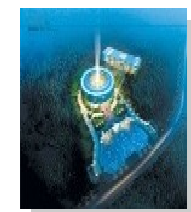


中国国家网格环境



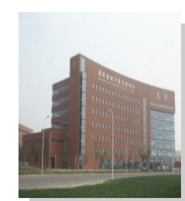
NSCC- 广州 ,2013 天河 2

NSCC- 无锡， 2016 太湖之光

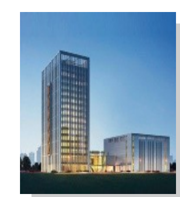


NSCC- 长沙 ,2012 天河 1A

NSCC- 济南 ,2012 神威蓝光



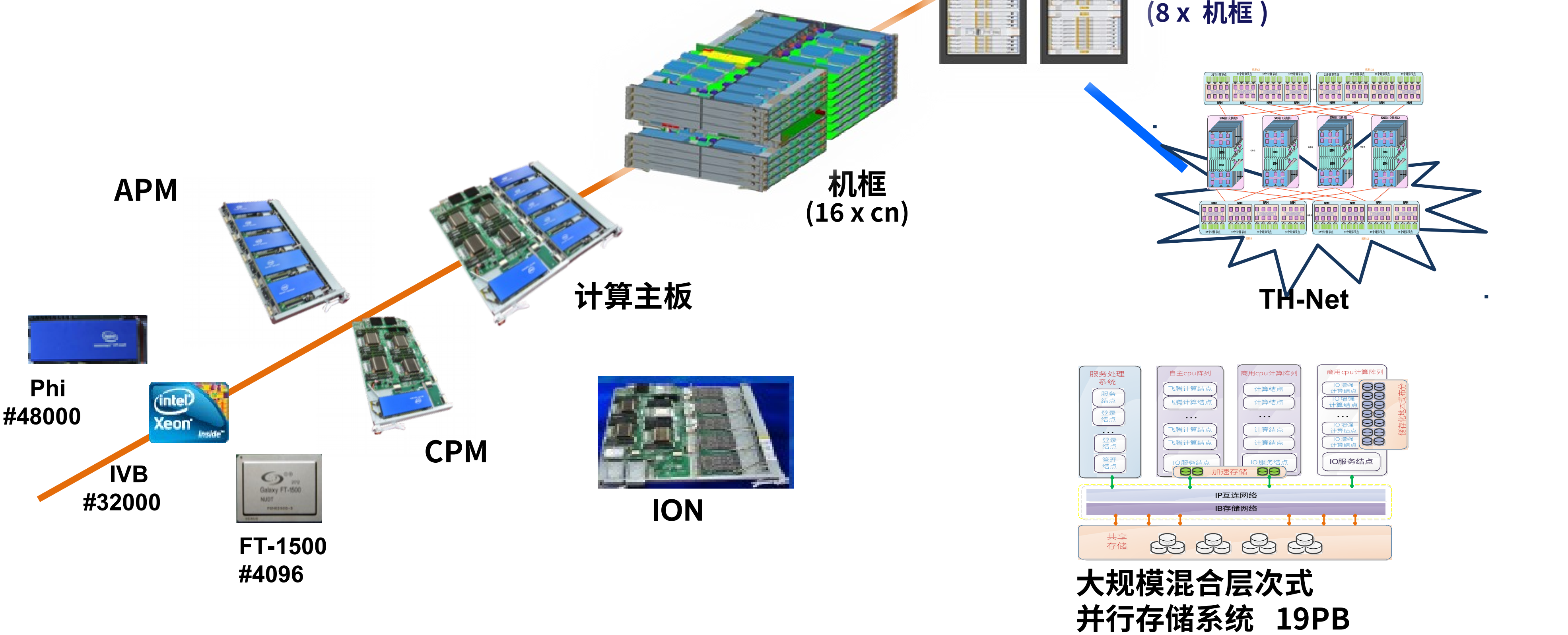
NSCC- 天津 ,2010 天河 1A



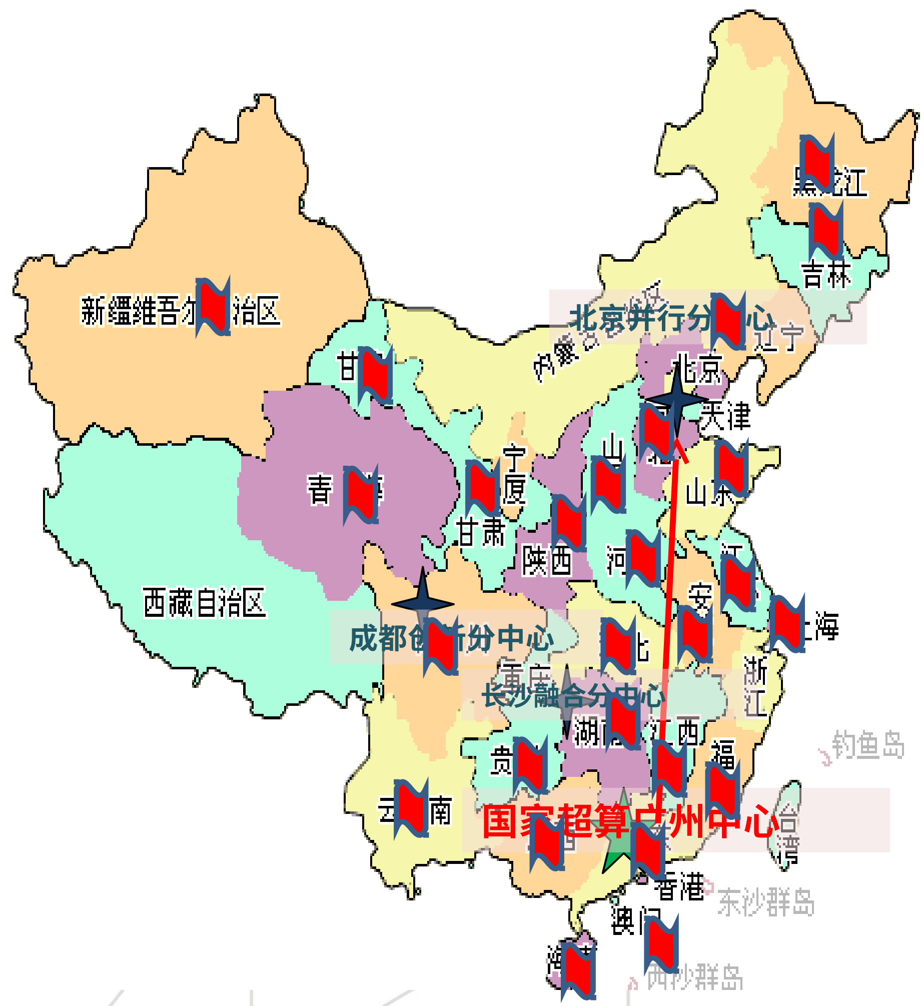
NSCC- 深圳 ,2011 曙光 6000

Tianhe-II

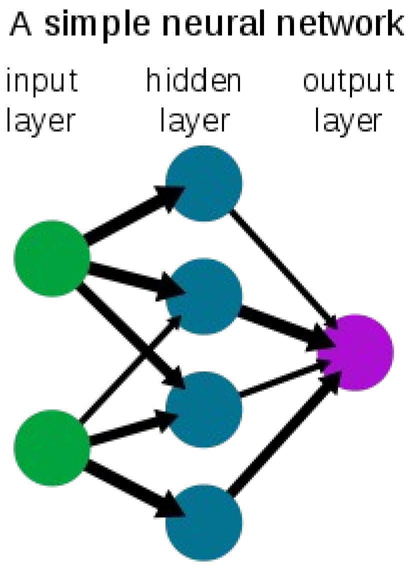
性能	100.7PFlops
系统	>1.6 万节点，1.4PB 内存 ,19PB 分布式存储
机柜	125+8+13+24=170 (720m²)
能耗	17.8 MW (1902MFlops/W)
制冷	密闭水风冷



The Greater Bay Area



AI & Machine learning basics

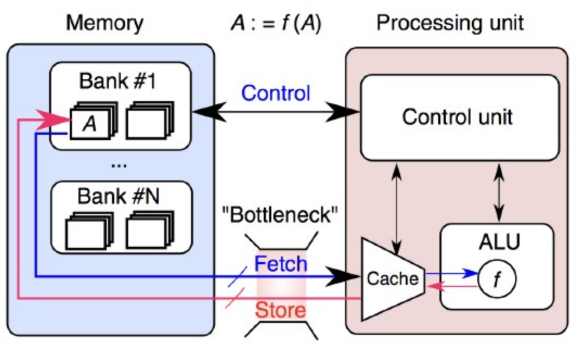


Challenges 1: models are more complicated

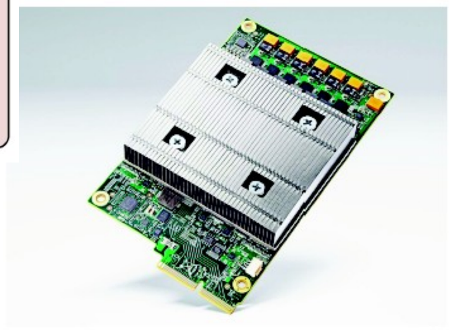
~ 100 layers, ~ 10^6 weights/parameters

Challenges 2: memory bottleneck

Data fetch is much expensive than data process

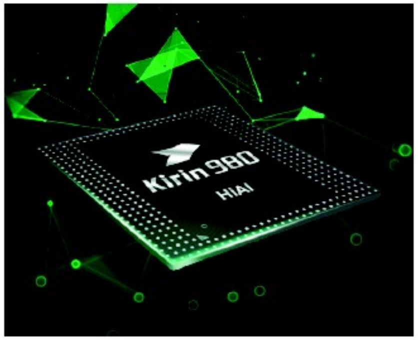


Neural processing unit / AI-accelerators



TPU by Google

A12 Bionic by Apple



Kirin 980 by Huawei

AI & Machine learning basics

Challenges 3: computing power consumption

AlphaGo:
- ❑ 176 GPUs, 1202 CPUs
- ❑ 150, 000 Watts

Jie Ke:
- ❑ 1.2L Human Brain
- ❑ ~20 Watts

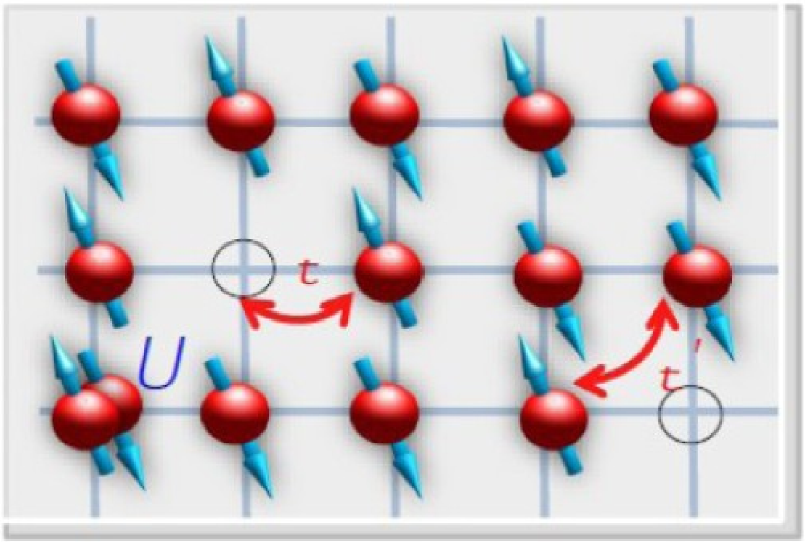
Huge power gap between human brain and CMOS-based AI system

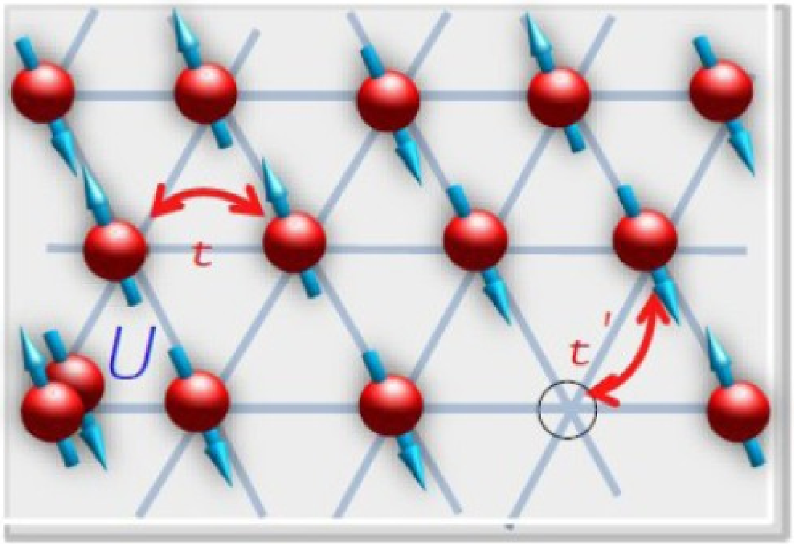
➢ It is much needed to develop **new hardware** with **new device** and **new architecture** **(new algorithms)**

Which one is better

	Supercomputer	Personal Computer	Human Brain
Computational Units	32,000 Xeon CPUs 10^12 transistors	4 CPUs, 10^9 transistors	10^11 neurons
Storage units	10^14 bits RAM 10^15 bits Storage	10^11 bit RAM 10^13 bit Storage	10^11 neurons 10^14 synapses
Cycle time	10^-9 sec	10^-9 sec	10^-3 sec
Operations/sec	10^15	10^10	10^17
Memory updates/sec	10^14	10^10	10^14
Power consumption	500 megawatt	100 watt	20 watt

Monte Carlo



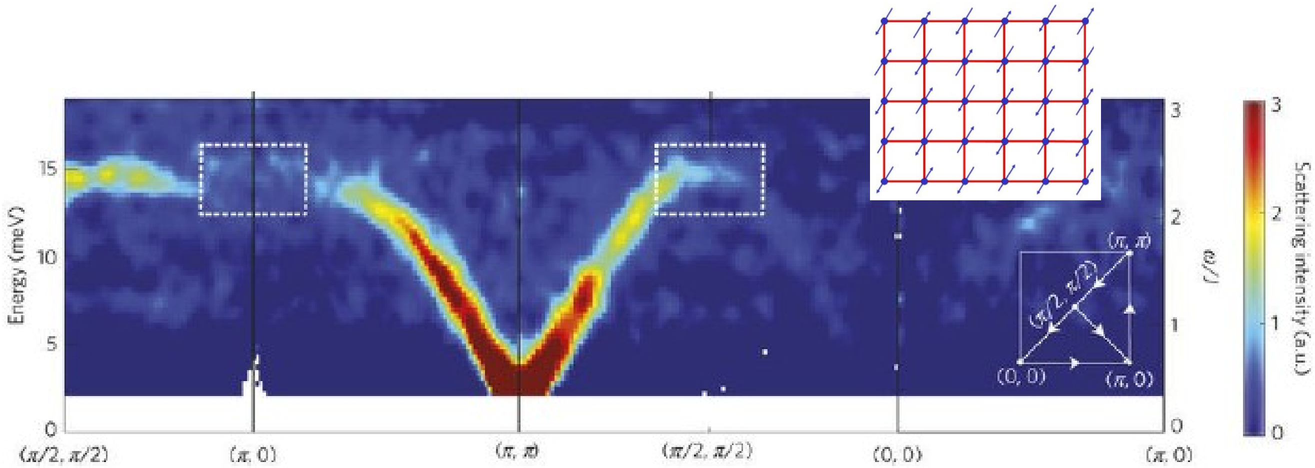


Partition function: $$Z = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \sum_n \langle n| e^{-\beta(\hat{H}-\mu\hat{N})} |n\rangle$$

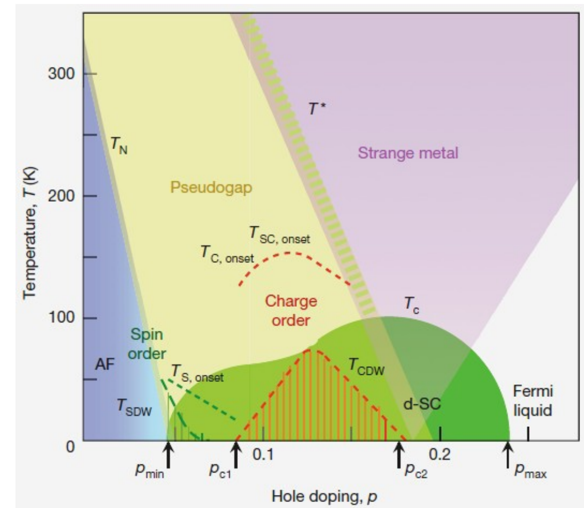
Observables: $$\langle \hat{A} \rangle = \frac{\mathrm{Tr}\left[\hat{A} e^{-\beta(\hat{H}-\mu\hat{N})}\right]}{\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]} = \frac{\sum_n \langle n|\hat{A} e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle}{\sum_n \langle n| e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle}$$

Fock space: $$\{|n\rangle\} \sim 2^{N_e} \; (e^{N_e \ln(2)}) \qquad 4^{N_e} \; (e^{N_e \ln(4)})$$

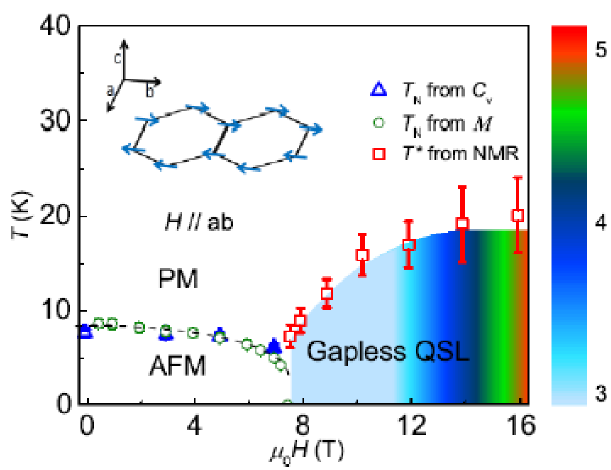
Quantum many-body system - Bosons

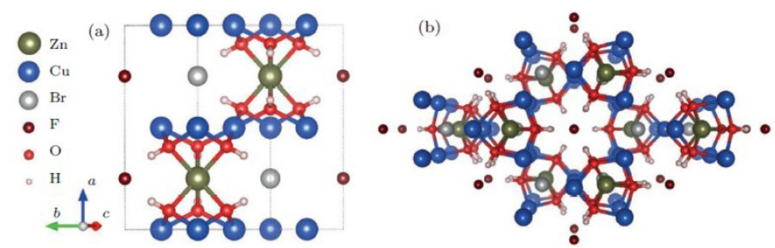


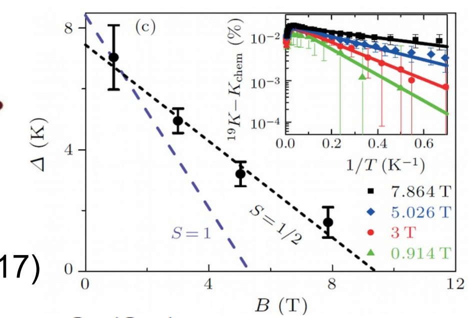
$Cu(DCOO)_2 \cdot 4D_2O$ ➢ Nat. Phys. 11, 62 (2015)



➢ Nature 518, 179 (2015)

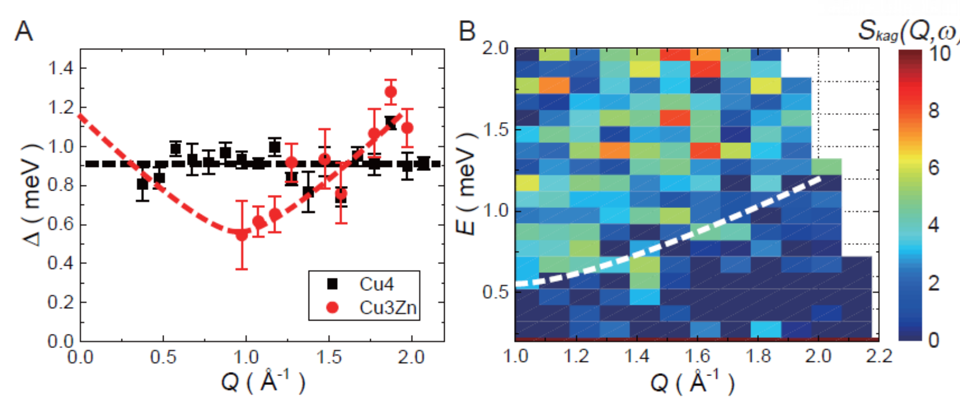






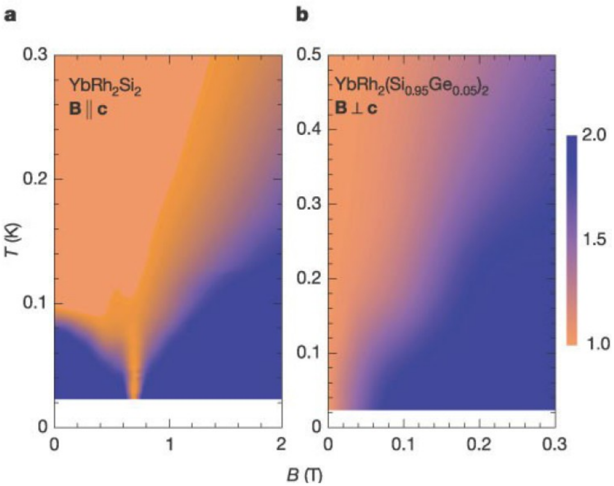
➢ CPL 34, 077502 (2017)

alpha-$RuCl_3$ ➢ PRL 119, 227208 (2017)

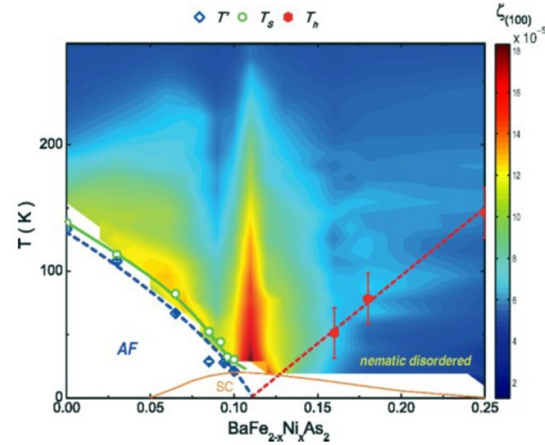


➢ Science, under review

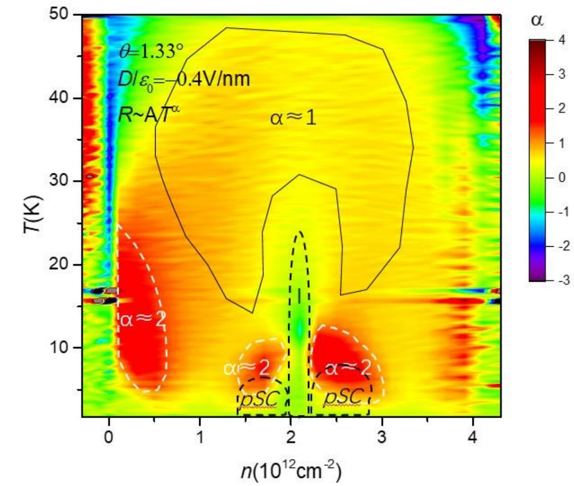
Quantum many-body system - Fermions



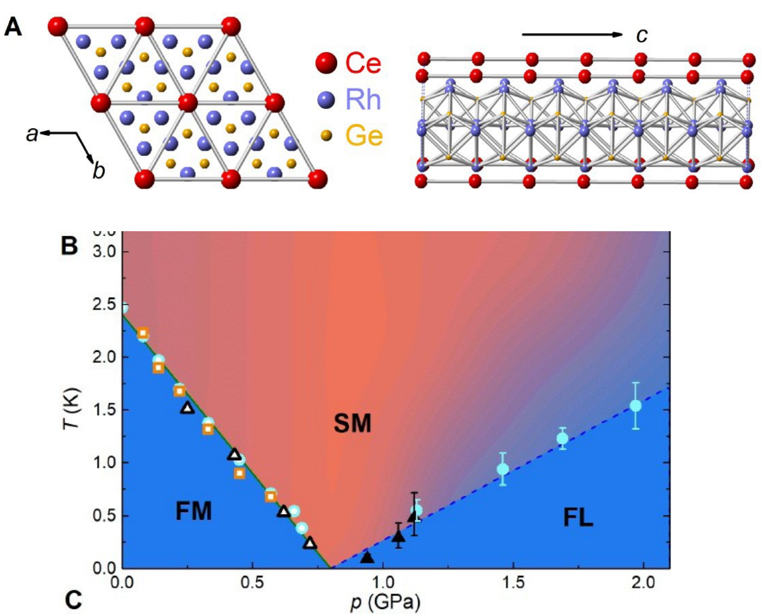
Nature 424, 524-527 (2003)

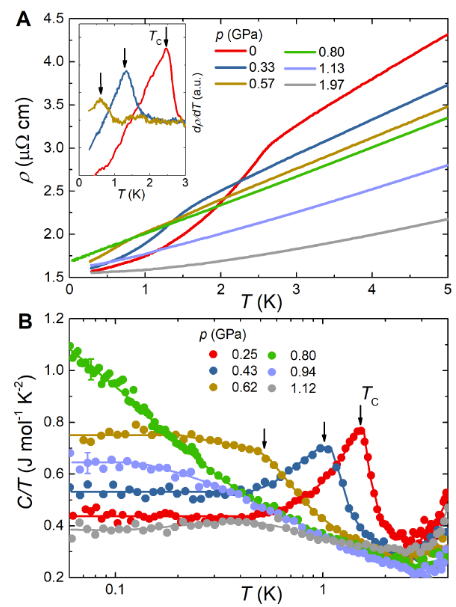


Phys. Rev. Lett. 117, 157002 (2016)



Twisted double bilayer Graphene
IOP, CAS Group
Ferromagnetic fluctuations
arXiv:1903.06952



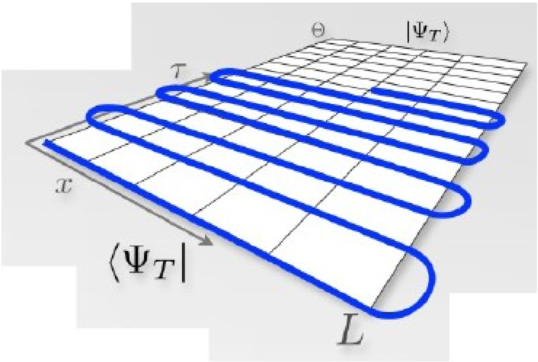


Ce-based heavy fermion metal, arXiv:1907.10470
Huiqiu Yuan’s group at Zhejiang University

- FM / AFM / Nematic fluctuations of itinerant electron systems
- Non-Fermi liquid, fluctuation induced superconductivity
- Fermionic QCP

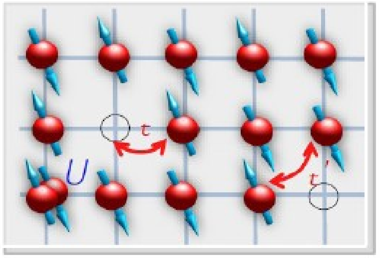
Quantum Monte Carlo

- Determinantal QMC for fermions $O(\beta N^3)$

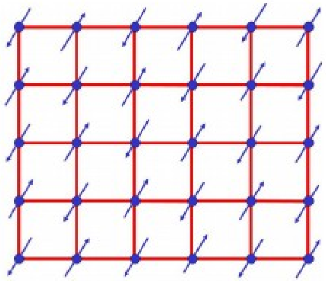


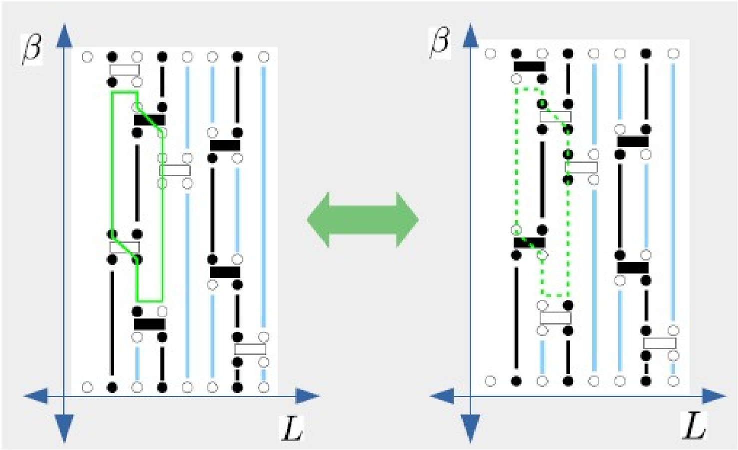
Hubbard model:
- Metal-Insulator transition
- Magnetic order
- Spectral properties
- Unconventional superconductivity

……



- World-line/SSE QMC for bosons/spins $O(\beta N)$





Heisenberg model:
- Quantum magnetism / Optical lattice
- Phase transition and critical phenomena
- Spectral properties
- Quantum spin liquids

……

Quantum Monte Carlo

- Computation effort scales linearly with βN^3

  System sizes: $N = L^2$ $L = 4, 6, 8, 10, 16, \cdots, 40$

  Time discretization: $\beta t \propto L, \Delta\tau t = 0.05$

  Parallelization: ~ 10^3 CPUs, ~ 10^6 CPU hours

NSCC 国家超级计算天津中心
National Supercomputer Center in Tianjin

国家超级计算广州中心
NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

Determinant quantum Monte Carlo

$$H = -t \sum_{\langle i,j \rangle, \sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

- Path-integral & Trotter-Suzuki decomposition

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] \approx \mathrm{Tr}\left[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\right] \qquad \Delta\tau = \frac{\beta}{m}, m \to \infty$$

- Free fermion (Slater) determinant

$$\mathrm{Tr}\left[e^{-\sum_{i,j} c_i^{\dagger} A_{i,j} c_j + c_i^{\dagger} B_{i,j} c_j}\right] = \mathrm{Det}\left[\mathbf{1} + e^{-\mathbf{A}} e^{-\mathbf{B}}\right]$$

Determinant quantum Monte Carlo

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

- Path-integral & Trotter-Suzuki decomposition

$$Z = \text{Tr}\{e^{-\beta \hat{H}}\} \approx \text{Tr}\big[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\big] \qquad \Delta\tau = \frac{\beta}{m}, m \to \infty$$

- Discrete Hubbard-Stratonovich transformation

$$e^{-\Delta\tau U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})} = C \sum_{s_1,\ldots,s_N = \pm 1} e^{\alpha \sum_{i=1}^{N} s_i (n_{i,\uparrow} - n_{i,\downarrow})}$$

$$(C, \alpha)(U, N, \Delta\tau)$$

$$\int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$$

- Blankenbecler et. al., Phys. Rev. D 24, 2278 (1981)
- Hirsch, Phys. Rev. B 28, 4059(R) (1983)
- Hirsch, Phys. Rev. B 31, 4403 (1985)

$$\int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}x^2 + bx} = \int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}(x - \frac{b}{a})^2 + \frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}$$

Determinant quantum Monte Carlo

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}) + \frac{U}{2} \sum_{i=1}^{N} (n_{i,\uparrow} + n_{i,\downarrow} - 1)^2$$

- Path-integral & Trotter-Suzuki decomposition

$$Z = \text{Tr}\left[e^{-\beta \hat{H}}\right] \approx \text{Tr}\left[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\right] \qquad \Delta\tau = \frac{\beta}{m}, m \to \infty$$

- Discrete Hubbard-Stratonovich transformation

$$e^{-\Delta\tau \frac{U}{2}(n_{i,\uparrow}+n_{i,\downarrow}-1)^2} = \frac{1}{4} \sum_{s_1, s_2, \cdots, s_N = \pm 1, \pm 2} \gamma(s_i) e^{i\sqrt{\Delta\tau \frac{U}{2}} \eta(s_i)(n_{i,\uparrow}+n_{i,\downarrow}-1)} + O[(\Delta\tau)^4]$$

$$\int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$$

- Blankenbecler et. al., Phys. Rev. D 24, 2278 (1981)
- Hirsch, Phys. Rev. B 28, 4059(R) (1983)
- Hirsch, Phys. Rev. B 31, 4403 (1985)
- Assaad, Phys. Rev. B 71, 075103 (2005)
- Assaad and Evertz, Lec. Notes. In Phys. 739 (2008)

$$\int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}x^2 + bx} = \int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}(x - \frac{b}{a})^2 + \frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}$$

Determinant quantum Monte Carlo

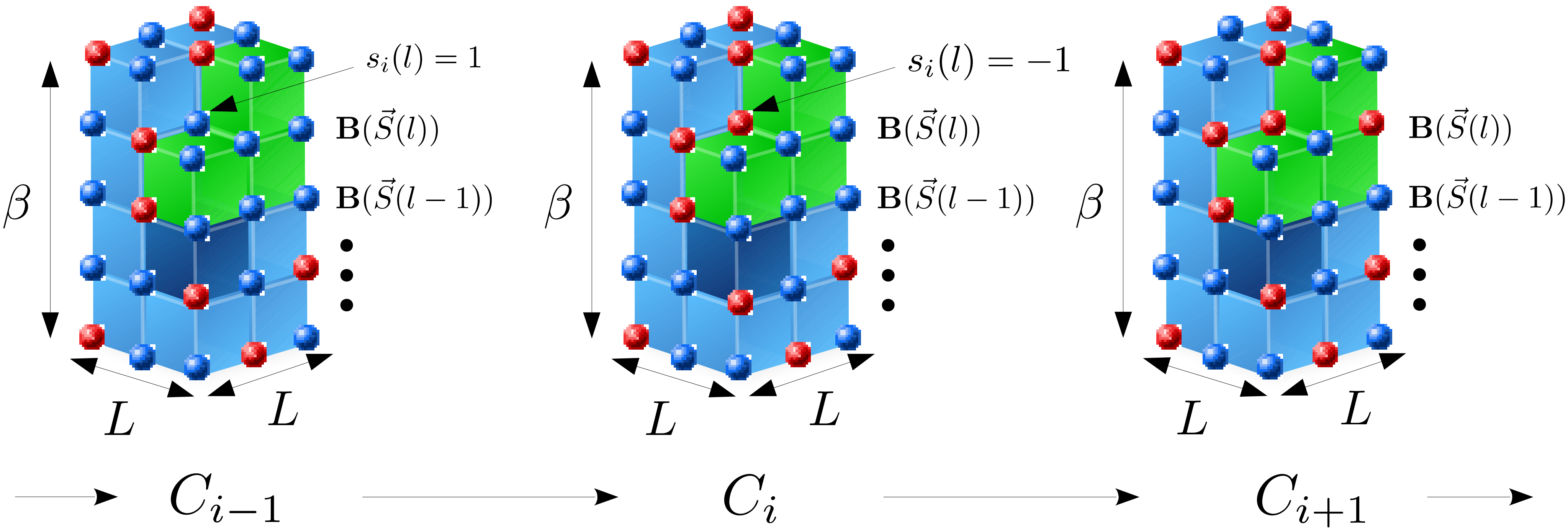
- Write Path-integral into determinant

$$Z = \mathrm{Tr}\left[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\right] = C^m \sum_{\vec{s}_1, \vec{s}_2, \ldots, \vec{s}_m} \det[\mathbf{1} + \mathbf{P}^\dagger \mathbf{B}_m \mathbf{B}_{m-1} \ldots \mathbf{B}_1 \mathbf{P}]$$

$$\mathbf{B}_l = e^{-\Delta\tau \mathbf{H_t}} e^{-\Delta\tau \mathbf{H_U}(\vec{s}(l))}$$

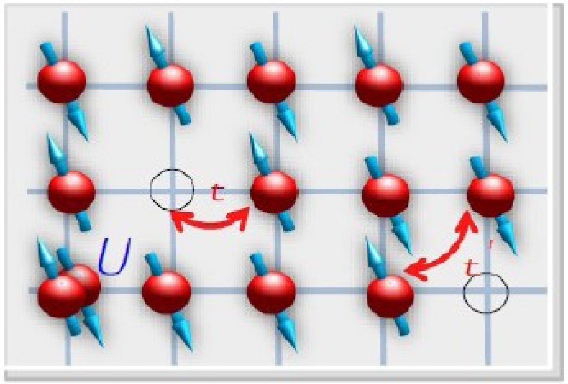
- Monte Carlo sampling in configuration space

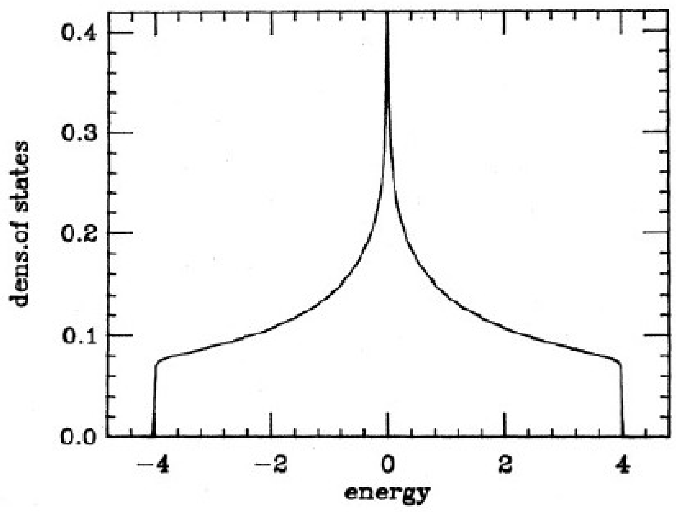
$$\mathbf{H_U}(\vec{s}(l)) \propto \alpha \vec{s}(l)$$

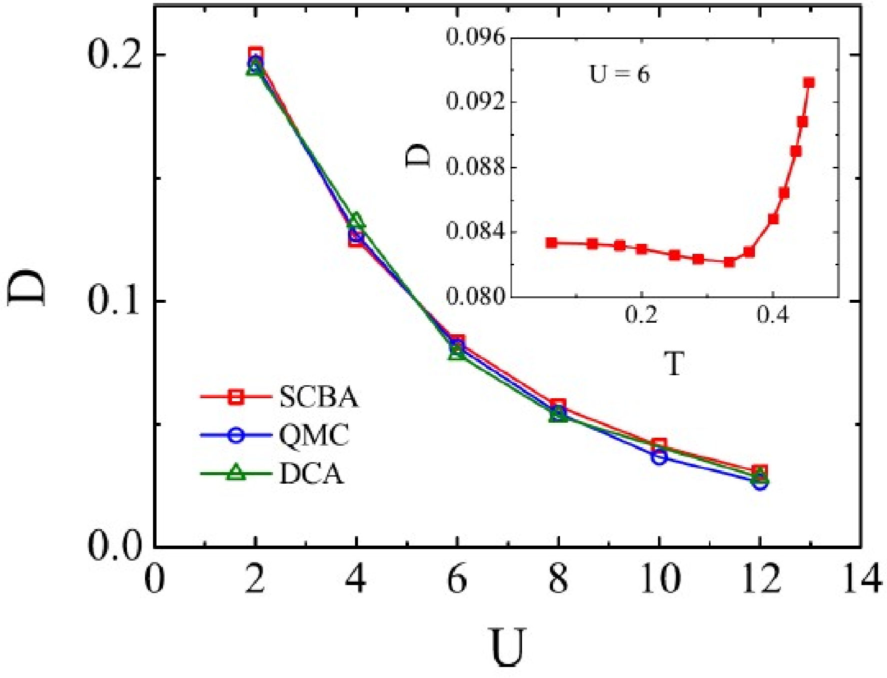


Square lattice Hubbard model

$$H = -t \sum_{\langle i,j \rangle, \sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \mathrm{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$



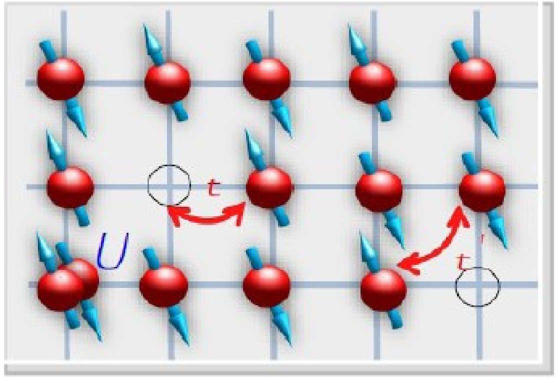


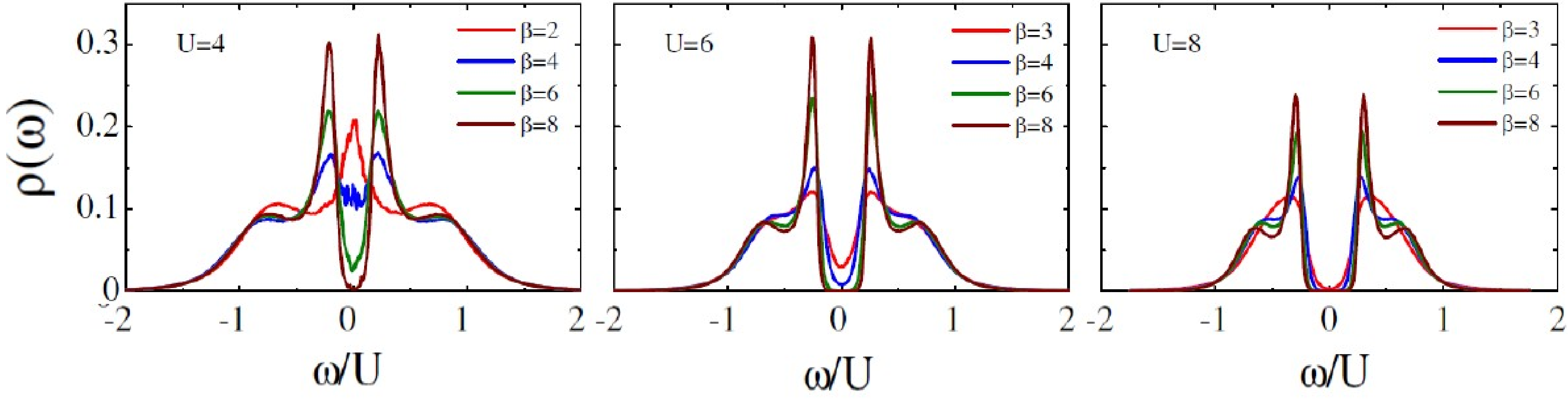


- C. Chen, Bachelor Thesis (2016)
- X.-J. Han et al., PRB 99, 245150 (2019)

Square lattice Hubbard model

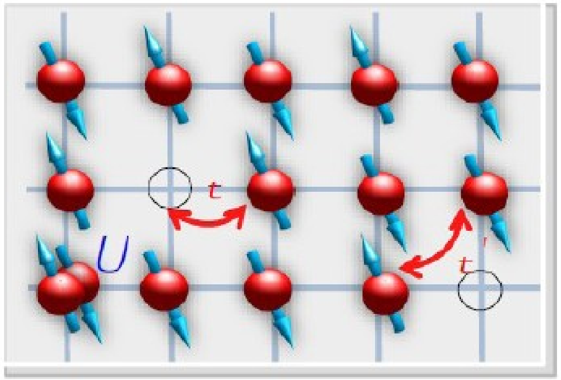
$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

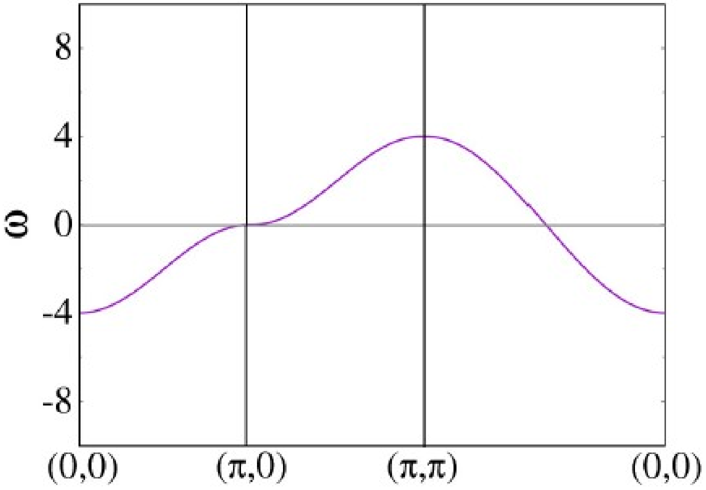


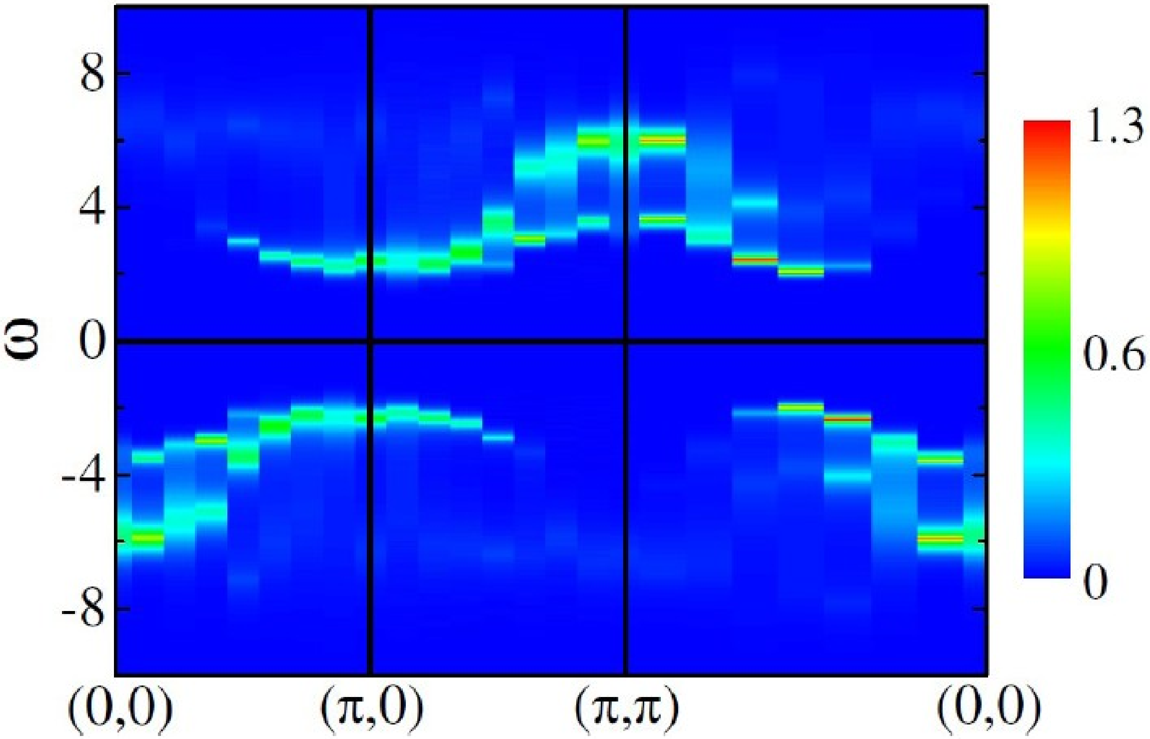


- C. Chen, Bachelor Thesis (2016)
- X.-J. Han et al., PRB 99, 245150 (2019)

Square lattice Hubbard model

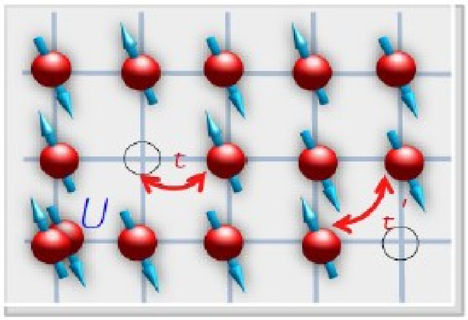


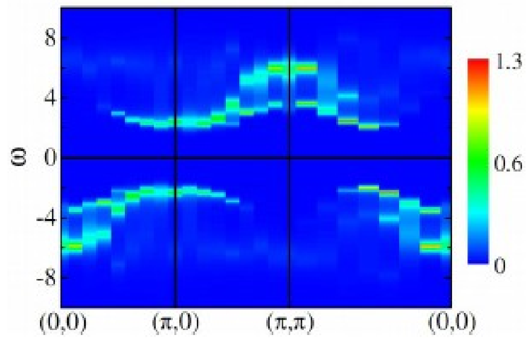




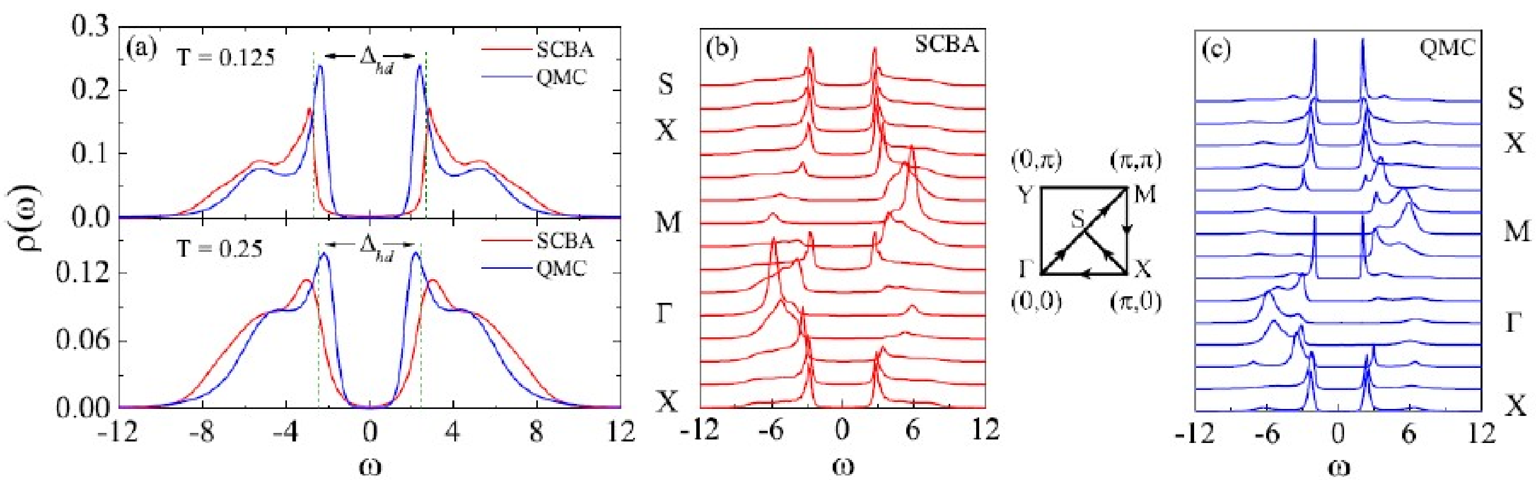
- C. Chen, Bachelor Thesis (2016)
- X.-J. Han et al., PRB 99, 245150 (2019)

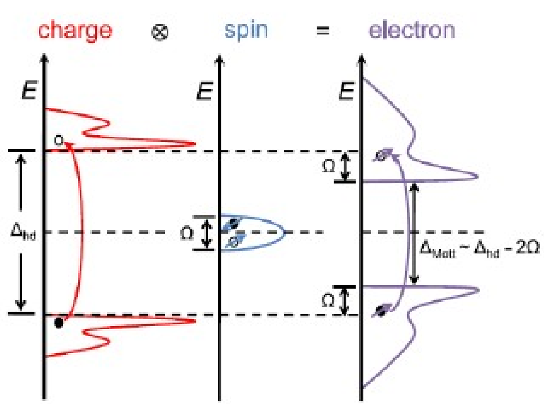
Square lattice Hubbard model

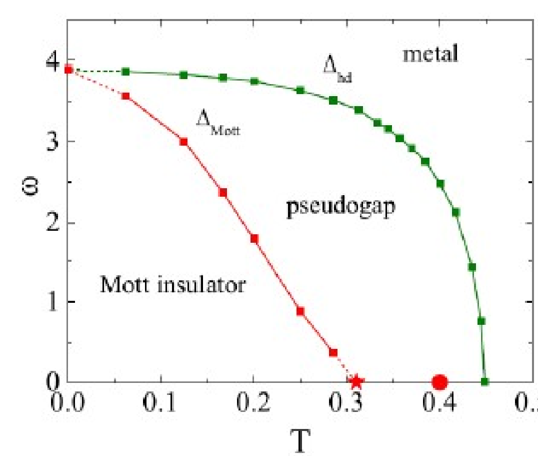




- C. Chen, Bachelor Thesis (2016)
- X.-J. Han et al., PRB 99, 245150 (2019)

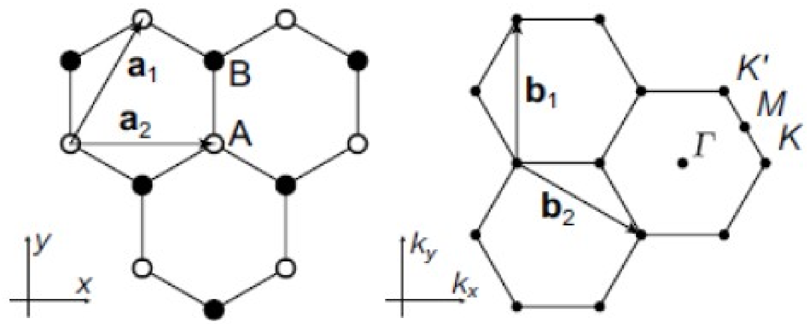


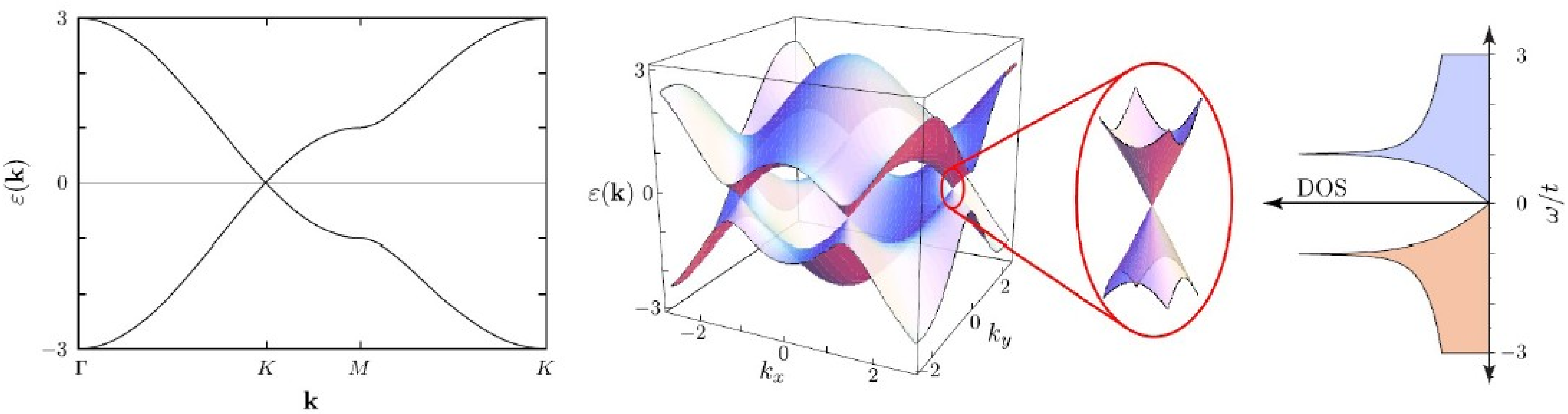




Honeycomb lattice Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \mathrm{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$



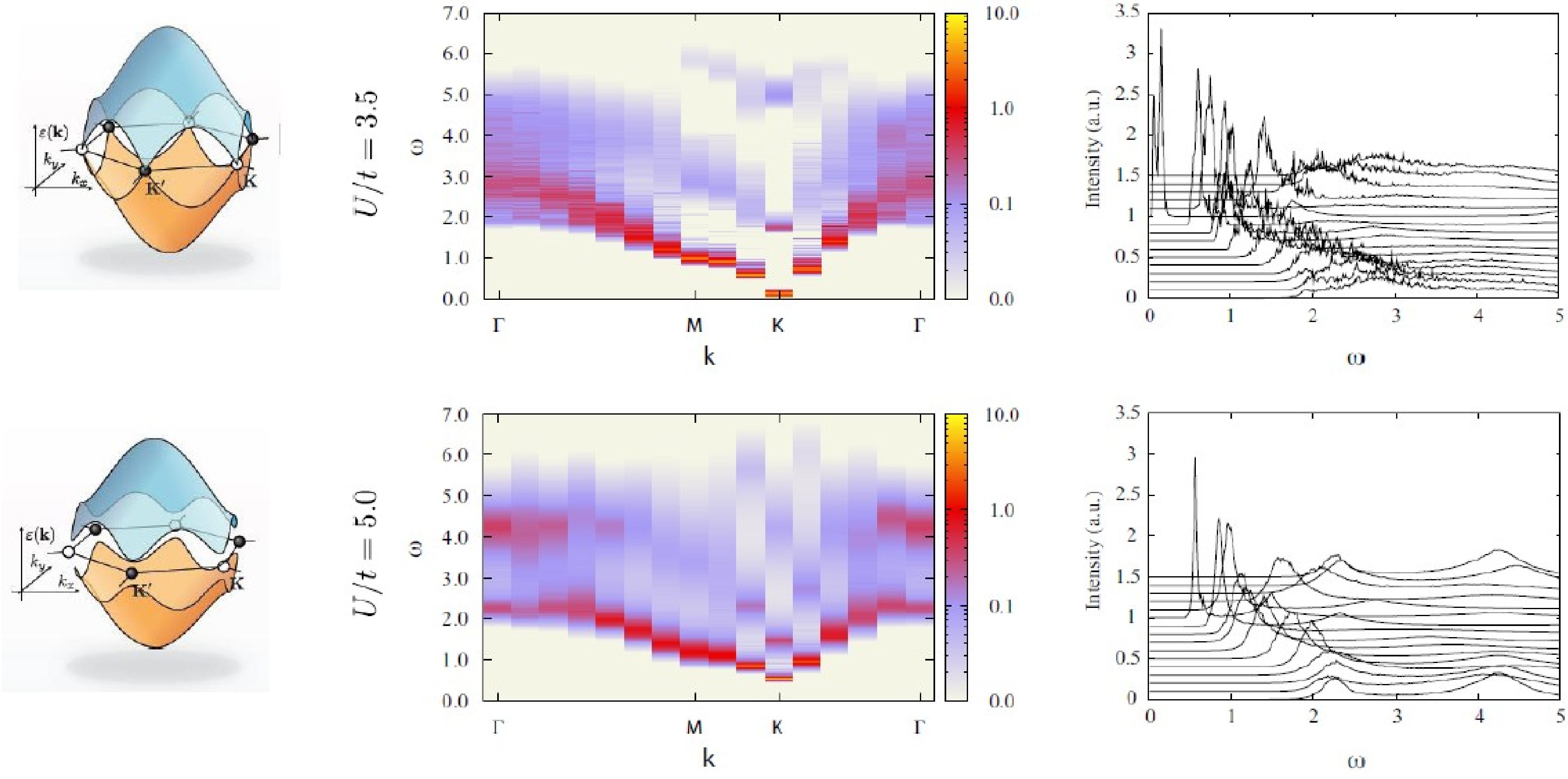


➢ ZYM, Phd Thesis (2011)

Honeycomb lattice Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \mathrm{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

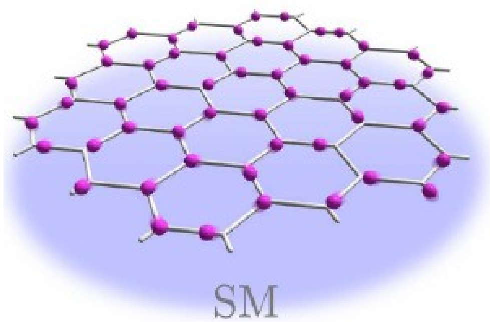
$A(\mathbf{k},\omega)$

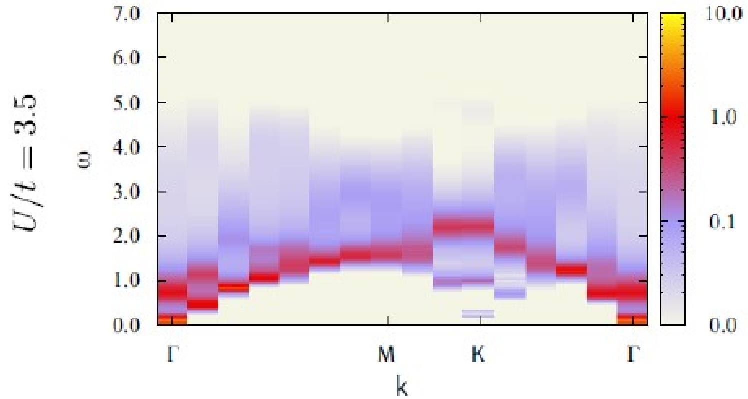


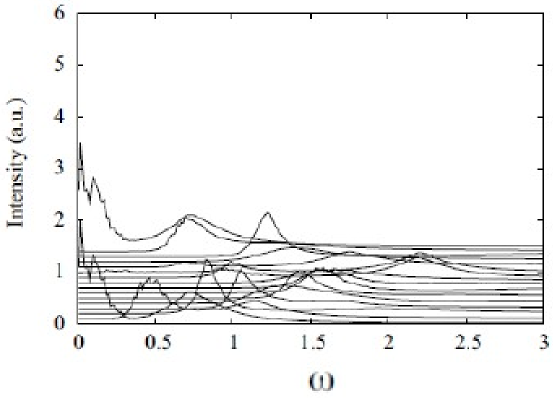
Honeycomb lattice Hubbard model

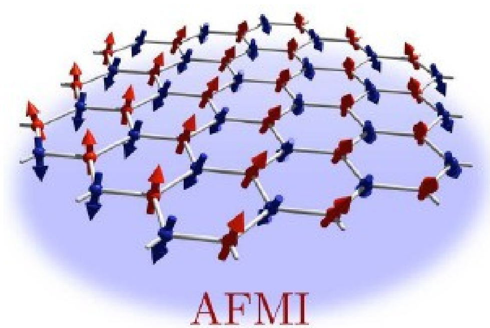
$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

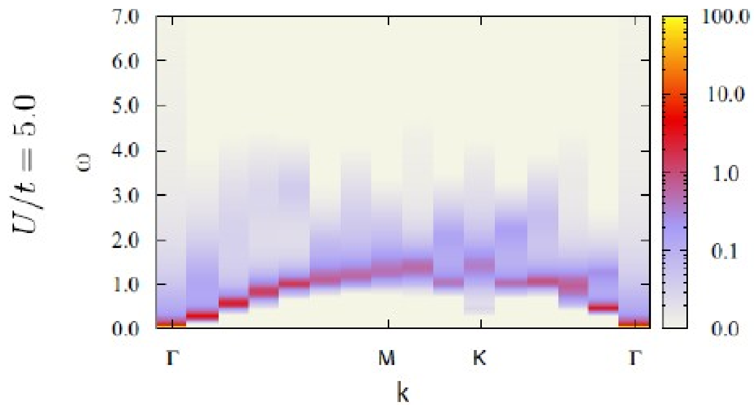
$\chi_s(\mathbf{k}, \omega)$

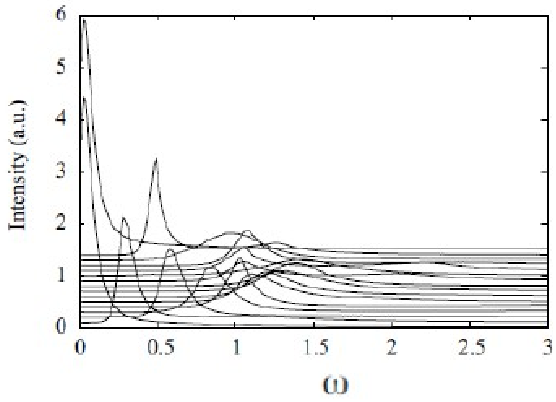










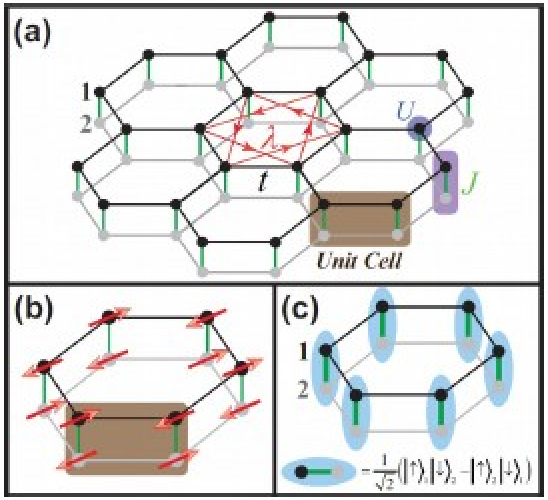


Determinantal quantum Monte Carlo

- Hubbard-Stratonovich Transformation

$$\exp\{-\Delta\tau \frac{J}{8}(D_{i,j} - D_{i,j}^{\dagger})^2\} = \frac{1}{4}\sum_{t_{i,j}=\pm 1,\pm 2} \gamma(t_{i,j}) e^{i\sqrt{\Delta\tau \frac{J}{8}}\eta(t_{i,j})(D_{i,j}-D_{i,j}^{\dagger})}$$

$$\exp\{-\Delta\tau U(Q_{\hexagon} - 4)^2\} = \frac{1}{4}\sum_{s_{\hexagon}=\pm 1,\pm 2} \gamma(s_{\hexagon}) e^{\alpha\eta(s_{\hexagon})(Q_{\hexagon}-4)}$$



➢ PRX 7, 031052 (2017)

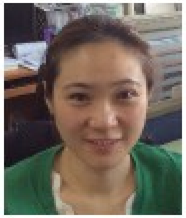
- Measurements

$$G(\mathbf{k},\tau) \propto Z_{sp}(\mathbf{k})e^{-\tau\Delta_{sp}(\mathbf{k})} \quad \mathbf{k} = \mathbf{k}_F$$

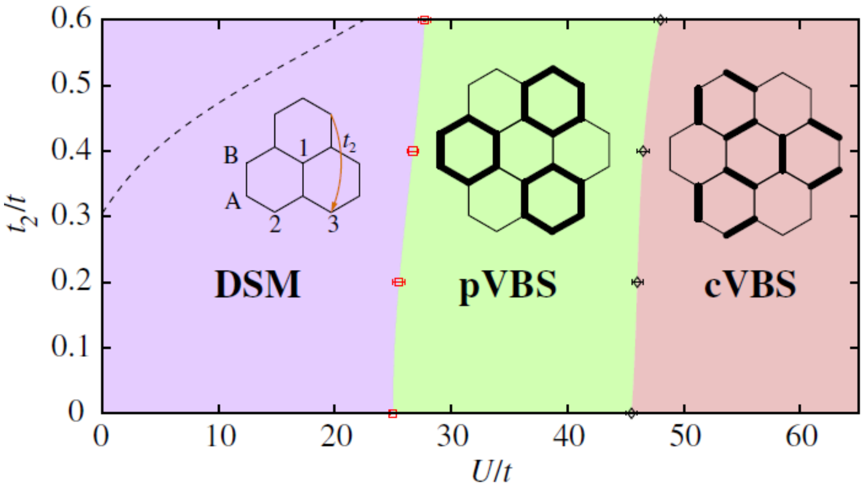
$$S(\mathbf{q},\tau) \propto Z_s(\mathbf{q})e^{-\tau\Delta_s(\mathbf{k})} \quad \mathbf{q} = \mathbf{Q}_{AF}$$

SAC $\longrightarrow A(\mathbf{k},\omega)$

SAC $\longrightarrow S(\mathbf{q},\omega)$



H. Shao A. Sandvik



➢ PRL in press (1901.11424)

Learning materials

https://www.physics.hku.hk/~mengziyang/teaching.html

Tutorial and Code Demonstration

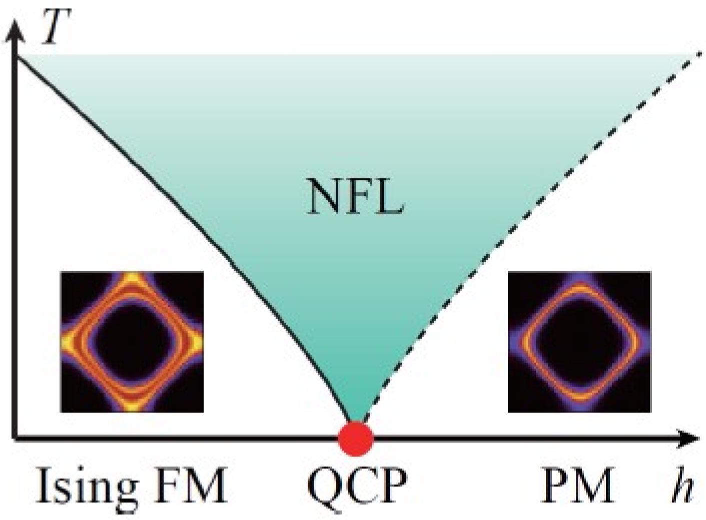
Time: 10:00 Friday (Oct.11)

Venue:CPD-3.16, 3/F, Run Run Shaw Tower, Centennial Campus

Gaopei, PAN and Chuhao, LI
Institute of Physics
Chinese Academy of Science

Tidbits from Monte Carlo

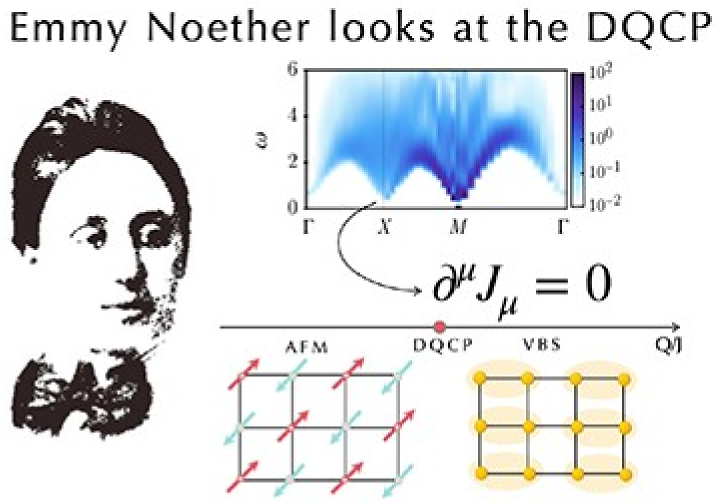
- Fermions couple to critical bosonic modes



- Itinerant quantum critical point
- Non-Fermi-liquid
- Self-learning Monte Carlo methods
- Matter fields couple to guage fields
- Alegbraic spin liquid, orthogonal metal

……

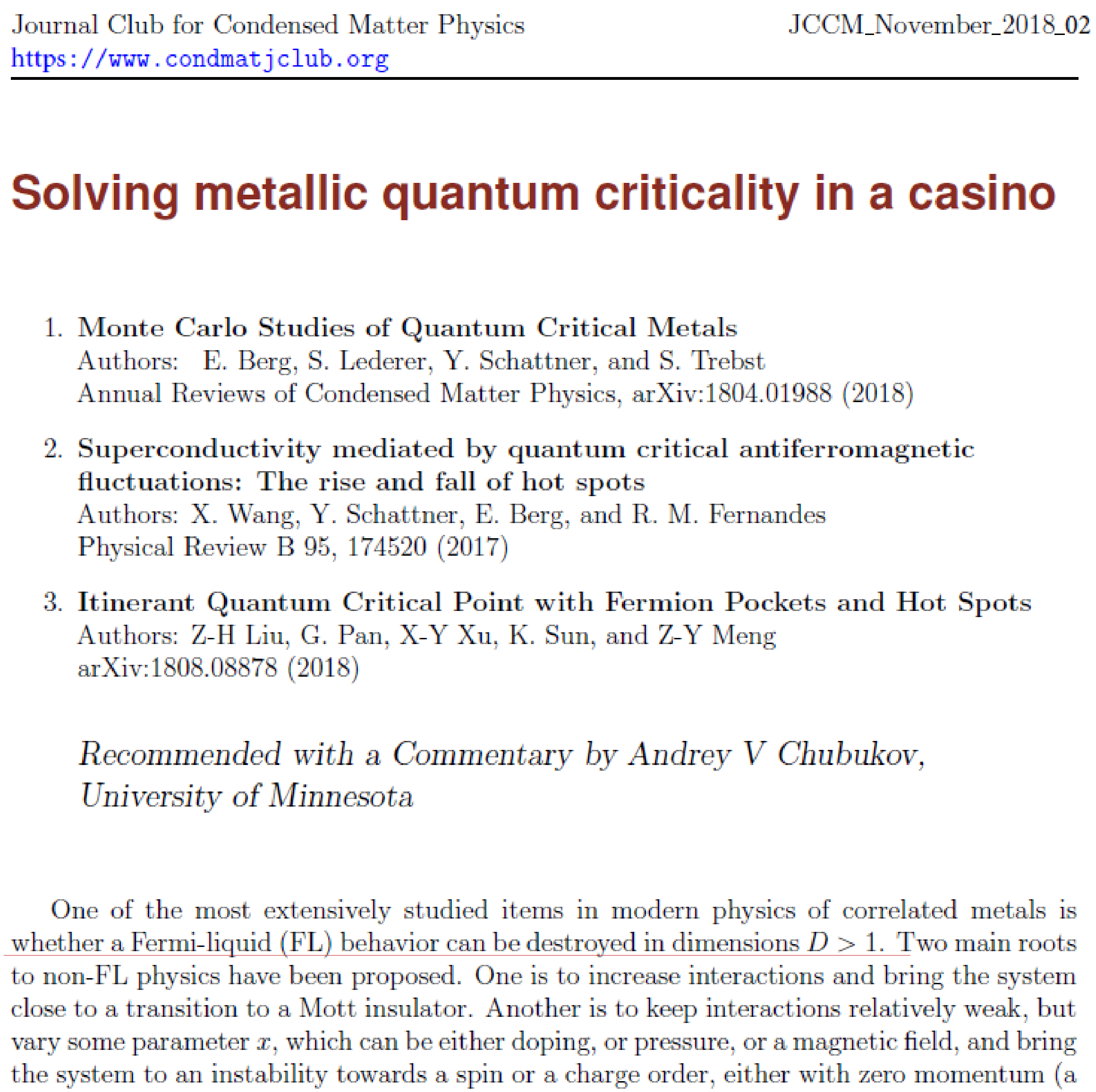
- Designer spin/boson models QMC



- DQCP & Gauge and matter fields
- Emergent continuous symmetry
- Dynamical signatures of topological order and spin liquids
- Duality between SPT transitions and DQCP

……

- Rich analytic literature, sum particular series of diagrams
- The ultimate desire is to obtain the exact non-FL forms of fermionic and bosonic propagators in D>1
- Alternative numerical approaches QMC
- Lattice models, large sizes and low T
- Numerics and Analytics would converge



Journal Club for Condensed Matter Physics JCCM_November_2018_02
https://www.condmatjclub.org

Solving metallic quantum criticality in a casino

1. **Monte Carlo Studies of Quantum Critical Metals**
   Authors: E. Berg, S. Lederer, Y. Schattner, and S. Trebst
   Annual Reviews of Condensed Matter Physics, arXiv:1804.01988 (2018)
2. **Superconductivity mediated by quantum critical antiferromagnetic fluctuations: The rise and fall of hot spots**
   Authors: X. Wang, Y. Schattner, E. Berg, and R. M. Fernandes
   Physical Review B 95, 174520 (2017)
3. **Itinerant Quantum Critical Point with Fermion Pockets and Hot Spots**
   Authors: Z-H Liu, G. Pan, X-Y Xu, K. Sun, and Z-Y Meng
   arXiv:1808.08878 (2018)

Recommended with a Commentary by Andrey V Chubukov, University of Minnesota

One of the most extensively studied items in modern physics of correlated metals is whether a Fermi-liquid (FL) behavior can be destroyed in dimensions $D > 1$. Two main roots to non-FL physics have been proposed. One is to increase interactions and bring the system close to a transition to a Mott insulator. Another is to keep interactions relatively weak, but vary some parameter x, which can be either doping, or pressure, or a magnetic field, and bring the system to an instability towards a spin or a charge order, either with zero momentum (a

People

Xiao Yan Xu

Zi Hong Liu

Chuang Chen

Gao Pei Pan

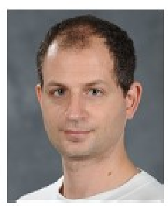
Yang Qi

Kai Sun

Revealing Fermionic Quantum Criticality from New Monte Carlo Techniques

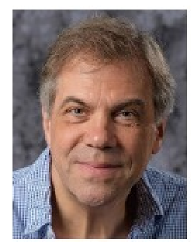
Topical Review, J. Phys.: Condens. Matter 31, 463001 (2019)

Fakher Assaad



Erez Berg

Cenke Xu



Andrey Chubukov

Subir Sachdev

Model

$$H = \sum_{k,\sigma} \mathbf{v}_k \cdot (\mathbf{k} - \mathbf{k}_F) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_q \chi_0^{-1}(\mathbf{q}) \mathbf{S}_q \cdot \mathbf{S}_{-q}$$
$$+ g \sum_{k,q,\alpha,\beta} c^\dagger_{\mathbf{k}+\mathbf{q},\alpha} \sigma_{\alpha,\beta} c_{\mathbf{k},\beta} \cdot \mathbf{S}_{-q}$$

$$S = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{k,\alpha} c^\dagger_{\mathbf{k},\sigma} G_0^{-1}(\mathbf{k}, \tau - \tau') c_{\mathbf{k},\sigma}(\tau')$$
$$+ \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sum_q \chi_0^{-1}(\mathbf{q}) \mathbf{S}_q(\tau) \cdot \mathbf{S}_{-q}(\tau')$$
$$+ g \int_0^\beta d\tau \sum_q \mathbf{s}_q(\tau) \cdot \mathbf{S}_{-q}(\tau)$$

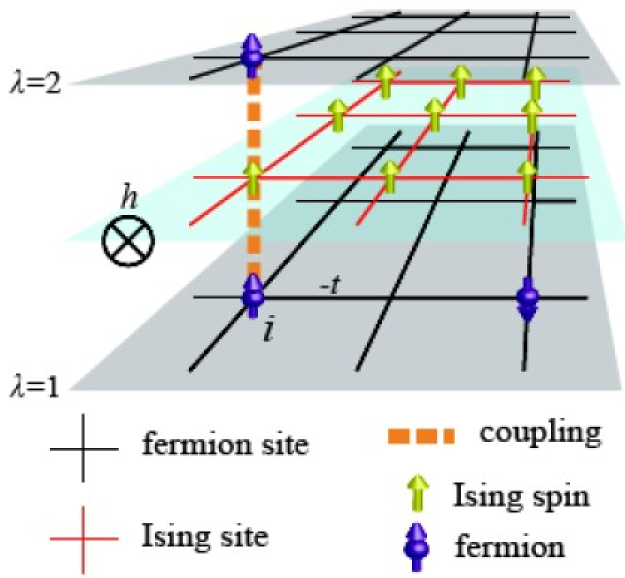
$$\chi_0(\mathbf{q}, \omega) = \frac{\chi_0}{\xi^{-2} + (\mathbf{q} - \mathbf{Q})^2 - (\omega/v_s)^2}$$

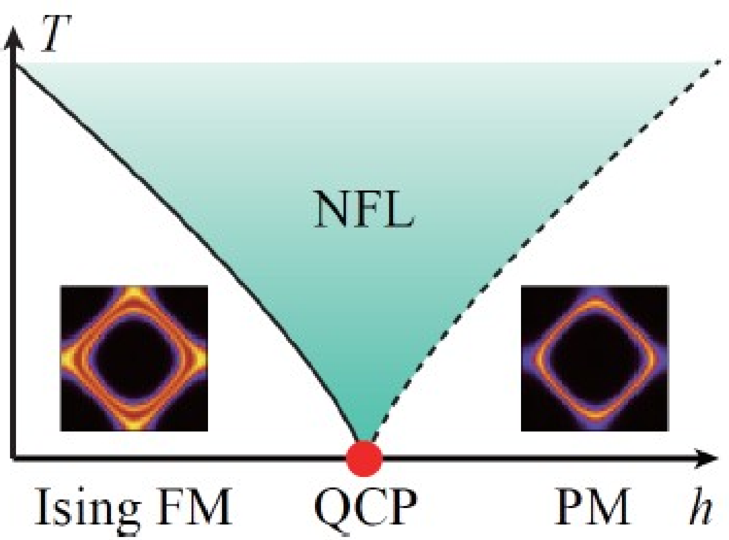
$$G_0^{-1}(\mathbf{k}, \tau) = \partial_\tau - \mathbf{v}_k \cdot (\mathbf{k} - \mathbf{k}_F)$$

- Abanov, Chubukov, Schmalian, Adv. in Phys. 52, 119 (2003)
- Metlitski, Sachdev, PRB 82, 075127 (2010)
- Metlitski, Sachdev, PRB 82, 075128 (2010)
- Sung-Sik Lee, Annu. Rev. Condens. Matter Phys 9, 227 (2018)

Model

➢ PRX 7, 031101 (2017)



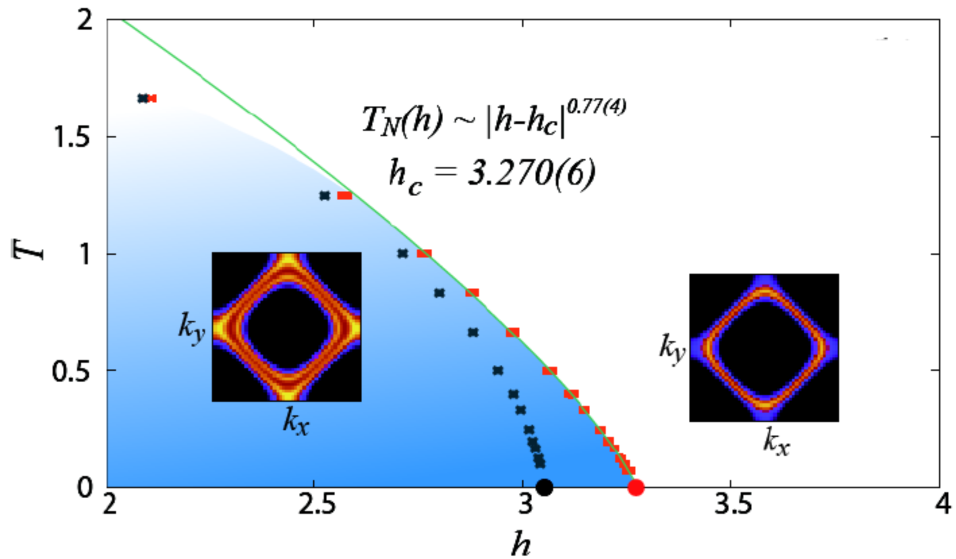


$$\hat{H} = \hat{H}_f + \hat{H}_s + \hat{H}_{sf}$$

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

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

$$\hat{H}_{sf} = -\xi \sum_{i\lambda} s^z_i (n_{i\lambda\uparrow} - n_{i\lambda\downarrow})$$



SLMC

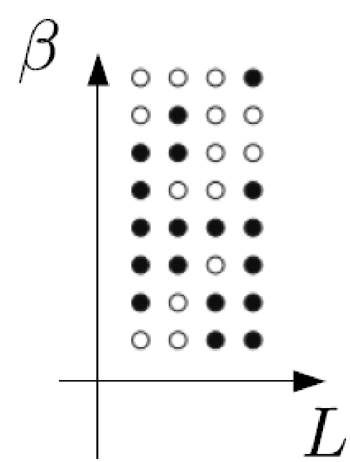
$$Z = \mathrm{Tr}\{e^{-\beta H}\} = \mathrm{Tr}\{(e^{-\Delta\tau H_{\mathrm{fermion}}} e^{-\Delta\tau H_{\mathrm{boson}}} e^{-\Delta\tau H_{\mathrm{coupling}}})^M\} + O(\Delta\tau^2)$$

$$= \mathrm{Tr}_f\{\sum_{\{S_z\}} \langle S_z^M | e^{-\Delta\tau H_{\mathrm{fermion}}} e^{-\Delta\tau H_{\mathrm{boson}}} e^{-\Delta\tau H_{\mathrm{coupling}}} | S_z^{M-1}\rangle \cdots \cdots \langle S_z^2 | e^{-\Delta\tau H_{\mathrm{fermion}}} e^{-\Delta\tau H_{\mathrm{boson}}} e^{-\Delta\tau H_{\mathrm{coupling}}} | S_z^1 \rangle\}$$

$$= \sum_{\{S_z\}} \underbrace{(\prod_{\tau}\prod_{\langle i,j\rangle} e^{-\Delta\tau J \sum_{\langle i,j\rangle} s^z_{i,\tau} s^z_{j,\tau}})(\prod_i \prod_{\langle \tau,\tau'\rangle} \Lambda e^{\gamma \sum_i s^z_{i,\tau} s^z_{i,\tau'}})}_{\mathcal{W}_{\mathcal{C}}^{\mathrm{boson}}} \cdot \underbrace{\mathrm{Tr}_f\{\prod_\tau e^{-\Delta\tau H_{\mathrm{fermion}}} e^{-\Delta\tau H_{\mathrm{coupling}}(\{s^z_\tau\})}\}}_{\mathcal{W}_{\mathcal{C}}^{\mathrm{fermion}}}$$

$$= \sum_{\{S_z\}} \mathcal{W}_{\mathcal{C}}{}^{\mathrm{boson}} \mathrm{Tr}_f\{\prod_\tau (e^{-\Delta\tau c^\dagger T c} \prod_i e^{c^\dagger V\{s^z_{i,\tau}\} c})\}$$

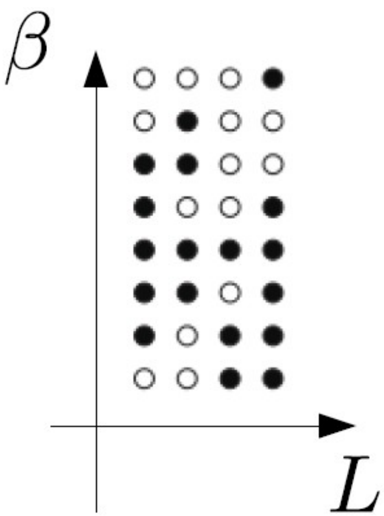
$$= \sum_{\{S_z\}} \mathcal{W}_{\mathcal{C}}{}^{\mathrm{boson}} \left| \det[\mathbf{1} + \prod_\tau (e^{-\Delta\tau T} \prod_i e^{V\{s^z_{i,\tau}\}})] \right|^2$$

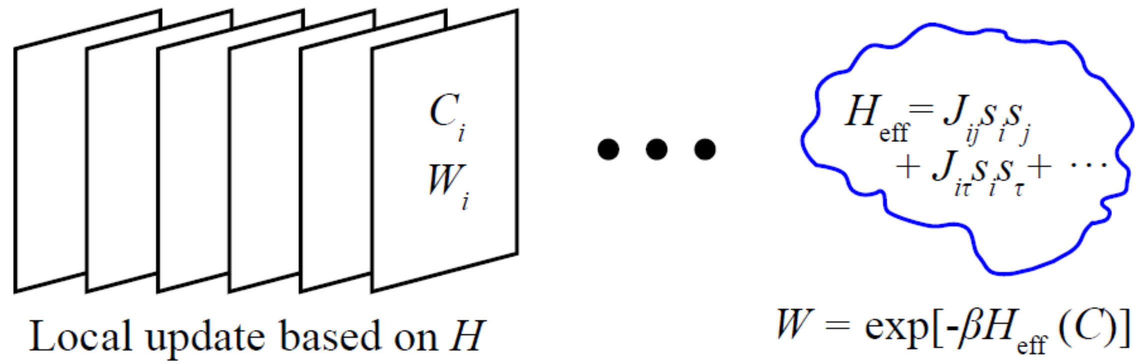


- Self-learning Monte Carlo Method

O(N) speedup, large lattice is possible

SLMC

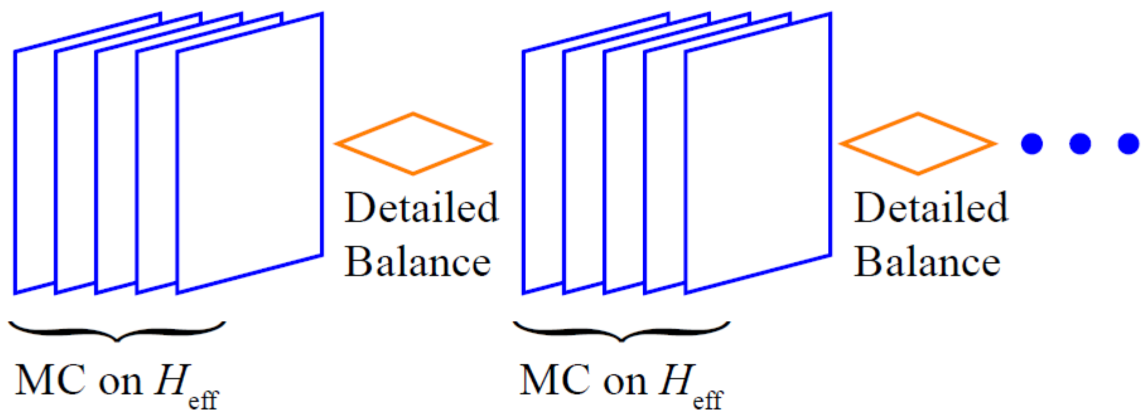




$$H_{\text{eff}}[\mathcal{C}] = E_0 + \sum_{(i,\tau);(j,\tau')} J^{\text{eff}}_{(i,\tau);(j,\tau')} s^z_{i,\tau} s^z_{j,\tau'} + \cdots$$

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

$$-\beta H_{\text{eff}}[\mathcal{C}] = \ln(\omega[\mathcal{C}])$$



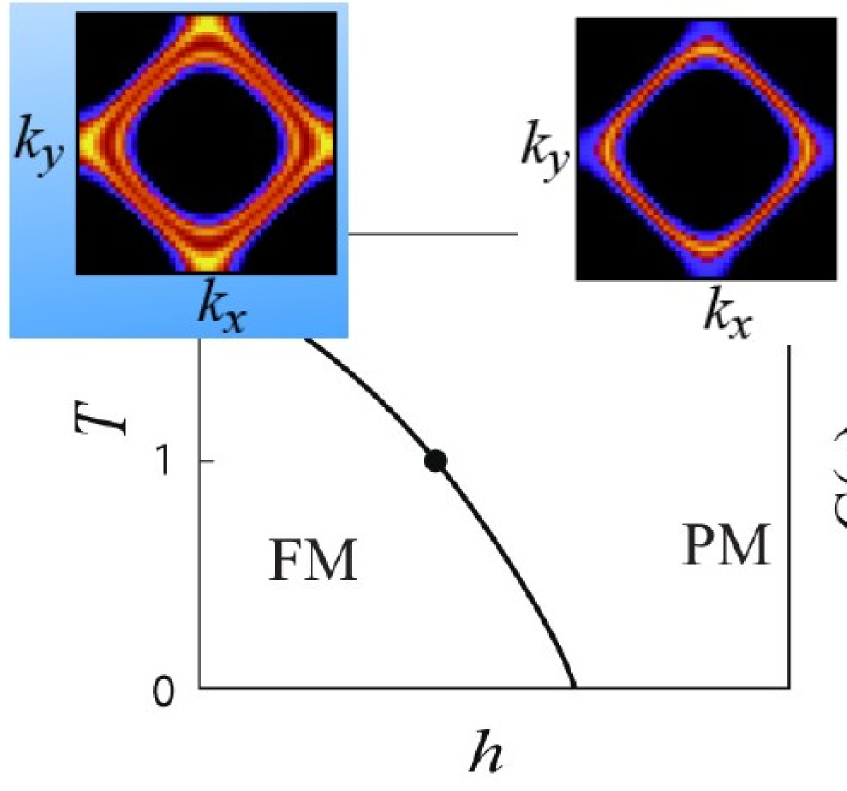
- PRB 95, 041101 (2017)
- PRB 96, 041119 (2017)
- PRL 122, 077601 (2019)

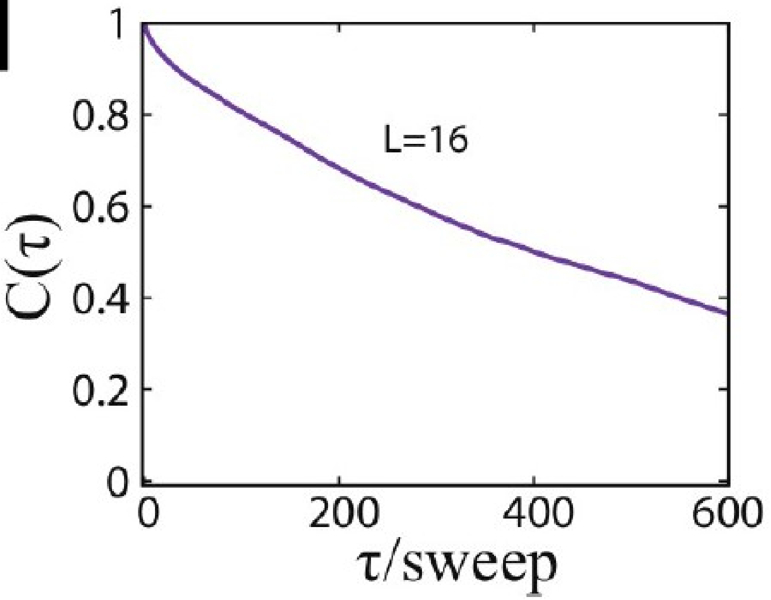
$$A(\mathcal{C} \to \mathcal{C}') = \min\{1, e^{-\beta\left((H(\mathcal{C}') - H_{\text{eff}}(\mathcal{C}')) - (H(\mathcal{C}) - H_{\text{eff}}(\mathcal{C}))\right)}\}$$

SLMC

Fermions coupled to bosonic mode

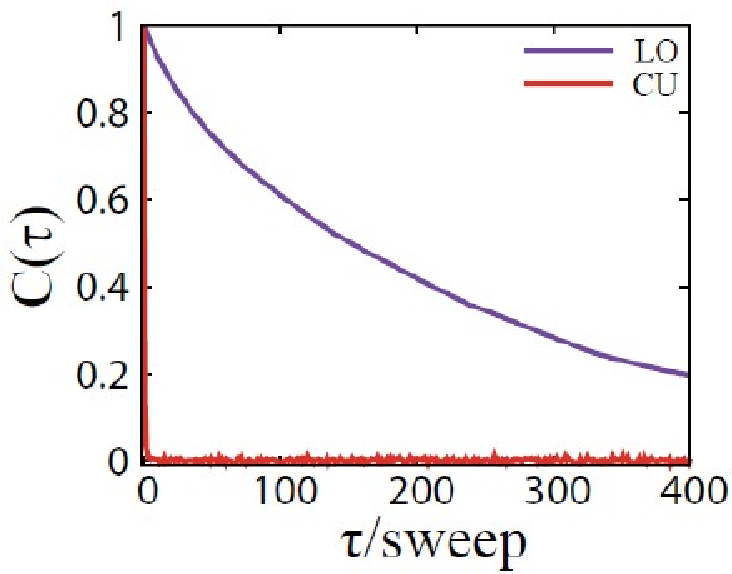
- Itinerant quantum critical point
- Non-Fermi-liquid
- Electron-phonon coupling

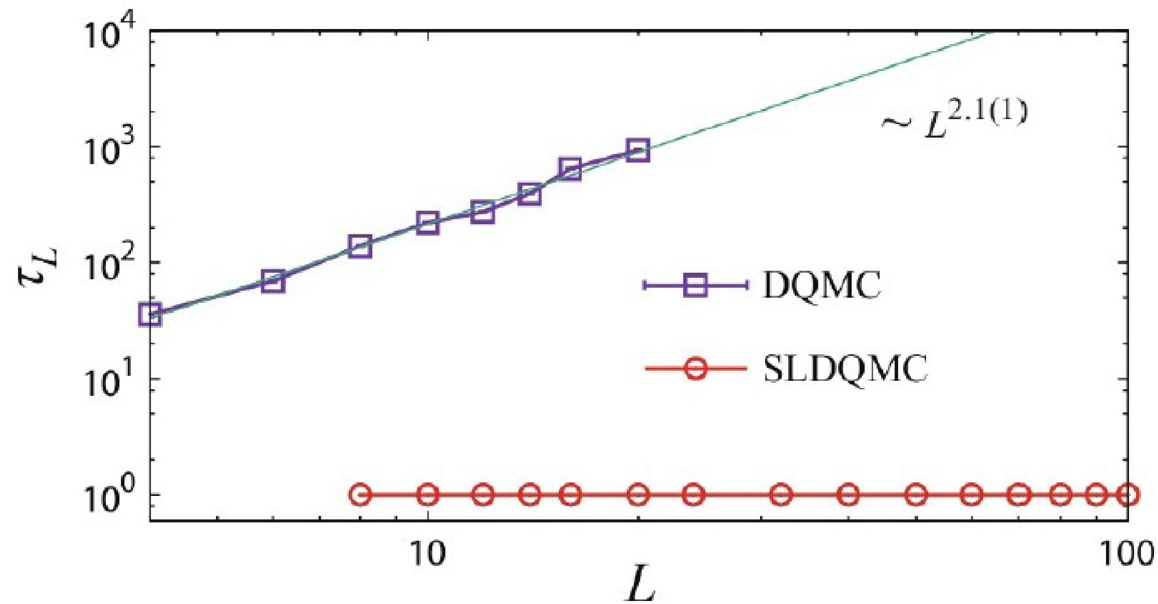




Complexity for getting an independent configuration: $\beta N^3 \tau_L$

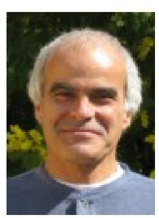
SLMC





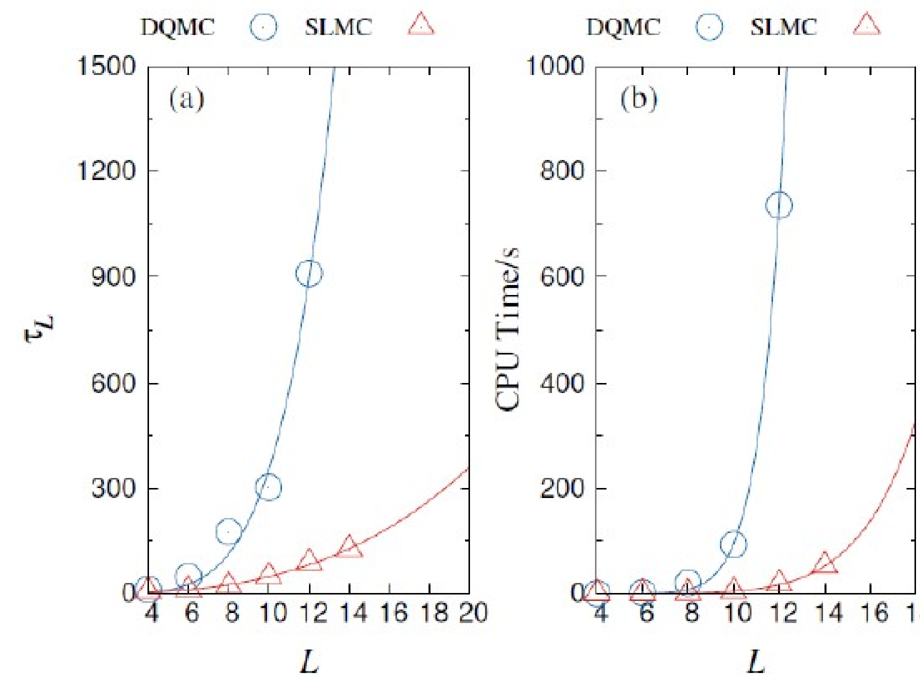
- Self-Learning on electron-phonon model
  Phys. Rev. B 98, 041102(R) (2018)

Chuang Chen



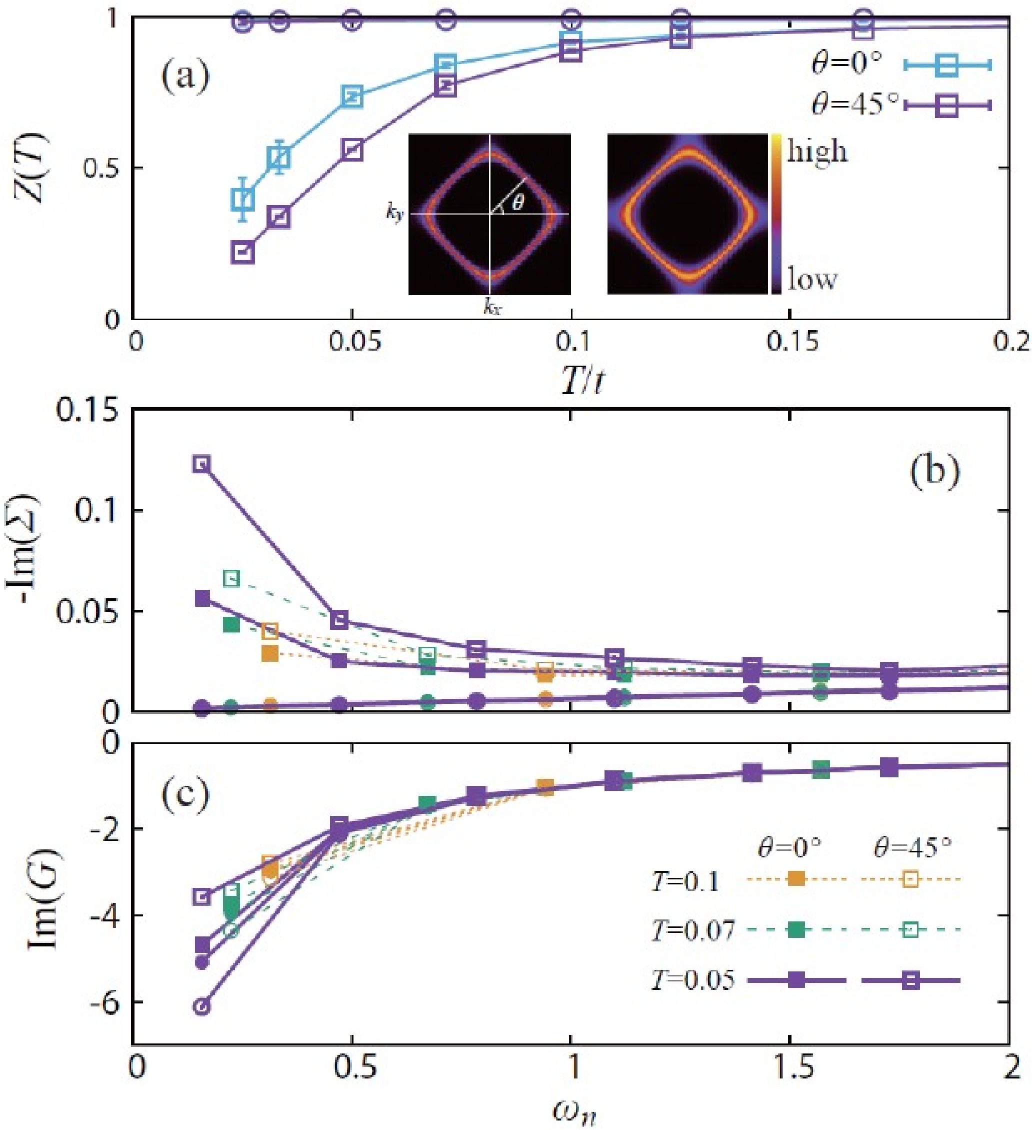
George Batrouni

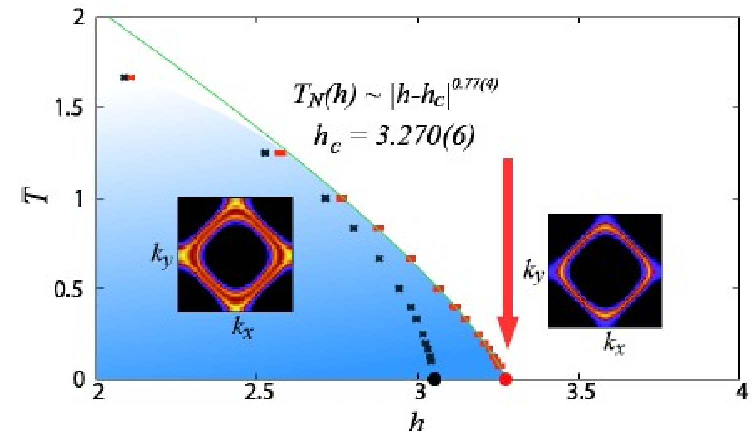
Richard Scalettar



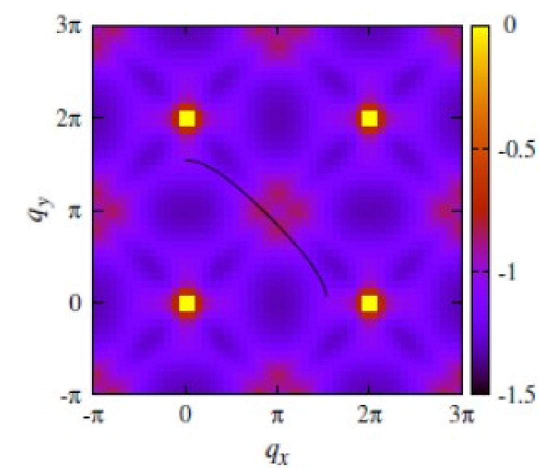
- Dirac Fermions Coupled to Phonons
  Phys. Rev. Lett. 122, 077601 (2019)

Non-Fermi-liquid





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

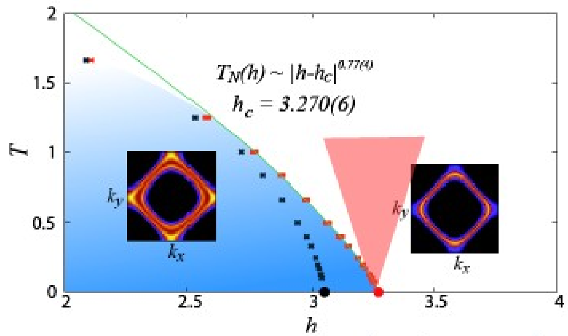


➢ PRX 7, 031101 (2017)

FM-QCP

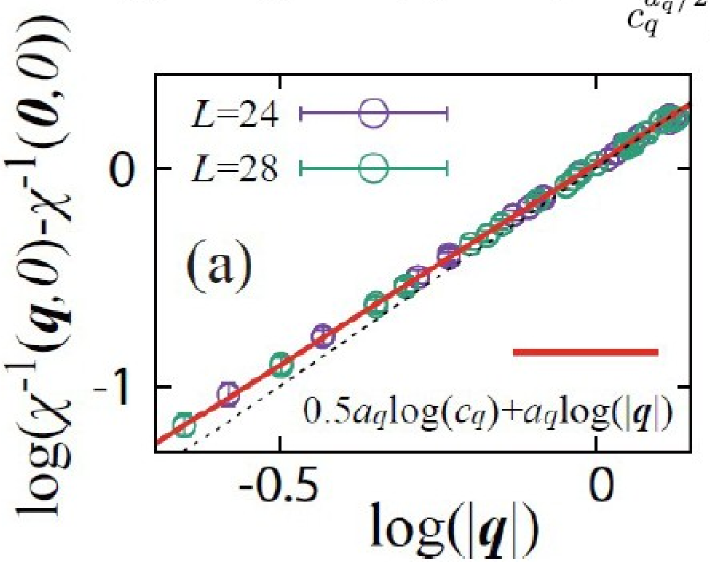
$$\chi(h,T,\mathbf{q},i\omega_n) = \frac{1}{L^2}\sum_{ij}\int_0^\beta d\tau e^{i\omega_n\tau - i\mathbf{q}\cdot\mathbf{r}_{ij}}\langle s_i(\tau)s_j(0)\rangle$$

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



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

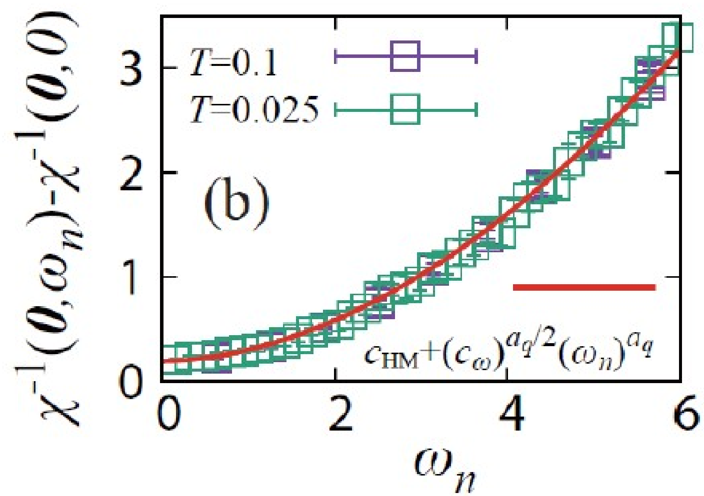
$$\chi(h=h_c, T=0, \mathbf{q}=0, \omega) = \frac{1}{c_\omega^{a_q/2}(\omega_n)^{a_q} + c_{HM}}$$



$a_q = 2 - \eta$

$a_q = 1.85(3)$

$\nu = \gamma / a_q$

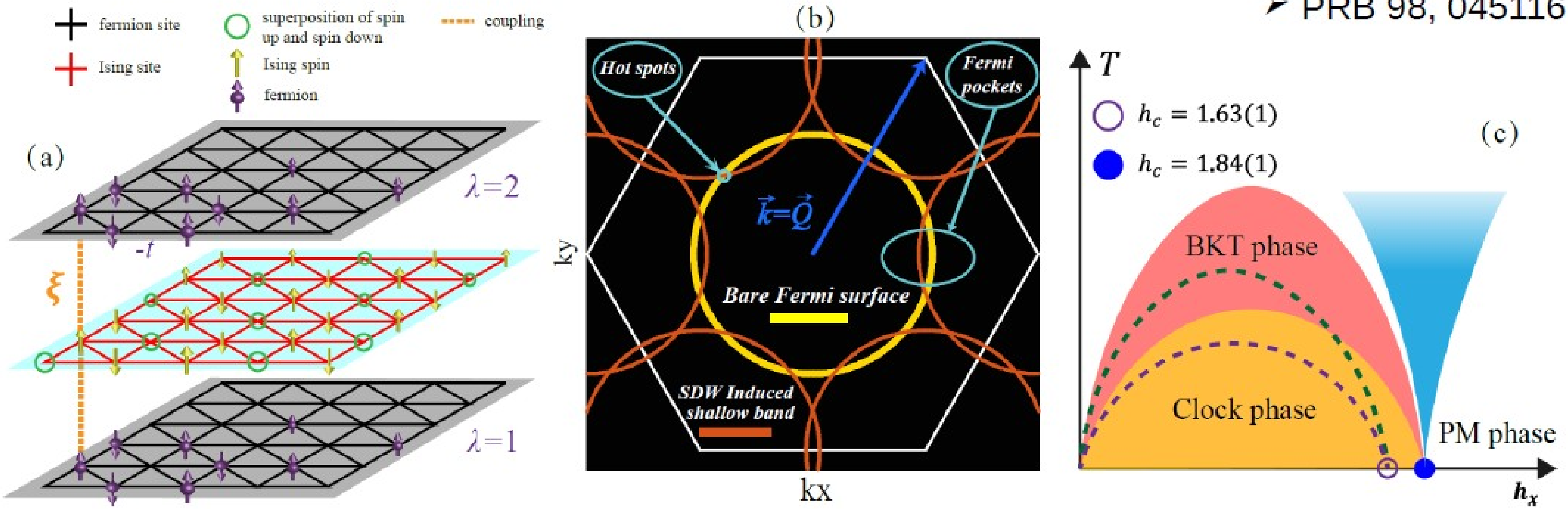


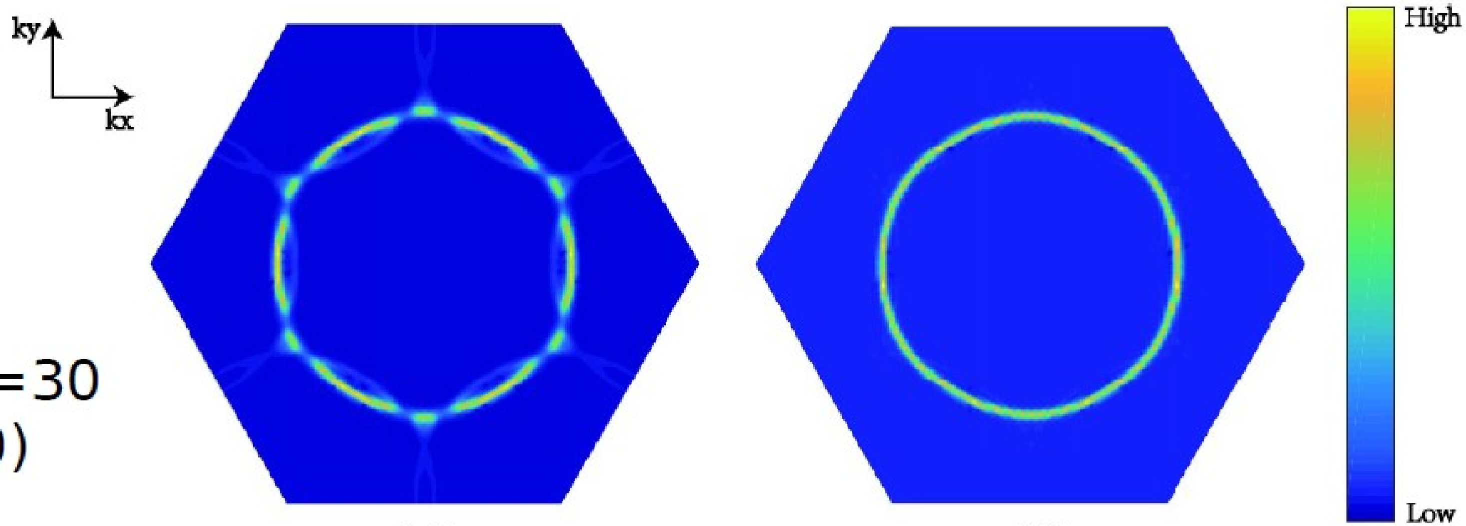
$\eta = 0$	$\nu = 0.5$	$\gamma = 1$	$z = 3$	Hertz-Millis-Moriya
$\eta = 0.04$	$\nu = 0.63$	$\gamma = 1.24$	$z = 1$	(2+1)d Ising model
$\eta = 0.15(3)$	$\nu = 0.64(3)$	$\gamma = 1.18(4)$		Our model

- PRX 7, 031101 (2017)

AFM-QCP

➢ PRB 98, 045116 (2018)



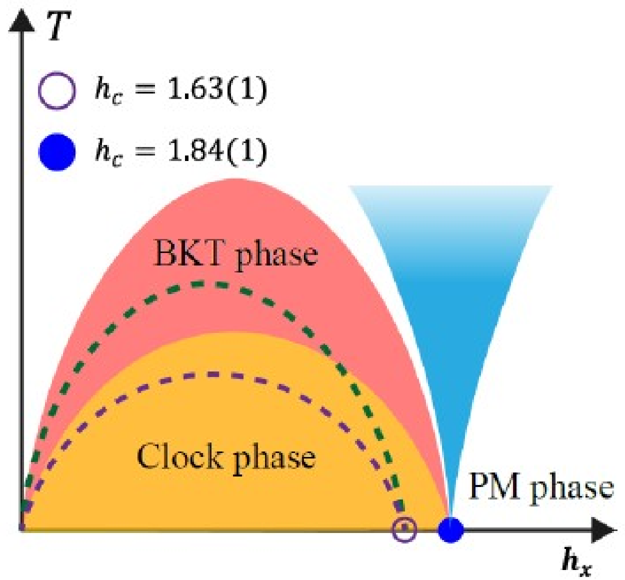


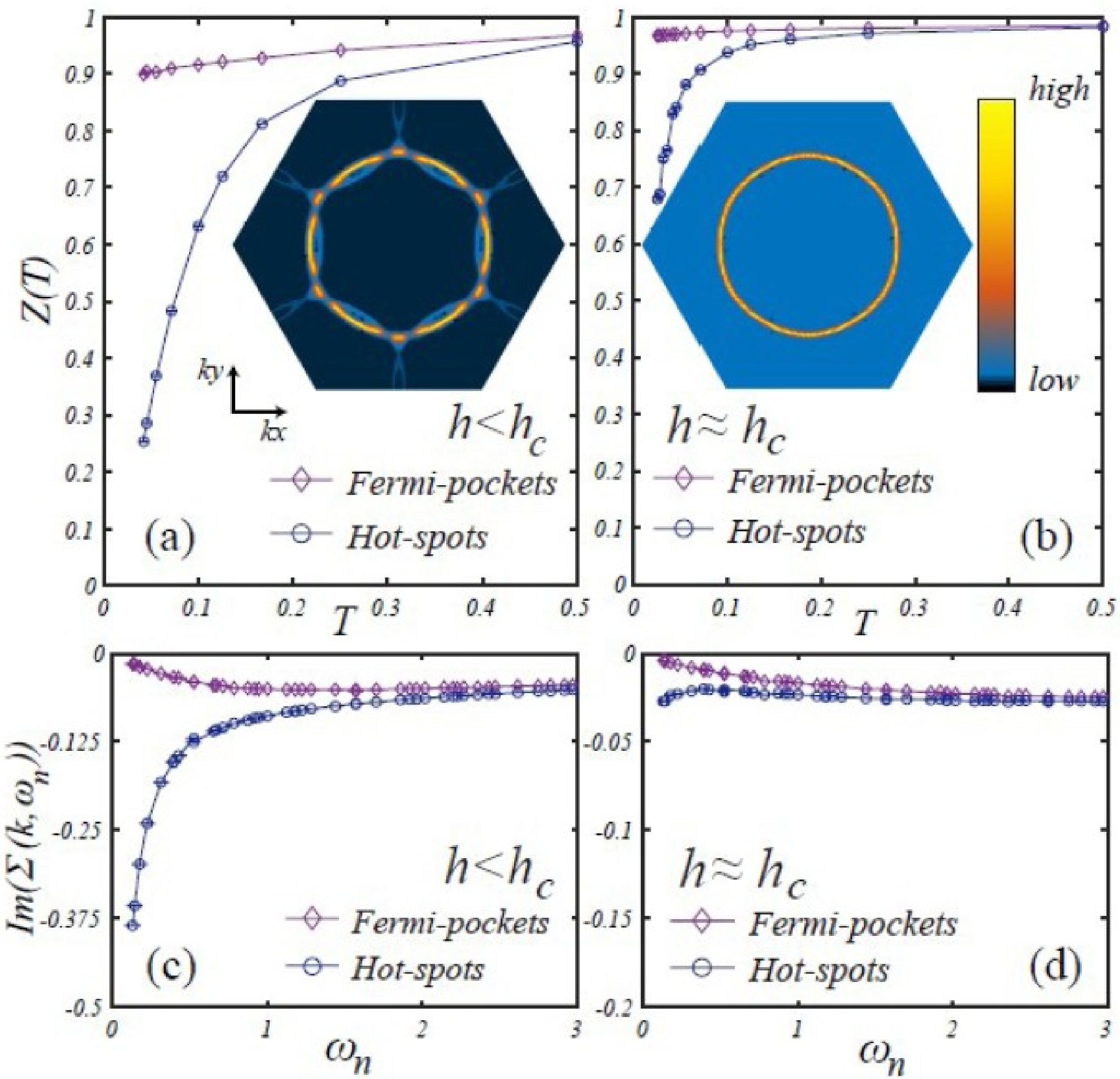
(a) (b)

L=30, beta=30
(30x30x600)

AFM-QCP

- PRB 98, 045116 (2018)



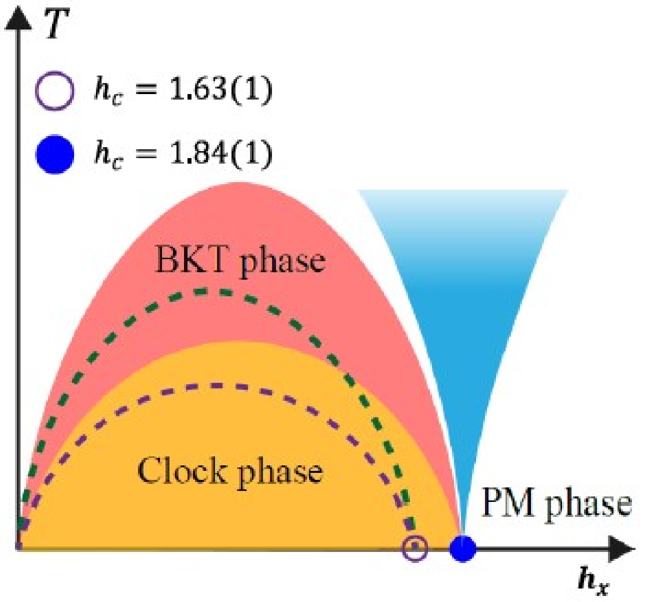


L=30, beta=30
(30x30x600)

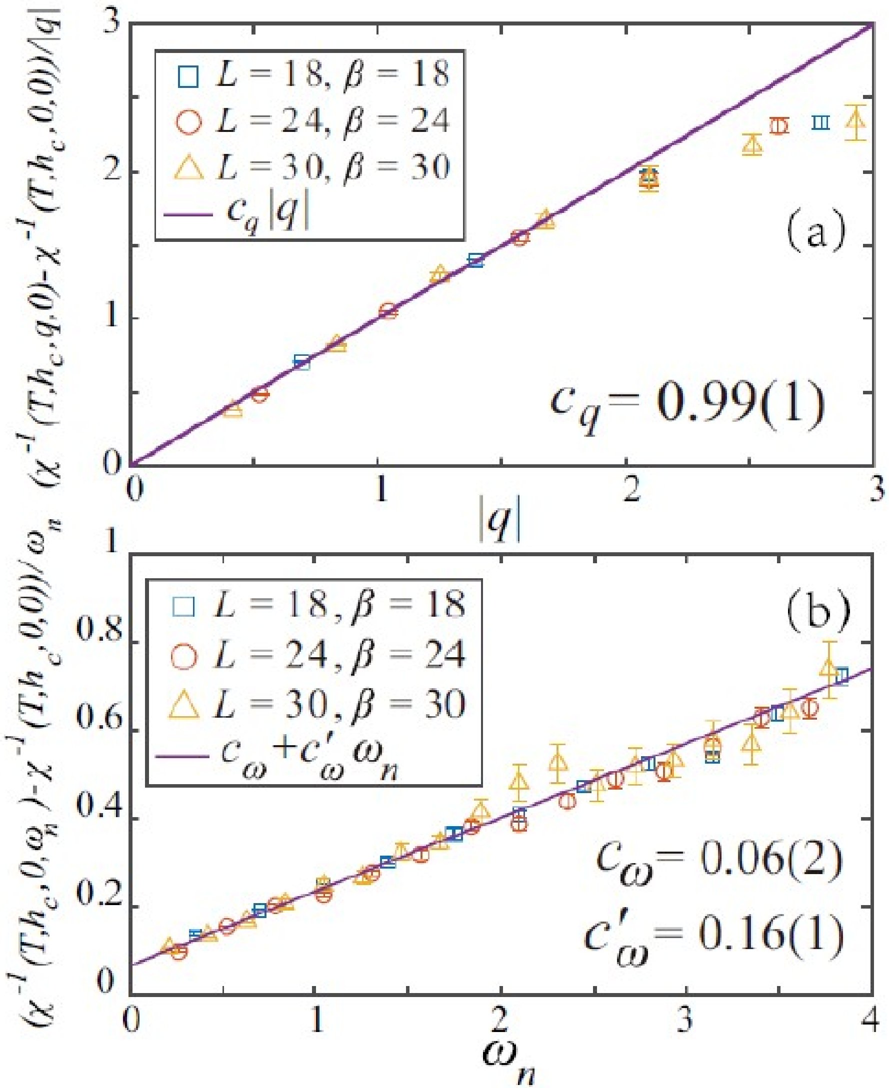
AFM-QCP

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

- PRB 98, 045116 (2018)

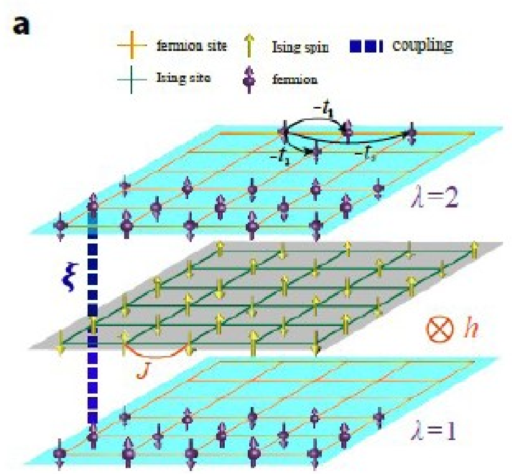


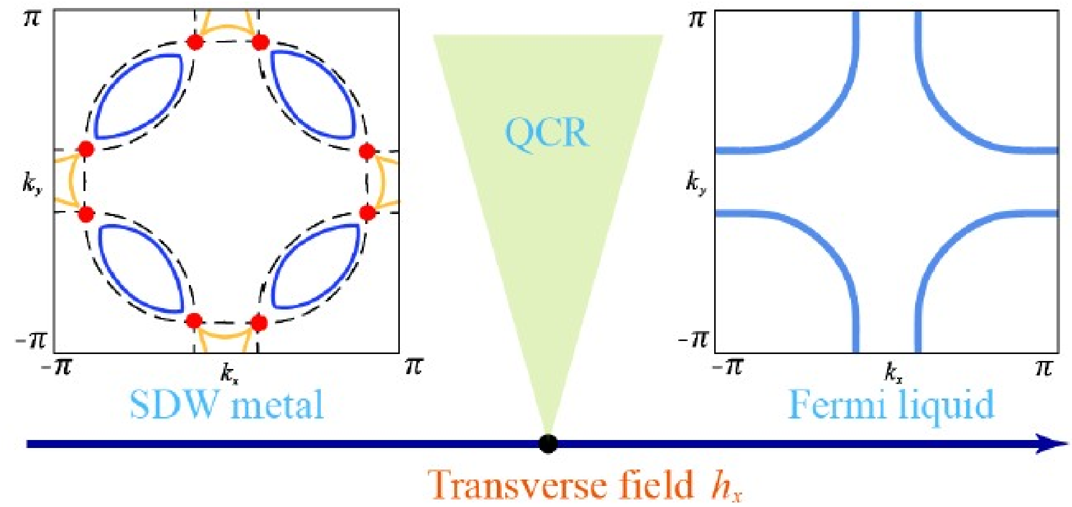
L=30, beta=30
(30x30x600)

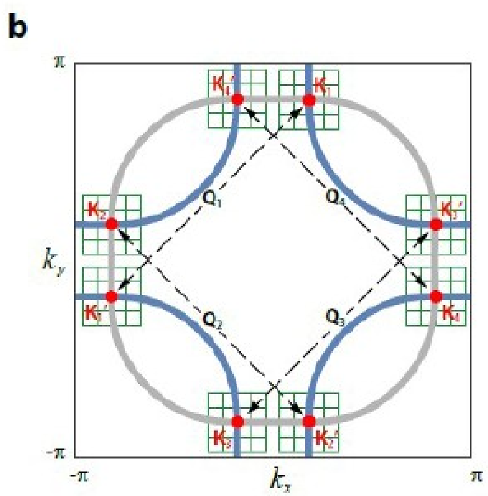


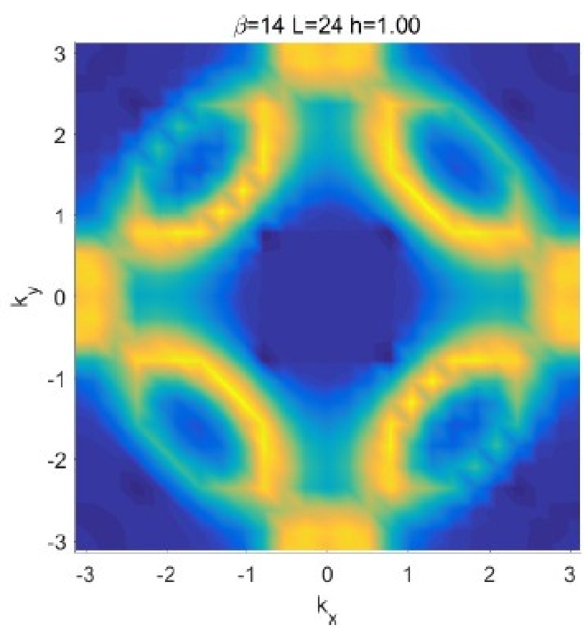
AFM-QCP

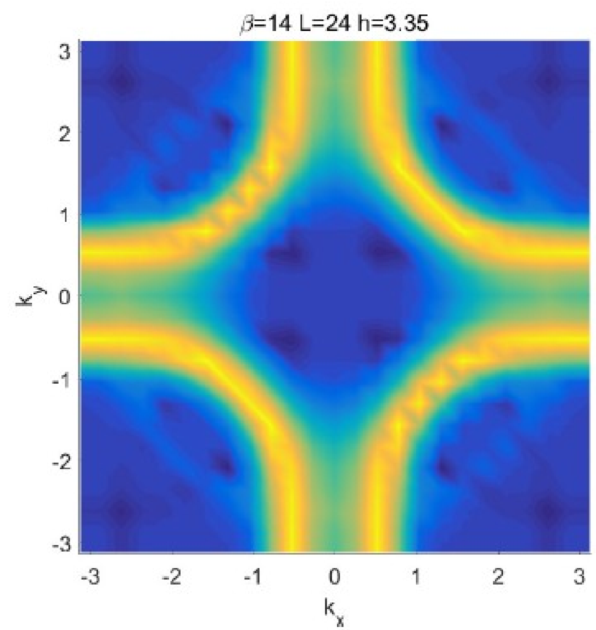
- PNAS 116 (34), 16760-16767 (2019)











EMUS

➢ PRB 99, 085114 (2019)

$$H = H_f + H_b + H_{fb}$$

r-space

$$H_f = \sum_{i,j,a} t_{ij}(c^\dagger_{i,a}c_{j,a} + \text{h.c.})$$

$$H_b = J\sum_{\langle i,j\rangle} s^z_i s^z_j - h\sum_i s^x_i$$

$$H_{fb} = \sum_{i,a,b} \xi_{a,b}\ s^z_i c^\dagger_{i,a}c_{i,b}$$

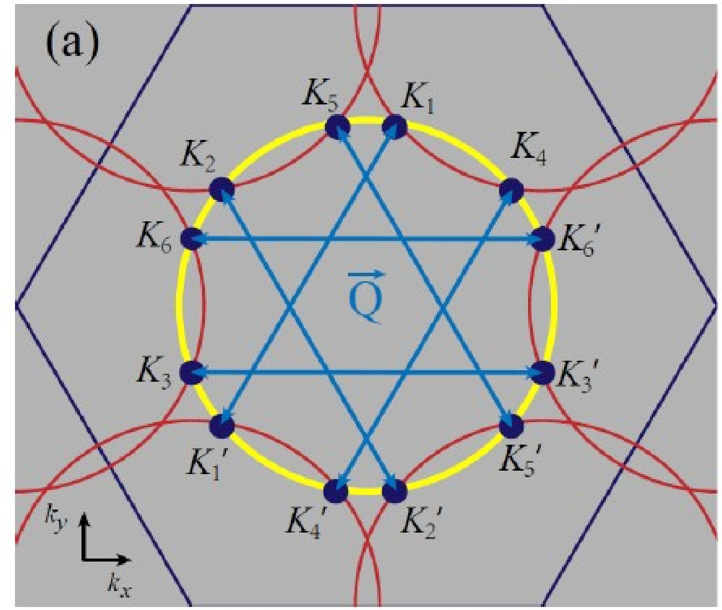
k-space

$$H_f = \sum_{\mathbf{q},l=1,a}^{6} [\epsilon(\mathbf{q}+\mathbf{K}_l) - \mu]c^\dagger_{\mathbf{q},l,a}c_{\mathbf{q},l,a}$$

$$H_b = J\sum_{\langle i,j\rangle} s^z_i s^z_j - h\sum_i s^x_i$$

$$H_{fb} = \sum_{\mathbf{q},\mathbf{q}',l=1,a,b}^{6} s^z(\mathbf{q}-\mathbf{q}'+\mathbf{Q}_l)\ c^\dagger_{\mathbf{q},l,a}c_{\mathbf{q}',l,b}$$

$$s^z(\mathbf{k}) = \frac{1}{N}\sum_i s^z_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}$$



$$\text{Hotspot pairs}: \ \{\mathbf{K}_l, \mathbf{K}'_l\},\ l = 1,\cdots,6$$

$$\text{AF wavevector}: \ \pm\mathbf{Q}_l = \mathbf{K}_l - \mathbf{K}'_l$$

$$\mathbf{k} - \mathbf{k}' = (\mathbf{q}+\mathbf{K}_l) - (\mathbf{q}'+\mathbf{K}'_l) = (\mathbf{q}-\mathbf{q}') + \mathbf{Q}_l$$

SLAC fermion, Lang & Laeuchli

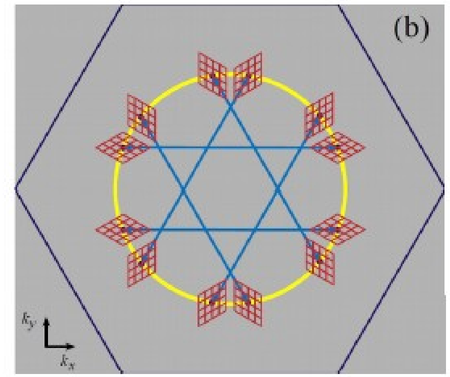
➢ PRL 123, 137602 (2019)

EMUS

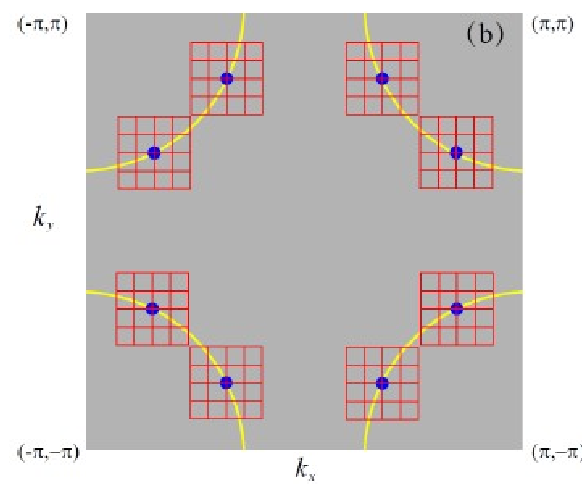
➢ PRB 99, 085114 (2019)

$$\mathbf{T} = \begin{bmatrix} t_1 & & & \\ & t_2 & & \\ & & \ddots & \\ & & & t_6 \end{bmatrix}_{N} \quad t_1 \rightarrow \begin{bmatrix} \epsilon(\mathbf{q}+\mathbf{K}_1)-\mu & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & \epsilon(\mathbf{q}'+\mathbf{K}'_1)-\mu & 0 \\ 0 & 0 & 0 & \ddots \end{bmatrix}_{N_f}$$

$$\mathbf{V} = \begin{bmatrix} v_1 & & & \\ & v_2 & & \\ & & \ddots & \\ & & & v_6 \end{bmatrix}_{N} \quad v_1 \rightarrow \begin{bmatrix} 0 & 0 & s^z(\mathbf{q}-\mathbf{q}'+\mathbf{Q}_1) & \cdots \\ 0 & 0 & \vdots & \ddots \\ s^z(\mathbf{q}'-\mathbf{q}-\mathbf{Q}_1) & \cdots & 0 & 0 \\ \vdots & \ddots & 0 & 0 \end{bmatrix}_{N_f}$$



- Computational complexity $O(\beta N^3) \rightarrow O(\beta N_f^3)$
- Naturally integrated in SLMC
- Generic in finite Q models



AFM-QCP

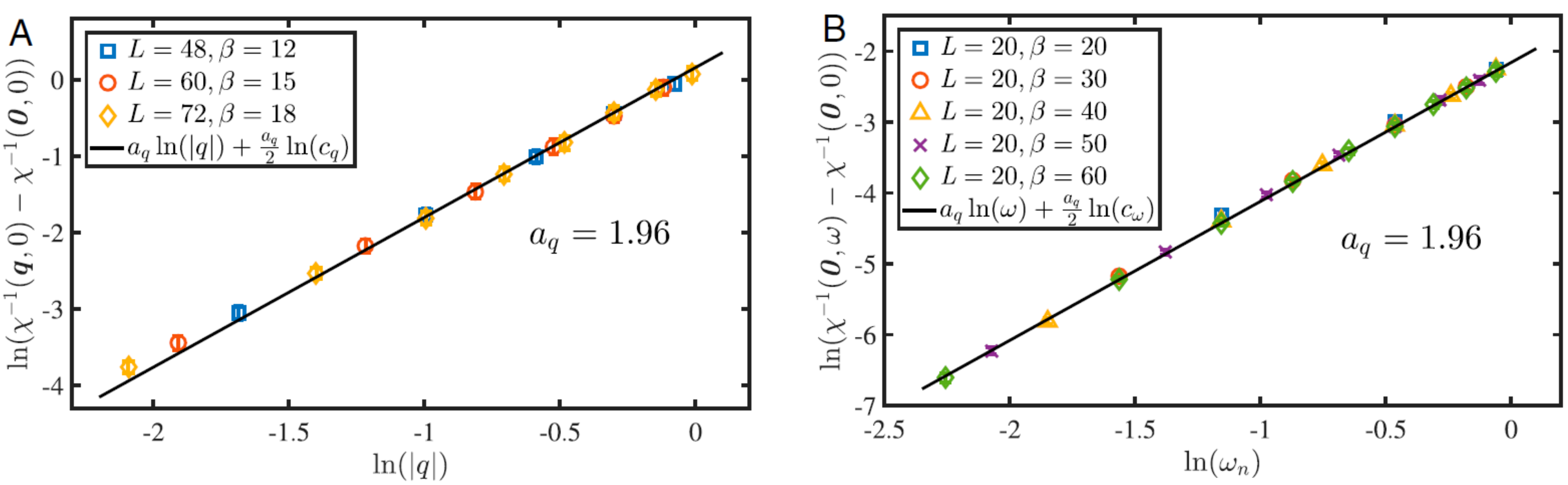
➢ PNAS 116 (34), 16760-16767 (2019)

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

$$\chi(T,h_c,\mathbf{q},\omega_n) = \frac{1}{c_t T^2 + (c_q|\mathbf{q}|^2 + c_\omega \omega^2)^{a_q/2}}$$

Bare boson (2+1)D Ising

$$a_q = 2 - \eta = 1.96$$



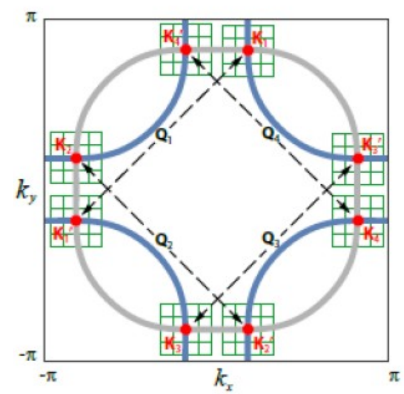
AFM-QCP

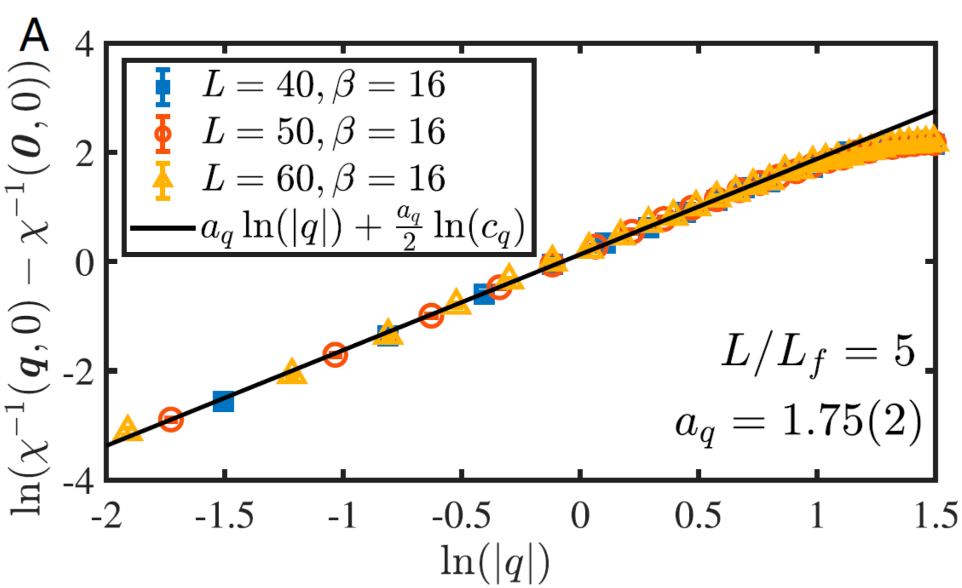
- A. Abanov, A. Chubukov, J. Schmalian, Adv. in Phys., 52, 119 (2003)
- PNAS 116 (34), 16760-16767 (2019)

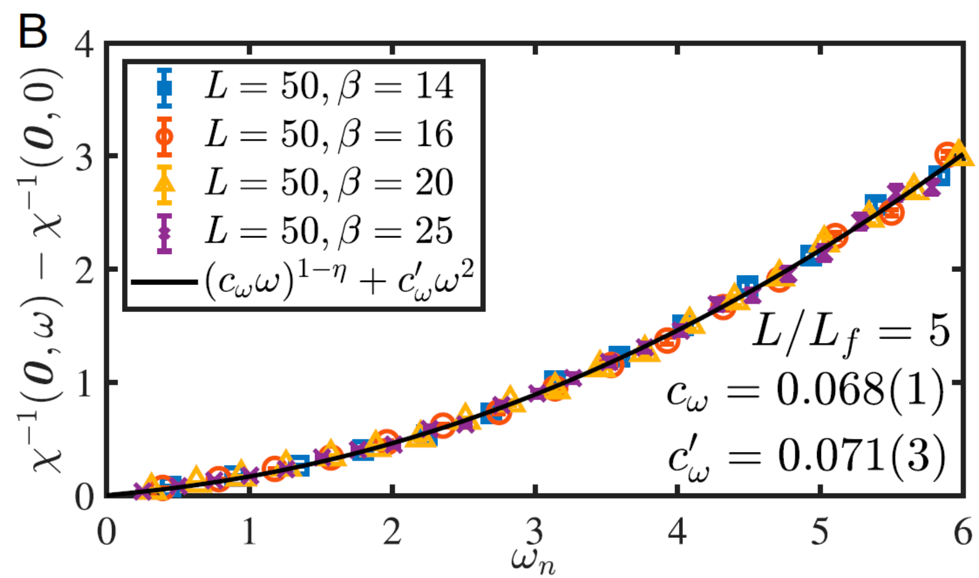
$$\chi(\mathbf{q},\omega_n) \propto \frac{1}{(c_q|\mathbf{q}|^2 + c_\omega \omega)^{a_q/2} + c'_\omega \omega^2}$$

$$a_q = 2(1-\eta) \qquad \eta = \frac{2}{N_{hs}} = 0.125 \text{ (with } N_{hs} = 16)$$

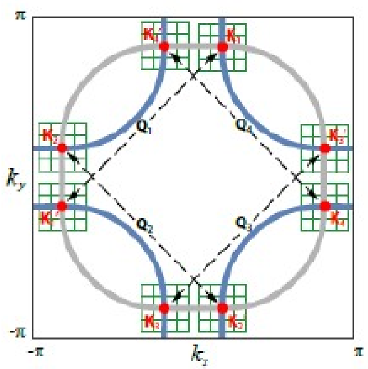
RG calculations seem to predict $\eta = 1/N_{hs}$?







AFM-QCP



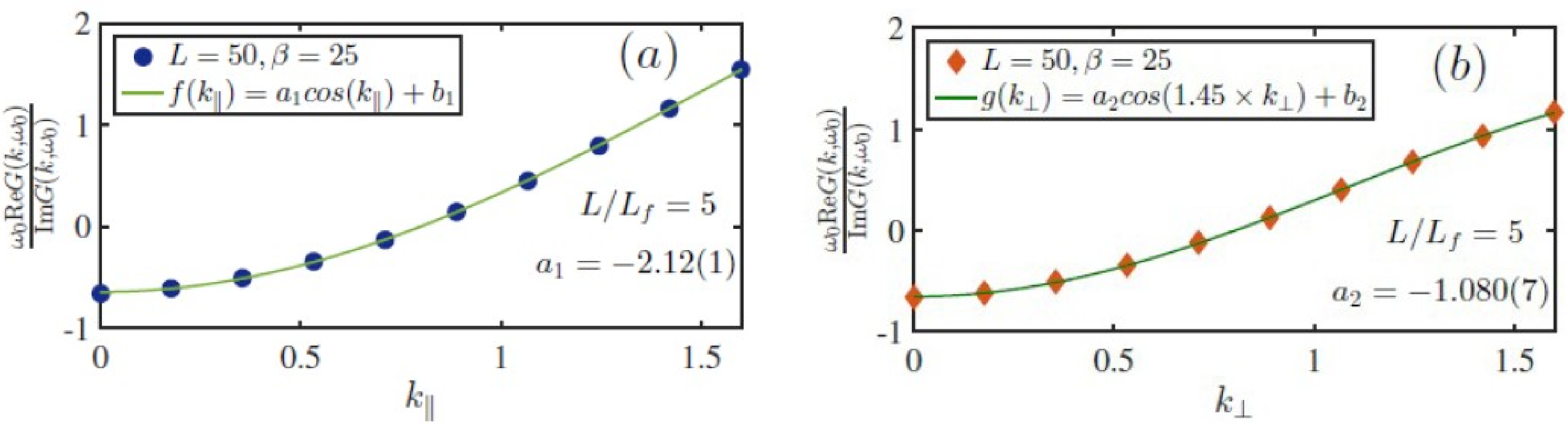
- M. Metlitski, S. Sachdev, PRB 82, 075128 (2010)

rotation of fermi velocity ?

$$\mathbf{v}_F = \frac{\partial}{\partial_{\mathbf{k}}} \frac{\omega_0 \mathrm{Re}G(k,\omega_0)}{\mathrm{Im}G(k,\omega_0)}\bigg|_{\mathbf{k}=\mathbf{k}_F}$$

Hot spots location	k_x	k_y
	2.5800	0.5615

v_F at hot spots	$v_\parallel$	$v_\perp$
Near QCP	1.523(8)	1.435(8)
Free fermion	1.506	1.468



- PNAS 116 (34), 16760-16767 (2019)

Fermion QCPs with QMC

- Ferromagnetic/nematic QCP zero $\mathbf{Q}$

➢ PRX 7, 031101 (2017)

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

$$a_q = 2 - \eta \text{ with } \eta = 0.15(3)$$

- Antiferromagnetic QCP finite $\mathbf{Q}$
  - Triangle lattice $3\mathbf{Q}_{\mathrm{AF}} = \Gamma$

➢ PRB 98, 045116 (2018)

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

  - Square lattice $2\mathbf{Q}_{\mathrm{AF}} = \Gamma$

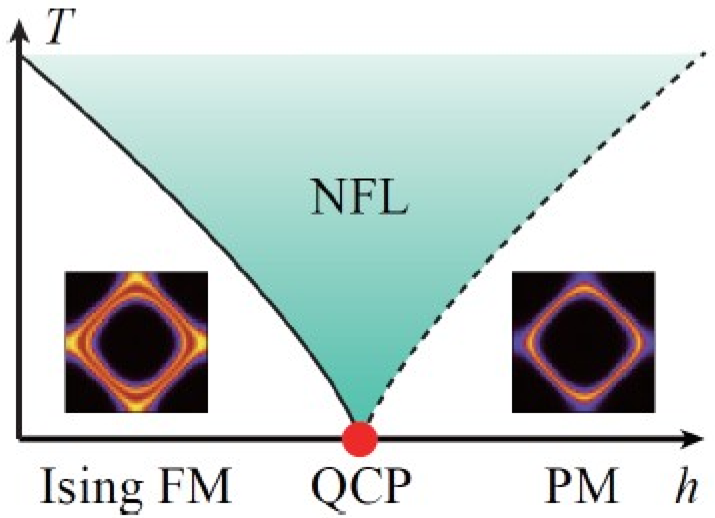
➢ PNAS 116 (34), 16760 (2019)

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

$$\eta = \frac{2}{N_{hs}} = 0.125 \text{ (with } N_{hs} = 16)$$

Tidbits from Monte Carlo

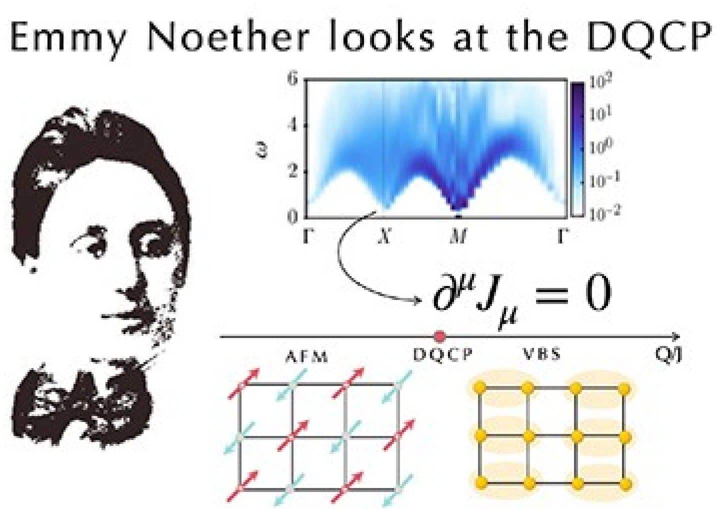
- Fermions couple to critical bosonic modes



- Itinerant quantum critical point
- Non-Fermi-liquid
- Self-learning Monte Carlo methods
- Matter fields couple to guage fields
- Alegbraic spin liquid, orthogonal metal

……

- Designer spin/boson models QMC



- DQCP & Gauge and matter fields
- Emergent continuous symmetry
- Dynamical signatures of topological order and spin liquids
- Duality between SPT transitions and DQCP

……

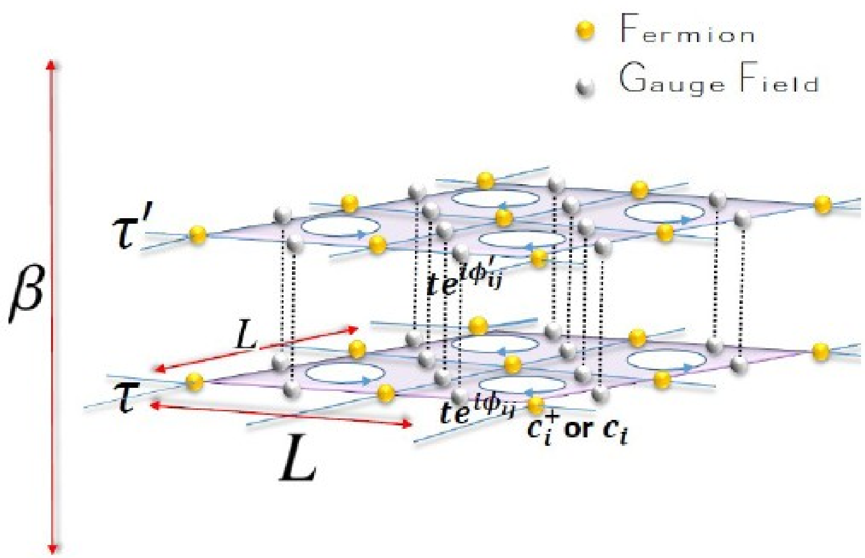
PHYSICAL REVIEW X **9**, 021022 (2019)

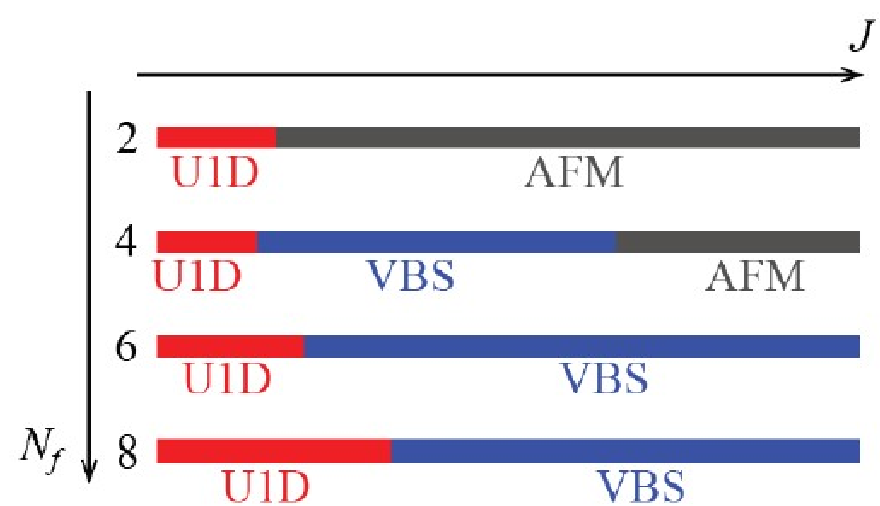
Monte Carlo Study of Lattice Compact Quantum Electrodynamics with Fermionic Matter: The Parent State of Quantum Phases

Xiao Yan Xu,[1,*] Yang Qi,[2–4,†] Long Zhang,[5] Fakher F. Assaad,[6] Cenke Xu,[7] and Zi Yang Meng[8,9,10,11,‡]

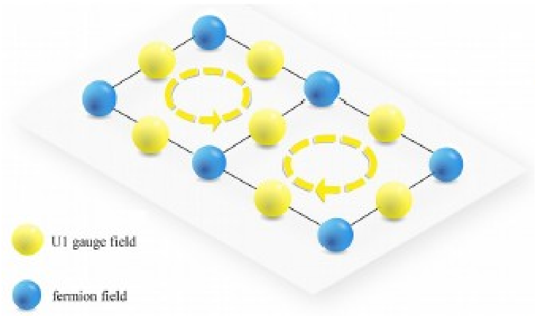
Directly simulate U(1) gauge field couples to fermionic matter

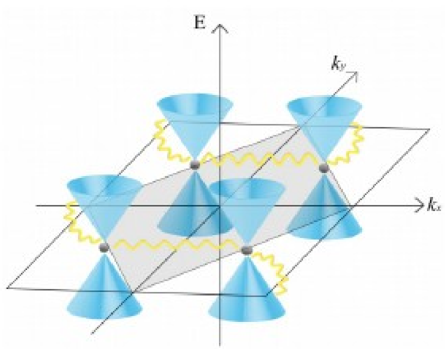
$$H=\frac{1}{2}JN_f\sum_{\langle i,j\rangle}\frac{1}{4}\hat{L}_{ij}^2-t\sum_{\langle i,j\rangle\alpha}\left(\hat{c}_{i\alpha}^{\dagger}e^{i\hat{\theta}_{ij}}\hat{c}_{j\alpha}+\text{h.c.}\right)+\frac{1}{2}K\,N_f\sum_{\square}\cos\left(\text{curl}\hat{\theta}\right)$$





U1 gauge field couple to matter field



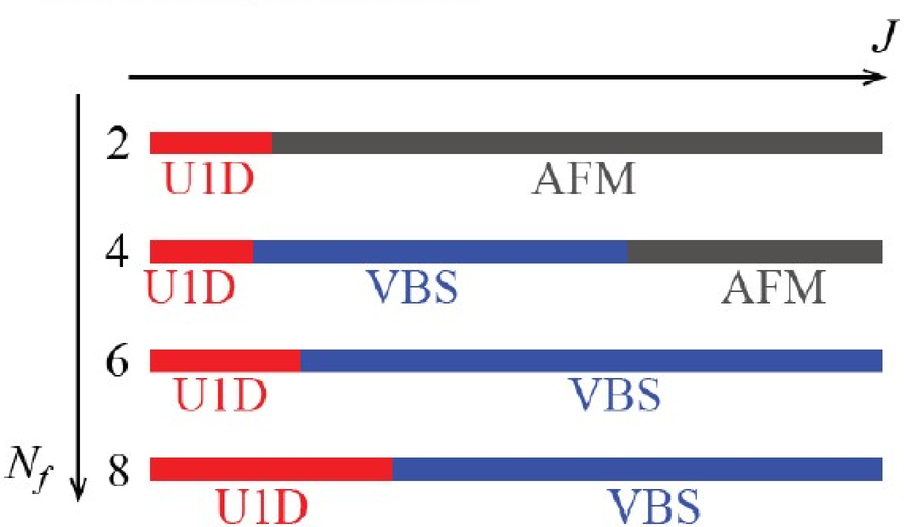


$$Z=\int D(\phi,\bar{\psi},\psi)e^{-(S_\phi+S_F)} \quad S=S_F+S_\phi=\int_0^\beta d\tau(L_F+L_\phi)$$

$$L_F=\sum_{\langle i,j\rangle\alpha}\psi^\dagger_{i\alpha}\left[(\partial_\tau-\mu)\delta_{ij}-te^{i\phi_{ij}}\right]\psi_{j\alpha}+\text{h.c.},$$

$$L_\phi=\frac{4}{JN_f\Delta\tau^2}\sum_{\langle i,j\rangle}\left(1-\cos(\phi_{ij}(\tau+1)-\phi_{ij}(\tau))\right)+\frac{1}{2}KN_f\sum_{\square}\cos\left(\text{curl}\phi\right)$$

See the Chap. 6 in Xiao-Gang Wen's Book



$$Z=\int D(\phi,\bar{\psi},\psi)e^{-(S_\phi+S_F)}=\int D\phi e^{-S_\phi}\text{Tr}_\psi\left[e^{-S_F}\right]$$

$$\text{Tr}_\psi\left[e^{-S_F}\right]=\left[\det\left(I+\prod_{z=1}^{L_\tau}B_z\right)\right]^{N_f}$$

➢ PRX 9, 021022 (2019)

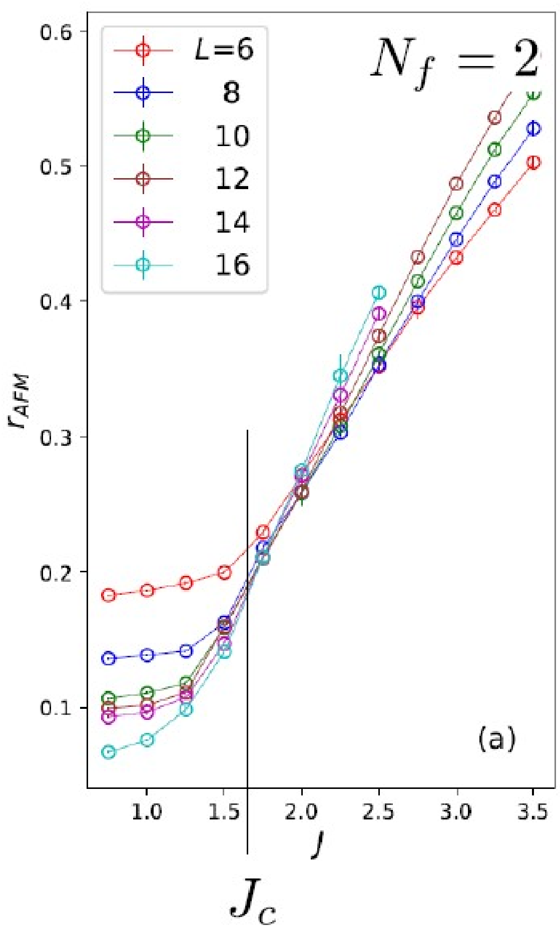
U1 gauge field couple to matter field

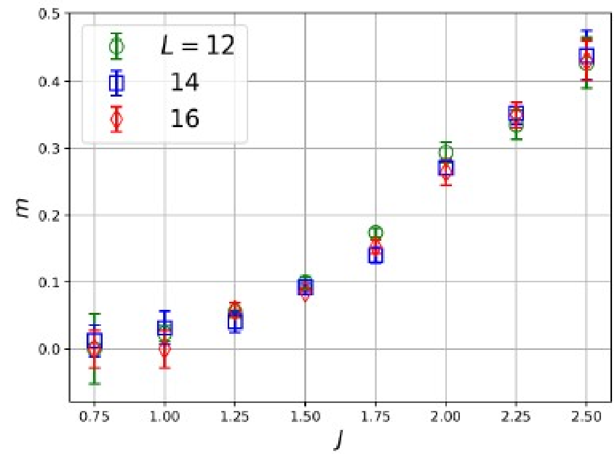
$$\chi_S(\mathbf{k}) = \frac{1}{L^4}\sum_{ij}\sum_{\alpha\beta}\langle S^{\alpha}_{\beta}(i)S^{\beta}_{\alpha}(j)\rangle e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$$

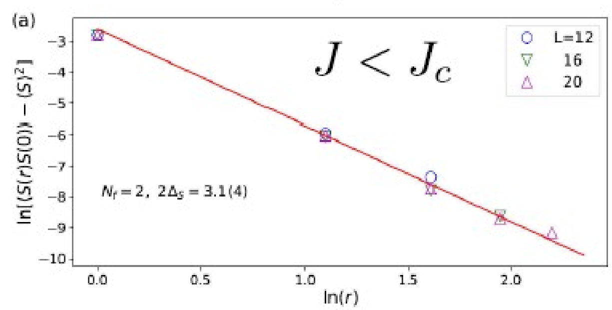
$$r_{\mathrm{AFM}} = 1 - \frac{\chi_S(\mathbf{X}+\delta\mathbf{q})}{\chi_S(\mathbf{X})}$$

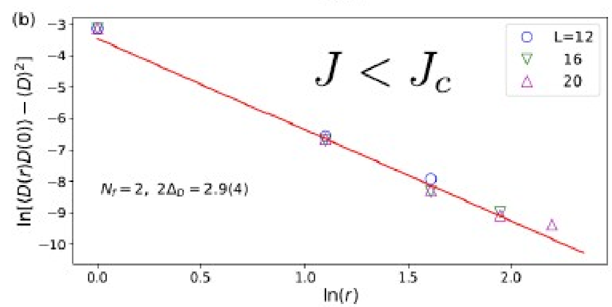
$$\chi_D(\mathbf{k}) = \frac{1}{L^4}\sum_{ij}(\langle D_i D_j\rangle - \langle D_i\rangle\langle D_j\rangle)e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$$

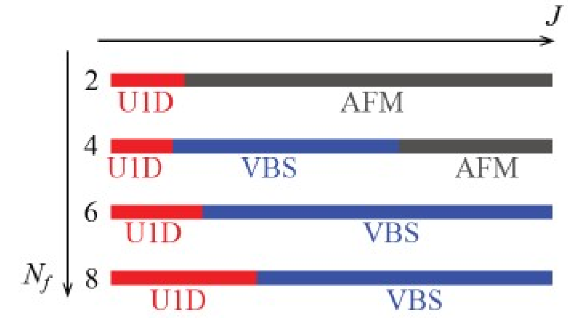
$$r_{\mathrm{VBS}} = 1 - \frac{\chi_D(\mathbf{M}+\delta\mathbf{q})}{\chi_D(\mathbf{M})}$$

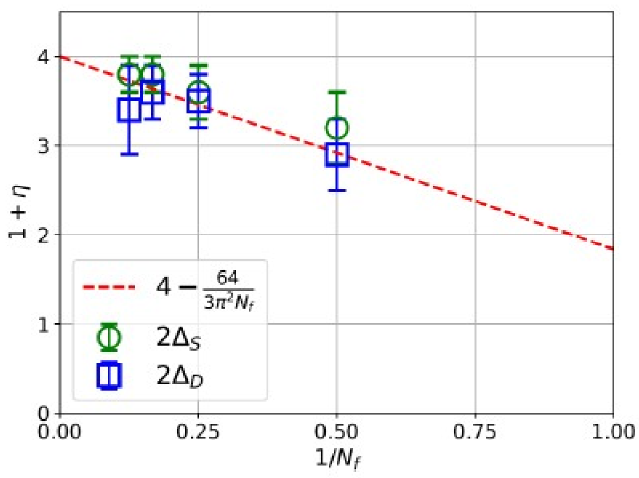












➢ PRX 9, 021022 (2019)

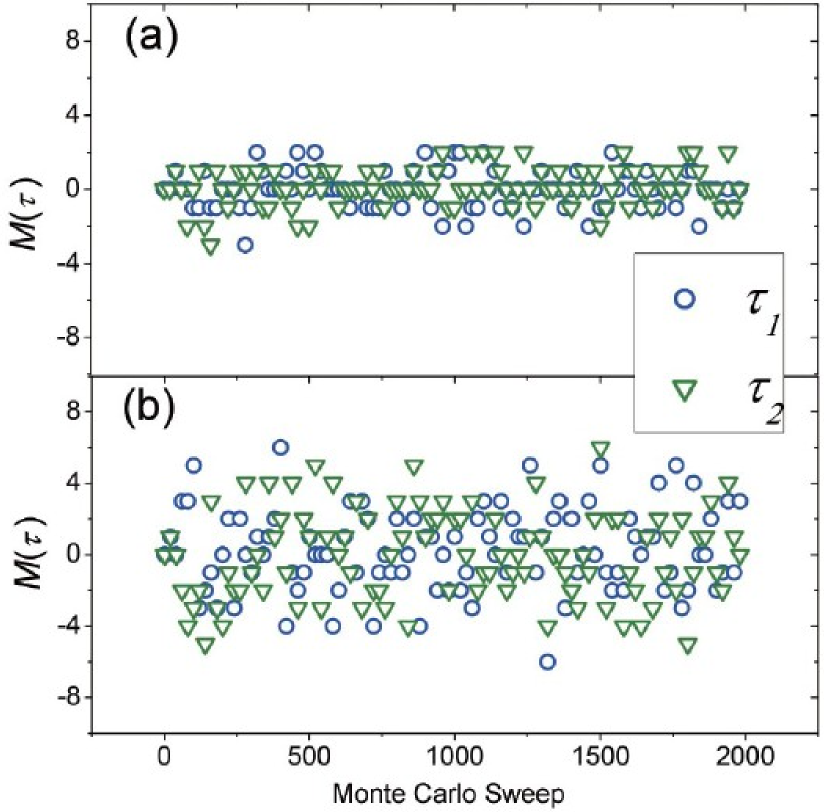
U1 gauge field couple to matter field

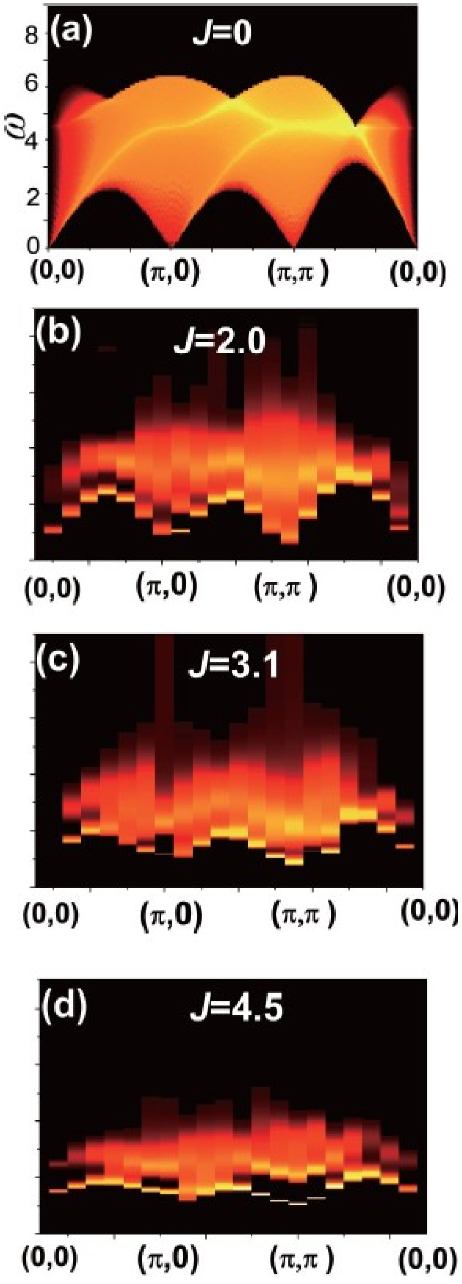
$$\sum_{b\in\square}\phi_b = \Phi_\square + 2\pi m_\square \qquad M(\tau) = \sum_{\square} m(\tau)$$

$$L = 12, \beta = 2L$$

$J = 1.8$

$J = 3.5$





Monopole proliferation leads to confinement of gauge field

- Wei Wang, et. al. PRB 100, 085123 (2019)

U1 gauge field couple to matter field

QED3-Gross-Neveu at O(1/Nf) and O(1/Nf^2), three loops, four loops, epsilon-expansion

- J. A. Gracey, Phys. Rev. D 98, 085012 (2018)
- B. Ihrig, L. Janssen, L. N. Mihaila, and M. M. Scherer, Phys. Rev. B 98, 115163 (2018)
- N. Zerf, P. Marquard, R. Boyack, and J. Maciejko, Phys. Rev. B 98, 165125 (2018)
- R. Boyack, A. Rayyan, and J. Maciejko, Phys. Rev. B 99, 195135 (2019)

1/N Aslamazov-Larkin digrams

- N. Zerf, R. Boyack, P. Marquard, J. A. Gracey, and J. Maciejko, arXiv:1905.03719

Monopoles in QED3-Gross-Neveu theory

- X.-Y. Song, Y.-C. He, A. Vishwanath, and C. Wang, arXiv:1811.11182 (2018)
- X.-Y. Song, C. Wang, A. Vishwanath, and Y.-C. He, arXiv:1811.11186 (2018)
- E. Dupuis, M. Paranjape, and W. Witczak-Krempa, arXiv:1905.02750

Z2 gauge field couple to matter field

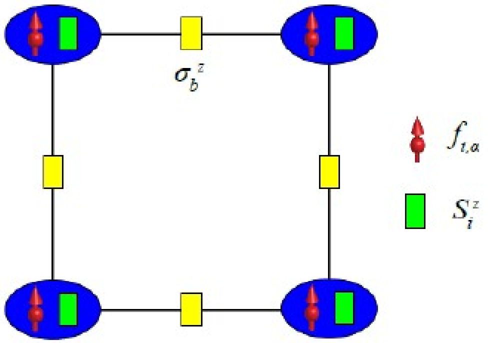
$$H = H_f + H_z + H_g$$

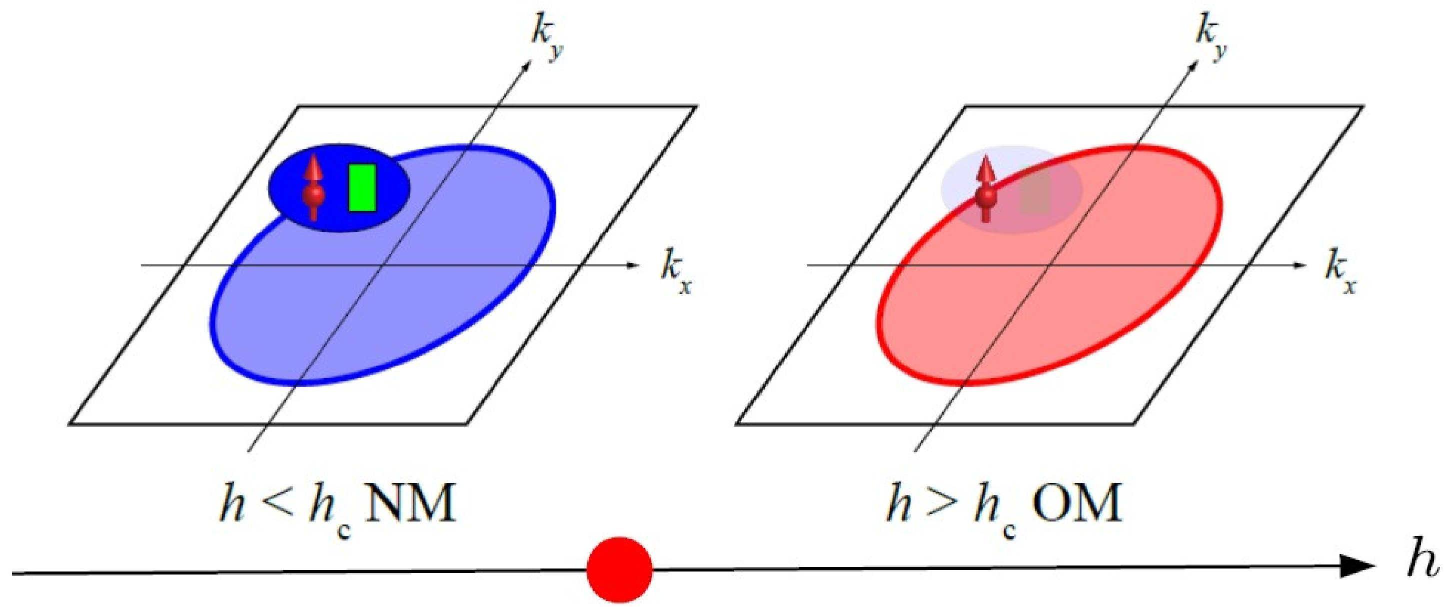
composite fermion: $c_{i,\alpha} = f_{i,\alpha} S_i^z$

$$H_f = -t\sum_{\langle i,j\rangle}(f^\dagger_{i,\alpha}\sigma^z_{b_{\langle i,j\rangle}} f_{j,\alpha} + h.c.) - \mu\sum_i f^\dagger_{i,\alpha} f_{i,\alpha}, \qquad t=1$$

$$H_z = -J\sum_{\langle i,j\rangle} S^z_i \sigma^z_{b_{\langle i,j\rangle}} S^z_j - h\sum_i S^x_i, \qquad J=1$$

$$H_g = -K\sum_{\square}\prod_{b\in\square}\sigma^z_b - g\sum_b \sigma^x_b. \qquad K=1, g=0.5$$

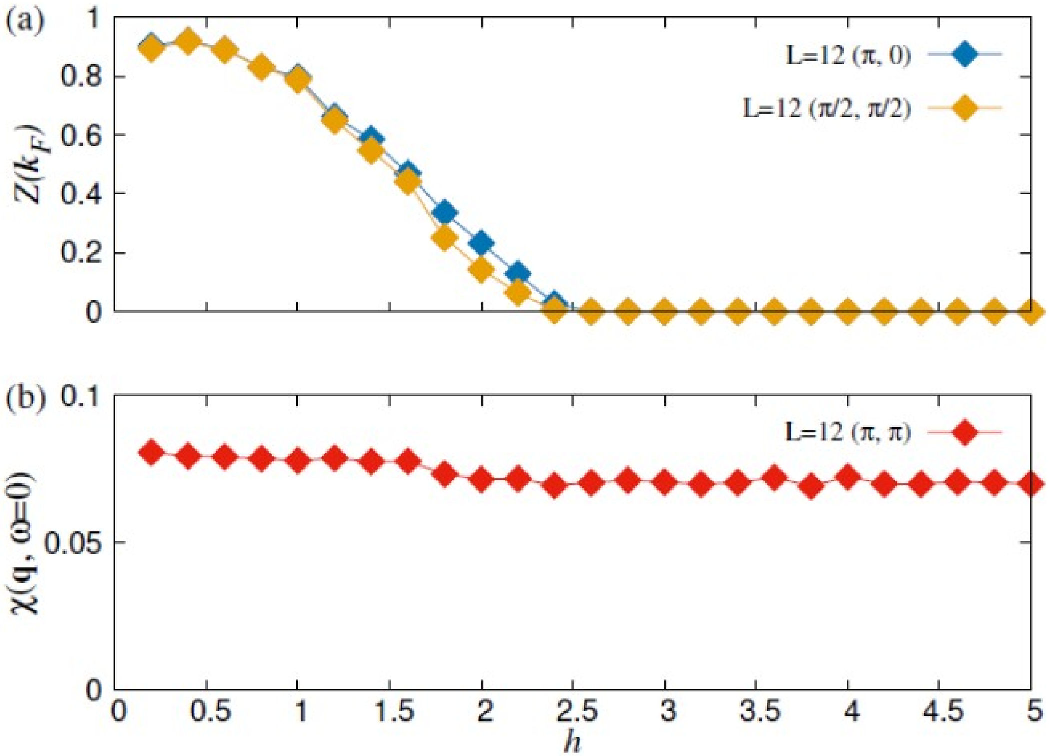




- Chuang Chen et al., arXiv:1904.12872
- Gazit, Assaad, Sachdev, arXiv:1906.11250
- Hohenadler, Assaad, PRL 121, 086601 (2018)
- Hohenadler, Assaad, PRB 100, 125133 (2019)

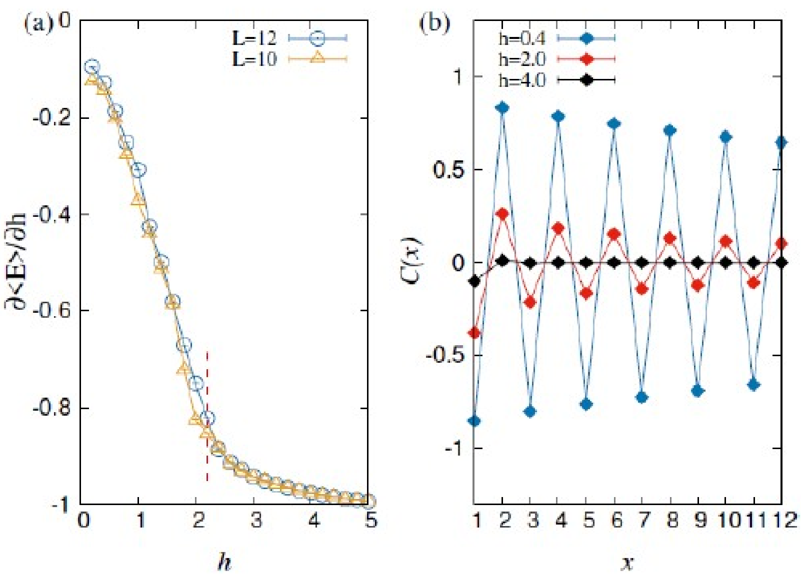
Z2 gauge field couple to matter field

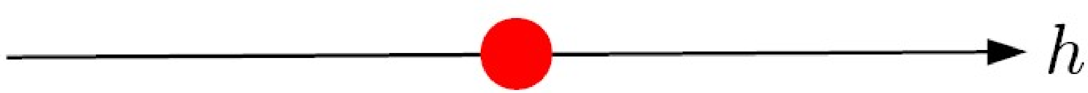
Continuous phase (Higgs) transition between NM and OM without symmetry breaking



Gauge-invariant string operator

$$C(\mathbf{r}) = \langle S_i^z \prod_i^{i+\mathbf{r}} \sigma^z_{b\in \text{path}\mathbf{r}} S^z_{i+\mathbf{r}} \rangle$$





Normal metal

Orthogonal metal

NM Z2 gauge field confined

OM Z2 gauge field deconfined

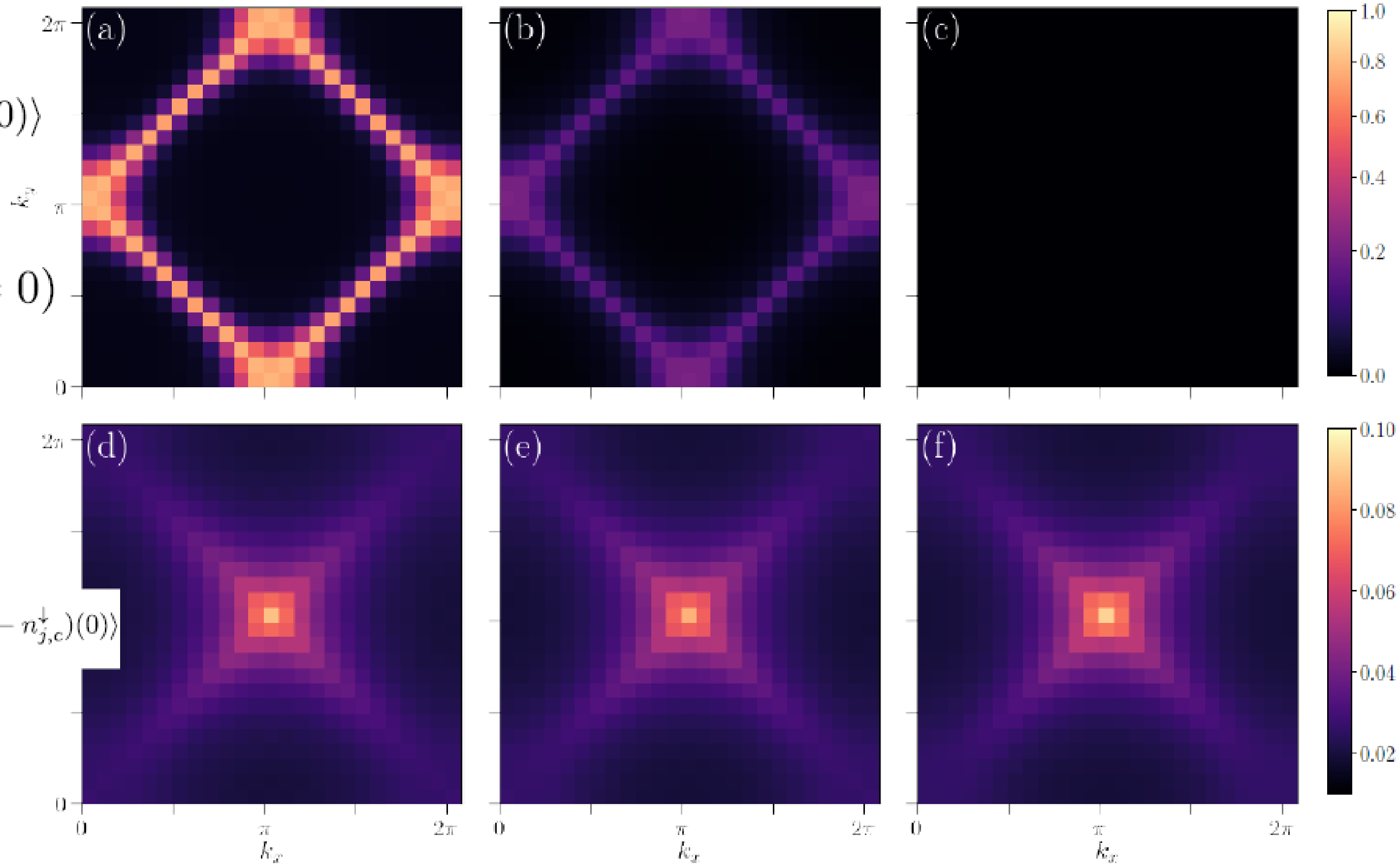
➢Chuang Chen et al., arXiv:1904.12872

Z2 gauge field couple to matter field

$$G(\mathbf{k},\tau) = \frac{1}{N}\sum_{i,j,\alpha} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}\langle c^\dagger_{i,\alpha}(\tau)c_{j,\alpha}(0)\rangle$$

$$G(\mathbf{k},\beta/2) \propto A(\mathbf{k},\omega=0)$$

$$\chi(\mathbf{q},\omega=0) = \frac{1}{\beta N}\int_0^\beta d\tau \sum_{i,j}\langle(n^\uparrow_{i,c}-n^\downarrow_{i,c})(\tau)(n^\uparrow_{j,c}-n^\downarrow_{j,c})(0)\rangle$$



$$\langle n_{i,c}\rangle = 1$$

$$L = 24, T = 0.1$$

h

$h = 0.4$ Normal metal

$h_c \approx 2$

$h = 4$ Orthogonal metal

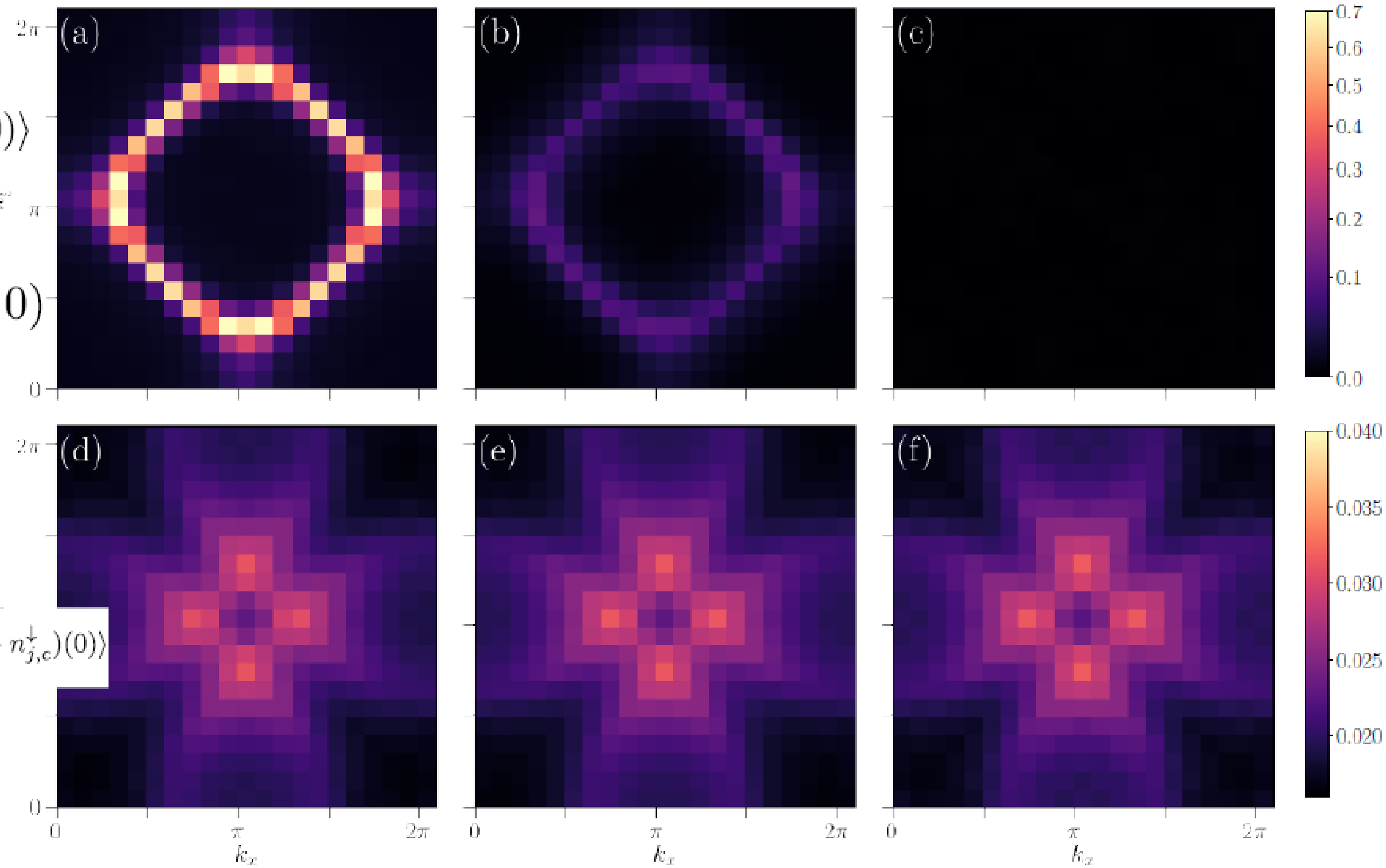
➢ Chuang Chen et al., arXiv:1904.12872

Z2 gauge field couple to matter field

$$G(\mathbf{k},\tau) = \frac{1}{N}\sum_{i,j,\alpha} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}\langle c^{\dagger}_{i,\alpha}(\tau)c_{j,\alpha}(0)\rangle$$

$$G(\mathbf{k},\beta/2) \propto A(\mathbf{k},\omega=0)$$

$$\chi(\mathbf{q},\omega=0) = \frac{1}{\beta N}\int_0^{\beta} d\tau \sum_{i,j}\langle (n^{\uparrow}_{i,c}-n^{\downarrow}_{i,c})(\tau)(n^{\uparrow}_{j,c}-n^{\downarrow}_{j,c})(0)\rangle$$



$$\langle n_{i,c}\rangle = 0.7$$

$$L = 20, T = 0.1$$

h

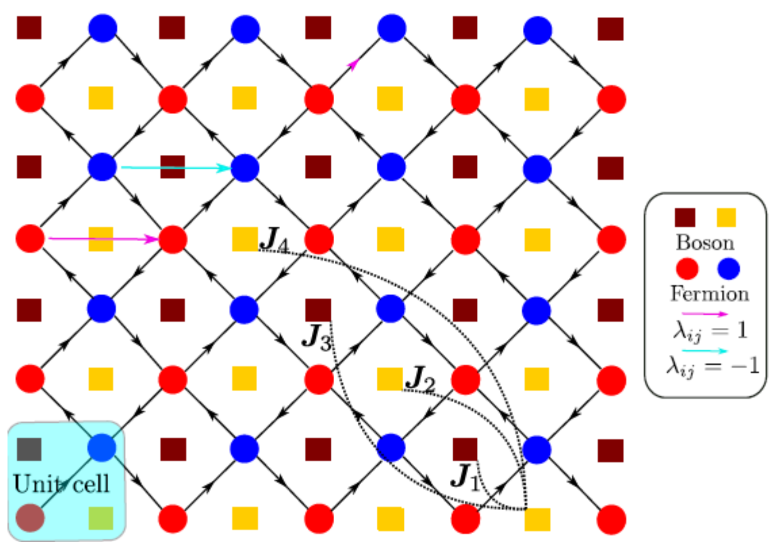
$h = 0.5$
Normal metal

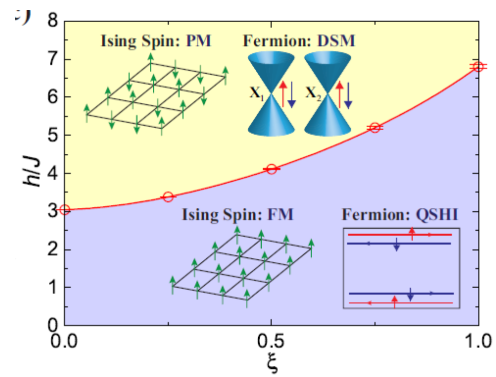
$h_c \approx 2$

$h = 4$
Orthogonal metal

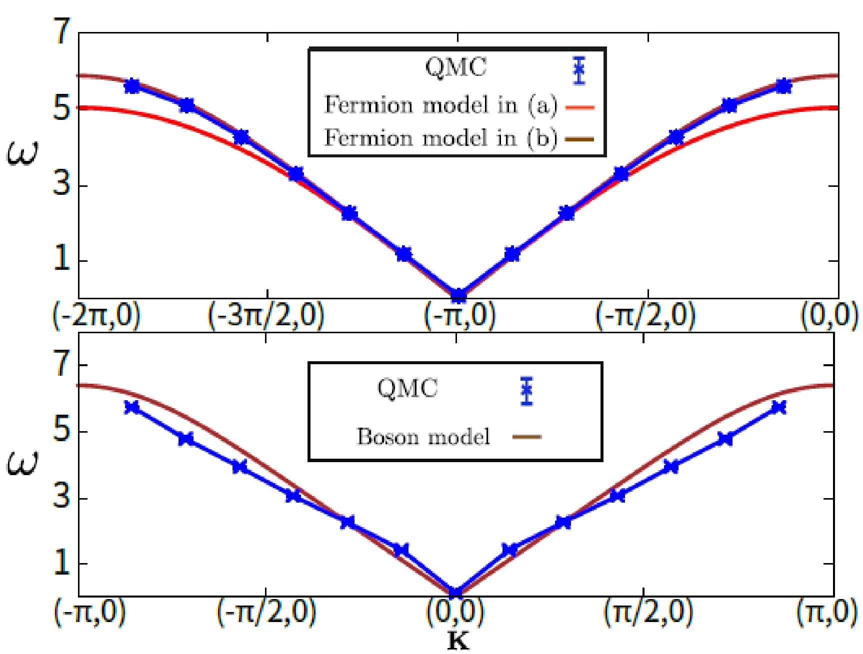
➢Chuang Chen et al., arXiv:1904.12872

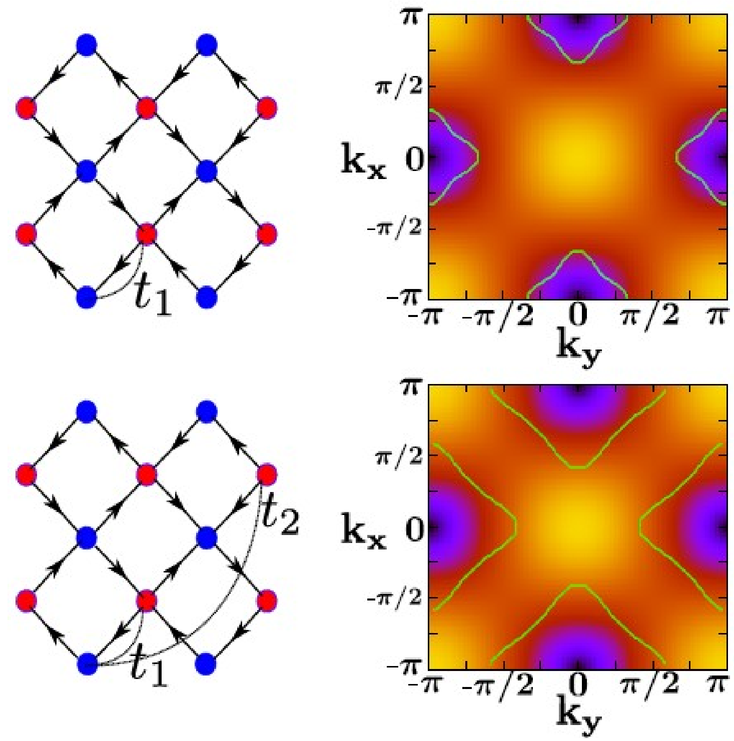
Designer Hamiltonian for Chiral Ising GN





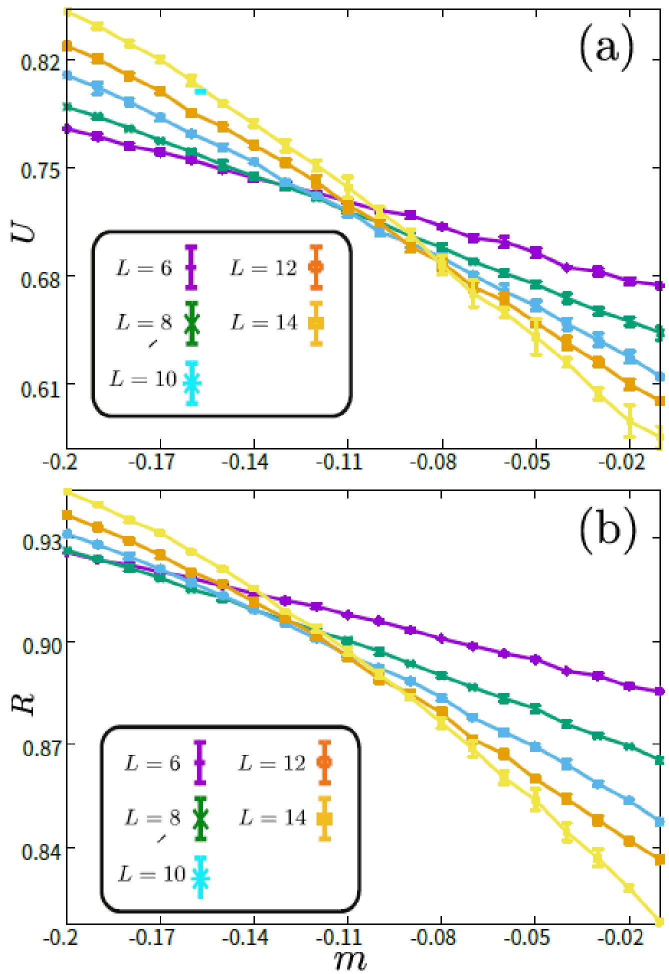
- PRB 97, 081110 (2018)



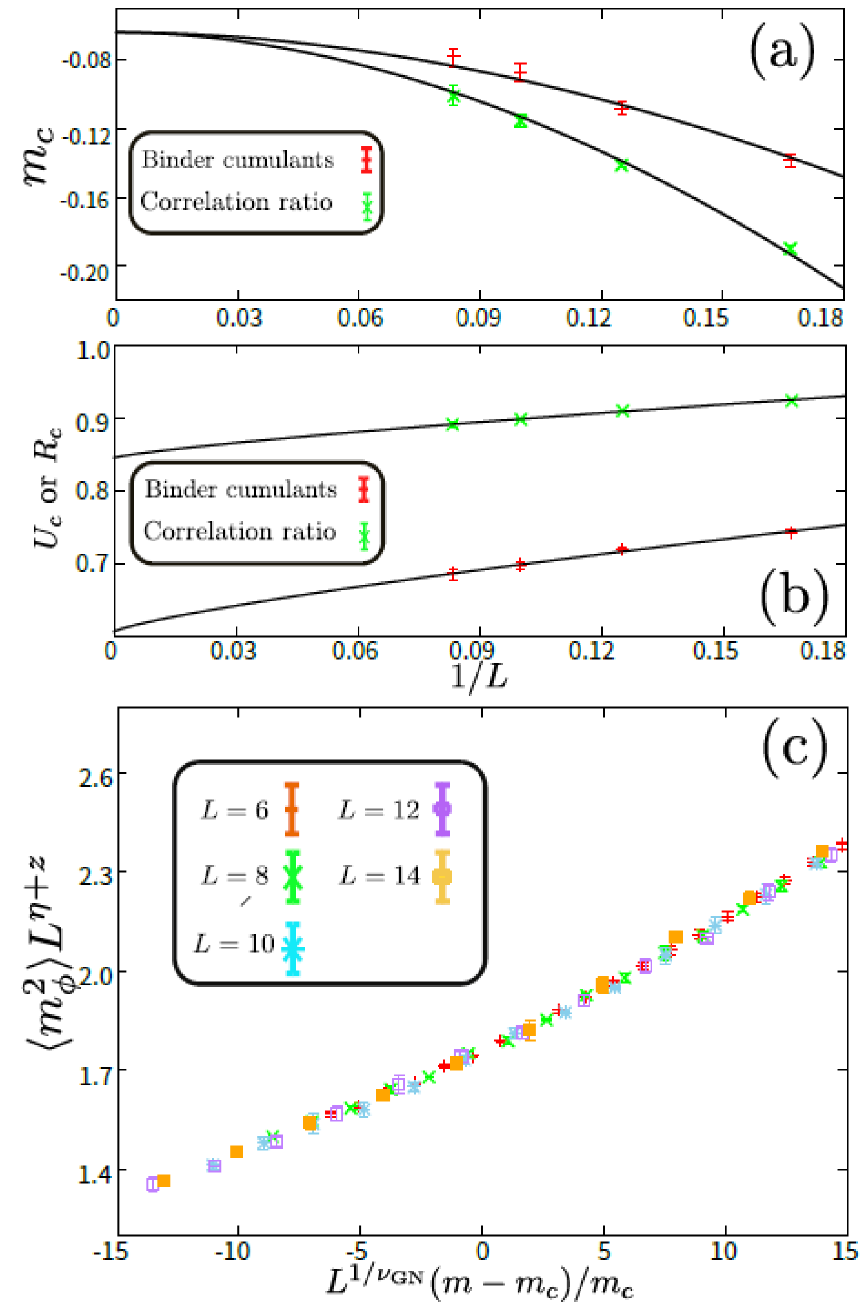


3 times larger linear dispersion area

- Yuzhi Liu, Kai Sun, ZYM, in preparation

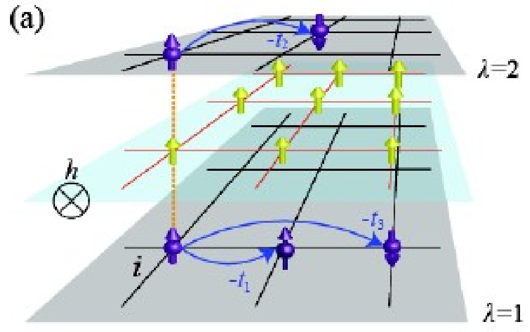


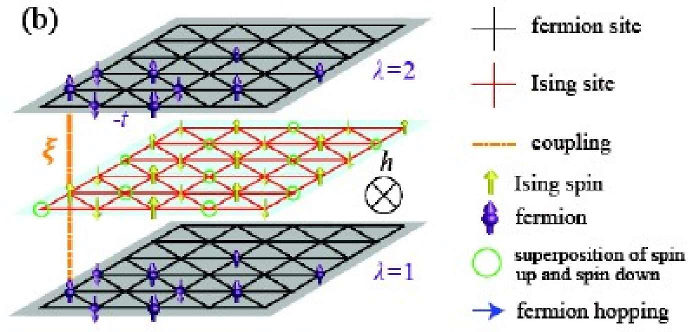
	$1/\nu_{GN}$	η_ϕ	η_ψ	ω
this work	1.1(1)	0.60(2)		0.78(6)
previous QMC [20]	1.2(1)	0.65(3)		
previous QMC [21]	1.20(1)	0.62(1)	0.38(1)	
Perturbative RG [18]	0.931	0.7079	0.0539	0.794
Bootstrap rough bound [29]	0.88	0.742	0.044	



➢ Yuzhi Liu, Kai Sun, ZYM, in preparation

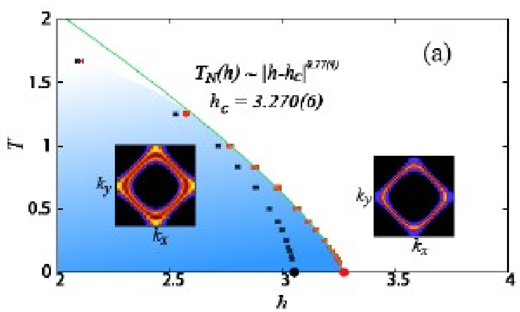
Tidbit from Monte Carlo

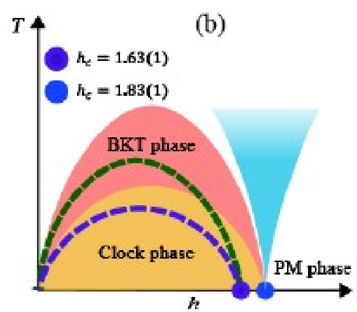


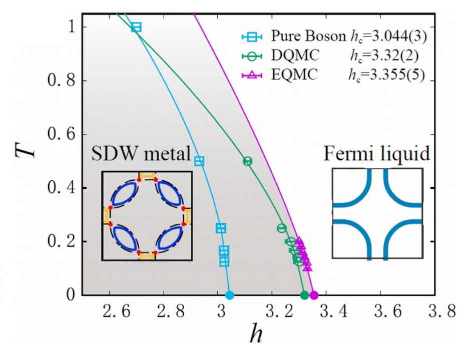


Difficult questions

- PRX 7, 031101 (2017)
- PRB 98, 045116 (2018)
- PNAS 116 (34), 16760 (2019)

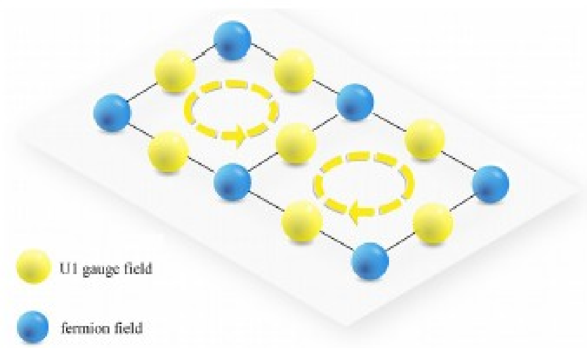


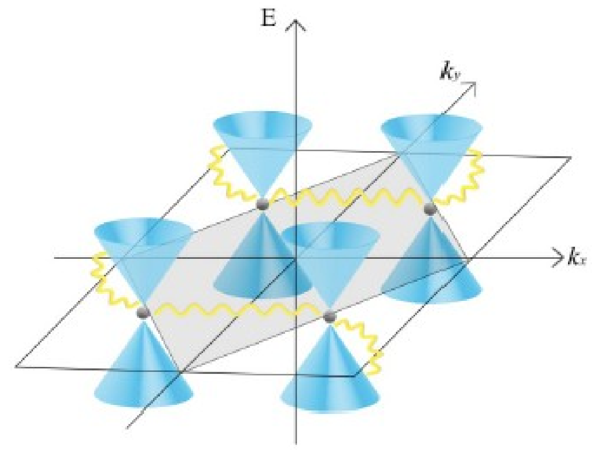




Methodologies

- PRB 95, 041101 (R) (2017)
- PRB 96, 041119 (R) (2017)
- PRB 98, 041102 (R) (2018)
- PRL 122, 077601 (2019)
- PRB 99, 085114 (2019)





New paradigms in quantum matter

- PRX 9, 021022 (2019)
- arXiv: 1904.12872
- PRB 100, 085123 (2019)