Gauge theory of optimal doping criticality in the cuprates

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Subir Sachdev

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LETTER TO THE EDITOR

Scaling at the percolation threshold above six dimensions

Amnon Aharony, Yuval Gefen and Aharon Kapitulnik
Department of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel

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Abstract. The fractal dimensionality of the infinite cluster at the percolation threshold for dimensionalities \( d > 6 \) is shown to be \( D = 4 \) (rather than the naive finite size scaling prediction \( D = d - 2 \)). Similarly, the conductivity of a sample of size \( L \) scales as \( L^{-d} \) (rather than \( L^{-6} \)). This anomalous behaviour is related to a dangerous irrelevant variable, associated with the probability to have vertices of three bonds. The crossover to the 'homogeneous' behaviour occurs at length scales which are short compared with the correlation length. The 'links and blobs' picture is confirmed for \( d > 6 \), and the size of the latter is estimated.

encountered in their growth, a similar temperature-doping phase diagram of superconductivity are made difficult by the severe difficulties associated with the proper selection of the doping range. Although similar studies of antiferromagnetism and inelastic neutron scattering demonstrate that there is no long-range antiferromagnetic order for the reduced samples in the doping range from 0.13–0.18 but that the large magnetic fluctuations in electron-doped cuprates and may be absent (and perhaps charge-density waves, while only hole-type carriers are observed for hole-doped cuprates).

Unfortunately, these competing phases can lead to many erroneous conclusions and the resulting structural impacts. One can also observe the pseudogap line as the directional growth of millimeter size high-quality single crystals. We will then discuss the reduction conditions and epitaxial thin films. We should underline that Sr in SrCuO$_2$ has been inserted successfully in (CaCuO$_2$)$_x$Sr$_{1-x}$CuO$_4$. We underline in particular the results of isotopic substitution with the presence of superconductivity up to 70 K.

Post-annealing required for the reduction is tricky as it involves the directional growth of millimeter size high-quality single crystals. The first group of techniques involves the use of solvent floating zone (TSFZ). The second group of techniques consists of solidification and favours the growth of small Ca contents with superconductivity. One can also observe the pseudogap line as the addition of Ca allows one to stabilize the IL crystal structure as shown first by Siegrist et al.

We should underline that Sr in SrCuO$_2$ has been inserted successfully in (CaCuO$_2$)$_x$Sr$_{1-x}$CuO$_4$. We underline in particular the results of isotopic substitution with the presence of superconductivity up to 70 K. Moreover, the stability of other related oxide phases that may be competitors in the temperature-composition phase diagram. These compounds, namely single crystals and IL compounds, namely single crystals and polycrystalline samples has been gathered by Ishawata et al.

In the light blue region above the superconducting dome, strong magnetic correlations are present, suggesting that the mechanism modifying the electronic properties of electron-doped cuprates is generally irrelevant for the mechanism of superconductivity. In electron-doped cuprates and may be absent. Moreover, the physical properties are quite different in electron- and hole-doped cuprates. There are solid evidence of two-band-like behaviours in the transport properties of electron-doped cuprates and may be absent.}

In the case of thin films, the growth phase diagram involves also oxygen pressure. In the light blue region above the superconducting dome, strong magnetic correlations are present, suggesting that the mechanism modifying the electronic properties of electron-doped cuprates is generally irrelevant for the mechanism of superconductivity. In electron-doped cuprates and may be absent.
Antiferromagnetism in the Hubbard Model

\[
H = -\sum_{i<j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right) \left(n_{i\downarrow} - \frac{1}{2}\right) - \mu \sum_i c_{i\alpha}^\dagger c_{i\alpha}
\]

\(t_{ij} \rightarrow \) “hopping”. \(U \rightarrow \) local repulsion, \(\mu \rightarrow \) chemical potential

Mean-field theory with a spin density wave (SDW) order parameter \(\tilde{\Phi}_i = (-1)^{i_x + i_y} \langle c_{i\alpha}^\dagger \bar{\sigma}_{\alpha\beta} c_{i\beta} \rangle / 2\)

\(\tilde{\Phi} \neq 0\): SDW LRO

\(\langle \tilde{\Phi} \rangle \neq 0\): Reconstructed Fermi surface

\(\langle \tilde{\Phi} \rangle = 0\): SDW SRO

Large Fermi surface.

Symmetry breaking phase transition

\(U/t\)
Symmetry breaking and topological phase transition

SDW SRO
Defects in local SDW order are suppressed ("Hedgehogs" in Neel order in spacetime)
Reconstructed Fermi surface.
\[ \langle \Phi \rangle = 0 \]

Symmetry breaking phase transition

SDW LRO
Reconstructed Fermi surface
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Topological phase transition

SDW SRO
Large Fermi surface.
\[ \langle \Phi \rangle = 0 \]
Symmetry breaking and topological phase transition

SDW SRO
Emergent gauge fields and “topological order”.
Reconstructed Fermi surface.
\[ \langle \Phi \rangle = 0 \]

SDW LRO
Reconstructed Fermi surface
\[ \langle \Phi \rangle \neq 0 \]

Symmetry breaking phase transition

Topological phase transition

SDW SRO
Large Fermi surface.
\[ \langle \Phi \rangle = 0 \]
Square lattice Hubbard model with electron doping

\[ \langle \Phi \rangle \neq 0 \]
and large

Metal with electron pockets

Metal with electron and hole pockets

Metal with “large” Fermi surface

\[ \langle \Phi \rangle \neq 0 \]
and small

\[ \langle \Phi \rangle = 0 \]
Nd$_{2-x}$Ce$_x$CuO$_{4+\delta}$

Doping Dependence of an n-Type Cuprate Superconductor Investigated by Angle-Resolved Photoemission Spectroscopy


Correlation between Fermi surface transformations and superconductivity in the electron-doped high-$T_c$ superconductor Nd$_{2-x}$Ce$_x$CuO$_4$

T. Helm,$^{1,*}$ M. V. Kartsovnik,$^{1,†}$ C. Proust,$^2$ B. Vignolle,$^2$ C. Putzke,$^{3,‡}$ E. Kampert,$^3$ I. Sheikin,$^4$ E.-S. Choi,$^5$ J. S. Brooks,$^5$ N. Bittner,$^{1,§}$ W. Biberacher,$^1$ A. Erb,$^{1,6}$ J. Wosnitza,$^3$ and R. Gross$^{1,6,||}$

- Quantum oscillations show the presence of small hole pockets up to a doping $x = 0.175$
Correlation between Fermi surface transformations and superconductivity in the electron-doped high-$T_c$ superconductor Nd$_{2-x}$Ce$_x$CuO$_4$


- Quantum oscillations show the presence of small hole pockets up to a doping $x = 0.175$

Although antiferromagnetic order disappears near $x = 0.14$, perhaps there is field-induced antiferromagnetic order up to $x = 0.175$?
Fermi surface reconstruction in electron-doped cuprates without antiferromagnetic long-range order


- New photoemission measurements at zero magnetic field show Fermi surfaces in quantitative agreement with quantum oscillation measurements.
Fermi surface reconstruction in electron-doped cuprates without antiferromagnetic long-range order


- New photoemission measurements at zero magnetic field show Fermi surfaces in quantitative agreement with quantum oscillation measurements.

- The energy gap between the electron and hole pockets collapses near $x = 0.17$ like an order parameter.
Fermi surface reconstruction in electron-doped cuprates without antiferromagnetic long-range order


- New photoemission measurements at zero magnetic field show Fermi surfaces in quantitative agreement with quantum oscillation measurements.

- The energy gap between the electron and hole pockets collapses near $x = 0.17$ like an order parameter.

- “The totality of the data points to a mysterious order between $x = 0.14$ and $x = 0.17$, whose appearance favors the FS reconstruction and disappearance defines the quantum critical doping. A recent topological proposal provides an ansatz for its origin.”
Figure 1 | Fermi surface reconstruction in optimal-doped NCCO.

(a) Schematic diagram of a reconstructed Fermi surface with electron-like pockets near antinode and hole-like pockets near node. The dashed lines indicate the antiferromagnetic Brillouin zone.

(b) Schematic band dispersion along a momentum cut on the electron-like pocket (near hotspot), marked by the red arrow in (a).

The original dispersion is split into conduction and valence bands by an AFM energy gap. The reconstructed bands bend back at the AFMZB.

(c) Schematic band dispersion along a momentum cut on the hole-like pocket (nodal cut), marked by the blue arrow in (a).

The AFM energy gap is slightly above $E_F$, but the folded band (back-bent hole band) disperses below $E_F$. The gray (dashed) line in (b,c) represents the original (folded) band.

(d-f) the same as (a-c), but for the original Fermi surface without reconstruction.

(g-i) Photoemission intensity plot (g), second derivative image with respect to energy (h) and raw energy distribution curves (EDCs) (i) for optimal-doped NCCO, measured along a momentum cut on the electron-like pocket (near hotspot, labelled by the red arrow in the inset of (h)).

Conduction and valence bands extracted from the EDCs (blue triangles in i) are also presented in (g,h) (black circles and white circles). The EDC at the AFMZB is shown in red (i).

The main band and folded band are marked by “MB” and “FB”, respectively.

(j-l) the same as (g-i), but for the nodal cut (labelled by the blue arrow in the inset of (h)).
S. Sachdev, Topological order and Fermi surface reconstruction, arXiv:1801.01125

SDW SRO
Defects in local SDW order are suppressed ("Hedgehogs" in Neel order in spacetime)
Reconstructed Fermi surface.
\(\langle \tilde{\Phi} \rangle = 0\)

Symmetry breaking and
topological phase transition

SDW LRO
Reconstructed Fermi surface
\(\langle \tilde{\Phi} \rangle \neq 0\)

Symmetry breaking phase transition

SDW SRO
Large Fermi surface.
\(\langle \tilde{\Phi} \rangle = 0\)
Defects in local SDW order are suppressed ("Hedgehogs" in Neel order in spacetime) reconstructed Fermi surface.

\[ \langle \Phi \rangle = 0 \]

Increasing SDW order

\[ x = 0.14 \]

\[ x = 0.17 \]

Symmetry breaking phase transition

\[ U/t \]

SDW LRO

\[ \langle \Phi \rangle \neq 0 \]

Reconstructed Fermi surface

SDW SRO

\[ \langle \Phi \rangle = 0 \]

Large Fermi surface.
Constraints on volume enclosed by the Fermi surface

- In a conventional Fermi liquid state, Fermi volume must equal $1 + x \pmod{2}$.
- When the unit cell is doubled by SDW order, total Fermi volume must equal $x \pmod{1}$. 
Constraints on volume enclosed by the Fermi surface

- In a conventional Fermi liquid state, Fermi volume must equal \( 1 + x \pmod{2} \).
- When the unit cell is doubled by SDW order, total Fermi volume must equal \( x \pmod{1} \).
- A state with Fermi volume \( x \pmod{2} \), but no translational symmetry breaking, must have non-quasiparticle excitations with vanishing energy on a torus i.e. emergent gauge fields

Anti-ferromagnet with $p$ holes per square
Spin liquid with density $p$ of spinless, charge $+e$ (or $-e$) "chargons".

$$= (|↑↓⟩ - |↓↑⟩) / \sqrt{2}$$
Spin liquid with density \( p \) of spinless, charge +e (or -e) “chargons”.

\[
\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)
\]
Spin liquid with density $p$ of spinless, charge $+e$ (or $-e$) "chargons".

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Spin liquid with density $p$ of spinless, charge $+e$ (or $-e$) "chargons", and charge 0, spin 1/2 "spinons"

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Spin liquid with density $p$ of spinless, charge $+e$ (or $-e$) “chargons”, and charge 0, spin 1/2 “spinons”

$$= \frac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{\sqrt{2}}$$

Metal with electron-like quasiparticles on a Fermi surface of size $p$, and emergent gauge fields

\[
\frac{1}{\sqrt{2}} \left( |\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle \right)
\]

\[
\frac{1}{\sqrt{2}} \left( |\uparrow \circ\rangle + |\circ \uparrow\rangle \right)
\]
\[
\mathbf{FL}^* \\
= \frac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{\sqrt{2}} \\
= \frac{(|\uparrow\circ\rangle + |\circ\uparrow\rangle)}{\sqrt{2}}
\]

Metal with electron-like quasiparticles on a Fermi surface of size \(p\), and emergent gauge fields

Metal with electron-like quasiparticles on a Fermi surface of size \( p \), and emergent gauge fields.

\[
\begin{align*}
\text{Metal} & \quad = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \\
\text{Emergent gauge fields} & \quad = \frac{1}{\sqrt{2}} \left( |\uparrow\circ\rangle + |\circ\uparrow\rangle \right)
\end{align*}
\]

Metal with electron-like quasiparticles on a Fermi surface of size $p$, and emergent gauge fields.

\[ (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \]

\[ (|\uparrow \circ\rangle + |\circ \uparrow\rangle)/\sqrt{2} \]

Metal with electron-like quasiparticles on a Fermi surface of size $p$, and emergent gauge fields

FL*
Metal with electron-like quasiparticles on a Fermi surface of size $p$, and emergent gauge fields

$$FL^*$$

$$= (|↑↓⟩ - |↓↑⟩) / \sqrt{2}$$

$$= (|↑⊙⟩ + |⊙↑⟩) / \sqrt{2}$$

Metal with electron-like quasiparticles on a Fermi surface of size $p$, and emergent gauge fields

$$\text{FL}^*$$

$$= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$$

$$= (|\uparrow\circ\rangle + |\circ\uparrow\rangle) / \sqrt{2}$$

Metal with electron-like quasiparticles on a Fermi surface of size $p$, and emergent gauge fields

\[
\left| \uparrow \downarrow \right\rangle - \left| \downarrow \uparrow \right\rangle = \frac{1}{\sqrt{2}}
\]

\[
\left( \left| \uparrow \circ \right\rangle + \left| \circ \uparrow \right\rangle \right) = \frac{1}{\sqrt{2}}
\]
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Emergent gauge fields and "topological order".
Reconstructed Fermi surface.
\[ \langle \Phi \rangle = 0 \]

Symmetry breaking and topological phase transition

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SU(2) gauge theory
SDW theory

We can (exactly) transform the Hubbard model to the “spin-fermion” model: **electrons** $c_{i\alpha}$ on the square lattice with dispersion

$$\mathcal{H}_c = -\sum_{i,\rho} t_{\rho} \left( c_{i,\alpha}^\dagger c_{i+\mathbf{v}_\rho,\alpha} + c_{i+\mathbf{v}_\rho,\alpha}^\dagger c_{i,\alpha} \right) - \mu \sum_i c_{i,\alpha}^\dagger c_{i,\alpha} + \mathcal{H}_{\text{int}}$$

are coupled to a magnetic moment order parameter $\Phi^p(i), p = x, y, z$

$$\mathcal{H}_{\text{int}} = -\lambda \sum_i \Phi^p(i) c_{i,\alpha}^\dagger \sigma_{\alpha\beta}^p c_{i,\beta} + V_\Phi$$
For (fluctuating) SDW SRO, we transform to a rotating reference frame using the SU(2) rotation $R_i$

$$
\begin{pmatrix}
    c_i^\uparrow \\
    c_i^\downarrow
\end{pmatrix} = R_i \begin{pmatrix}
    \psi_i^+, \\
    \psi_i^-
\end{pmatrix},
$$

in terms of fermionic “chargons” $\psi_s$ and a **Higgs field** $H^a(i)$

$$
\sigma^p \Phi^p(i) = R_i \sigma^a H^a(i) R_i^\dagger
$$

The Higgs field is the SDW order in the rotating reference frame.

S. Sachdev, M. A. Metlitski, Y. Qi, and C. Xu, PRB **80**, 155129 (2009)
For (fluctuating) SDW SRO, we transform to a rotating reference frame using the SU(2) rotation $R_i$

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\begin{pmatrix}
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\[
\sigma^p \Phi^p(i) = R_i \sigma^a H^a(i) R_i^\dagger
\]

The Higgs field is the SDW order in the rotating reference frame. Note that this representation is ambiguous up to a SU(2) gauge transformation, $V_i$

\[
\begin{pmatrix}
  \psi_{i,+} \\
  \psi_{i,-}
\end{pmatrix}
\rightarrow V_i \begin{pmatrix}
  \psi_{i,+} \\
  \psi_{i,-}
\end{pmatrix}
\]

$R_i \rightarrow R_i V_i^\dagger$

$\sigma^a H^a(i) \rightarrow V_i \sigma^b H^b(i) V_i^\dagger$.  

S. Sachdev, M. A. Metlitski, Y. Qi, and C. Xu, PRB **80**, 155129 (2009)
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**Spin density wave theory**
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$SU(2)$ gauge theory: fractionalize the SDW order parameter into the Higgs field ($H$) and the spinons ($R$); fractionalize the electron ($c$) into chargons ($\psi$) and spinons. Such a theory was used to model the photoemission and the cluster DMFT results in the intermediate phase.

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**SU(2) gauge theory for quantum criticality:** Fractionalize the SDW order parameter into the Higgs field ($H$) and the spinons ($R$); but do not fractionalize the electron ($c$) into chargons ($\psi$) and spinons. The hopping $t$ leads to a strong attraction between $\psi$ and $R$, leading to an electron-like bound state i.e. assume all the low energy fermionic excitations have the quantum numbers of an electron.
We can (exactly) transform the Hubbard model to the “spin-fermion” model: \textbf{electrons} $c_{i\alpha}$ on the square lattice with dispersion

$$\mathcal{H}_c = -\sum_{i,\rho} t_\rho \left( c_{i,\alpha}^\dagger c_{i+\rho,\alpha} + c_{i+\rho,\alpha}^\dagger c_{i,\alpha} \right) - \mu \sum_i c_{i,\alpha}^\dagger c_{i,\alpha} + \mathcal{H}_{\text{int}}$$

are coupled to a magnetic moment order parameter $\Phi^p(i)$, $p = x, y, z$

$$\mathcal{H}_{\text{int}} = -\lambda \sum_i \Phi^p(i) c_{i,\alpha}^\dagger \sigma_{\alpha\beta}^p c_{i,\beta} + V_\Phi$$
SU(2) gauge theory

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$$\mathcal{H}_{\text{int}} = -\lambda \sum_i \Phi^p(i) c_{i,\alpha}^\dagger \sigma_{\alpha\beta}^p c_{i,\beta} + V_\Phi$$

Express $\Phi^{\ell}$ in terms the Higgs field

$$\sigma^p \Phi^p(i) = R_i \sigma^a H^a(i) R_i^\dagger$$

Integrate out high energy $c_\alpha$ and spinons $R$, to obtain effective theory for $H^a$ and low energy $c_\alpha$ near the Fermi surface.
SU(2) gauge theory

We obtain different numbers of adjoint Higgs scalars, $N_f$, depending upon the spatial dependence of the local spin correlations:

Neel correlations: $N_f = 1$,

$$K = (\pi, \pi),$$

$$H^a(i) = H^a_1(\mathbf{r}) e^{i K \cdot \mathbf{r}_i}$$

Unidirectional incommensurate correlations: $N_f = 2$,

$$K = (\pi, \pi - \delta),$$

$$H^a(i) = \text{Re} \left\{ [H^a_1(\mathbf{r}) + i H^a_2(\mathbf{r})] e^{i K \cdot \mathbf{r}_i} \right\}$$

Bidirectional incommensurate correlations: $N_f = 4$,

$$K_y = (\pi, \pi - \delta), \quad K_x = (\pi - \delta, \pi),$$

$$H^a(i) = \text{Re} \left\{ [H^a_1(\mathbf{r}) + i H^a_2(\mathbf{r})] e^{i K_x \cdot \mathbf{r}_i} + [H^a_3(\mathbf{r}) + i H^a_4(\mathbf{r})] e^{i K_y \cdot \mathbf{r}_i} \right\}$$
SU(2) gauge theory

SU(2) gauge theory with $N_f$ adjoint Higgs fields with potential $V(H_a^\ell)$, $a = 1, 2, 3$, $\ell = 1 \ldots N_f$

$$- \sum_{i, \rho} t_\rho \left( c_{i, \alpha}^\dagger c_{i+\nu_\rho, \alpha} + c_{i+\nu_\rho, \alpha}^\dagger c_{i, \alpha} \right) - \mu \sum_i c_{i, \alpha}^\dagger c_{i, \alpha}$$

$$+ \sum_i c_{i, \alpha}^\dagger c_{i, \alpha} H^a(i) H^a(i)$$

$$V(H_a^\ell) = s H_a^\ell H_a^\ell + u_1 (H_a^\ell H_a^\ell)^2 + u_2 H_a^\ell H_a^a H_b^b H_m^b + \ldots$$
\[ N_f = 1 \]

**Phase diagrams of SU(2) gauge theory**

Exponentially large confinement length

Reconstructed Fermi surfaces at distances smaller than the confinement length

Fermi liquid with large Fermi surface

Phase diagrams of SU(2) gauge theory

$N_f = 2$

**Higgs**

Emergent deconfined $Z_2$ gauge field

$\langle H_1^a H_2^a \rangle = 0$

Reconstructed Fermi surfaces

Ising* or Deconfined critical SU(2) gauge theory

Confinement

Fermi liquid with large Fermi surface
$N_f = 2$

Phase diagrams of SU(2) gauge theory

**Higgs**

Charge density wave order
Exponentially large confinement length

Gauge invariant order parameter

$$\langle H_\ell^a H_m^a - \delta_{\ell m} (H_n^a H_n^a) / N_f \rangle \neq 0$$

breaks $O(N_f)$ symmetry

Reconstructed Fermi surfaces at distances smaller than the confinement length

**Confinement**

Fermi liquid with large Fermi surface

**XY Wilson-Fisher or Deconfined critical SU(2) gauge theory**
Phase diagrams of SU(2) gauge theory

\( N_f = 2 \)

Charge density wave order
Exponentially large confinement length

Gauge invariant order parameter

\[ \langle H_{\ell}^a H_{m}^a - \delta_{\ell m} (H_{n}^a H_{n}^a) / N_f \rangle \neq 0 \]

breaks \( O(N_f) \) symmetry

Reconstructed Fermi surfaces at distances smaller than the confinement length

Transition between conventional phases with and without broken symmetry need not be of the LGW type!

XY Wilson-Fisher or Deconfined critical
SU(2) gauge theory
Phase diagrams of SU(2) gauge theory

\[ N_f = 4 \]

\[ V(H^a_{\ell}) \]
\[ \langle H^a_{\ell} \rangle \neq 0 \]
\[ H^a_{\ell} \]

**Higgs**

Emergent deconfined
Z$_2$ gauge field
and/or
Charge density wave order
and/or
Ising-nematic order
(Reconstructed Fermi surfaces)

**Deconfined critical**
SU(2) gauge theory

**Confinement**

(Fermi liquid with
large Fermi surface)
Fermi surface reconstruction in electron-doped cuprates


S. Sachdev, Topological order and Fermi surface reconstruction, arXiv:1801.01125

SDW SRO

**Higgs phase**
Emergent deconfined $\mathbb{Z}_2$ gauge field/
CDW/Ising-nematic

\[
\langle H^a \rangle \neq 0 \quad \langle \Phi^p \rangle = 0 \\
\langle R \rangle = 0
\]

\[
\langle \Phi^p \rangle \neq 0 \\
\langle H^a \rangle \neq 0, \quad \langle R \rangle \neq 0
\]

SDW LRO

Confinement
No topological order.

\[
\langle H^a \rangle = 0, \quad \langle R \rangle \neq 0
\]

\[
\langle \Phi^p \rangle = 0
\]

$g$

$U/t$
**Higgs phase**
Emergent deconfined $Z_2$ gauge field/CDW/Ising-nematic

\[ \langle H^a \rangle \neq 0, \quad \langle \Phi^p \rangle = 0 \]
\[ \langle R \rangle = 0 \]

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**Confinement**
No topological order.

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SU(2) gauge theory with $N_f = 1, 2, 4$ adjoint Higgs fields

\[ \langle H^a \rangle = 0, \quad \langle R \rangle \neq 0 \]
\[ \langle \Phi^p \rangle = 0 \]