SU(2) gauge theory of the pseudogap phase in the two-dimensional Hubbard model

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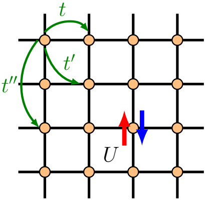
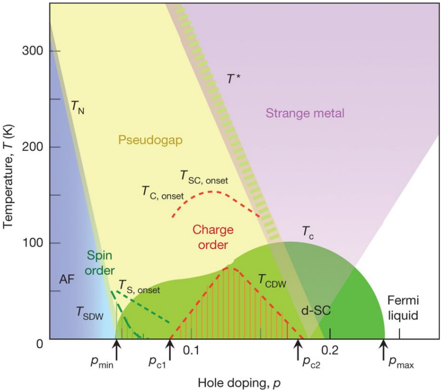
Introduction

The cuprates and the Hubbard Model

$$\mathcal{H} = \sum_{j,j',\sigma} t_{jj'} \, c^\dagger_{j,\sigma} \, c_{j',\sigma} + U \sum_j c^\dagger_{j,\uparrow} \, c_{j,\uparrow} \, c^\dagger_{j,\downarrow} \, c_{j,\downarrow}$$



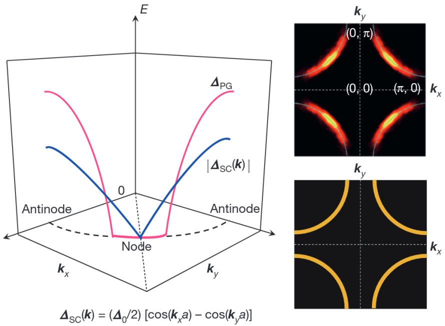


from Keimer *et al.*, Nature **518**, 179 (2015)

It captures the main features of the cuprates phase diagram

The pseudogap regime

Spectral function shows Fermi arcs

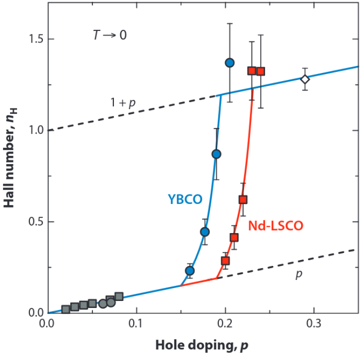


from Keimer *et al.*, Nature **518**, 179 (2015)

Hall number $n_H = \frac{1}{|e|R_H}$

$\propto$ charge carrier density

$\rightarrow$ crossover from p to $1+p$



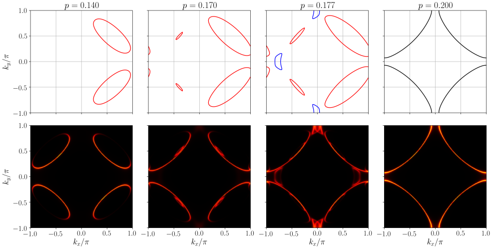
from Proust & Taillefer, Nature **518**, 179 (2015)

Mean-field for spiral magnetism

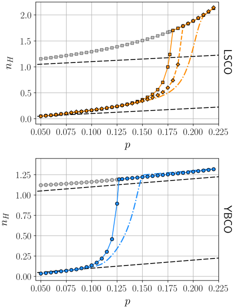
In the pseudogap regime assume a long-range ordered state

$$\frac{1}{2}\langle c_j^* \vec{\sigma} c_j \rangle = m \left[\cos\left(\mathbf{Q}\cdot\mathbf{r}_j\right) \hat{e}_x + \sin\left(\mathbf{Q}\cdot\mathbf{r}_j\right) \hat{e}_y \right]$$

single band $\xi_{\mathbf{k}}$ gets reconstructed into $E^{\pm}_{\mathbf{k}} = \frac{\xi_{\mathbf{k}+\mathbf{Q}}+\xi_{\mathbf{k}}}{2} \pm \sqrt{\left(\frac{\xi_{\mathbf{k}+\mathbf{Q}}-\xi_{\mathbf{k}}}{2}\right)^2 + (Um)^2}$



from Bonetti *et al.*, PRB **101**, 165142 (2020)



from Bonetti *et al.*, PRB **101**, 165142 (2020)

- Fermi arcs
- charge carrier drop

BUT no evidence for magnetic order in the pseudogap!

Method & Results

Motivation

Spiral magnetism provides a good description of the pseudogap phase

BUT it spontaneously breaks the SU(2)-spin symmetry
$\rightarrow$ not observed in the experiments

IDEA: consider a fluctuating magnet

Fractionalization of the e^-: $$c_{j,\sigma} = \sum_{\eta=\uparrow,\downarrow} R_{j,\sigma\eta}\psi_{j,\eta}$$

[Schulz, in *The Hubbard model* (1995), Borejsza & Dupuis, PRB **69**, 085119 (2004), Scheurer *et al.*, PNAS **115**, E3665 (2018)]

- $R_j \in \mathrm{SU}(2)$ describe spin fluctuations (bosonic spinons)
- ψ_j are fermionic fields carrying only charge (chargons)
- $\mathrm{SU}(2)$ gauge freedom $R_j \rightarrow R_j V_j$ & $\psi_j \rightarrow V_j^\dagger \psi_j$ $\rightarrow$ gauge theory
- if $\langle \psi_j^* \vec{\sigma} \psi_j \rangle \neq 0$ but $\langle R_j \rangle = 0$ no SSB

SU(2) gauge theory

Hubbard model coupled to a SU(2) gauge field $A_{\mu,j} = (-R_j^\dagger \partial_\tau R_j, iR_j^\dagger \boldsymbol{\nabla} R_j)$

$$\mathcal{S}[\psi,\psi^*,R] = \int_0^\beta d\tau \Big\{ \sum_{j,j'} \psi_j^* \left[(\partial_\tau - \mu - A_{0,j})\, \delta_{jj'} + t_{jj'} e^{-\mathbf{r}_{jj'}\cdot(\boldsymbol{\nabla} - i\mathbf{A}_j)} \right] \psi_j + U \sum_j n^\psi_{j\uparrow} n^\psi_{j\downarrow} \Big\}$$

Integration of the chargon degrees of freedom

$$e^{-\mathcal{S}_{\text{eff}}[R]} = \int \mathcal{D}\psi \mathcal{D}\psi^* \, e^{-\mathcal{S}[\psi,\psi^*,R]}$$

Integral has to be performed by means of approximate methods to derive low-energy theory for the spinon d.o.f. R

Effective field theory

Gradient expansion $=$ expansion in powers of $A_\mu(x)$ $\to$ retain only lowest order

$$\mathcal{S}_{\text{eff}}[R] \approx \int_{\mathbb{R}^2\times[0,\beta]} dx \left\{ \frac{1}{2} \mathcal{J}_{\mu\nu}^{ab} A_\mu^a(x) A_\nu^b(x) \right\}$$

here $A_\mu(x) = \sum_{a=1}^{3} A_\mu^a(x) \frac{\sigma^a}{2}$

Re-expressing $A_\mu(x)$ in terms of $R(x)$, we obtain the

$\mathrm{O}(3)\times\mathrm{O}(2)/\mathrm{O}(2)$ nonlinear sigma model

[Azaria *et al.*, PRL **64**, 3175 (1990)]

$$\mathcal{S}_{\text{NL}\sigma\text{M}}[\mathcal{R}] = \int_{\mathbb{R}^2\times[0,\beta]} dx \left\{ \frac{1}{2} \operatorname{tr}\left[\mathcal{P}_{\mu\nu} (\partial_\mu \mathcal{R})^T (\partial_\nu \mathcal{R}) \right] \right\}$$

with $\mathcal{R}^{ab}(x) = \frac{1}{2}\operatorname{Tr}\left[R^\dagger(x)\sigma^a R(x)\sigma^b\right] \in \mathrm{SO}(3)$ the adjoint representation of R

and $\mathcal{P}_{\mu\nu} = \frac{1}{2}\operatorname{Tr}\left[\mathcal{J}_{\mu\nu}\right]\mathbb{1} - \mathcal{J}_{\mu\nu}$ $\qquad$ $\mathcal{J}_{\mu\nu}$ is the spin stiffness tensor

Chargon condensates

Different possible "magnetic" orders of the chargons

- $\langle \psi_j^* \vec{\sigma} \psi_j \rangle = 0 \rightarrow \mathcal{J}_{\mu\nu}^{ab} = 0$

- Néel order $\langle \psi_j^* \vec{\sigma} \psi_j \rangle \propto (-1)^{\mathbf{r}_j} \hat{v} \quad \rightarrow \quad \mathcal{J}_{\mu\nu} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & J_{\mu\nu} & 0 \\ 0 & 0 & J_{\mu\nu} \end{pmatrix}$

  effective model reduces to

$$\mathcal{S}_{\mathrm{NL}\sigma\mathrm{M}}[\hat{n}] = \int_{\mathbb{R}^2 \times [0,\beta]} dx \, \frac{1}{2} \Big\{ Z |\partial_\tau \hat{n}|^2 + J |\boldsymbol{\nabla} \hat{n}|^2 \Big\}, \qquad \hat{n}^a = \mathcal{R}^{a1}, \qquad |\hat{n}|^2 = 1$$

  2 equivalent Goldstone modes encoded in $\hat{n}$

- spiral order $\langle \psi_j^* \vec{\sigma} \psi_j \rangle \propto \cos(\mathbf{Q} \cdot \mathbf{r}_j) \hat{v}_1 + \sin(\mathbf{Q} \cdot \mathbf{r}_j) \hat{v}_2$, $\quad \mathcal{J}_{\mu\nu} = \begin{pmatrix} J_{\mu\nu}^{\perp} & 0 & 0 \\ 0 & J_{\mu\nu}^{\perp} & 0 \\ 0 & 0 & J_{\mu\nu}^{\square} \end{pmatrix}$

  $\mathbf{Q} = (\pi - 2\pi\eta, \pi)$ breaking of lattice C_4 symmetry

  3 Goldstone modes: two out-of-plane ($J_{\mu\nu}^{\perp}$) and one in-plane ($J_{\mu\nu}^{\square}$)

Computation of parameters I

Goal: compute the spin stiffness tensor

Technique: fRG+MF [Yamase *et al.*, PRL **116**, 096402 (2016)] on the chargon d.o.f.

Symmetric Phase $\to$ temperature flow [Honerkamp & Salmhofer, PRB **64**, 184516 (2001)]

$\psi \to T^{\frac{3}{4}}\psi, \quad G_0^T(\mathbf{k}\,\nu) = T^{\frac{1}{2}}(i\nu + \xi_\mathbf{k})^{-1}$

1-loop truncation with static approximation on the vertex
$\to$ tU-fRG [Husemann & Salmhofer, PRB **79**, 195125 (2009), Lichtenstein *et al.*, CPC **213**, 100 (2017)]

$$\Sigma^\psi(\mathbf{k},\nu) = 0$$

$$\begin{aligned} V^\psi_{\uparrow\downarrow\uparrow\downarrow}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3;\cancel{\nu_1,\nu_2,\nu_3}) = U &- \phi^p_{\mathbf{k}_1,\mathbf{k}_3}(\mathbf{k}_1+\mathbf{k}_2) \\ &+ \phi^m_{\mathbf{k}_1,\mathbf{k}_3}(\mathbf{k}_2-\mathbf{k}_3) \\ &- \frac{1}{2}\phi^c_{\mathbf{k}_1,\mathbf{k}_4}(\mathbf{k}_3-\mathbf{k}_1) + \frac{1}{2}\phi^m_{\mathbf{k}_1,\mathbf{k}_4}(\mathbf{k}_3-\mathbf{k}_1) \end{aligned}$$

ϕ^p, ϕ^m, ϕ^c: pairing, magnetic and charge channels

$$\phi^X_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) = \sum_{\ell,\ell'} \phi^X_{\ell\ell'}(\mathbf{q}) f^\ell_\mathbf{k} (f^\ell_{\mathbf{k}'})^*$$

$f^0_\mathbf{k} = 1,\ f^1_\mathbf{k} = \cos k_x + \cos k_y,\ f^2_\mathbf{k} = \cos k_x - \cos k_y,\ f^3_\mathbf{k} = \sqrt{2}\sin k_x,\ f^4_\mathbf{k} = \sqrt{2}\sin k_y,\ \ldots$

Computation of parameters II

The flow is run until a temperature T^* where $V^{\psi, T\to T^*} \to \infty$

Symmetry-Broken Phase: allow for order parameter of the type $\langle \psi^*_{\mathbf{k},\uparrow} \psi_{\mathbf{k}+\mathbf{Q},\downarrow} \rangle$

Gap equation for $T \leq T^*$

$$\boxed{\Delta_{\mathbf{k}} = \int_{\mathbf{k}'} \bar{V}^m_{\mathbf{k},\mathbf{k}'}(\mathbf{Q}) \, \frac{f(E^-_{\mathbf{k}'}) - f(E^+_{\mathbf{k}'})}{E^+_{\mathbf{k}'} - E^-_{\mathbf{k}'}}}$$

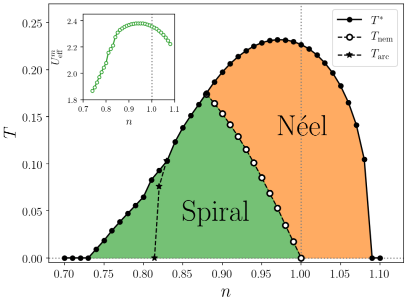
$\bar{V}^m_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) \to$ 2PI vertex in the ph-crossed channel at $T = T^*$

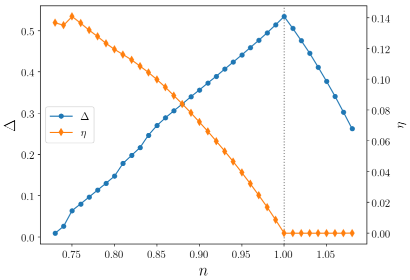
Optimal $\mathbf{Q}$-vector is found minimizing the free energy

$$F(\mathbf{Q}) = -T \int_{\mathbf{k}} \sum_{\ell=\pm} \ln\left(1 + e^{-E^\ell_{\mathbf{k}}(\mathbf{Q})/T}\right) + \int_{\mathbf{k},\mathbf{k}'} \Delta_{\mathbf{k}} \left[\bar{V}^m_{\mathbf{k},\mathbf{k}'}(\mathbf{Q})\right]^{-1} \Delta_{\mathbf{k}'} + \mu \cdot n$$

for simplicity, we assume $\bar{V}^m_{\mathbf{k},\mathbf{k}'}(\mathbf{q}) \approx U^m_{\text{eff}} [= \int_{\mathbf{k},\mathbf{k}'} \bar{V}^m_{\mathbf{k},\mathbf{k}'}(\mathbf{Q}_c)] \to \Delta_{\mathbf{k}} \approx \Delta$

Chargon mean-field phase diagram





- $U^m_{\rm eff}$=1.8t÷2.4t strongly renormalized w.r.t. $U = 4t$
- pseudogap regime extends from $n \approx 0.73$ to $n \approx 1.08$
- 1st order transition on the e^- doped side & 2nd order on the h-doped side
- nematic transition *inside* the pseudogap (Néel to spiral)
- $T_{\rm arc}$ divides Fermi arcs from large FS
- gap function maximal at $n = 1$
- incommensurability $\eta \to$ $\mathbf{Q} = (\pi - 2\pi\eta, \pi)$ grows with decreasing n

Spin stiffnesses I

Temporal component of the stiffnesses $\mathcal{J}_{00}^{ab}$ is given by the dynamic limit of the spin susceptibility χ^{ab}

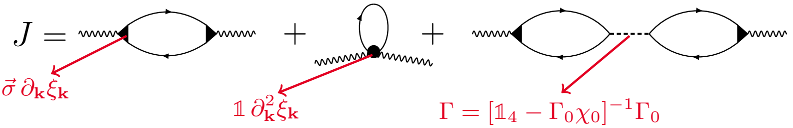
$$\mathcal{J}_{00}^{ab} = \chi_{\mathrm{dyn}}^{ab} \equiv \lim_{\omega \to 0} \chi^{ab}(\mathbf{q} = \mathbf{0}, \omega)$$

[Bonetti, arXiv:2204.04132 (2022)]

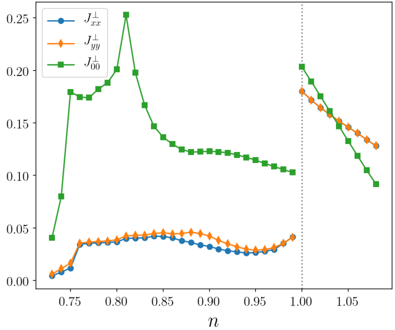
fRG+MF $\rightarrow$ RPA formula for coupled charge-spin susceptibilities [Kampf, PRB **53**, 747 (1996)]

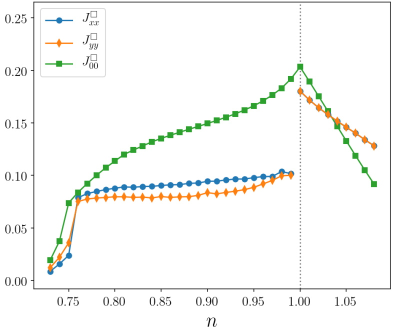
$$\chi(\mathbf{q},\omega) = \chi_0(\mathbf{q},\omega)\left[\mathbb{1}_4 - \Gamma_0(\mathbf{q})\chi_0(\mathbf{q},\omega)\right]^{-1} \quad \Gamma_0(\mathbf{q}) = \mathrm{diag}(-U_{\mathrm{eff}}^{c}(\mathbf{q}), U_{\mathrm{eff}}^{m}, U_{\mathrm{eff}}^{m}, U_{\mathrm{eff}}^{m})$$

Spatial stiffnesses $\mathcal{J}_{\alpha\beta}^{ab}$ computed coupling the system to an external SU(2) gauge field



Spin stiffnesses II





- strong e^{-}-h asymmetry
- appearance of hole pockets causes a sudden jump in J_{xx}^{a} & J_{yy}^{a}
- $J_{00}^{\perp}$ peaks at $n \approx 0.82$ where two hole pockets merge ($\rightarrow$ large FS)
- quantum fluctuations stronger on the hole-doped side

Massive CP^1 model [Azaria *et al.*, Nucl. Phys. **455**, 648 (1995)]

CP^1 representation: $R = \begin{pmatrix} z_1 & -z_2^* \\ z_2 & z_1^* \end{pmatrix}$ with $|z_1|^2 + |z_2|^2 = 1$ 2 Schwinger bosons

$$\mathcal{S}_{\mathrm{CP}^1}[z, z^*] = \int dx \left[2J^{\perp}_{\mu\nu}(\partial_\mu z^*)(\partial_\nu z) - 2(J^{\perp}_{\mu\nu} - J^{\square}_{\mu\nu}) j_\mu j_\nu\right]$$

$j_\mu = (i/2)[z^*(\partial_\mu z) - (\partial_\mu z^*)z]$ current operator

Lagrange multiplier λ to enforce $|z|^2 = 1$ & U(1) gauge field $\mathcal{A}_\mu$ to decouple $j_\nu j_\nu$

$$\mathcal{S}_{\mathrm{CP}^1}[z, z^*, \lambda, \mathcal{A}_\mu] = \int dx \left[2J^{\perp}_{\mu\nu}(D_\mu z^*)(D_\nu z) + i\lambda\left(|z|^2 - 1\right) + \frac{1}{2} M_{\mu\nu}\mathcal{A}_\mu \mathcal{A}_\nu\right]$$

covariant derivative $D_\mu = \partial_\mu + i\mathcal{A}_\mu$, gauge field mass $M = 4J^\perp[J^\perp - J^\square]^{-1}J^\square$

Here, Landau damping of the spinons neglected $\to$ out-of-plane modes are underdamped [Bonetti & Metzner, PRB **105**, 134426 (2022)]

Large-N spin gap equation

extend $z = (z_1, z_2)$ to $z = (z_1, z_2, \dots, z_N)$ & consider the limit $N \to \infty$

integrating out $z \to \mathcal{S}_{\mathrm{CP}^{N-1}} = N\mathcal{S}_0[\lambda, \mathcal{A}_\mu]$, solve $\frac{\delta \mathcal{S}_0}{\delta \lambda} = 0$ & $\frac{\delta \mathcal{S}_0}{\delta \mathcal{A}_\mu} = 0$

$$\frac{1}{J^\perp_{00}} \int_{|\mathbf{q}|<\Lambda_{\mathrm{uv}}} \frac{1}{2\sqrt{\epsilon^2_{\mathbf{q}} + m_s^2}} \coth\left(\frac{\sqrt{\epsilon^2_{\mathbf{q}} + m_s^2}}{2T}\right) = 1$$

spin gap $m_s = \sqrt{-i\langle\lambda(x)\rangle / J^\perp_{00}}$, $\epsilon_{\mathbf{q}} = \sqrt{c^2_{\alpha\beta} q_\alpha q_\beta}$ velocity tensor $c_{\alpha\beta} = \sqrt{J^\perp_{\alpha\beta}/J^\perp_{00}}$

solution $\boxed{m_s \approx T^{-1} e^{-\frac{2\pi}{T}(J - J_c)}}$ $\to$ **Mermin-Wagner theorem**, $J = \sqrt{\det J^\perp_{\alpha\beta}}$, $J_c \propto \Lambda_{\mathrm{uv}}$

at $T = 0$

$$n_0 + \frac{1}{J^\perp_{00}} \int_{|\mathbf{q}|<\Lambda_{\mathrm{uv}}} \frac{1}{2\sqrt{\epsilon^2_{\mathbf{q}} + m_s^2}} = 1 \qquad n_0 = \langle z_1 \rangle^2 \text{ condensate fraction}$$

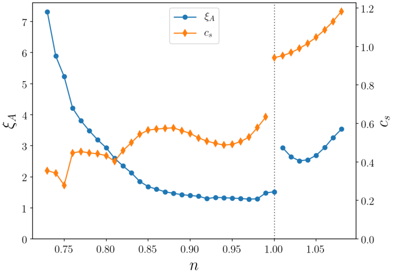
$\boxed{n_0 = 1 - \frac{J_c}{J}}$ $\to$: if $J > J_c \to$ LRO, if $J < J_c \to$ quantum disordered phase

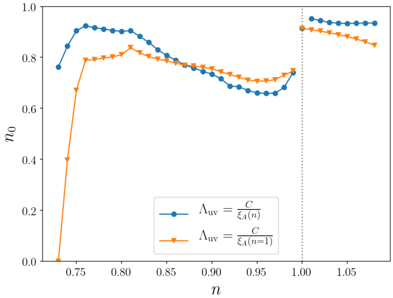
uv cutoff & spinon fluctuations

estimate uv cutoff as $\boxed{\Lambda_{\mathrm{uv}} = \frac{C}{\xi_A}}$ ξ_A magnetic coherence length $\sim 1/$(amplitude mass)

constant C is fixed by imposing $n_0 \approx 0.6$ at half-filling for $U/t \to +\infty$ (Heisenberg limit)

2 choices: $\xi_A(n)$ & fix $\xi_A(n=1)$





- for both cutoff choices the GS is LRO
- spinon fluctuations stronger in the hole-doped regime ($n < 1$)
- average velocity $c_s = \sqrt{\det c_{\alpha\beta}}$ weakly filling-dependent

Applying $c_j(\tau) = R_j(\tau)\psi_j(\tau)$, we have

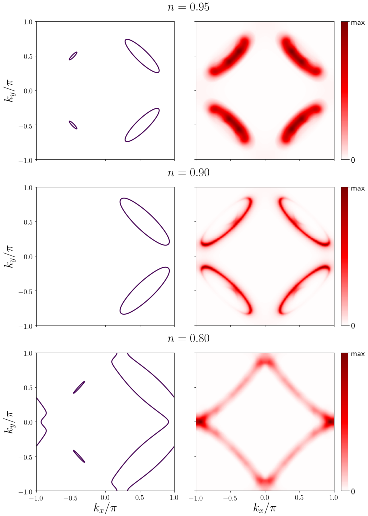
$$G = G^R \circ G^\psi$$

$$G^R_{N\to\infty}(\mathbf{q},\omega) = \frac{1/J^\perp_{00}}{-\omega^2 + c^2_{\alpha\beta} q_\alpha q_\beta + m_s^2}$$

$$G^\psi(\mathbf{k},\omega) = \begin{pmatrix} \omega - \xi_\mathbf{k} & -\Delta \\ -\Delta & \omega - \xi_{\mathbf{k}+\mathbf{Q}} \end{pmatrix}^{-1}$$

- if $n_0 = 0$, $G \propto \mathbb{1}$ $\rightarrow$ NO SSB (at $T \neq 0$ $\forall J$ & at $T = 0$ for $J < J_c$)
- Fermi arcs survive
- large FS for small filling
- transport properties not affected by spinons $\rightarrow$ charge carrier drop

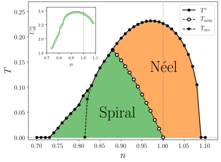
chargon FS *vs* e^- spectral function



Summary

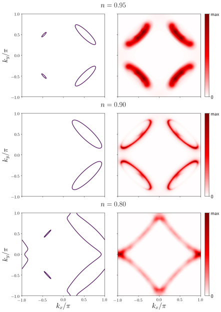
fRG+MF+fluctuations method

- fractionalization of the electron $c_j(\tau) = R_j(\tau)\psi_j(\tau)$
- fRG+MF on $\psi_j(\tau) \to$ compute spin stiffnesses
- derive effective NLσM for $R_j(\tau)$ + large-N expansion



Results

- finite temperature pseudogap regime below T^*
- nematic transition *inside* the pseudogap
- spectral function always displays Fermi arcs
- transport coefficients reproduce the charge carrier density drop



[preprint: Bonetti & Metzner arXiv:2207.00829 (2022)]

Thank you for your attention