Variational wavefunctions for the pseudogap metal

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May 23, 2023

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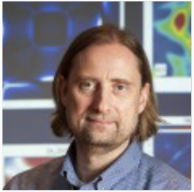
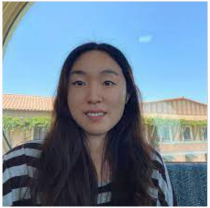


Dirk Morr

Darshan Joshi

Maine Christos

Alexander Nikolaenko



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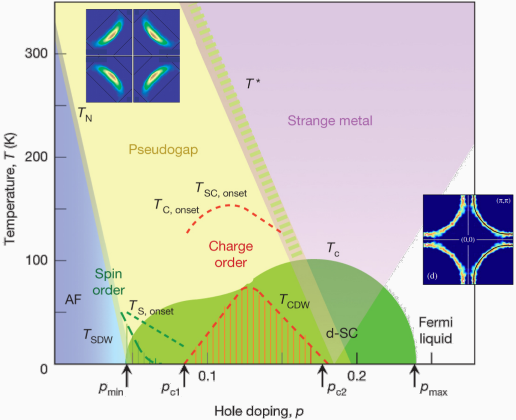
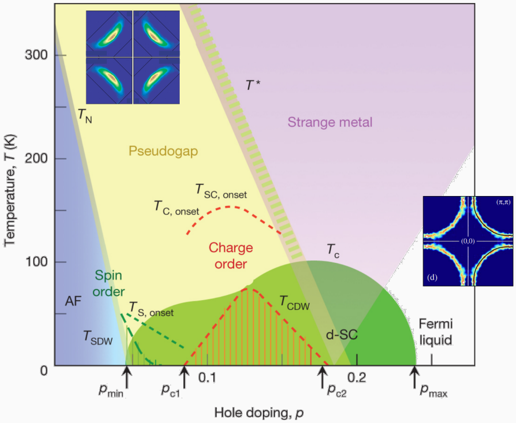
Long-standing mystery in cuprates - the nature of the pseudogap



Keimer et al. 2015.

Long-standing mystery in cuprates - the nature of the pseudogap

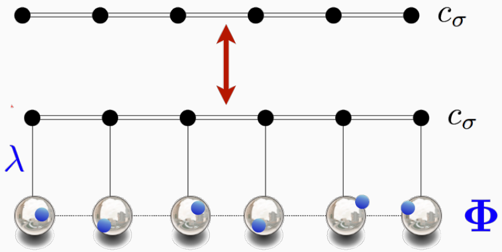


View the pseudogap metal as a quantum state, which could be stable at $T = 0$ under suitable conditions

Goal: construct a mean-field theory that captures both FL and psuedo-gap metals

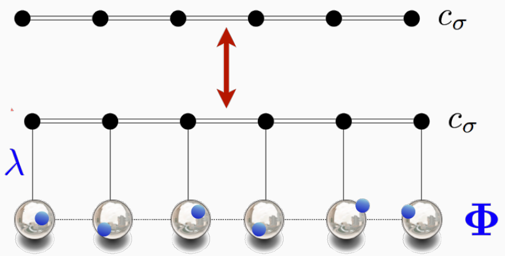
Keimer et al. 2015.

Paramagnon theory of the Hubbard model



$$H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Paramagnon theory of the Hubbard model



$$H_{sf} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} - \lambda \sum_i c^\dagger_{i\alpha} \frac{\sigma_{\alpha\beta}}{2} c_{i\beta} \cdot \mathbf{\Phi}_i + J_\perp \mathbf{P}^2_{\mathbf{\Phi} i}$$

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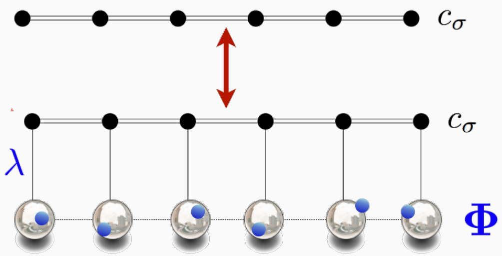

AFQMC connection: re-formulate $e^{-\tau H}|\psi_0\rangle$ as 2D free fermions coupled to (2+1)D classical fields. "Re-quantizing" classical fields gives $e^{-\tau H_{sf}}|\psi_0\rangle \otimes |a\rangle$

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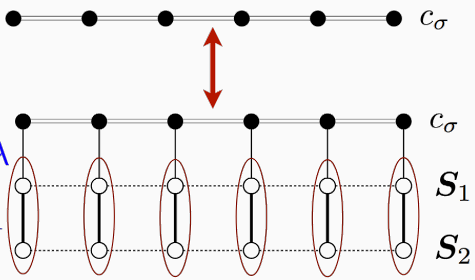

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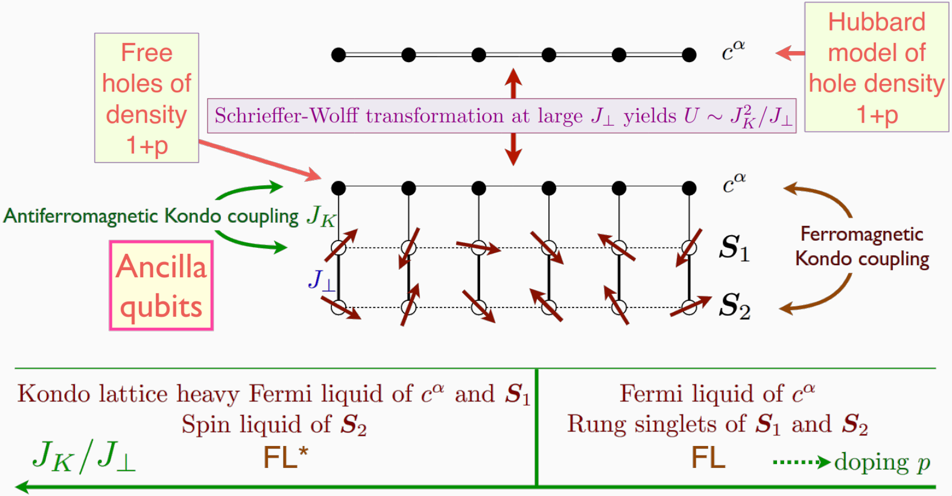
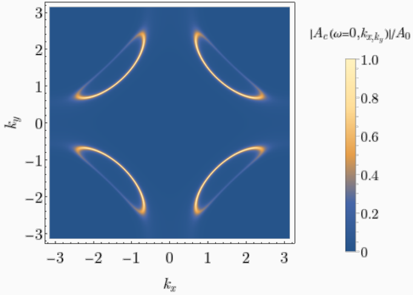
Represent $\ell = 0\,, 1$ excitations as antiferromagnetic spin pair, $\mathbf{\Phi}_i = \frac{1}{\sqrt{3}}\left(\mathbf{S}_{2i} - \mathbf{S}_{1i}\right)$

Mean-field phase diagram of the pseudogap metal



FL* phase qualitatively captures pseudogap features



Mean-field calculation reproduces small hole pockets with weak back-side spectral weight

Mascot et al. 2022; Nikolaenko et al. 2023; Christos et al. 2023.

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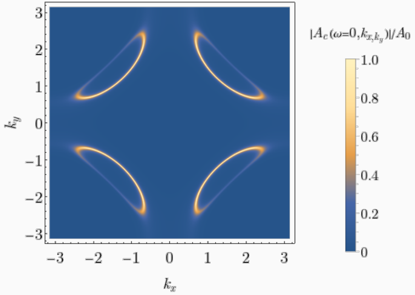

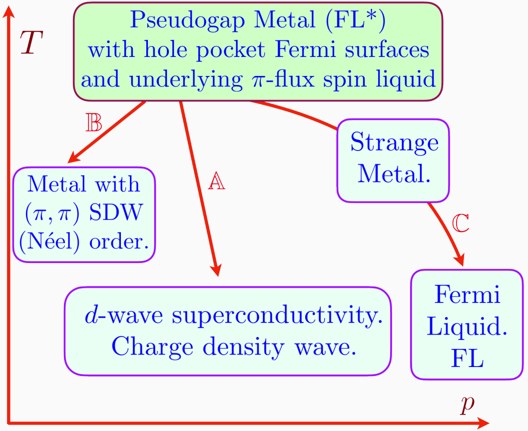

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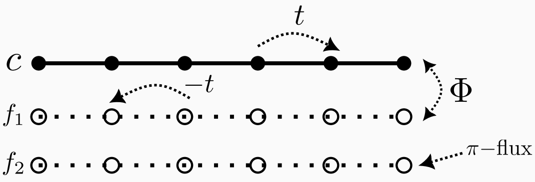
Paramagnon fractionalization admits trial wavefunctions



$$|\psi\rangle \equiv \underbrace{\prod_i \left(f_{1i\uparrow} f_{2i\downarrow} - f_{1i\downarrow} f_{2i\uparrow}\right)}_{\text{Rung singlet projection}} |\psi_{\mathrm{MF}}\rangle$$

- How do these states fare energetically?
- Can they reproduce (static) correlation functions?

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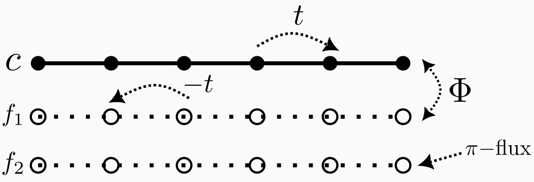

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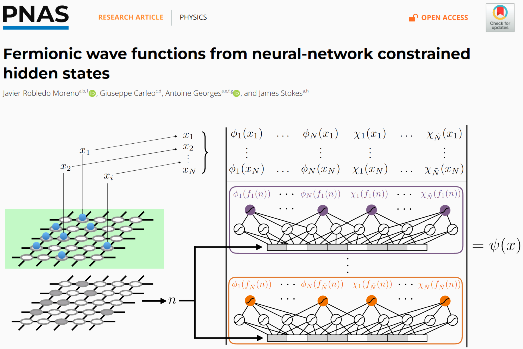
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Fermionic wave functions from neural-network constrained hidden states

Javier Robledo Moreno[a,b,1], Giuseppe Carleo[c,d], Antoine Georges[a,e,f,g], and James Stokes[a,h]

Spin singlet projection implementation

$$\psi(R) \equiv \underbrace{(\langle R| \otimes \langle\uparrow\downarrow|)\,|\psi_{\mathrm{MF}}\rangle}_{\text{Scales exponentially}}$$

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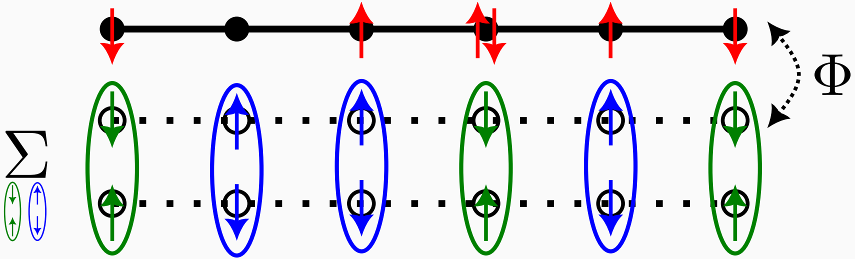

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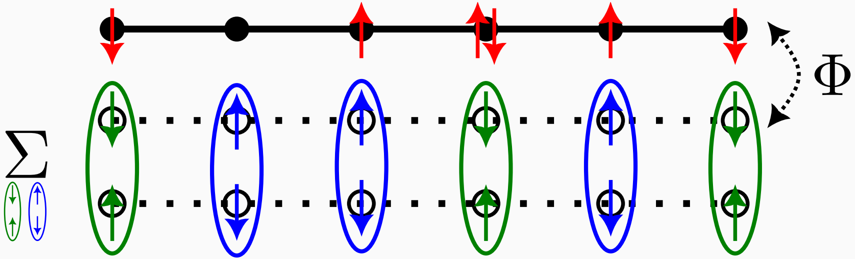
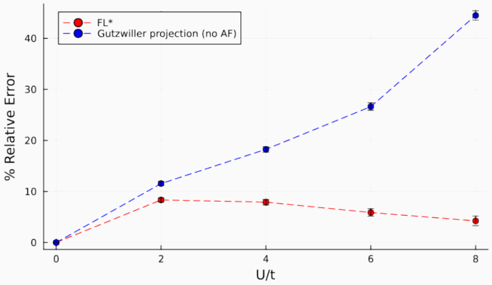


$$\frac{\langle\psi|\,H\,|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{R,x,x'} \psi^*(R,x')\psi(R,x)E(R,x,x')}{\sum_{R,x,x'} \psi^*(R,x')\psi(R,x)}$$

$p(R,x,x')s(R,x,x')$

Results at half filling, 4×4 lattice



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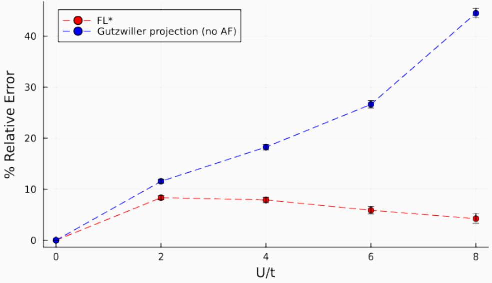
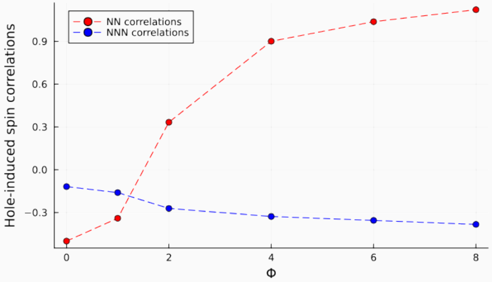


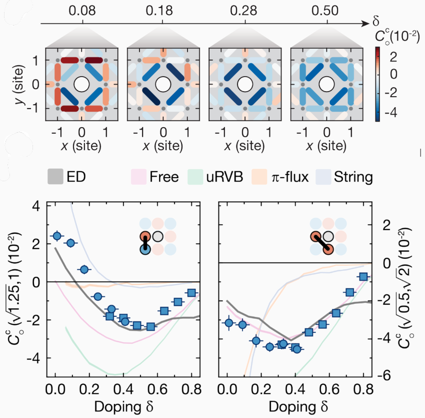


RESEARCH

QUANTUM SIMULATION

Microscopic evolution of doped Mott insulators from polaronic metal to Fermi liquid

Joannis Koepsell[1,2]*, Dominik Bourgund[1,2], Pimonpan Sompet[1,2], Sarah Hirthe[1,2], Annabelle Bohrdt[2,3]†‡, Yao Wang[4,5], Fabian Grusdt[2,6], Eugene Demler[4]§, Guillaume Salomon[1,2,7,8], Christian Gross[1,2,9], Immanuel Bloch[1,2,6]



Future directions

For pseudogap:

- Careful finite size analysis - average over BCs, extrapolate to thermodynamic limit, etc
- Non-zero doping - at $U/t = 8$, energetic favourability vanishes around $p \approx 0.25$
- GA for simplifying wavefunctions?

General perspectives:

- Using "quantum" auxiliary fields for trial variational wavefunctions - how optimizable is a more general projection?