Quantum Critical Points On Graphene's Honeycomb Lattice

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Half-filled Hubbard model on honeycomb lattice

• Hamiltonian:

$$H=H_0+H_1$$

• Hopping:

$$H_0 = -t \sum_{\vec{A}, i, \sigma = \pm 1} u_{\sigma}^{\dagger}(\vec{A}) v_{\sigma}(\vec{A} + \vec{\delta}_i) + h.c.$$



• Interaction:

$$H_{1} = \sum_{\vec{X}, \vec{Y}, \sigma, \sigma'} n_{\sigma}(\vec{X}) \left[\frac{U}{2} \delta_{\vec{X}, \vec{Y}} + \frac{e^{2}(1 - \delta_{\vec{X}, \vec{Y}})}{4\pi |\vec{X} - \vec{Y}|} \right] n_{\sigma'}(\vec{Y})$$

- *U*: on-site repulsion ("Hubbard-*U*")
- e^2 : long-range part of Coulomb interaction ("dim'less charge")

Low-energy effective theory

• Spectrum of *H*₀:

$$\varepsilon_{1,2}(\vec{q}) = \pm v_{\mathsf{F}} |\vec{q} - \vec{K}_{1,2}| + \mathcal{O}((\vec{q} - \vec{K}_{1,2})^2)$$

Dirac points:
$$\vec{K}_{1,2} = \pm \vec{K}$$

Fermi velocity: $v_{\rm F} = \frac{\sqrt{3}}{2}ta$

• Low energy:

[Semenoff, PRL 1984]

$$S_0 = \int d au dec x \sum_{\sigma=\uparrow,\downarrow} ar\psi_\sigma(ec x, au) \gamma_\mu \partial_\mu \psi_\sigma(ec x, au)$$

where

$$\psi_{\sigma}(\vec{q}) = \begin{pmatrix} u_{\sigma}(\vec{\kappa} + \vec{q}) \\ v_{\sigma}(\vec{\kappa} + \vec{q}) \\ u_{\sigma}(-\vec{\kappa} + \vec{q}) \\ v_{\sigma}(-\vec{\kappa} + \vec{q}) \end{pmatrix}, \qquad \{\gamma_{\mu}, \gamma_{\nu}\} = 2\delta_{\mu\nu} \mathbb{1}_{4}, \ (\mu, \nu = 0, 1, 2)$$



Interactions

• Charge is RG (marginally) irrelevant: [Gonzalez, Guinea, Vozmediano, NPB 1994 & PRB 1999]

$$-k\partial_k e^2 \propto -k\partial_k \left(\frac{e_{\mathsf{el}}^2}{v_{\mathsf{F}}}\right) < 0$$

• Lorentz symmetry emergent even with interactions:

dynamical critical exponent z = 1

k

[Herbut, PRL 2006] [Herbut, Juricic, Vafek, PRB 2009] [Juricic, Herbut, Semenoff, PRB 2009] [Elias et al., Nat. Phys. 2011]

Low-energy effective theory:

$$S_{1} = S_{0} + \int d\tau d\vec{x} \sum_{x} g_{x} \left(s_{\sigma\sigma'}^{x} \bar{\psi}_{\sigma} M_{x} \psi_{\sigma'} \right)^{2}$$

with $M_x \in \mathbb{C}^{4 \times 4}$, $s^x \in \mathbb{C}^{2 \times 2}$ and compatible with lattice symmetries [Herbut, Roy, Juricic, PRB 2009]

Schematic phase diagram

If interactions strong enough: (some) symmetry breaking



Transition is probably direct and continuous

[Assaad, Herbut, PRX 2013]

... but what are the universality class and the critical exponents?

Gross-Neveu-Yukawa effective theories

$$\mathcal{L} = \bar{\Psi}(\mathbb{1}_2 \otimes \gamma_{\mu})\partial_{\mu}\Psi + \frac{1}{2}\phi_{a}(\bar{m}^2 - \partial_{\mu}^2)\phi_{a} + \bar{\lambda}(\phi_{a}^2)^2 + \bar{g}\phi_{a}\bar{\Psi}(\sigma_{a} \otimes \mathbb{1}_4)\Psi$$

where $\Psi = \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix}$ 8-component, $\bar{\Psi} = \Psi^{\dagger}(\mathbb{1} \otimes \gamma_0)$

(1) "chiral Ising": $a \equiv 0, \sigma_0 \equiv \mathbb{1}_2$

$$\langle \phi_0
angle \propto \langle \bar{\Psi} \Psi
angle = \sum_{\vec{k}=\pm \vec{K}+\vec{q}} \sum_{\sigma=\uparrow,\downarrow} \left(\langle u_{\sigma}^{\dagger} u_{\sigma}
angle - \langle v_{\sigma}^{\dagger} v_{\sigma}
angle
ight)$$

 \Rightarrow CDW order parameter

(2) "chiral H'berg": $a = 1, 2, 3, \sigma_a$: Pauli matrices

$$\langle \vec{\phi} \rangle \propto \langle \bar{\Psi} (\vec{\sigma} \otimes \mathbb{1}_4) \Psi \rangle = \sum_{\vec{k}=\pm \vec{K}+\vec{q}} \sum_{\sigma=\uparrow,\downarrow} \left(\langle u_{\sigma}^{\dagger} \vec{\sigma}_{\sigma\sigma'} u_{\sigma'} \rangle - \langle v_{\sigma}^{\dagger} \vec{\sigma}_{\sigma\sigma'} v_{\sigma'} \rangle \right)$$

 \Rightarrow AF order parameter

Spontaneous symmetry breaking

Strong coupling $\frac{\bar{g}^2}{\bar{m}^2}$: expect finite order parameter

- $\begin{array}{l} \chi \ \text{lsing:} \ \langle \phi_0 \rangle \propto \langle \bar{\Psi} \Psi \rangle \neq 0 \ \text{breaks} \ \mathbb{Z}_2 \\ \text{sublattice-exchange} \end{array}$
 - SM to CDW transition (for large V_1)
 - in (standard) \mathbb{Z}_2 -Gross-Neveu universality



[Rose, Vitale, Wetterich, PRL 2001] [Hofling, Nowak, Wetterich, PRB 2002] [Braun, Gies, D. Scherer, PRD 2011]



 χ H'berg: $\langle \vec{\phi} \rangle \propto \langle \Psi(\vec{\sigma} \otimes \mathbb{1}_4) \Psi \rangle \neq \vec{0}$ breaks $\mathrm{SU}(2)_{\mathrm{sp}}$ to U(1)

- SM to AF transition (for large U)
- SU(2)–Gross-Neveu universality class not yet as well understood

however, ε-expansion: [Rosenstein, Yu, Kovner, PLB 1993] [Herbut, Juricic, Vafek, PRB 2009]

... and also aimed at in simulations: [Sorella, Otsuka, Yunoki, Sci. Rep. 2012] [Assaad, Herbut, PRX 2013]

We investigate both by means of FRG

 \ldots and use χ Ising to test validity of nonperturbative approximation

FRG approach

• Wetterich equation:

$$\partial_k \Gamma_k = \frac{1}{2} \operatorname{STr} \left[\partial_k R_k (\Gamma_k^{(2)} + R_k)^{-1} \right]$$



LPA' truncation:

$$\begin{split} \Gamma_{k} &= \int d^{D}x \left[Z_{\Psi,k} \bar{\Psi}(\mathbbm{1} \otimes \gamma_{\mu}) \partial_{\mu} \Psi - \frac{1}{2} Z_{\phi,k} \phi_{a} \partial_{\mu}^{2} \phi_{a} \right. \\ &+ U_{k}(\rho) + \bar{g}_{k} \phi_{a} \bar{\Psi}(\sigma_{a} \otimes \mathbbm{1}_{4}) \Psi \right], \qquad \qquad \left[\rho(x) \equiv \frac{1}{2} \phi_{a} \phi_{a} \right] \\ \chi \text{ lsing: } a \equiv 0 \qquad \qquad \text{OP } \phi_{a} \equiv \phi_{0} \in \mathbbmR \\ \chi \text{ H'berg: } a = 1, \dots, 3 \qquad \qquad \text{OP } (\phi_{a}) = \vec{\phi} \in \mathbbmR^{3} \end{split}$$

• includes all (perturbatively) relevant operators

[...also many more!]

• becomes exact near D = 4

[... we show it also becomes exact near D = 2 (for sharp cutoff)]

RG flow near D = 4

Flow equations complicated nonlinear functions but simplify considerably when $D = 4 - \epsilon$ with $\epsilon \ll 1!$

• β functions: [L.J. & Herbut, PRB **89**, 205403 (2014)]

$$\partial_t \lambda = (-\epsilon + 2\eta_\phi)\lambda + 4(S+9)\lambda^2 - 2g^4$$

$$\partial_t g^2 = (-\epsilon + \eta_\phi + 2\eta_\psi)g^2 - 2(S-1)g^4$$

anomalous dimensions:

$$\eta_{\phi} = 4g^2 \qquad \eta_{\psi} = rac{S+1}{2}g^2$$



[Herbut, Juricic, Vafek, PRB 2009]

- (χ lsing: S = 0, χ H'berg: S = 2)
- \Rightarrow exactly the flow equations in (4ϵ) -expansion (one-loop)!

Critical point in 2 < D < 4: Correlation-length exponent [L.J. & Herbut, PRB 89, 205403 (2014)] χ lsing: [SM-CDW transition] 2MC simulations $1/N_{\rm f}$ ([1/1] Padé) 1.8 $2 + \epsilon$ (1st order $2 + \epsilon$ (2nd order) 1.6 $2 + \epsilon$ (3rd order) $4 - \epsilon$ (1st order 1.4 $4 - \epsilon$ (2nd order) $P_{2,2}(D$ 1.2 $P_{3,2}(D)$ functional RG $1/\nu$ 1 1.10.81.050.60.40.950.20.92.92.953 3.053.10 3 2 2.22.42.62.83.23.43.63.84 D









 $D = 4 - \epsilon$: exact

 $D = 2 + \epsilon$: exact (sharp cutoff)

$$D = 3$$
: agrees within $\Delta \eta / \eta_{\phi} \simeq 3-6$ %
with best available results
... although $\eta_{\phi} \simeq O(1)$ large!

Conclusions

(1) QCPs on honeycomb lattice in two distinct (new) universality classes: χ lsing (SM-CDW) vs. χ H'berg (SM-AF)

(2) FRG in LPA' desribes critical behavior surprisingly wellagreement in mid-single-digit percent range (χ Ising)

(3) Similar accuracy in χ H'berg? ...however: β (FRG) $\simeq 1.3$ vs. β (QMC) $\simeq 0.8$? [Sorella, Otsuka, Yunoki, Sci. Rep. 2012]

(4) χ universality classes ideal testing ground for nonperturbative approximation schemes

... within FRG and beyond

Symmetries

- Sublattice-exchange symmetry $(u \leftrightarrow v)$: \mathbb{Z}_2 : $\Psi \mapsto (\mathbb{1} \otimes \gamma_2)\Psi, \quad \phi_a \mapsto -\phi_a$ (and $q_x \mapsto -q_x, \ q_y \mapsto q_y$)
- Rotations in spin space: $SU(2)_{sp}: \Psi \mapsto e^{i\theta \vec{n} \cdot (\vec{\sigma} \otimes \mathbb{1}_4)} \Psi, \quad \phi_0 \mapsto \phi_0, \quad \vec{\phi} \mapsto R\vec{\phi} \quad [R \in O(3)]$
- Charge conservation: $U(1)_{ch}: \Psi \mapsto e^{i\theta}\Psi, \quad \phi_a \mapsto \phi_a$
- Translational invariance ("chiral" symmetry): [Herbut, Juricic, Roy, PRB 2009] $U(1)_{\chi}: \Psi \mapsto e^{i\theta(\mathbb{1}_2 \otimes \gamma_{35})}\Psi, \quad \gamma_{35} \equiv -i\gamma_3\gamma_5$
- χ Ising model: elevated chiral symmetry $\operatorname{SU}(2)_{\chi}: \quad \Psi \mapsto e^{i\theta \vec{n}(\vec{\sigma} \otimes \gamma_{35})}\Psi, \quad \phi_0 \mapsto \phi_0$

(not in χ H'berg!)

- Together:
 - χ lsing: $\mathbb{Z}_2 \times \mathrm{U}(2) \times \mathrm{U}(2)$
 - χ H'berg: $\mathbb{Z}_2 \times \mathrm{U}(2) \times \mathrm{U}(1)$