Preempting Fermion Sign Problem: Unveiling Quantum Criticality through Nonequilibrium Dynamics

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「趁着 sign problem 还没反应过来，“抢先”把基态相图/量子临界性搞清楚」

Yin-Kai Yu, Zhi-Xuan Li, Shuai Yin, Zi-Xiang Li, arXiv:2410.18854 (2024)

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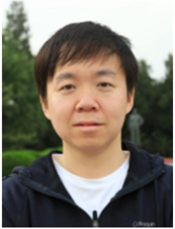

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费米子蒙卡与符号问题

- 行列式蒙特卡罗算法（Determinant Quantum Monte-Carlo, DQMC）——用于求解强关联费米子系统

$$Z = \sum_{\mathrm{c}} w(\mathrm{c})$$

符号问题 (sign promblem)：采样概率 $w(\mathrm{c})$ 非正定

- 强行采样 $w(\mathrm{c}) = |w(\mathrm{c})| \, \mathrm{sign}(\mathrm{c})$，$\langle \,\square\, \rangle_{|w|} = \frac{\sum_{\mathrm{c}} \,\square\, |w(\mathrm{c})|}{\sum_{\mathrm{c}} |w(\mathrm{c})|}$，得

$$\langle O \rangle = \frac{\sum_{\mathrm{c}} w(\mathrm{c}) O(\mathrm{c})}{\sum_{\mathrm{c}} w(\mathrm{c})} = \frac{\sum_{\mathrm{c}} |w(\mathrm{c})| \mathrm{sign}(\mathrm{c}) O(\mathrm{c}) / \sum_{\mathrm{c}} |w(\mathrm{c})|}{\sum_{\mathrm{c}} |w(\mathrm{c})| \mathrm{sign}(\mathrm{c}) / \sum_{\mathrm{c}} |w(\mathrm{c})|} = \frac{\langle O \rangle_{|w|}}{\langle \mathrm{sign} \rangle_{|w|}}.$$

指数级时间复杂度，NP-hard[1]

$$\Delta \langle O \rangle \sim \frac{1}{\langle \mathrm{sign}_c \rangle} \sim \mathrm{e}^{\tau N \Delta f}$$

[1] Troyer and Wiese, PRL, (2005).

费米子符号问题

- **传统求基态方法**，将试探波函数演化**足够长的虚时** τ，得到基态波函数，然后求可观测量：

$$\langle O\rangle_{\mathrm{GS}} = \lim_{\tau\to\infty} \frac{\langle\psi_{\mathrm{T}}|\, \mathrm{e}^{-\frac{\tau}{2}H}\ O\ \mathrm{e}^{-\frac{\tau}{2}H}\, |\psi_{\mathrm{T}}\rangle}{\langle\psi_{\mathrm{T}}|\, \mathrm{e}^{-\tau H}\, |\psi_{\mathrm{T}}\rangle}$$

  - 困难 1：🤔有符号问题，计算时间 $\mathrm{e}^{\tau\to\infty}$
  - 困难 2：🤔量子临界点附近，临界慢化

- 放弃求解基态波函数，考虑**非平衡态**

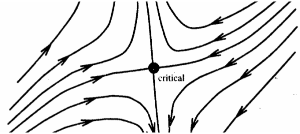
$$\langle O(\tau)\rangle = \frac{\langle\psi_0|\, \mathrm{e}^{-\frac{\tau}{2}H}\ O\ \mathrm{e}^{-\frac{\tau}{2}H}\, |\psi_0\rangle}{\langle\psi_0|\, \mathrm{e}^{-\tau H}\, |\psi_0\rangle} = ??$$

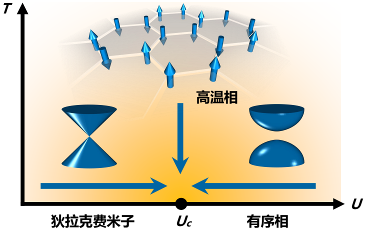
  - 困难 3：🤔基态量子临界点如何影响非平衡过程？

临界标度与非平衡动力学

- 1976, M. E. Fisher，有限尺寸标度[2]
- 1989, H. K. Janssen *et al.*，临界弛豫过程，非平衡标度[3]（经典）
- 2014, S. Yin *et al.*，虚时弛豫动力学，非平衡标度[4]（自旋）
- 2023, **Y.-K. Yu** *et al.*，推广到费米子系统[5]（sign-free system）

$$\langle O(\tau)\rangle = L^{-\kappa} f_O\left((U-U_c)L^{\frac{1}{\nu}}, \tau L^{-z}\right)$$





[2]Fisher, Reports on progress in physics, (1967).

[3]Janssen, Schaub, and Schmittmann, Z. Phys. B, (1989).

[4]Yin, Mai, and Zhong, PRL, (2014).

[5]Yin-Kai Yu, Zhi Zeng, Yu-Rong Shu, Zi-Xiang Li, and Shuai Yin, arXiv: 2310.10601, (2023).

Preempting the sign problem

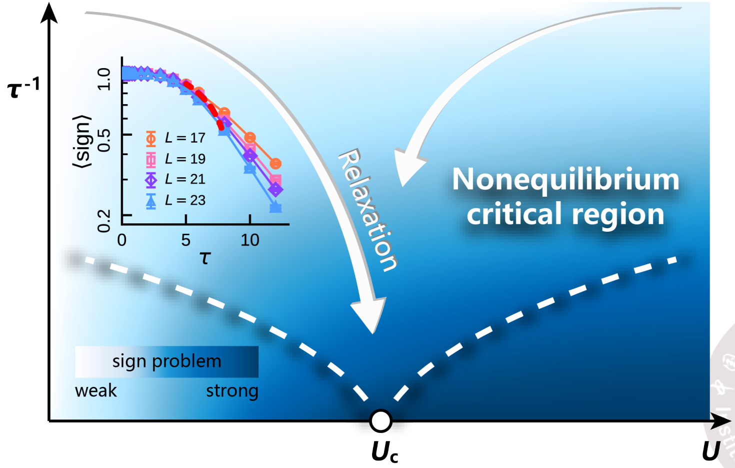
人们难以精确研究强关联费米子系统的量子临界性质与动力学，是因为：

- 困难 1：计算时间 $\mathrm{e}^{\tau N \Delta f}$ 🤔 (意味着缩短虚时可以指数级加速)
- 困难 2：发散的涨落模式 🤔 (非平衡标度行为)
- 困难 3：非平衡 🤔 (非平衡也可以体现基态临界性)

难 + 难 + 难 = 易：

😲 可以在符号问题比较弱的时候，就把基态临界性质算清楚！

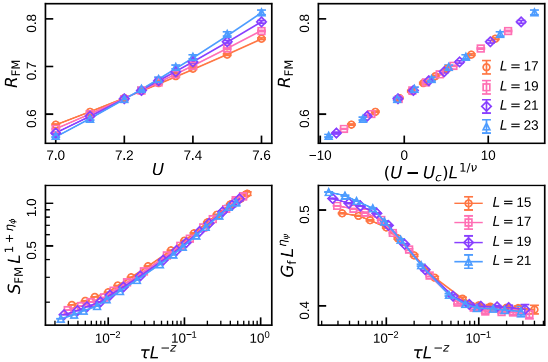
Preempting the sign problem



- 传统 PQMC 求基态，虚时 $\tau = 2L^z \sim 3L^z$，符号问题严重
- **非平衡 PQMC 方法**，比如取 $\tau = 0.3L^z$，符号问题不严重

应用实例一： single-Dirac-fermion Hubbard model

$$H = \sum_p c_p^\dagger \not{p}\, c_p + U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$



- $\tau = 0.3L^z$, FM correlation length ratio: $R_{\mathrm{FM}} = f_R\left((U - U_c)L^{1/\nu}\right)$
- $U = U_c$, FM structure factor: $S_{\mathrm{FM}} = L^{-(1+\eta_\phi)} f_S\left(\tau L^{-z}\right)$
- $U = U_c$, fermion correlation: $G_{\mathrm{f}} = L^{-\eta_\psi} f_G\left(\tau L^{-z}\right)$

应用实例一：single-Dirac-fermion Hubbard model

- 本工作使用**非平衡短时 PQMC 方法**
- 不同方法计算结果对比

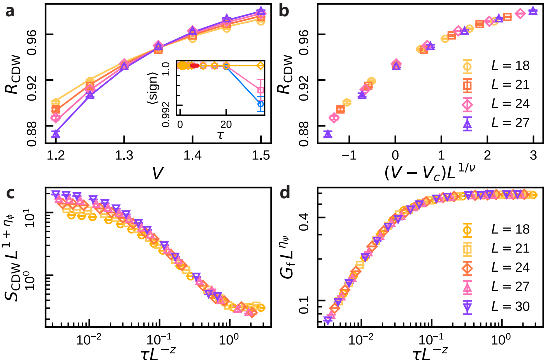
Method	U_c	ν^{-1}	η_ϕ	η_ψ
This work (from DSM, $\tau = 0.3L^z$)	7.220(37)	1.18(3)	0.33(2)	0.135(2)
This work (from FM, $\tau = 0.5L^z$)	7.214(44)	1.05(10)	0.34(5)	0.131(20)
Gutzwiller-PQMC (equilibrium)[6]	7.275(25)	1.19(3)	0.31(1)	0.136(5)
FRG[7]	-	1.229	0.372	0.131

[6] Tabatabaei, Negari, Maciejko, and Vaezi, Phys. Rev. Lett., (2022).

[7] Vacca and Zambelli, Phys. Rev. D, (2015).

应用实例二：spinless t-V model

$$H = -t\sum_{\langle ij\rangle} c_i^\dagger c_j + V\sum_{\langle ij\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right)$$

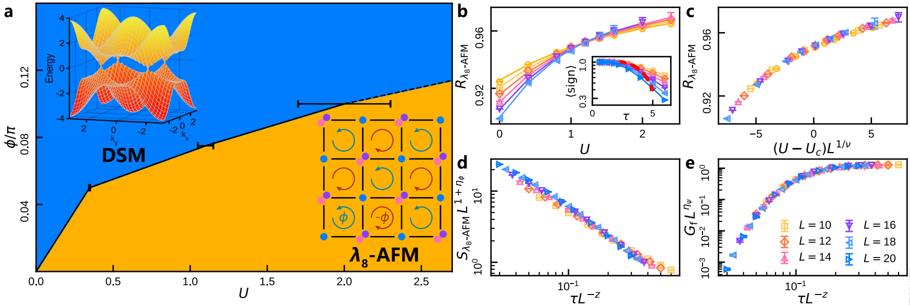


Method	V_c	ν	η_ϕ	η_ψ
This work (from CDW, $\tau = 0.3L^z$)	1.35(1)	0.77(12)	0.49(5)	0.073(4)
This work (from DSM, $\tau = 0.3L^z$)	1.37(2)	0.79(5)	0.44(2)	0.072(4)
Majorana QMC (equilibrium)	1.355(1)	0.77(2)	0.45(2)	-
Continuous-time QMC (equilibrium)	1.356(1)	0.80(3)	0.302(7)	-
FRG	-	0.929	0.602	0.069

对比：MQMC （Li, Jiang, Yao, NJP 2015), CTQMC （Wang, Corboz, Troyer, NJP 2014), FRG (Vacca, Zambelli, PRD 2015)

应用实例三：SU(3) Hubbard model

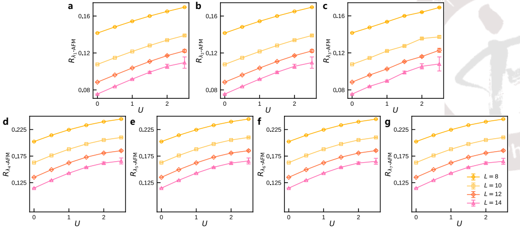
$$H = -\sum_{\langle ij\rangle\alpha} t_{ij} c^{\dagger}_{i\alpha} c_{j\alpha} + \frac{U}{2}\sum_i \left(\sum_\alpha n_{i\alpha} - \frac{3}{2}\right)^2,$$ 具有 SU(3) $\times$ Z_2 对称性



$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \begin{pmatrix} 1/\sqrt{3} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 \\ 0 & 0 & -2/\sqrt{3} \end{pmatrix}.$$



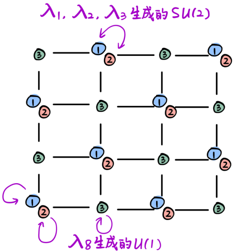
应用实例三：SU(3) Hubbard model

$$H=-\sum_{\langle ij\rangle\alpha}t_{ij}c_{i\alpha}^{\dagger}c_{j\alpha}+\frac{U}{2}\sum_i\left(\sum_\alpha n_{i\alpha}-\frac{3}{2}\right)^2$$，基态简并流形 $\frac{SU(3)\times Z_2}{SU(2)\times U(1)}$

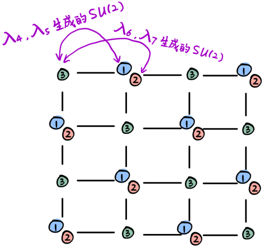
$$\lambda_1=\begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix},\quad \lambda_2=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix},\quad \lambda_3=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&0\end{pmatrix},$$

$$\lambda_4=\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix},\quad \lambda_5=\begin{pmatrix}0&0&-i\\0&0&0\\i&0&0\end{pmatrix},\quad \lambda_6=\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix},$$

$$\lambda_7=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix},\quad \lambda_8=\begin{pmatrix}1/\sqrt{3}&0&0\\0&1/\sqrt{3}&0\\0&0&-2/\sqrt{3}\end{pmatrix}.$$



SU(2)×U(1) gauged out



Goldstone×4

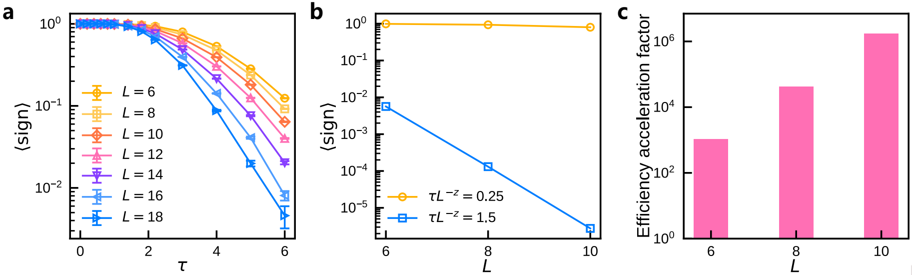
Universality class	ν^{-1}	η_ϕ	η_ψ
chiral $\frac{SU(3)\times Z_2}{SU(2)\times U(1)}$ (this work)	0.68(5)	0.55(5)	0.15(3)
chiral Heisenberg ($4-\epsilon$, 2nd order)[8]	1.478	1.023	0.058
chiral XY ($4-\epsilon$, 2nd order)[9]	1.809	0.698	0.082
chiral Ising ($4-\epsilon$, 2nd order)[9]	0.750	0.865	0.011
chiral Ising (FRG)[9]	0.993	0.912	0.013

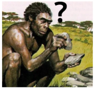
[8] Rosenstein, Hoi-Lai Yu, and Kovner, Phys. Lett. B, (1993).

[9] Janssen and Herbut, PRL, (2014).

应用实例三：SU(3) Hubbard model

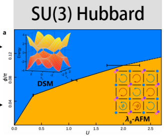
$$\text{Efficiency acceleration factor} = \frac{1/\langle \text{sign} \rangle_{\text{eq.}}}{1/\langle \text{sign} \rangle_{\text{neq.}}} \times \frac{\tau_{\text{eq.}}}{\tau_{\text{neq.}}}$$





本工作

算一星期



平衡态QMC

算一万年

cpu time

"Faster is different"

总结

1. **新的计算方法和理论框架——非平衡短时 PQMC：**

   在符号问题出现或者变得严重之前，就可以把量子临界性质算清楚。

2. **新的序和相变——λ_8-AFM：**

   在具有交错磁通的 SU(3) Hubbard 模型中，发现并研究了新奇的 chiral $\frac{SU(3)\times Z_2}{SU(2)\times U(1)}$ 普适类。

THANKS!

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