Fractionalized fermionic quantum criticality

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Complexity and Topology in Quantum Matter

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Outline

(1) Fractionalized quantum criticality

(2) Frustrated spins and spin-orbitals

(3) Square-lattice Kitaev-Ising spin-orbital model

(4) Honeycomb-lattice Kitaev-Heisenberg spin-orbital model

(5) Conclusions



Outline

Fractionalized quantum criticality (1)

Frustrated spins and spin-orbitals (2)

Square-lattice Kitaev-Ising spin-orbital model $\left(3\right)$

Honeycomb-lattice Kitaev-Heisenberg spin-orbital model $(\mathbf{4})$

(5) Conclusions



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$T \rightarrow 0$ $CoNb_2O_6$



[Kinross *et al.*, PRX '14] [Morris et al., Kaul, Armitage, Nat. Phys. '21]



Deconfined quantum criticality





Deconfined quantum criticality



Deconfined quantum criticality





[Senthil *et al.*, Science '04] [Pujari, Damle, Alet, PRL '13] [Block, Melko, Kaul, PRL '13] [Shao, Guo, Sandvik, Science '16]



Spin-liquid transitions







0



Quantum paramagnet

J

[Assaad & Grover, PRX '16] [Xu,, Qi, Zhang, Assaad, Xu, Meng, PRX '19] [LJ, Wang, Scherer, Meng, Xu, PRB '20]



[Metlitski, Mross, Sachdev, Senthil, PRB '15] [LJ & He, PRB '17] [Boyack, Lin, Zerf, Rayyan, Maciejko, PRB '18]

. . .



Example: Kagome-lattice Bose-Hubbard model

Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \left[b_i^{\dagger} b_j + b_i b_j^{\dagger} \right] + V \sum_{\bigcirc} (n_{\bigcirc})^2$$



... *b_i* hard-core bosons

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Phase diagram:





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Phase diagram:





... *b_i* hard-core bosons

Entanglement entropy: $S_n(A) = a\ell - \gamma + \dots$



[Isakov, Hastings, Melko, Nat. Phys. '11]





Quantum critical scaling: XY*

Superfluid density:



[Isakov, Hastings, Melko, Nat. Phys. '11]

 $\nu \approx 0.67 = \nu_{\rm XY}$

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Two-point superfluid correlator:



[Isakov, Melko, Hastings, Science '12]

 $\eta pprox 1.49
eq \eta_{
m XY} pprox 0.038$

Order parameter *composite* of fractionalized particles!

... cf. $\eta_T \approx 1.47$ from field theory [Calabrese, Pelissetto, Vicari, PRE '02]

Finite-size spectroscopy: Ising vs Ising*

Transverse-field Ising:

$$\mathcal{H} = -J\sum_{\langle ij
angle} \sigma^z_i \sigma^z_j - h\sum_i \sigma^x_i$$



Transverse-field toric code:

$$\mathcal{H} = -J\sum_{s}\prod_{i\in s}\sigma_i^x - J\sum_{p}\prod_{i\in p}\sigma_i^z - h\sum_i$$



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Kitaev spin-1/2 model

Hamiltonian:







[Kitaev, Ann. Phys. '06]



Kitaev spin-1/2 model

Hamiltonian:



Majorana representation:







[Kitaev, Ann. Phys. '06]



Kitaev spin-1/2 model

Hamiltonian:



Majorana representation:









Fractionalization:

with
$$\left[\hat{u}_{ij}, \tilde{\mathcal{H}}\right] = 0 \quad \Rightarrow \quad \text{static } \mathbb{Z}_2 \text{ gauge field}$$

Kitaev-Heisenberg spin-1/2 model

Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij
angle_{\gamma}} \sigma_{i}^{\gamma} \sigma_{j}^{\gamma} + J \sum_{\langle ij
angle} ec{\sigma}_{i} \cdot ec{\sigma}_{j}$$



... possible relevance to α -RuCl₃, Na₂IrO₃, Na₂Co₂TeO₆, ...



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Phase diagram:





... possible relevance to α -RuCl₃, Na₂IrO₃, Na₂Co₂TeO₆, ...





Kitaev-Heisenberg spin-1/2 model

Hamiltonian:

 $\mathcal{H} = K \sum \sigma_i^{\gamma} \sigma_j^{\gamma} + J \sum \vec{\sigma}_i \cdot \vec{\sigma}_j$ $\langle ij \rangle_{\gamma}$ $\langle ij \rangle$





... possible relevance to α -RuCl₃, Na₂IrO₃, Na₂Co₂TeO₆, ...

Technical challenge: Dynamical \mathbb{Z}_2 gauge field!



... from 24-site ED: [Chaloupka, Jackeli, Khaliullin, PRL '13]



'RB '21	
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Clifford algebra:

$$\{\Gamma^{\mu},\Gamma^{\nu}\}=2\delta^{\mu
u}$$

Representations:

$$\sigma^{lpha}$$
 2 × 2 γ^{i} 4 × 4





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$$\{\Gamma^{\mu},\Gamma^{\nu}\}=2\delta^{\mu
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$$\sigma^{lpha}$$
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Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij
angle_{\gamma}} \left(\Gamma^{\gamma}_{i} \Gamma^{\gamma}_{j} + \sum_{eta = \gamma_{\mathrm{m}} + 1}^{2q+3} \Gamma^{\gamma eta}_{i} \Gamma^{\gamma eta}_{j}
ight)$$





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Majorana representation: $\Gamma^{\alpha} = ib^{\alpha}c$ $\Gamma^{\alpha\beta} = ib^{\alpha}b^{\beta}$



Clifford algebra:

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u}\}=2\delta^{\mu
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Representations:

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Hamiltonian:

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ight)$$

Fractionalization:

$$\mathcal{H} \mapsto \tilde{\mathcal{H}} = iK \sum_{\langle ij \rangle_{\gamma}} \hat{u}_{ij} \left($$
with $\left[\hat{u}_{ij}, \tilde{\mathcal{H}} \right] = 0 \quad \Rightarrow$



Majorana representation: $\Gamma^{\alpha} = ib^{\alpha}c$ $\Gamma^{\alpha\beta} = ib^{\alpha}b^{\beta}$

$$\left(c_i c_j + \sum_{\beta=\gamma_m+1}^{2q+3} b_i^{\beta} b_j^{\beta}\right)$$

static \mathbb{Z}_2 gauge field!



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Kitaev spin-orbital models

Spin + orbital + ... degrees of freedom:



Γ^{μ} 8 \times 8

. . .

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Kitaev spin-orbital models

Spin + orbital + ... degrees of freedom:



Spin-orbital representation:

$$egin{aligned} &\gamma^1 = \sigma^y \otimes au^x = ib^1c \ &\gamma^2 = \sigma^y \otimes au^y = ib^2c \ &\gamma^3 = \sigma^y \otimes au^z = ib^3c \ &\gamma^4 = \sigma^x \otimes 1 = ib^4c \ &\gamma^5 = \sigma^z \otimes 1 = ib^5c \end{aligned}$$

Γ^{μ} 8 × 8

. . .

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Kitaev spin-orbital models

Spin + orbital + ... degrees of freedom:



Spin-orbital representation:

Example (square lattice):

$$egin{aligned} &\gamma^1 = \sigma^y \otimes au^x = ib^1c \ &\gamma^2 = \sigma^y \otimes au^y = ib^2c \ &\gamma^3 = \sigma^y \otimes au^z = ib^3c \ &\gamma^4 = \sigma^x \otimes 1 = ib^4c \ &\gamma^5 = \sigma^z \otimes 1 = ib^5c \ \end{aligned}$$



. . .

 $K\sum \left(\sigma_i^{\chi}\sigma_j^{\chi}+\sigma_i^{y}\sigma_j^{y}\right)\otimes\tau_i^{\gamma}\tau_j^{\gamma}$ $\langle ij
angle_{\gamma}$ Kitaev orbital



2 itinerant fermions

 $iK\sum \hat{u}_{ij}\left(c_ic_j+b_i^5b_j^5\right)$ $\langle ij \rangle_{\gamma}$

... recover known model for j = 3/2 spin liquid: [Yao, Zhang, Kivelson, PRL '09] [Nakai, Ryu, Furusaki, PRB '12]



Kitaev-Ising spin-orbital model

Ising perturbation:

$$H = H_{K} + J^{z} \sum_{\langle ij \rangle} \sigma_{i}^{z} \sigma_{j}^{z} \otimes \mathbb{1}_{i} \mathbb{1}_{j}$$





Kitaev spin-orbital liquid



Ising spin order



Kitaev-Ising spin-orbital model

Ising perturbation:

$$H = H_{K} + J^{z} \sum_{\langle ij \rangle} \sigma_{i}^{z} \sigma_{j}^{z} \otimes \mathbb{1}_{i} \mathbb{1}_{j}$$



0

Parton representation:







Kitaev spin-orbital liquid



Spin-orbital model \mapsto interacting fermions on π -flux lattice





Spinless fermions on π -flux lattice: QMC



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Charge density wave

V/t



[Li, Jiang, Yao, NJP '15]

[Huffman & Chandrasekharan, PRD '17; PRD '20]

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Spinless fermions on π -flux lattice: QMC





9







. . . .

Spinless fermions on π -flux lattice: QMC



1/
u = 1.12Gross-Neveu- \mathbb{Z}_2 universality:

Spin-orbital model:





00

Charge density wave



[Li, Jiang, Yao, NJP '15] [Huffman & Chandrasekharan, PRD '17; PRD '20]

9

2(1),
$$\eta_{\phi} = 0.51(3)$$

V/t

[LJ & Herbut, PRB '14] [Ihrig, Mihaila, Scherer, PRB '18] [Erramilli et al., JHEP '23]

N = 8: [Wang & Meng, arXiv:2304.00034]

[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]







Gross-Neveu vs Gross-Neveu*



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Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij
angle_{\gamma}} ec{\sigma}_i \cdot ec{\sigma}_j \otimes au_i^{\gamma} au_j^{\gamma} + J \sum_{\langle ij
angle_{\gamma}} ec{\sigma}_i$$



$\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j$

Hamiltonian:

$$\begin{aligned} \mathcal{H} &= \mathcal{K} \sum_{\langle ij \rangle_{\gamma}} \vec{\sigma_{i}} \cdot \vec{\sigma_{j}} \otimes \tau_{i}^{\gamma} \tau_{j}^{\gamma} + J \sum_{\langle ij \rangle_{\gamma}} \vec{\sigma_{ij}} \\ &\mapsto \hat{u}_{ij} \left(\begin{array}{c} c_{i}, \ b_{i}^{4}, \ b_{i}^{5} \end{array} \right) \cdot \begin{pmatrix} c_{j} \\ b_{j}^{4} \\ b_{j}^{5} \end{pmatrix} \\ &\equiv \hat{u}_{ij} c_{i}^{\top} c_{j} \end{aligned}$$



$ec{\sigma}_i\cdotec{\sigma}_j\otimes \mathbb{1}_i\mathbb{1}_j$

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$$\mathcal{H} = \mathcal{K} \sum_{\langle ij
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 $\mapsto \hat{u}_{ij} \left(c_{i}, b_{i}^{4}, b_{i}^{5}
ight) \cdot \begin{pmatrix} c_{j} \\ b_{j}^{4} \\ b_{j}^{5} \end{pmatrix}$
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with $[\hat{u}_{ij}, \mathcal{H}] = 0$ still static!

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Phase diagram:







with $[\hat{u}_{ij}, \mathcal{H}] = 0$ still static!



 $\bigotimes \left\langle c_{iA}^{\top} \vec{L} c_{iA} \right\rangle \neq \left\langle c_{jB}^{\top} \vec{L} c_{jB} \right\rangle$

"spin density wave"

Gross-Neveu-SO(3)* transition

iDMRG:



... on cylinder with $L_y = 4$ unit cells

[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]



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iDMRG:



... on cylinder with $L_y = 4$ unit cells

Effective field theory:

$$\mathcal{S} = \int d^2 \vec{x} d au \left[ar{\psi} \gamma'
ight]$$

0



[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]

 $\psi^{\mu}\partial_{\mu}\psi+gec{arphi}\cdotec{\psi}(\mathbb{1}_{2}\otimesec{L})\psi\Big|$

"Gross-Neveu-SO(3)"



Gross-Neveu-SO(3)* criticality

Critical exponents from ...

- 4 ε expansion @ 3 loop
- 1/N expansion @ $O(1/N^2)$
- Functional RG @ LPA'



N = 3	3		$1/\nu$	η_{ϕ}
$4-\epsilon$	expansion	naïve	0.97516	0.39181
		[1/2]	0.94472	0.40086
		[2/1]	sing.	0.36989
		[0/3]	1.09000	ne.
1/N expansion		naïve	2.67318	0.49833
		[1/1]	0.89397	0.46276
		[0/2]	sing.	0.51074
		naïve		
		[1/2]		
		[2/1]		
		[0/3]		
FRG	Taylor	linear	1.1901(10)	0.38781(6)
	-	sharp	1.209(4)	0.3434(5)
	pseudospectral	linear	1.18974	0.38781
		sharp	1.20465	0.34340

Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\lambda} c_{j\lambda} - J \sum_{i} \left(c^{\dagger}_{i\lambda} \vec{L} \tau^{z}_{\lambda\lambda'} c_{i\lambda'} \right)^{2}$$

... with $\mathsf{SO}(3) imes \mathsf{U}_\lambda(1) imes \mathsf{U}_\mathsf{c} imes \mathbb{Z}_2$ symmetry

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$$\mathcal{H} = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\lambda} c_{j\lambda} - J \sum_{i} \left(c^{\dagger}_{i\lambda} \vec{L} \tau^{z}_{\lambda\lambda'} c_{i\lambda'} \right)$$

QMC structure factors:

<u>ک</u>

... with SO(3) imes U $_{\lambda}(1) imes$ U $_{c} imes \mathbb{Z}_{2}$ symmetry

Phase diagram:

Symmetric semimetal

Phase diagram:

Symmetric semimetal $\bigcirc \heartsuit \bigtriangledown$

"Spin-orbital liquid"

Fermion spectral function:

1/
u = 0.906(35)

... cf. $1/\nu = 0.93(4)$ and $\eta_{\phi} = 0.83(4)$ from field theory [Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

Order parameter:

... cf. $1/\nu = 0.93(4)$ and $\eta_{\phi} = 0.83(4)$ from field theory [Ray, Ihrig, Kruti, Gracey, Scherer, LJ, PRB '21]

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0.6

 \diamond

Correlation ratios:

Critical couplings:

[Liu, Vojta, Assaad, LJ, PRL '22 (Editors' Suggestion)]

Free energy:

Correlation lengths:

 $\xi^{2} = \frac{1}{2d} \frac{\sum_{\vec{r}} |\vec{r}|^{2} S(\vec{r})}{\sum_{\vec{r}} S(\vec{r})}$

[Liu, Vojta, Assaad, LJ, PRL '22 (Editors' Suggestion)]

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Square-lattice Kitaev-Ising spin-orbital model:

Honeycomb-lattice Kitaev-Heisenberg spin-orbital model:

[Seifert, Dong, Chulliparambil, Vojta, Tu, LJ, PRL '20]

[Liu, Vojta, Assaad, LJ, PRL '22]

Conclusions

SO(*N*) Majorana-Hubbard models

[LJ & Seifert, PRB '22]

SU(*N*) Hubbard-Heisenberg models

[Affleck & Marston, PRB '88] [Read & Sachdev, NPB '89] [Lang, Meng, Muramatsu, Wessel, Assaad, PRL '13]