Insights from sign-problem-free QMC simulations

Overview

1) fermion sign problem
2) overcoming the sign problem
3) conceptual / quantitative insights
4) comparison to analytical theory (Hertz-Millis, Eliashberg, Sung-Sik Lee)
5) numerical improvements

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1) Fermion sign problem

Monte Carlo: $\langle O \rangle = \dfrac{\sum_c O(c) \cdot p(c)}{\sum_c p(c)}$

polynomial scaling in system size despite exp. growth of Hilbert space

QMC: $\langle O \rangle = \dfrac{\sum_c O(c) \cdot |p(c)| \cdot \sigma(c)}{\sum_c |p(c)| \cdot \sigma(c)} \cdot \dfrac{\sum_c |p(c)|}{\sum_c |p(c)|} = \dfrac{\langle O \cdot \sigma \rangle_{||}}{\langle \sigma \rangle_{||}}$

↳ but $\langle O \cdot \sigma \rangle$ and $\langle \sigma \rangle \sim \exp(-\beta N \Delta f)$

↳ back to exponential scaling

difference in free energy densities

Ways around sign problem? Popular route: change basis

but finding good basis is generally hard, actually NP-hard (Troyer, Wiese PRL '05).

2) Overcoming the sign problem

- auxiliary field QMC for strongly interacting fermions
  → unbiased approach

$$\mathrm{Tr}\; e^{-\beta \mathcal{H}} = \mathrm{Tr}\left(e^{-\Delta\tau \mathcal{H}}\right)^{L} \qquad \mathcal{H} = K + V$$

→ decouple quartic interaction via Hubbard - Stratonovich transform.
→ integrate out free fermions moving in a background field

$$Z = \sum_{s} \det U(s).$$

↑— sample HS field.

- avoiding sign problem
  → look for an anti-unitary symmetry $T^2 = -\mathbb{1}$
  ↳ eigenvalues of U come in complex - conjugate pairs
  ↳ $\det U$ is positive definite.

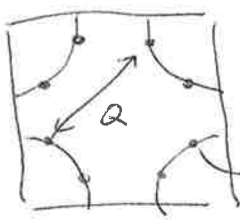
examples:
- attractive Hubbard model → HS transformed action has time - reversal symmetry
- spin<u>less</u> fermions do not → sign problem
- basis change : complex fermions → Majorana fermions ✓
- two band (= 2 flavors) models for effective actions → Berg, Metlitski, Sachdev

- low-energy effective two-band theory

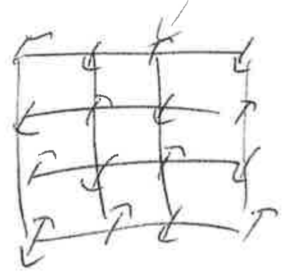
$$S = S_{\text{free fermion}} + S_{\text{boson } \phi^4} + S_{\text{boson-fermion-coupl}}$$

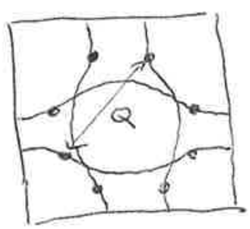
$$S_\varphi = r\vec{\varphi}^2 + \frac{1}{c^2}(\partial_t \vec{\varphi})^2 + \left[\nabla\left(e^{i\vec{Q}\vec{x}}\vec{\varphi}\right)\right]^2 + \frac{1}{2}u(\vec{\varphi}^2)^2$$

$$S_{int} = \lambda\vec{\varphi}\,(\psi^+ \vec{\sigma}\,\psi)$$



hot spots





deform FS <u>away</u> from hot spots

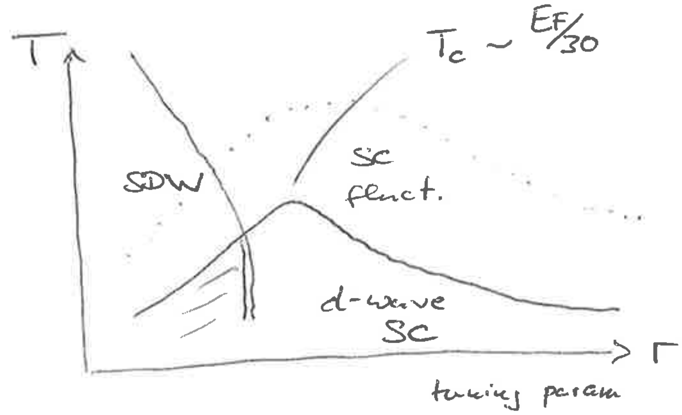
$\longrightarrow$ anti-unitary symmetry

$$S_{int} = \lambda\vec{\varphi}\,(\psi_1^+ \sigma\,\psi_2 + \psi_2^+ \sigma\,\psi_1)$$

3) Conceptual / quantitative insights

- consider an easy-plane O(2) AFM order parameter $\vec{\varphi} = (\varphi_x, \varphi_y)$

  $\hookrightarrow$ finite-T BKT transitions



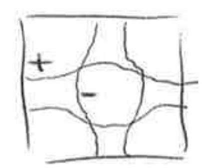
$\longrightarrow$ diamagnetism onsets at $T \sim 2T_c$

(paramag $\xrightarrow[\text{chg}]{\text{sign}}$ diamag $\rightarrow$ dram. increase of orbital susceptibility.)

$\longrightarrow$ reduction in tunneling d.o.s.

$$\tilde{N}(T) = \frac{1}{T} \int d\omega \, \frac{N(\omega)}{2\cosh\left(\frac{\beta\omega}{2}\right)}$$

$\longrightarrow$ SC is nodeless d-wave $\Psi = \psi_{1\uparrow}\psi_{1\downarrow} - \psi_{2\uparrow}\psi_{2\downarrow}$

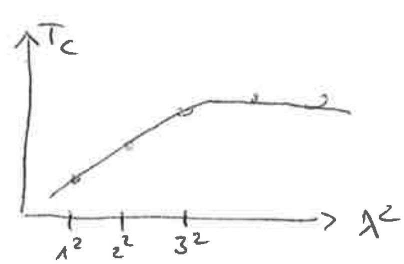


$\longrightarrow$ no signature of CDW formation

(weak enhancement of short-range CDW fluct. with d-wave form factor)

(arXiv: 1512.07257).

$\longrightarrow$ T_c depends on Yukawa coupling λ



(agreement with Eliashberg theory).

4) Comparison to analytical theory

QCP is masked by SC dome.

- └ suppress SC by magnetic field not possible → sign problem
- └ change Yukawa coupling

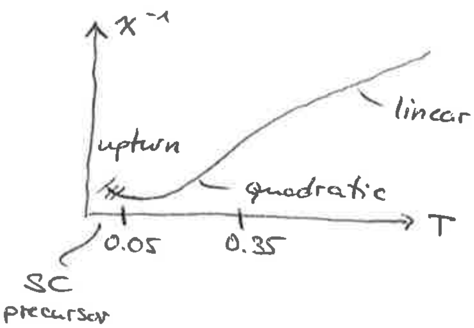
a) Hertz - Millis theory

(integrate out fermions, effective bosonic action, overdamped due to coupling to fermions → $z>1$, conventional RG techniques).

$$\chi^{-1}(\vec{q},\omega_n,r,T) = a_q \underbrace{(\vec{q}-\vec{Q})^2}_{z=2} + a_\omega \underbrace{|\omega_n|}_{\text{Landau damping}} + a_r(r-r_c) + \underbrace{f(r,T)}_{f\to 0 \text{ for } T\to 0}$$

Above T_c magnetic fluctuations mostly agree with Hertz-Millis theory.

But: $\chi^{-1} \sim T^2$ in disagreement



dynamical critical exponent $z=2$.

fermions: loss of single-fermion spectral weight at hot spots

non-FL behavior: finite QP lifetime, nearly independent of T,ω.

(arXiv: 1609.08620)

Summary: quite remarkable agreement with Hertz-Millis theory
(given that integrating out low-energy modes is dangerous → non-analytic terms in $\vec{q}$ and ω, 1/N expansion uncontrolled in $d=2$).

b) Eliashberg theory

(1-loop, bare GF, no self-consistency for bosonic prop.)
fermionic self-energies are then computed self-consistently, no vertex correction

1) $T_c \sim \lambda^2$ ✓

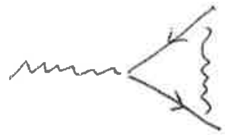
2) angular dependence

$$T_c \sim \lambda^2 \sin(\Theta_{hs}).$$

(arxiv: 1609.09568)

c) Sung-Sik Lee's theory (low-energy effective field theory)

Eliashberg theory does not treat vertex corrections, but if you include them you find



$\propto \quad (2 - N_b)$

bosonic flavors

i.e. the number of spin components does matter.

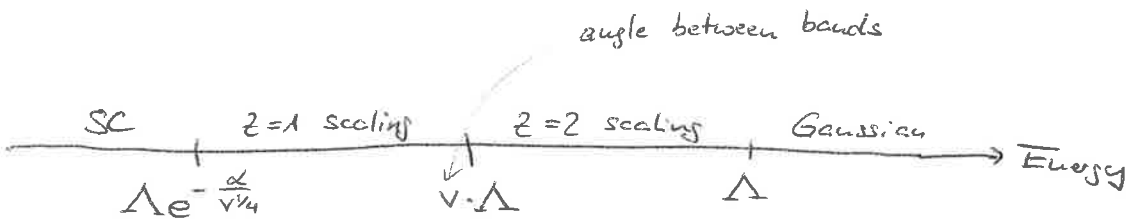
In fact, the previously studied O(2) model is rather special and certainly distinct from O(3) version.

↪ Similar picture for O(3) and O(2)
T_c peaked close to AFM QCP

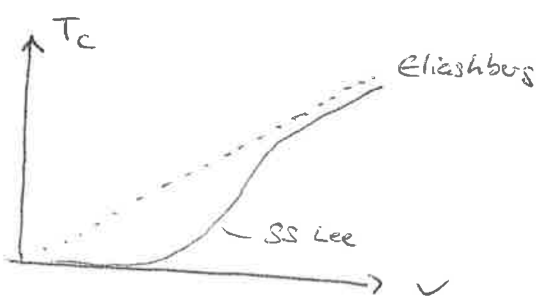
$$\chi^{-1} = a_q (\vec{q} - \vec{Q})^2 + a_\omega |\omega_n| + a_r (r - r_c) + f(r,T) .$$

↪ dynamical critical exponent $z = 1$?

O(3)



$$\left[\chi^{-1} = |q_x| + |q_y| + q^2 + |\omega|\right]$$



5) Numerical improvements

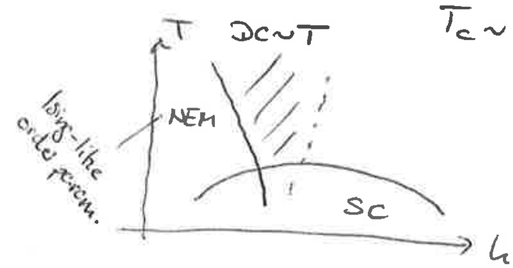
- scaling of algorithm

$$\mathcal{O}(\beta \cdot N_s^3 \cdot N_f^3 \cdot N_b^3)$$

system size — fermion flavors — boson flavors

- under the hood
  - parallel tempering + ensemble optimization
  - machine learning approaches ⟶ update accelerator

- DC resistivity
  - requires analytical continuation (imaginary → real time trafo)



$T_c \sim E_F/30$

(arxiv: 1612.01542)