The 12th Workshop on Quantum Many-Body Computation

Preempting fermion sign problem: Unveiling quantum criticality through non-equilibrium dynamics

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Take-home concepts

Fundamental & challenging question: quantum criticality for fermions

- Fermionic exchange statistics lead to a NP-hard fermion sign problem for numerical simulation of fermion systems [1].
- Due to critical slowing down, what is actually observed as critical behavior is dynamic critical behavior.

This work: D + D + D $\longrightarrow$ E

- **D**ifficulty 1: exponential calculation error $\sim 1/\langle \text{sign} \rangle$
- **D**ifficulty 2: divergent fluctuation modes
- **D**ifficulty 3: non-equilibrium
- **E**asiness: We can universally probe the fermionic quantum criticality via short-time dynamics before the fermion sign problem arises or becomes computationally prohibitive.

Universal imaginary-time relaxation dynamics

- Prepare ordered or disordered initial state.
- Quench them to the quantum critical point.
- Explore the imaginary-time relaxation by PQMC.
- For an observable P, its dynamic scaling should satisfy [2, 3]:

$$P\left(\tau, g, L, \{X\}\right) = \tau^{-\frac{\kappa}{z}} f_P\left(g\tau^{\frac{1}{\nu z}}, L^{-1}\tau^{\frac{1}{z}}, \{X\tau^{-\frac{c}{z}}\}\right),$$

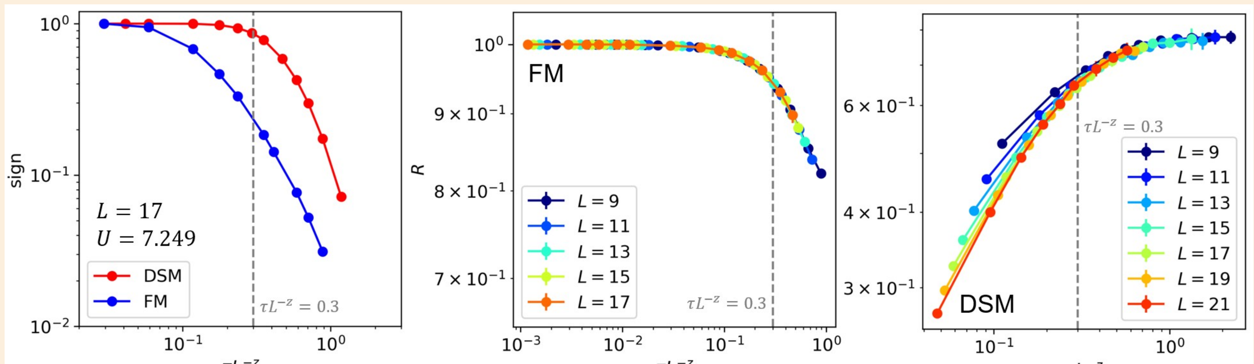
Example 1: SU(2) Hubbard model on single Dirac cone

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

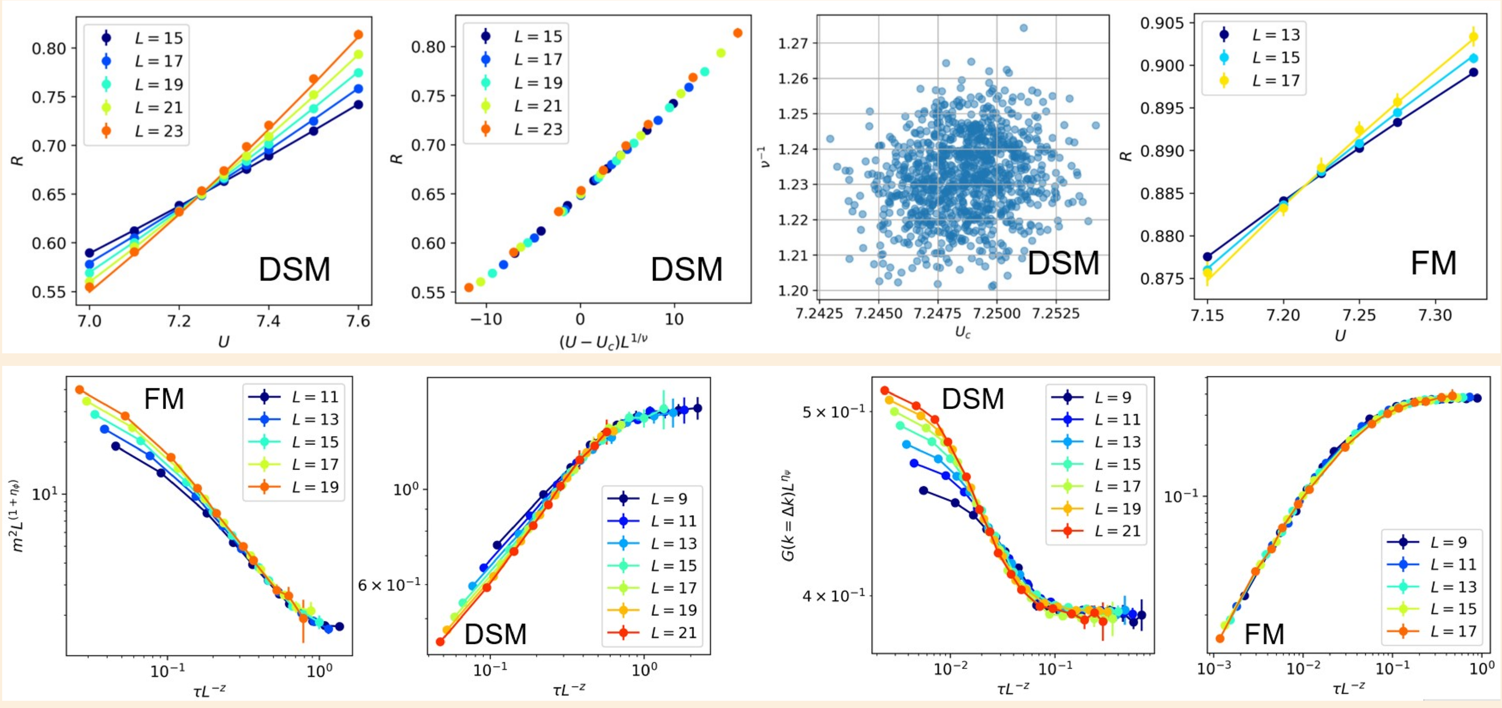
DSM-FM phase transition at critical point U_c ($N = 2$ chiral Ising universality class)

Correlation length ratio R has scaling as: $R\left(g, \tau, L\right) = f_R\left(gL^{1/\nu}, \tau^{-1}L^z\right)$

Acceptable sign problem at $\tau L^{-z} = 0.3$, within the range where the scaling works:



Probing the critical point and critical exponents via non-equilibrium dynamics:



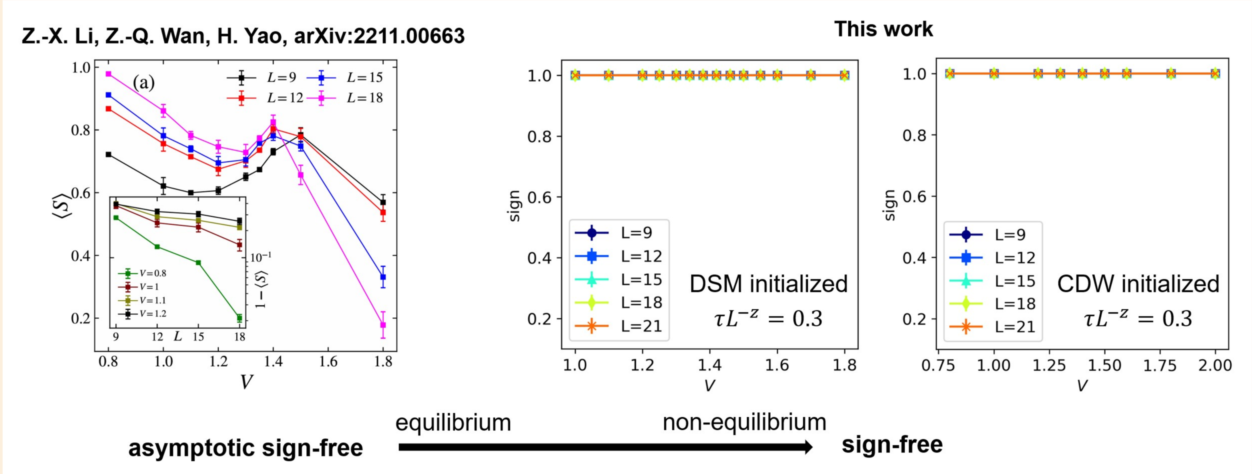
Benchmark with equilibrium results:

method	U_c	ν^{-1}	η_b	η_f
This work	7.249(4)	1.23(2)	0.395(17)	0.129(9)
Gutzwiller-PQMC (equilibrium) [4]	7.275(25)	1.19(3)	0.31(1)	0.136(5)
FRG [5]	-	1.229	0.372	0.131

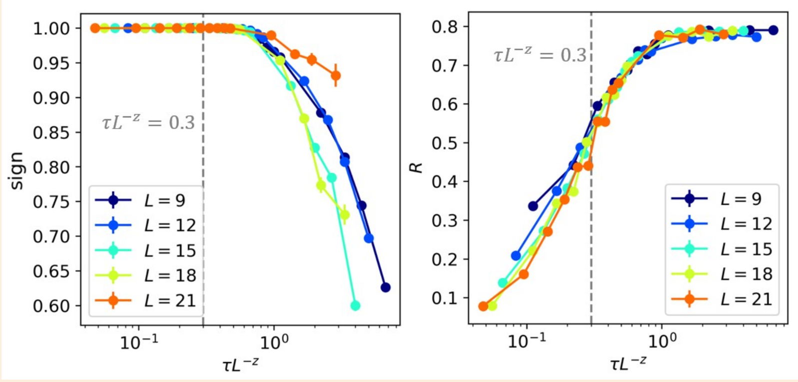
Example 2: "unnecessary" sign problem in t-V model

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

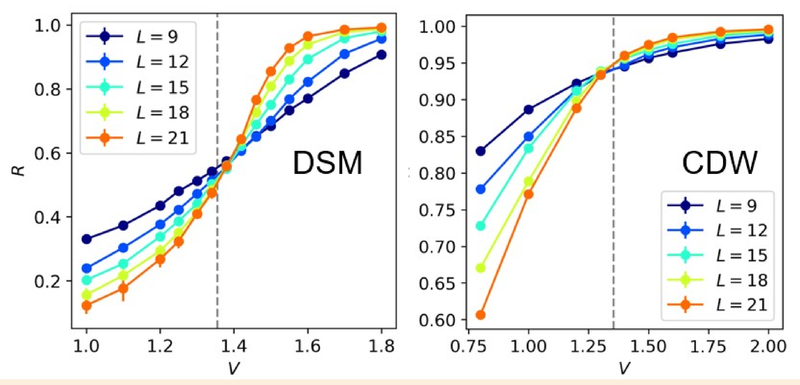
Non-equilibrium method extends the asymptotic sign-free [6] to complete sign-free:



Scaling and sign problem behaviors:



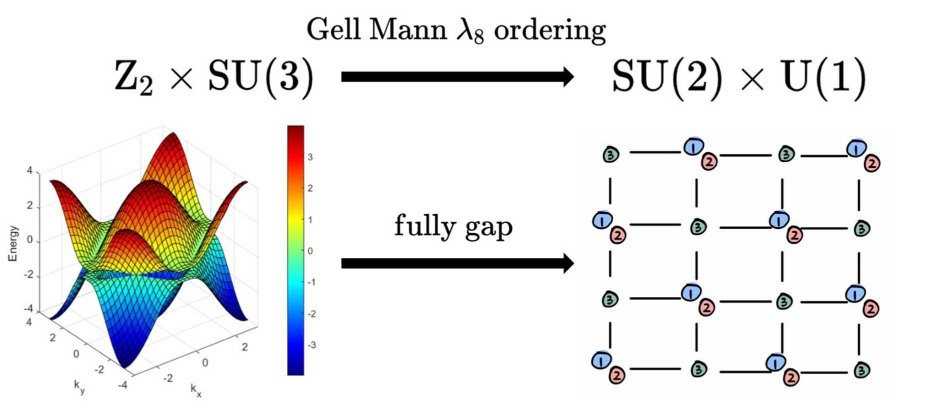
Benchmark with sign-free MQMC [7]:



Example 3: repulsive SU(3) Hubbard on anisotropic Dirac cone

Hamitonian: $H = -\sum_{\langle ij\rangle,\alpha} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U\sum_i\sum_{\alpha>\beta}(n_{i\alpha} - 1/2)(n_{i\beta} - 1/2)$, where $t_{ij} = te^{i\theta_{ij}}, \theta_{ij} = (-)^{i_x+i_y}\phi/4$.

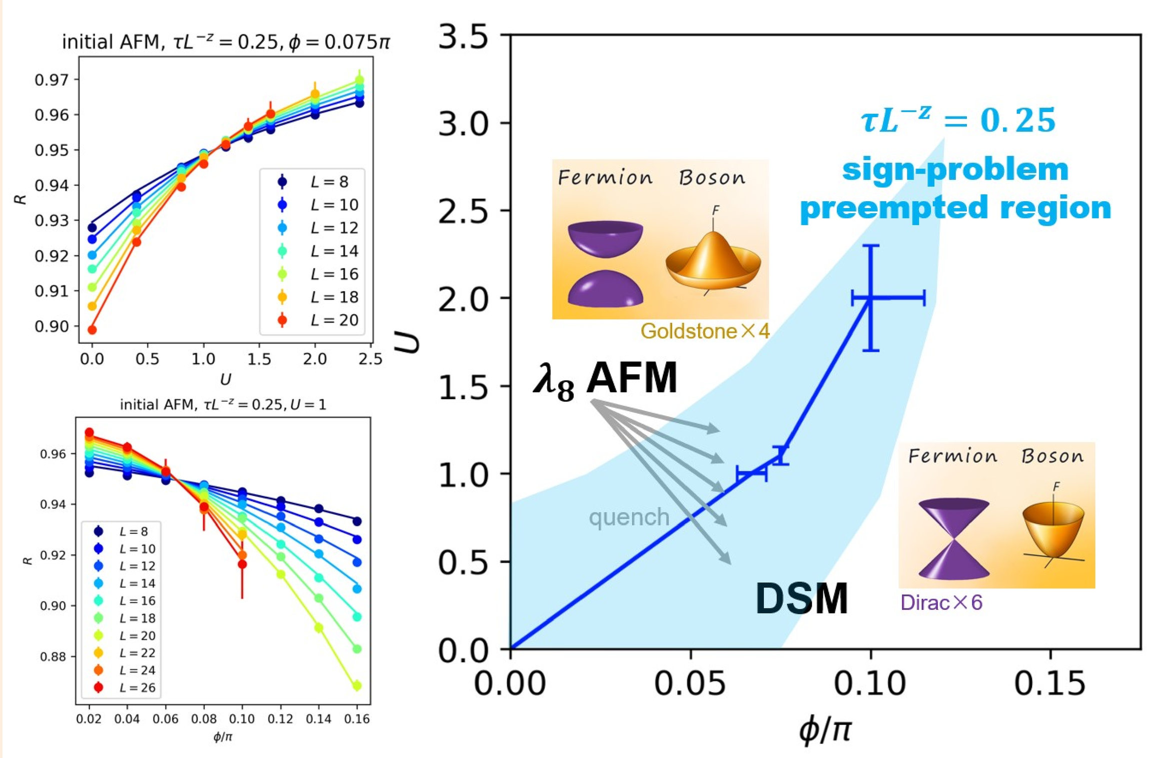
New universality class: a phase transition with Gell-Mann λ_8 order.



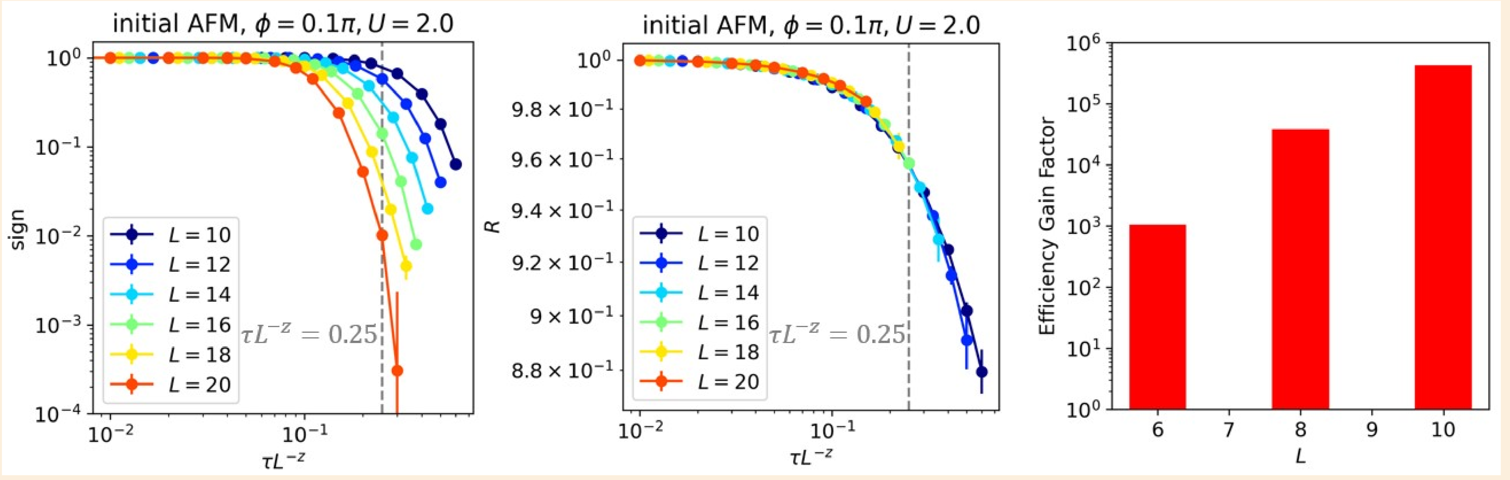
critical exponents:

- $\nu^{-1} = 0.68 \pm 0.05$
- $\eta_b = 0.65 \pm 0.10$

Phase diagram between Dirac semi-metal and λ_8 antiferromagnetic phase:



Efficiency increased by hundreds of thousands over the equilibrium method:



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Reference

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