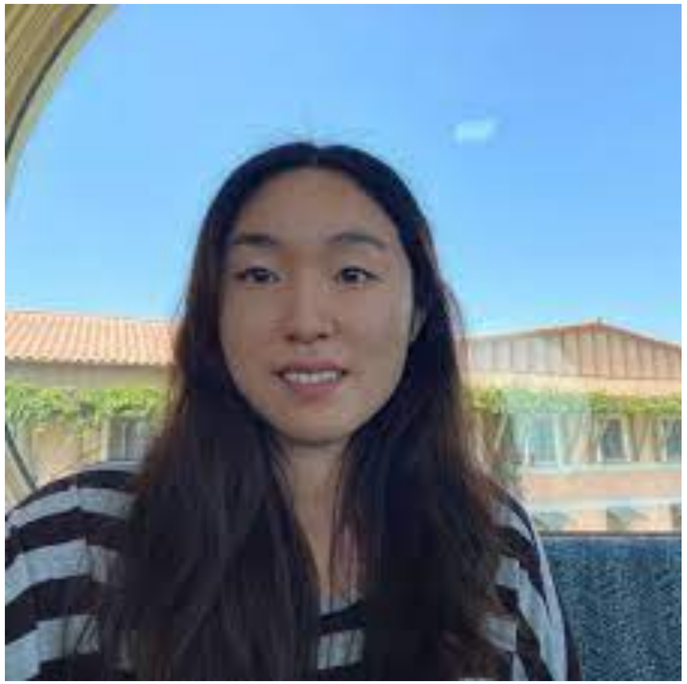
Ancilla theory of the pseudogap and of the cuprate phase diagram

Ringberg Castle
Max Planck Institute for Solid State Research, Stuttgart
November 16, 2023
Subir Sachdev

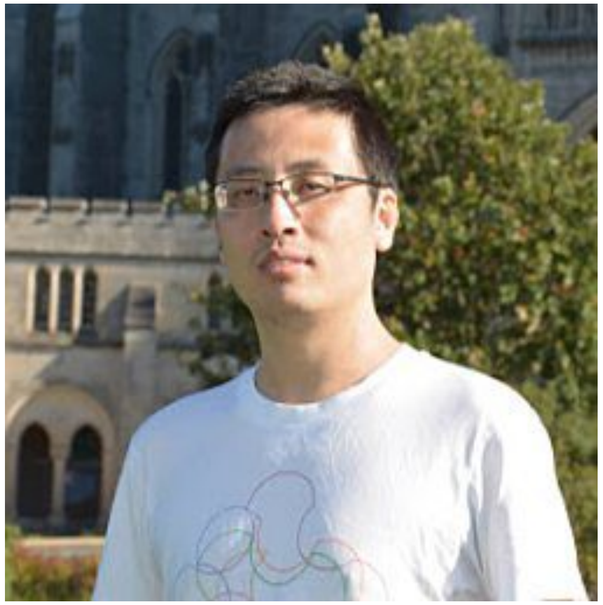
Maine Christos, Zhu-Xi Luo, Henry Shackleton, Ya-Hui Zhang,
Mathias Scheurer, and S. Sachdev, *Proc. Nat. Acad. Sci.* **120**, e2302701120 (2023)
Alexander Nikolaenko, Jonas v. Milczewski, Darshan G. Joshi,
and S.Sachdev, *Phys. Rev. B* **108**, 045123 (2023)
Maine Christos and S.Sachdev, arXiv:2308.03835

Maine Christos



Zhu-Xi Luo

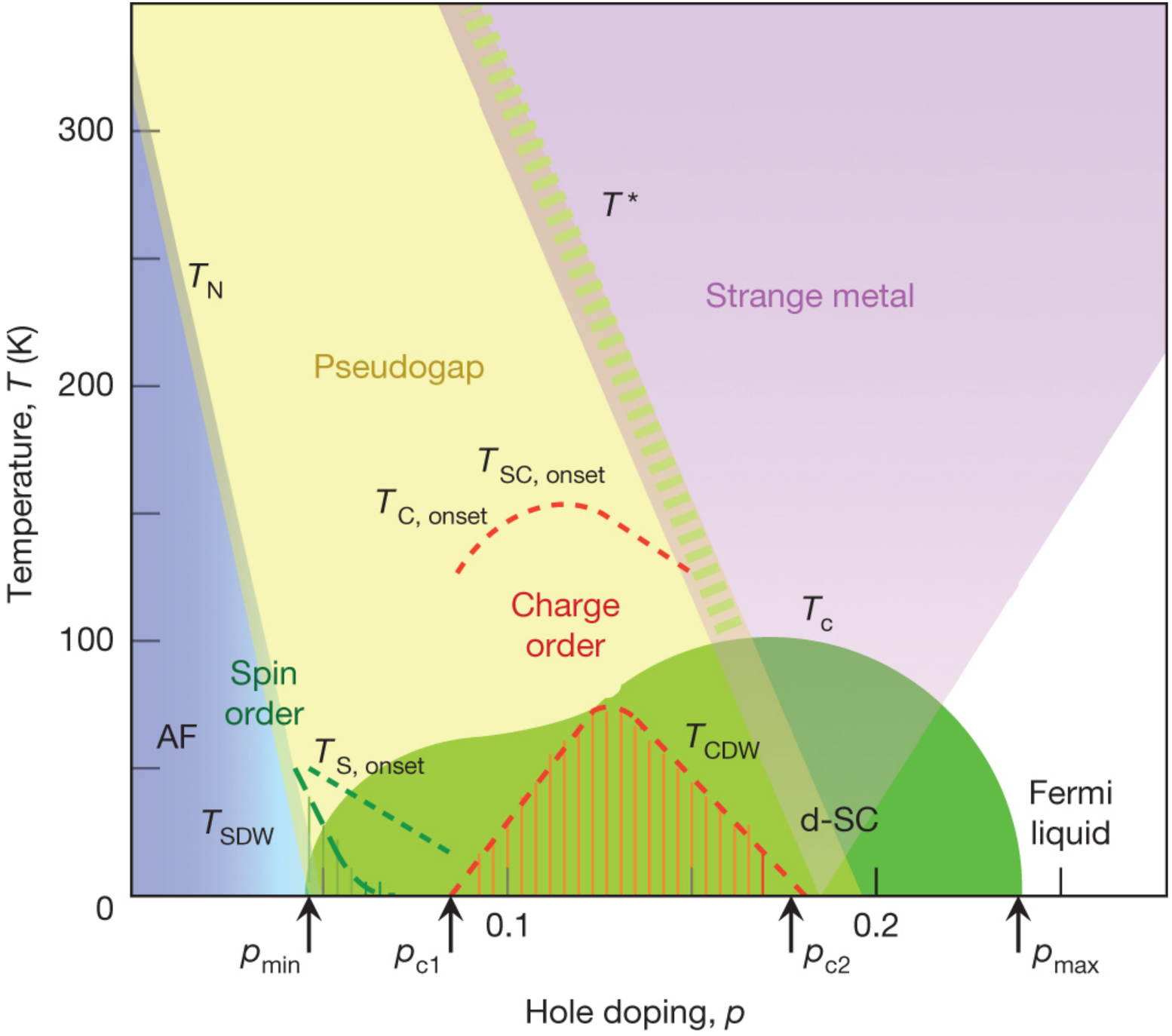
Mathias Scheurer

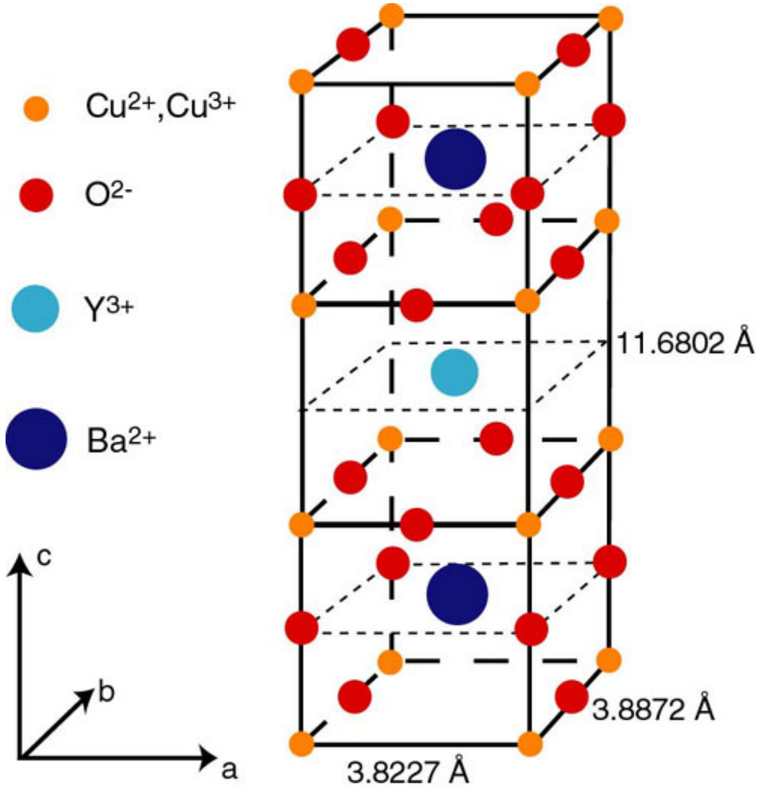


Ya-Hui Zhang

Henry Shackleton

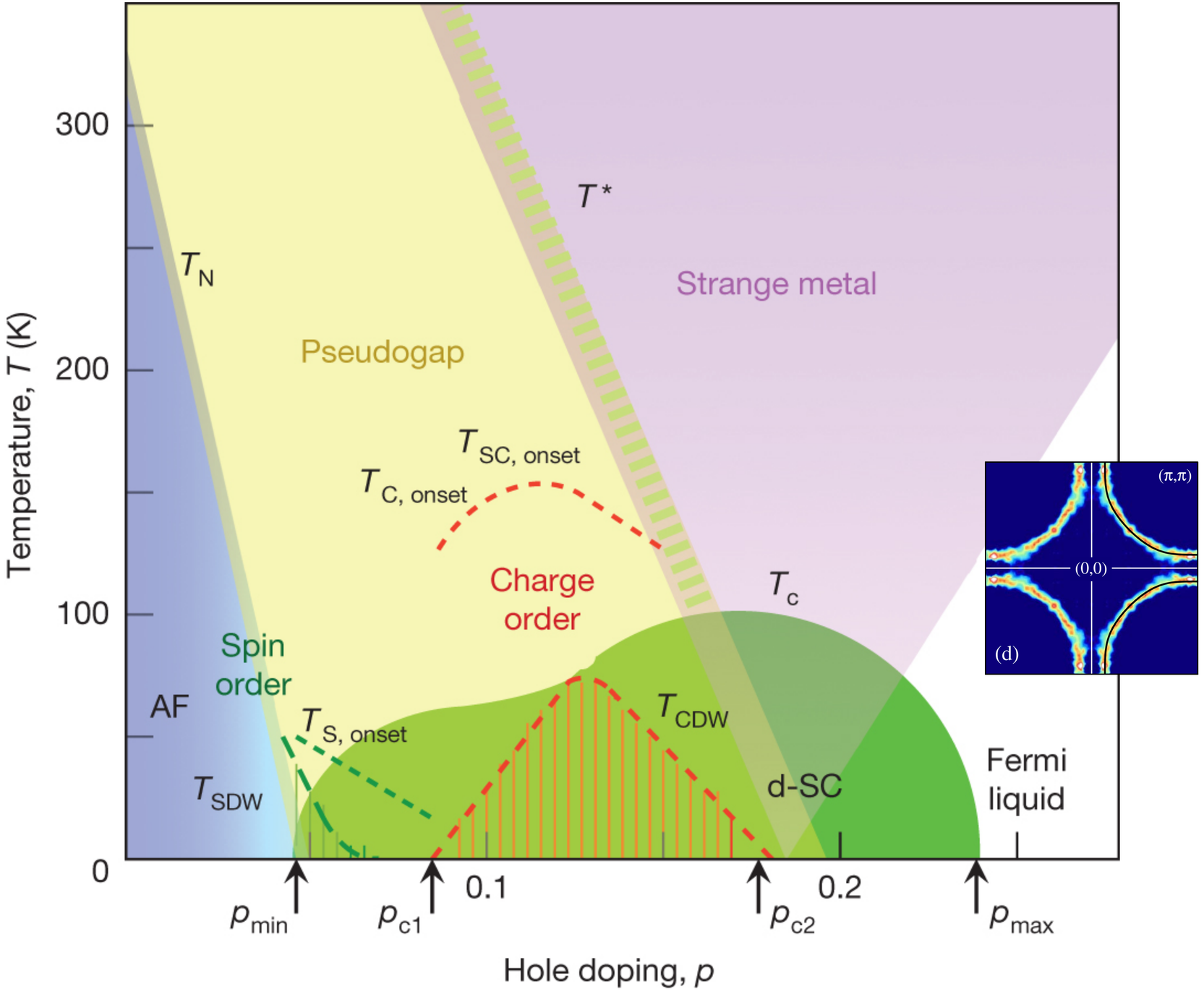
Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)





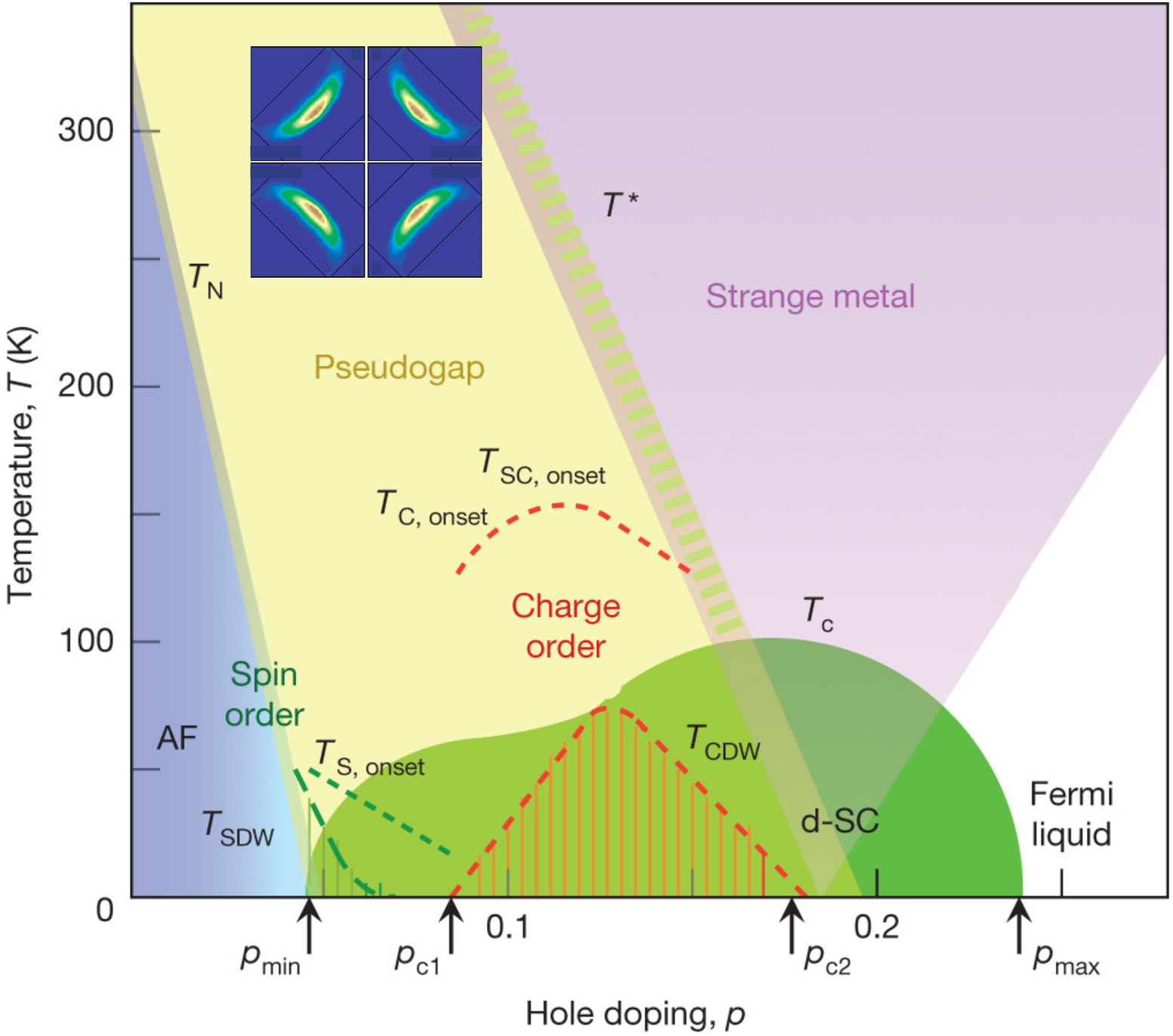
$YBa_2Cu_3O_{6+x}$

Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)



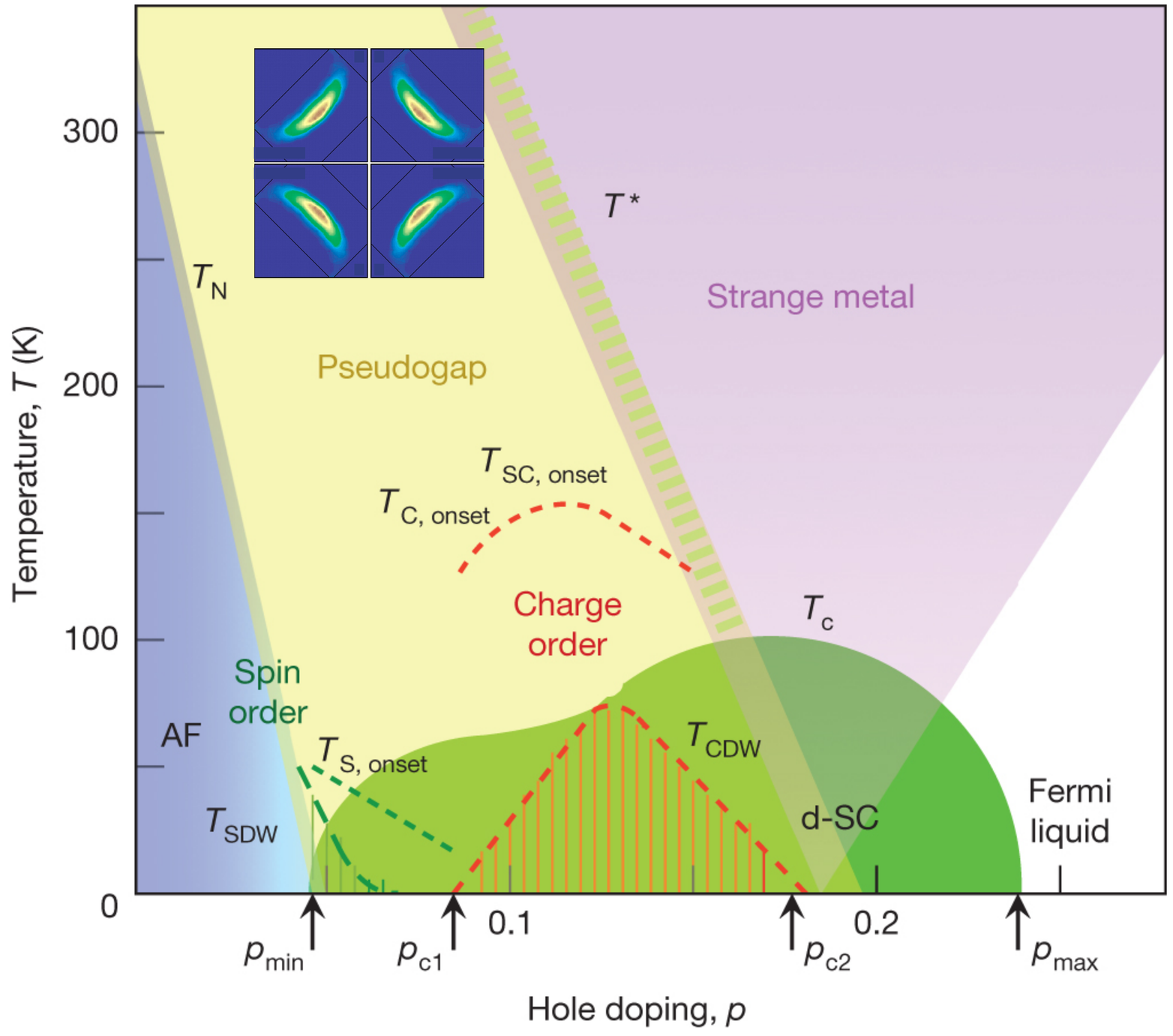
Fermi liquid in the overdoped metal

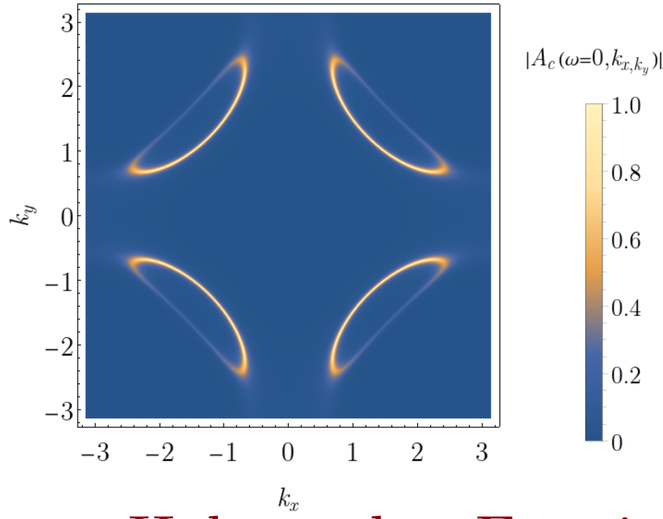
Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)



Pseudogap metal with "Fermi arcs"

Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)





Y. Qi and S. Sachdev *Phys. Rev. B* **81**, 115129 (2010)

E. Mascot, A. Nikolaenko, M. Tikhanovskaya, Ya-Hui Zhang, D. K. Morr, and S. Sachdev, *Phys. Rev. B* **105**, 075146 (2022)

Hole pocket Fermi surfaces of size p with charge e, spin-1/2 quasiparticles

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S. Sakai, Y. Motome, M. Imada, *Phys. Rev. Lett.* **102**, 056404 (2009).

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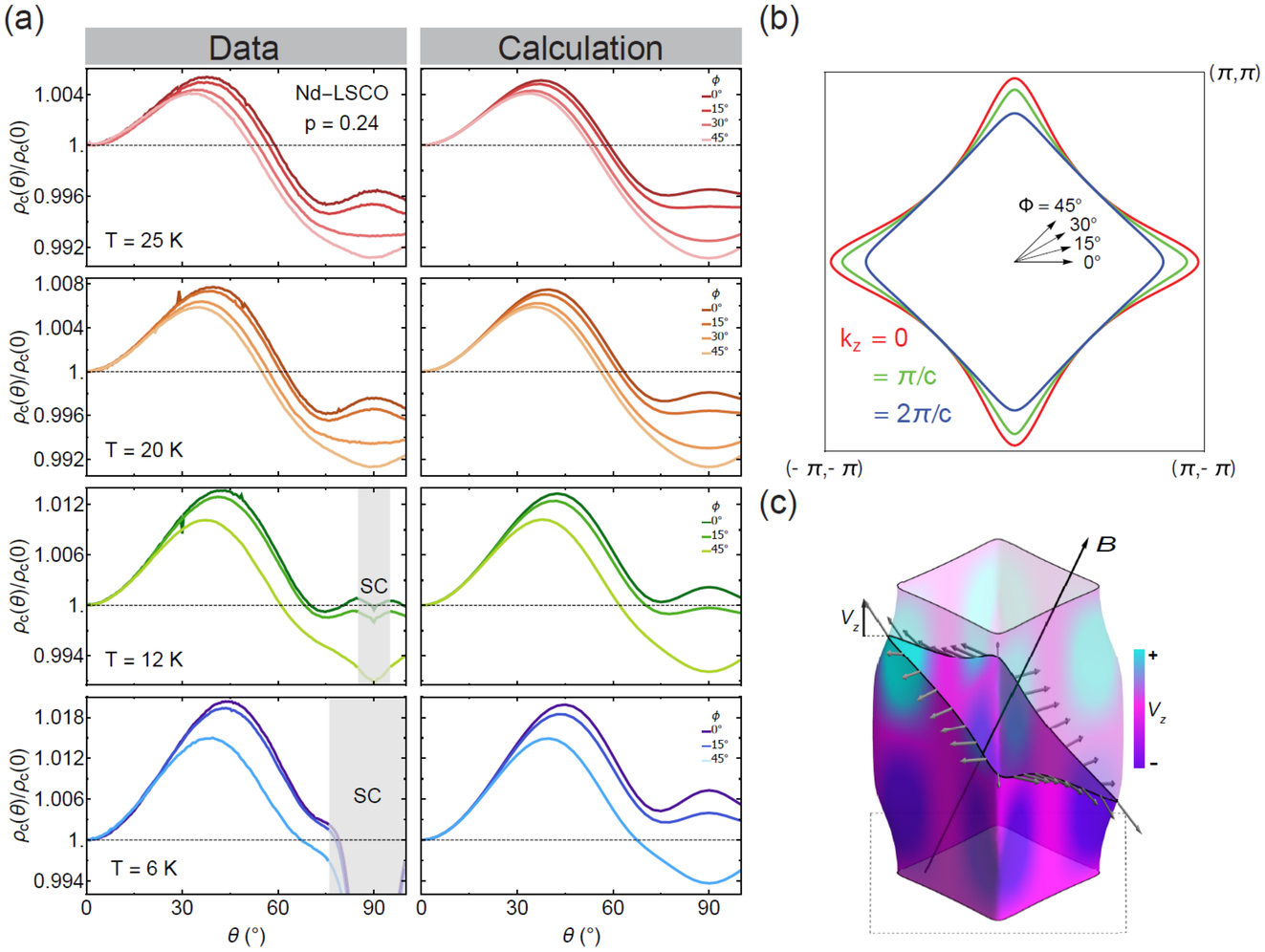
N. Wagner….A. Georges, G. Sangiovanni, arXiv:2301.05588

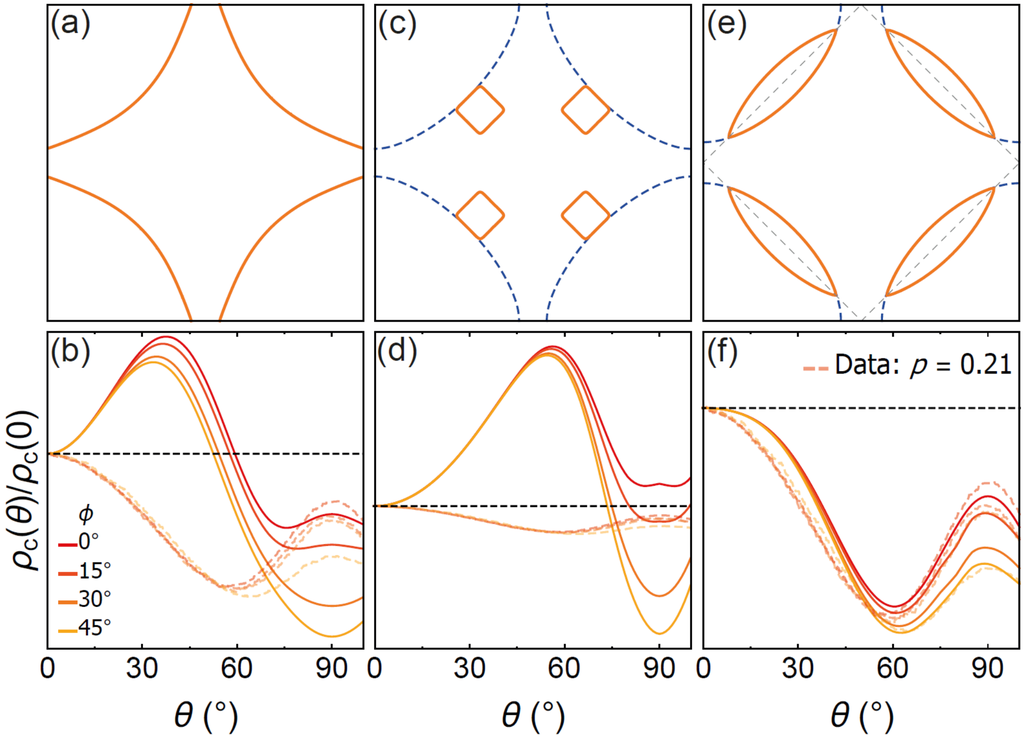
Jinchao Zhao, Gabriele La Nave, Philip Phillips, arXiv:2304.04787.

Fermi surface transformation at the pseudogap critical point of a cuprate superconductor

Yawen Fang, Gaël Grissonnanche, Anaëlle Legros, Simon Verret, Francis Laliberté, Clément Collignon, Amirreza Ataei, Maxime Dion, Jianshi Zhou, David Graf, M. J. Lawler, Paul Goddard, Louis Taillefer, and B. J. Ramshaw, *Nature Physics* **18**, 558 (2022)



$p > p_c$ Large Fermi surface



$p < p_c$ Reconstructed Fermi surface

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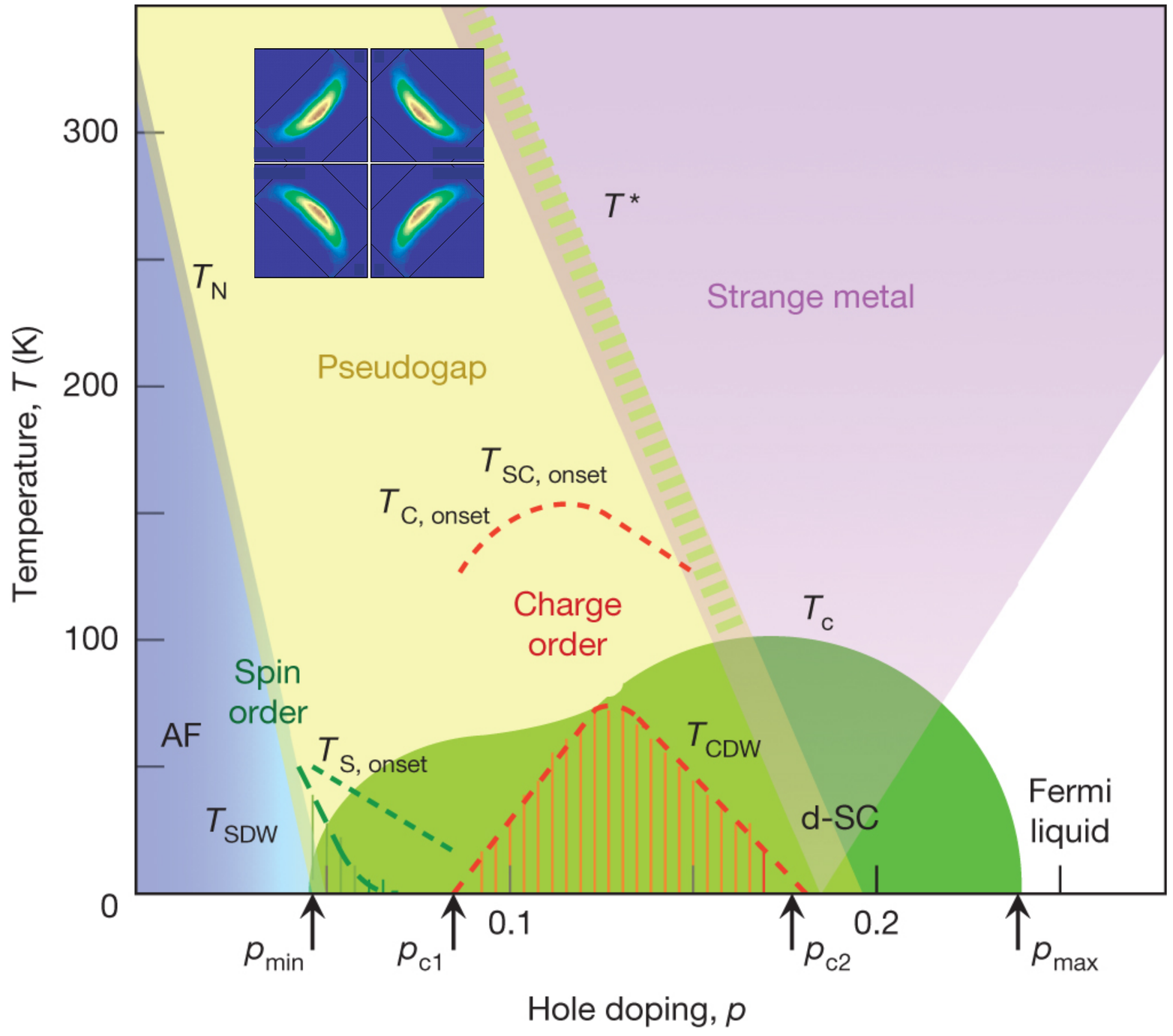

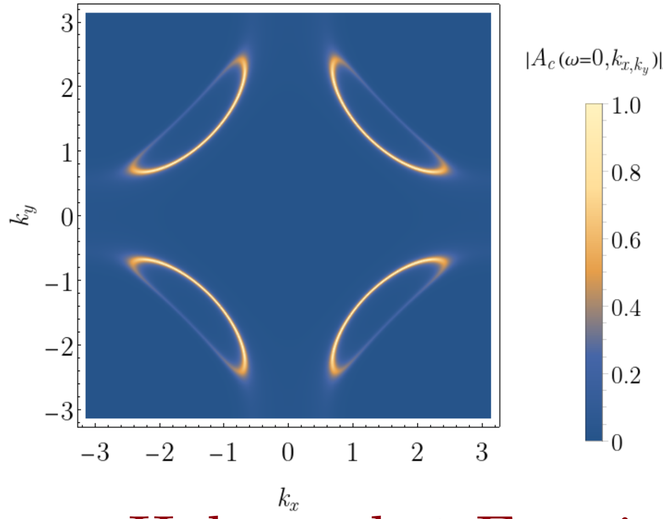

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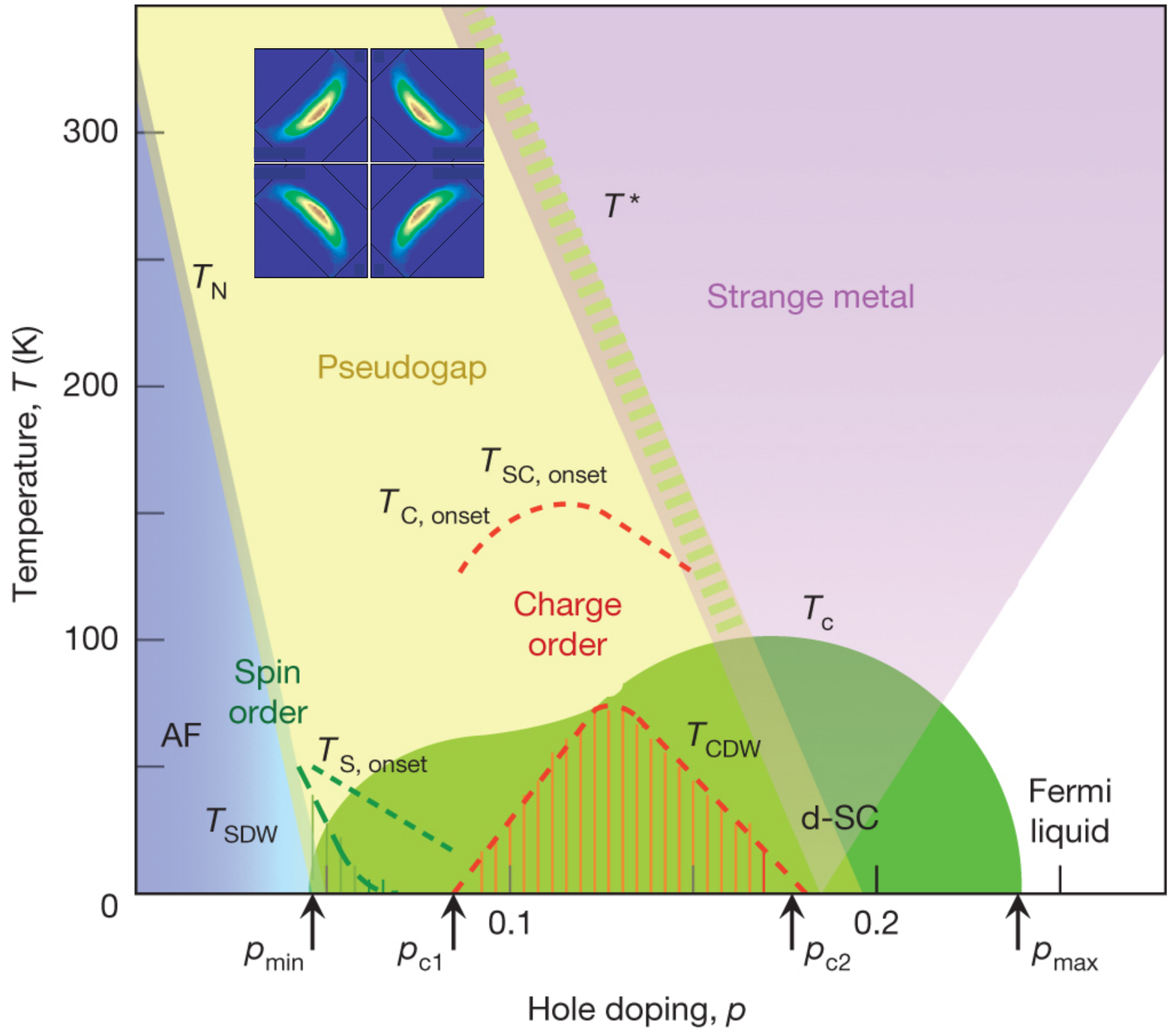

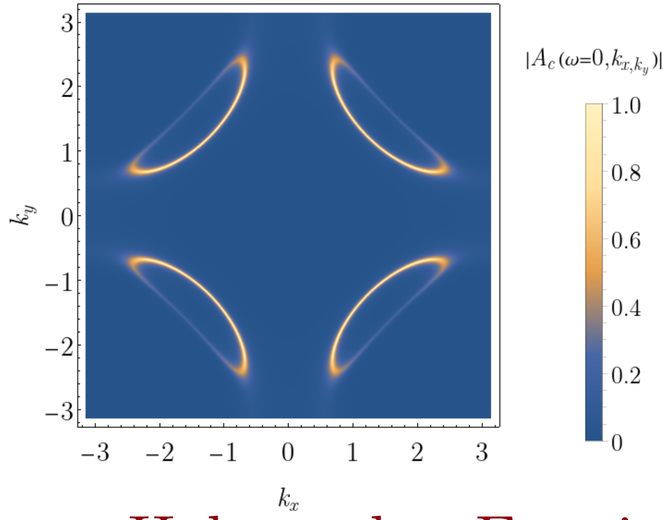

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arXiv:2304.04787.

Green's function zeros…..

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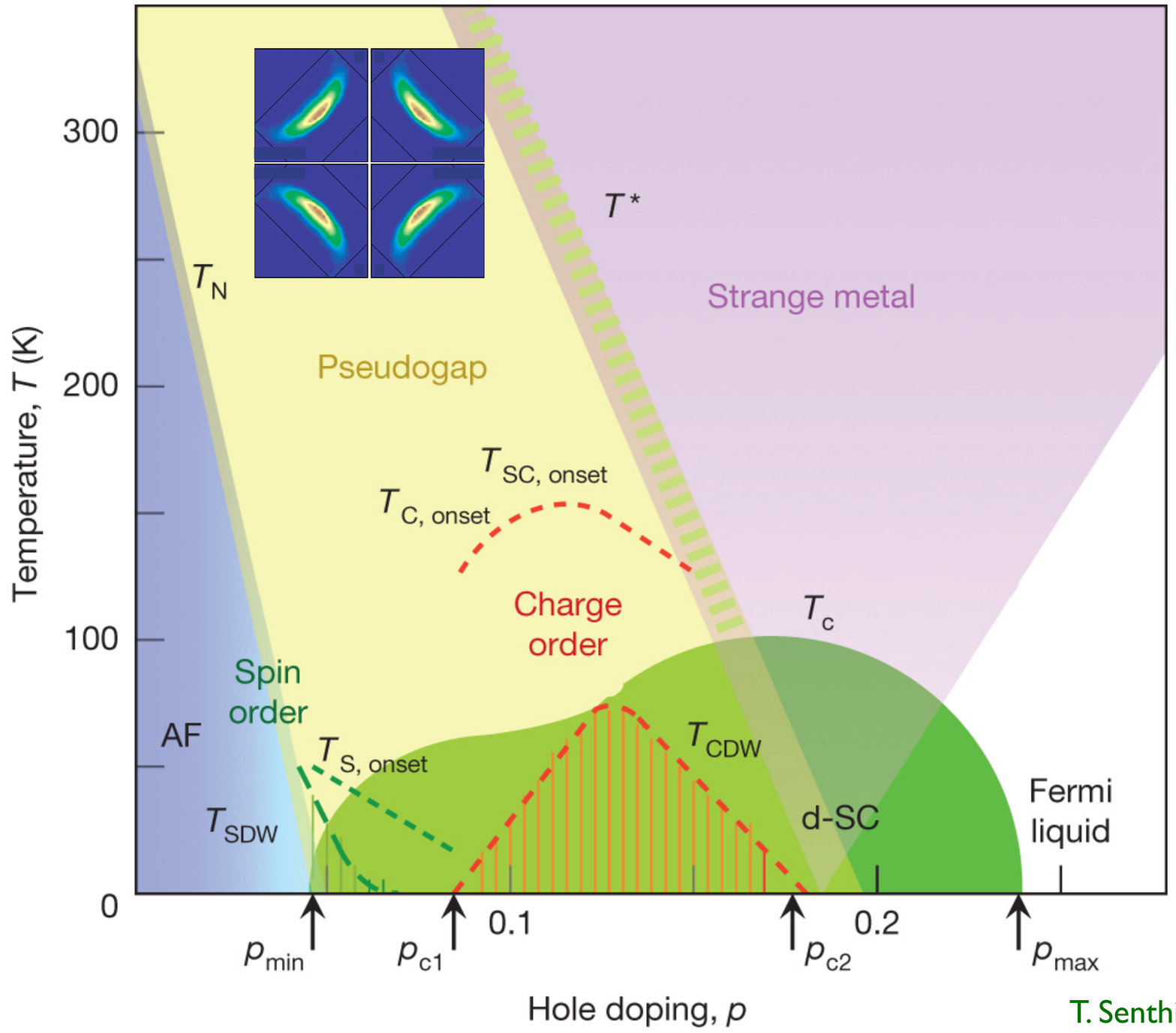

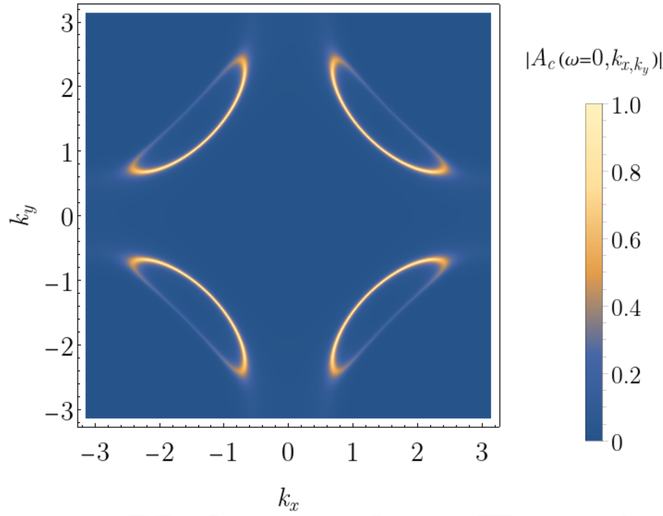

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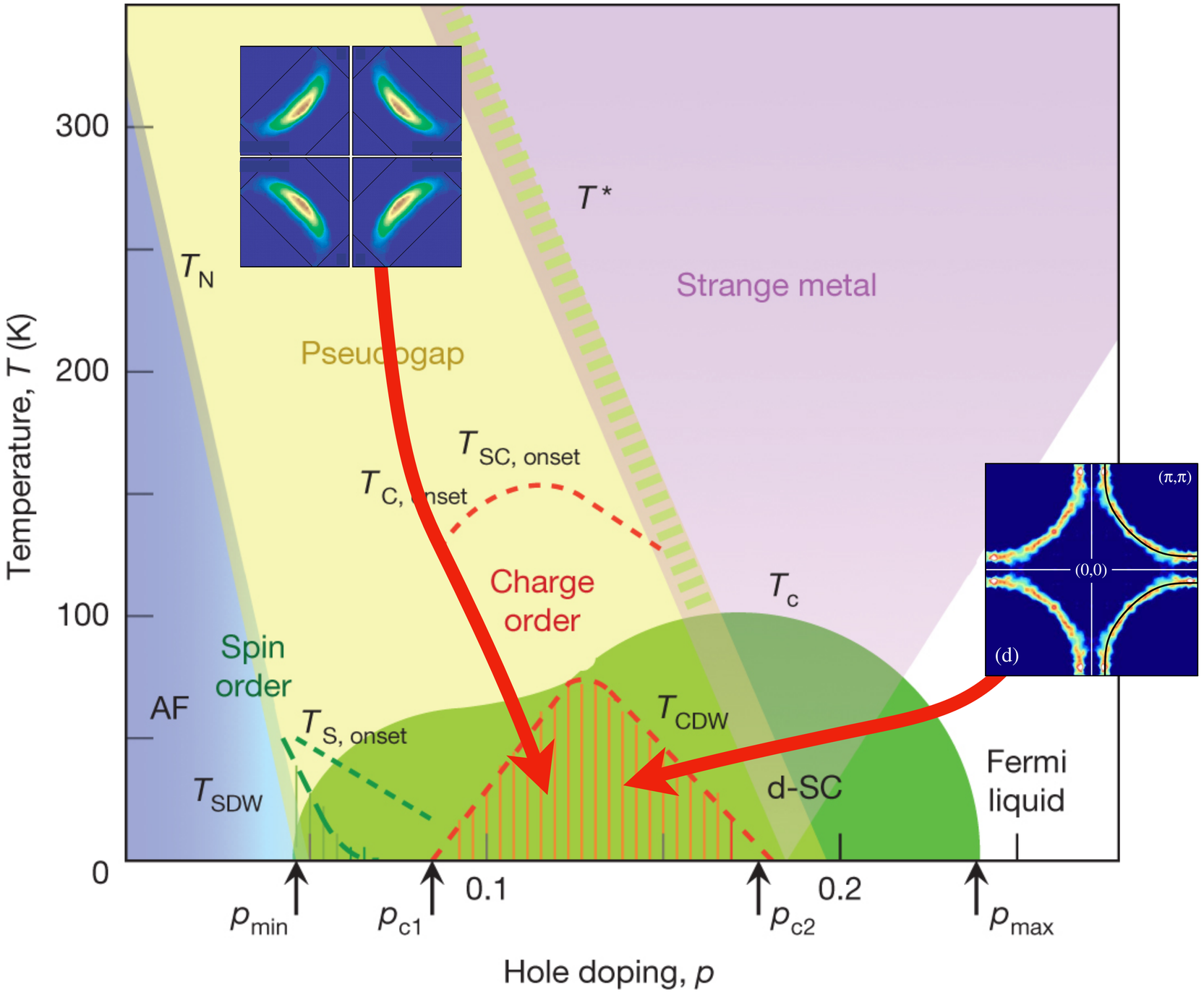
Hole pocket Fermi surfaces
of size p with
charge e, spin-1/2 quasiparticles
+
'spectator'
square lattice spin liquid
at half-filling.

FL*: Spin liquid is *required* because the Fermi surface does not enclose the Luttinger volume $(1+p)$.

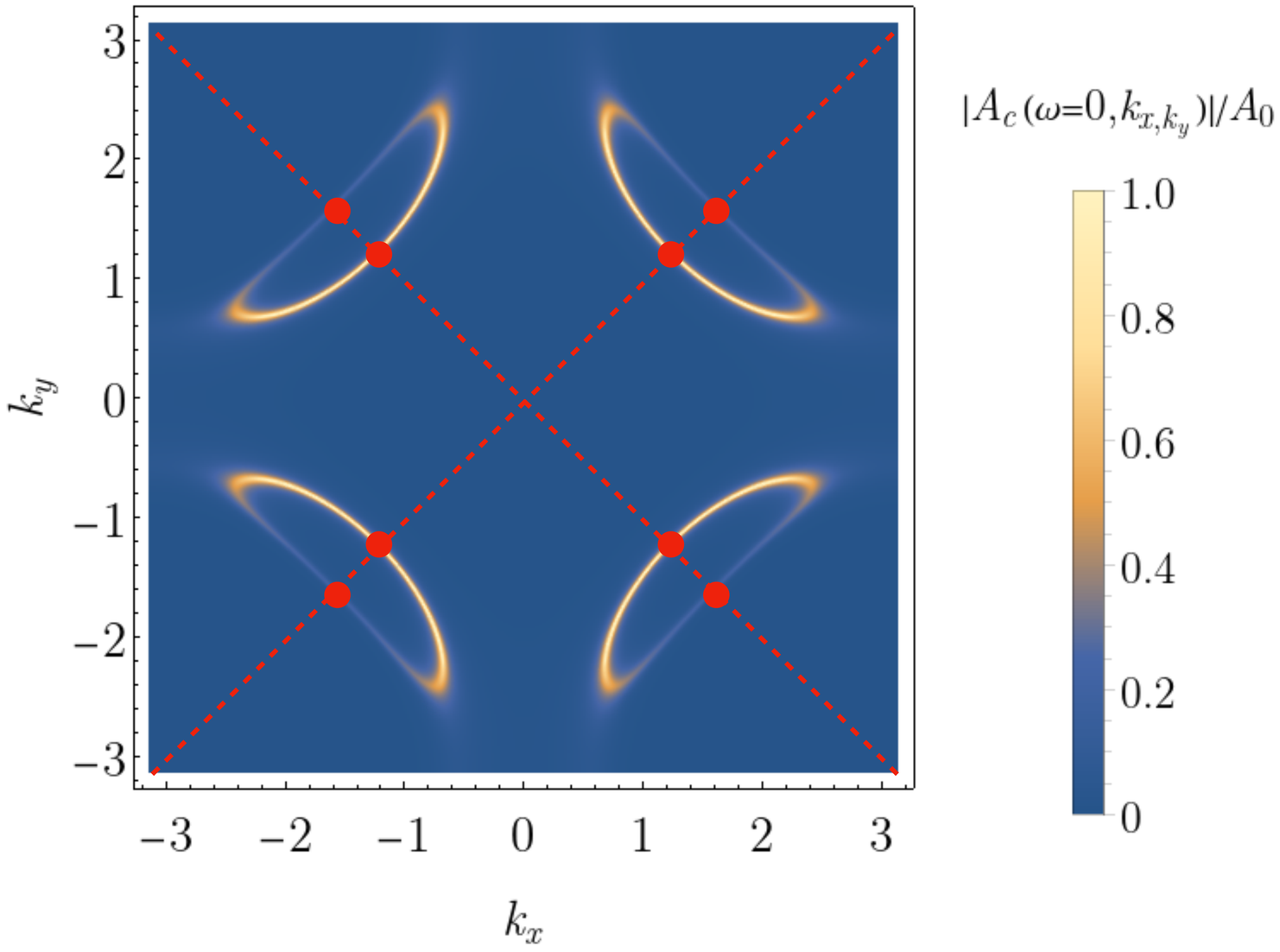
T. Senthil, M. Vojta, and S. Sachdev , *Phys. Rev. B* **69**, 035111 (2004)

Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)



Build a theory for the phase diagram from a theory of the pseudogap metal as a 'metastable' $T = 0$ quantum phase.

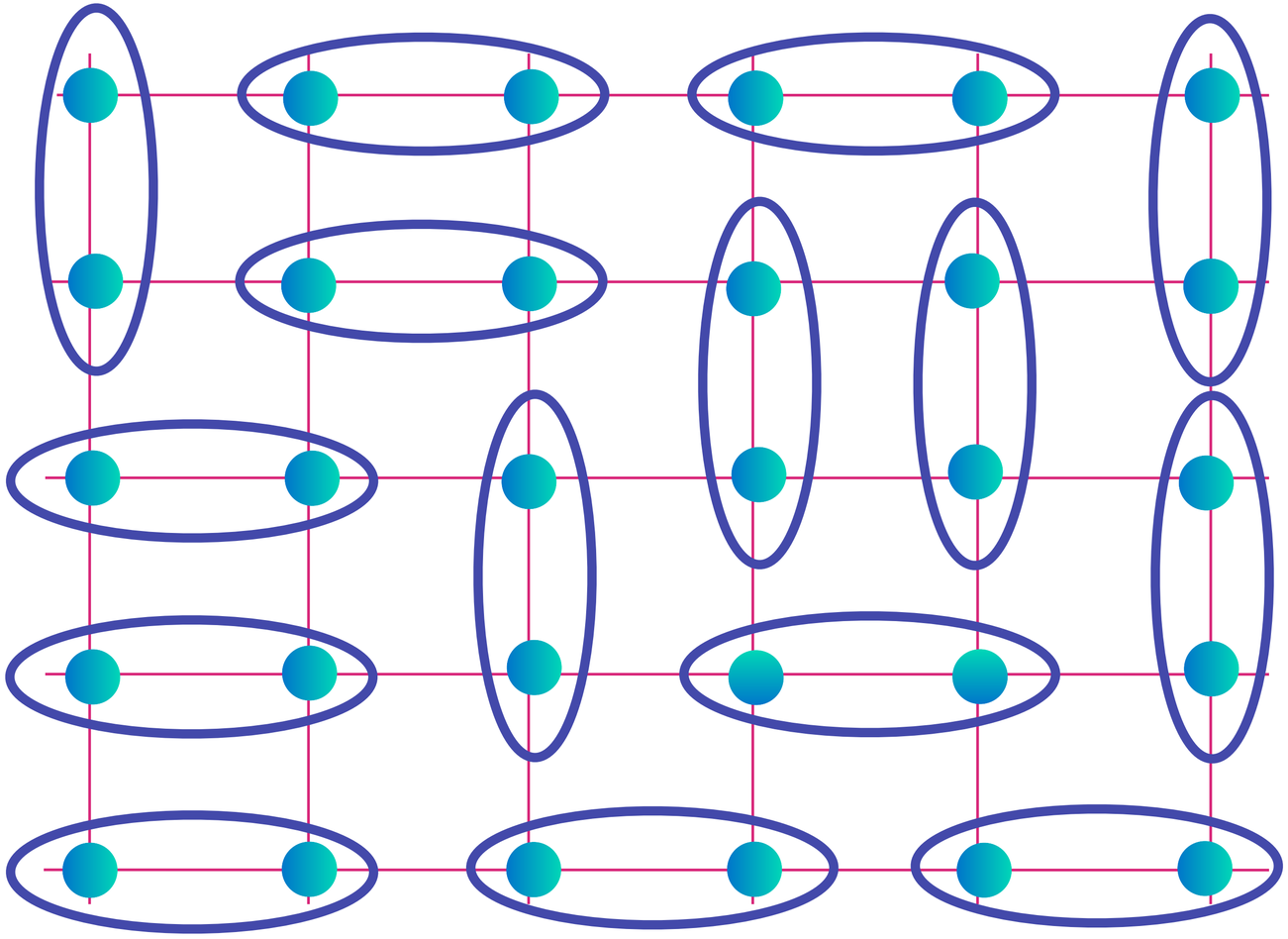
Lowest T phases obtained from pseudogap metal should connect smoothly to conventionally order phases obtained from the Fermi liquid.



Adding d-wave pairing
to the hole pockets
leads to 8 nodal points???

From FL*
to
a cuprate phase diagram

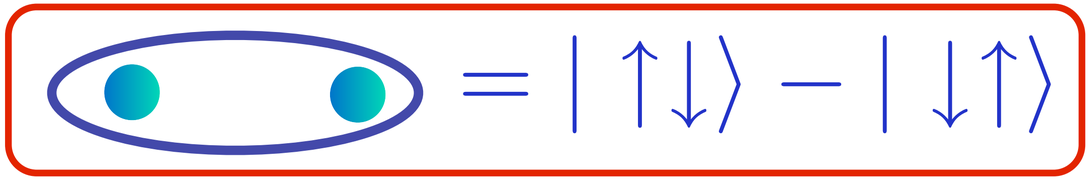
The dance of electrons on Cu atoms in YBCO



P.W. Anderson (1973)

Spin liquid

Electrons form entangled pairs, and the pairs entangle across the entire sample



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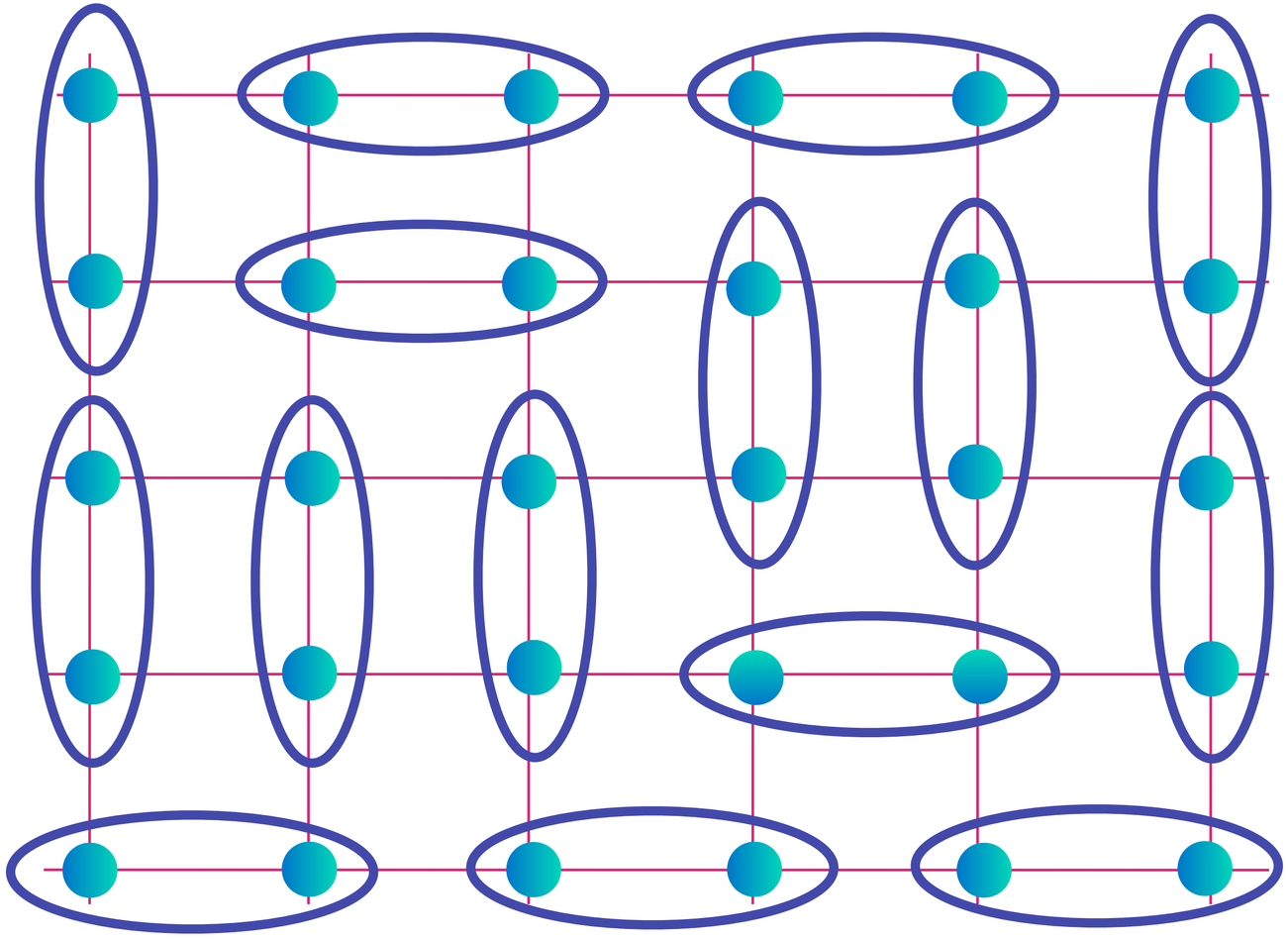

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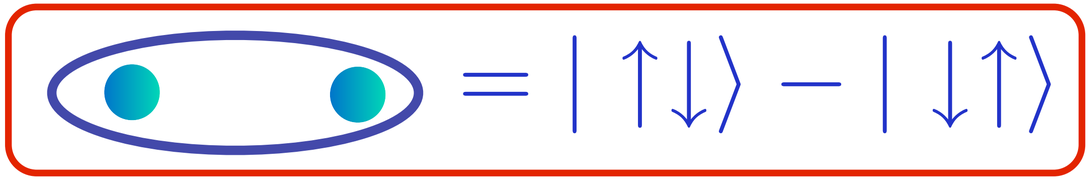

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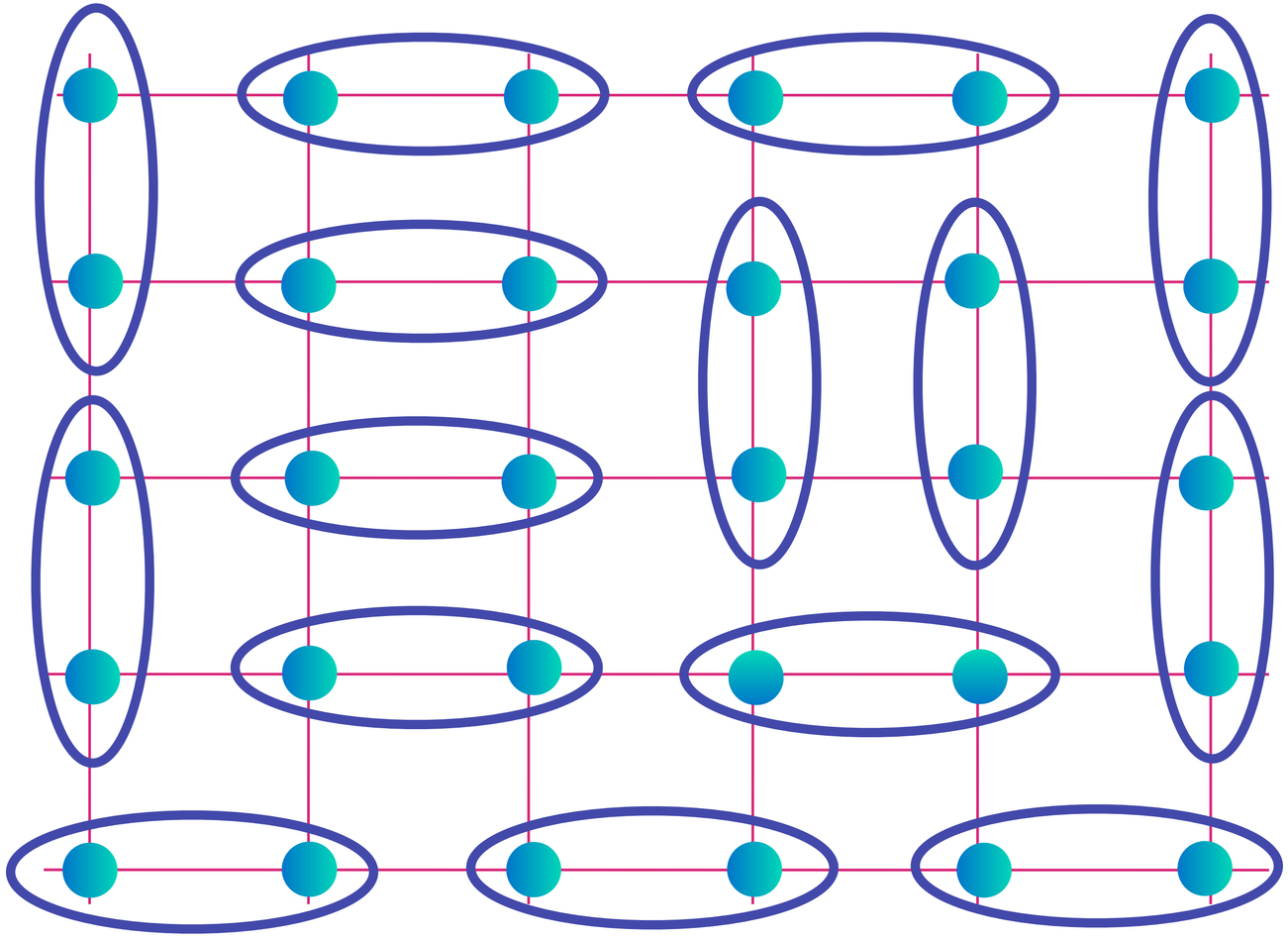

$$= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

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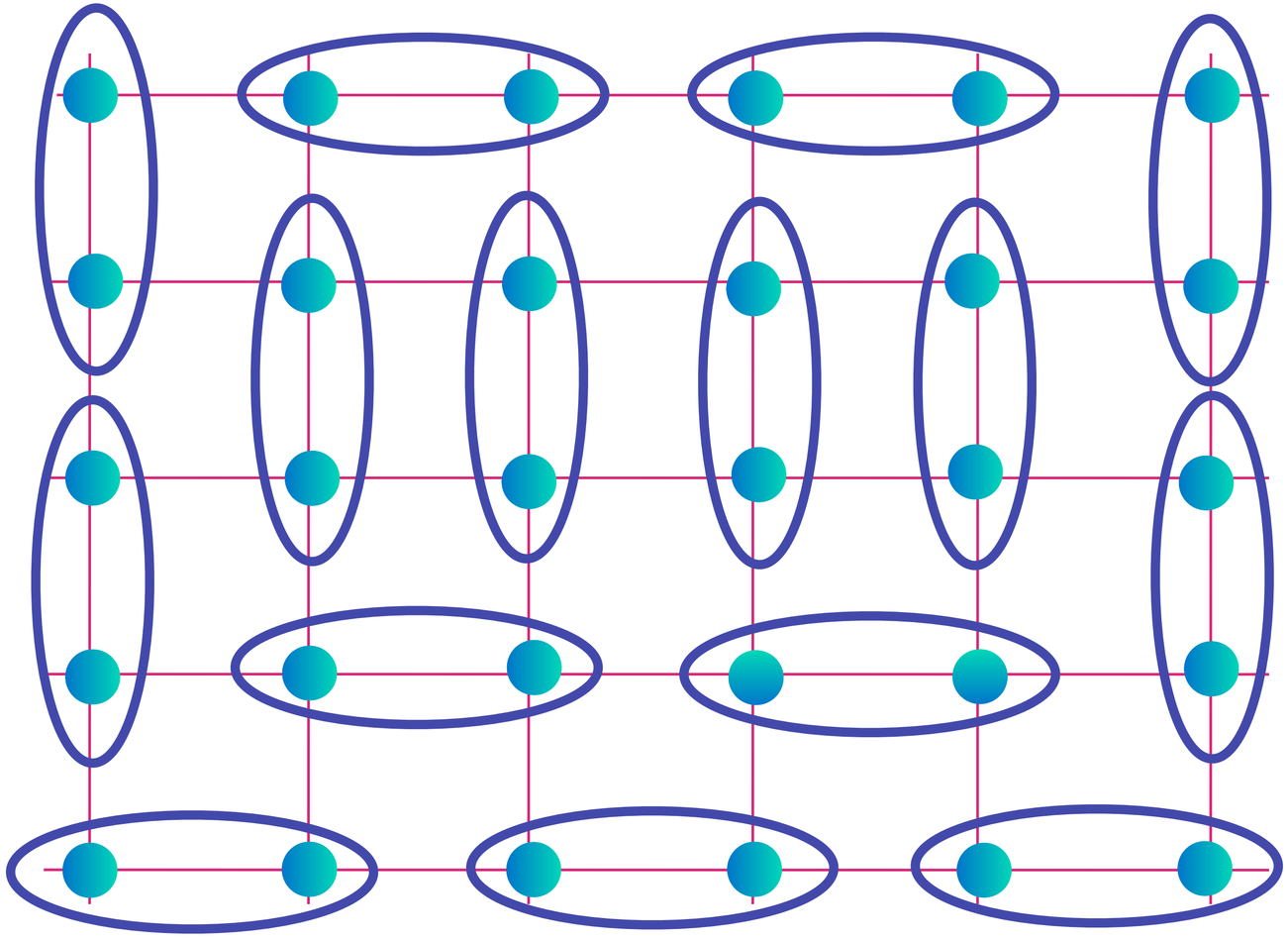

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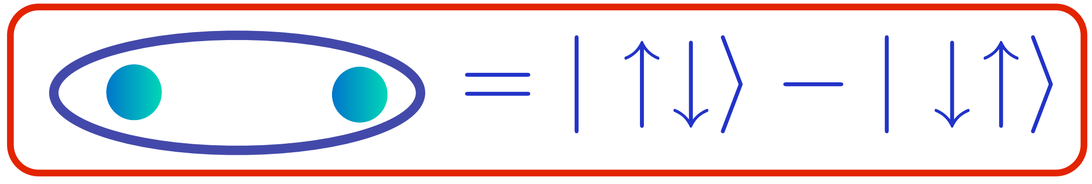

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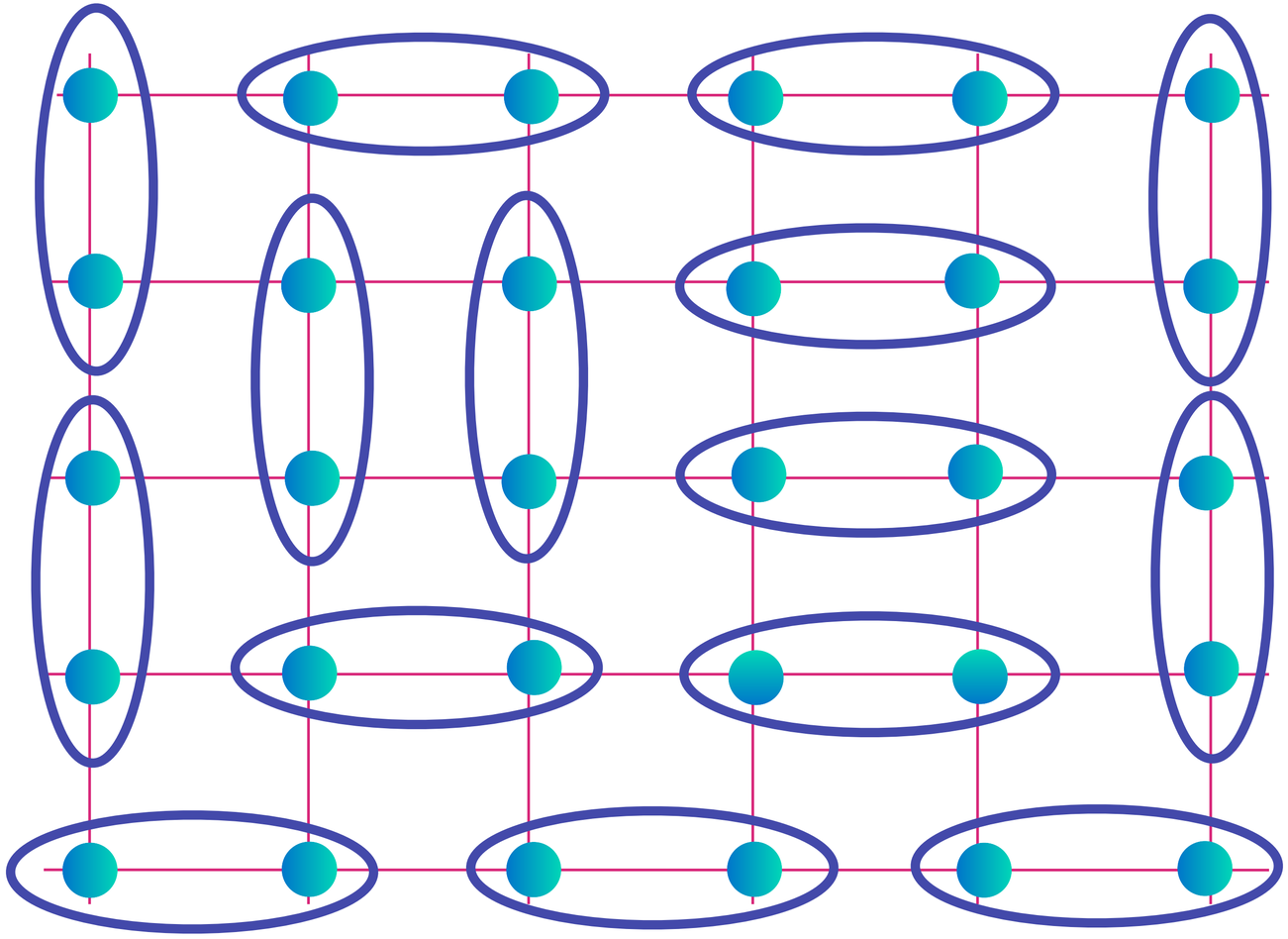

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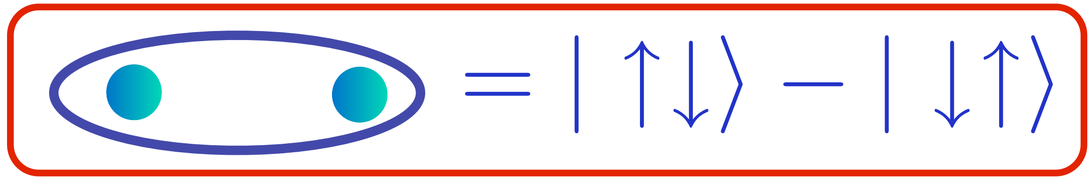

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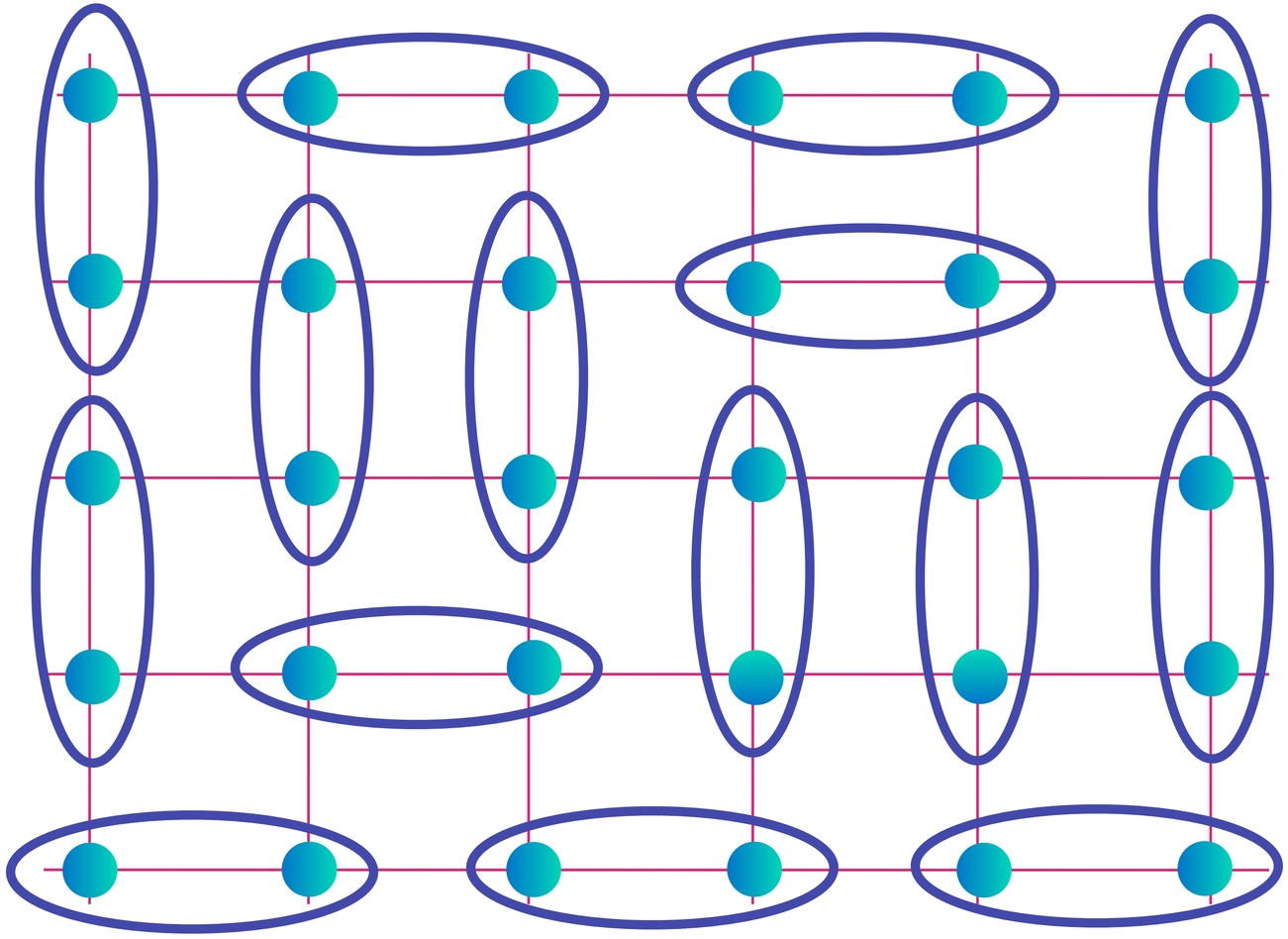

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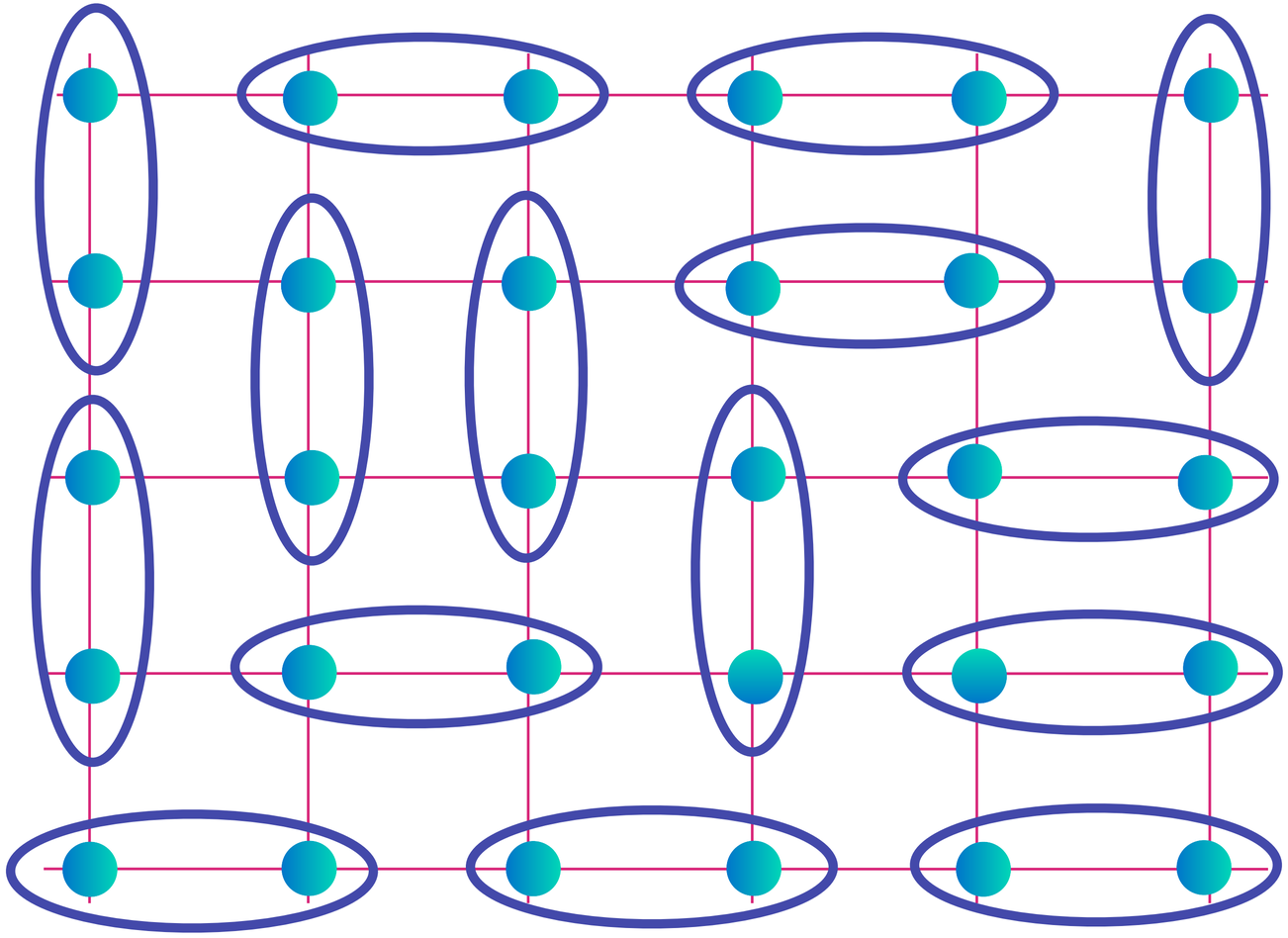

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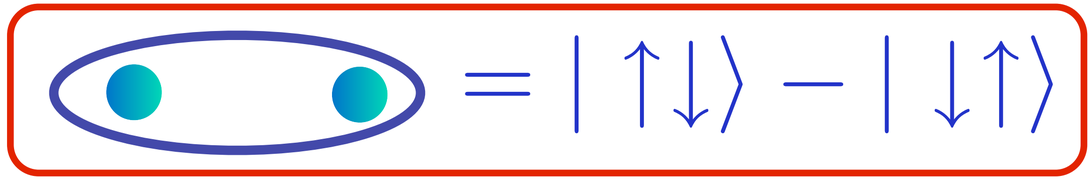

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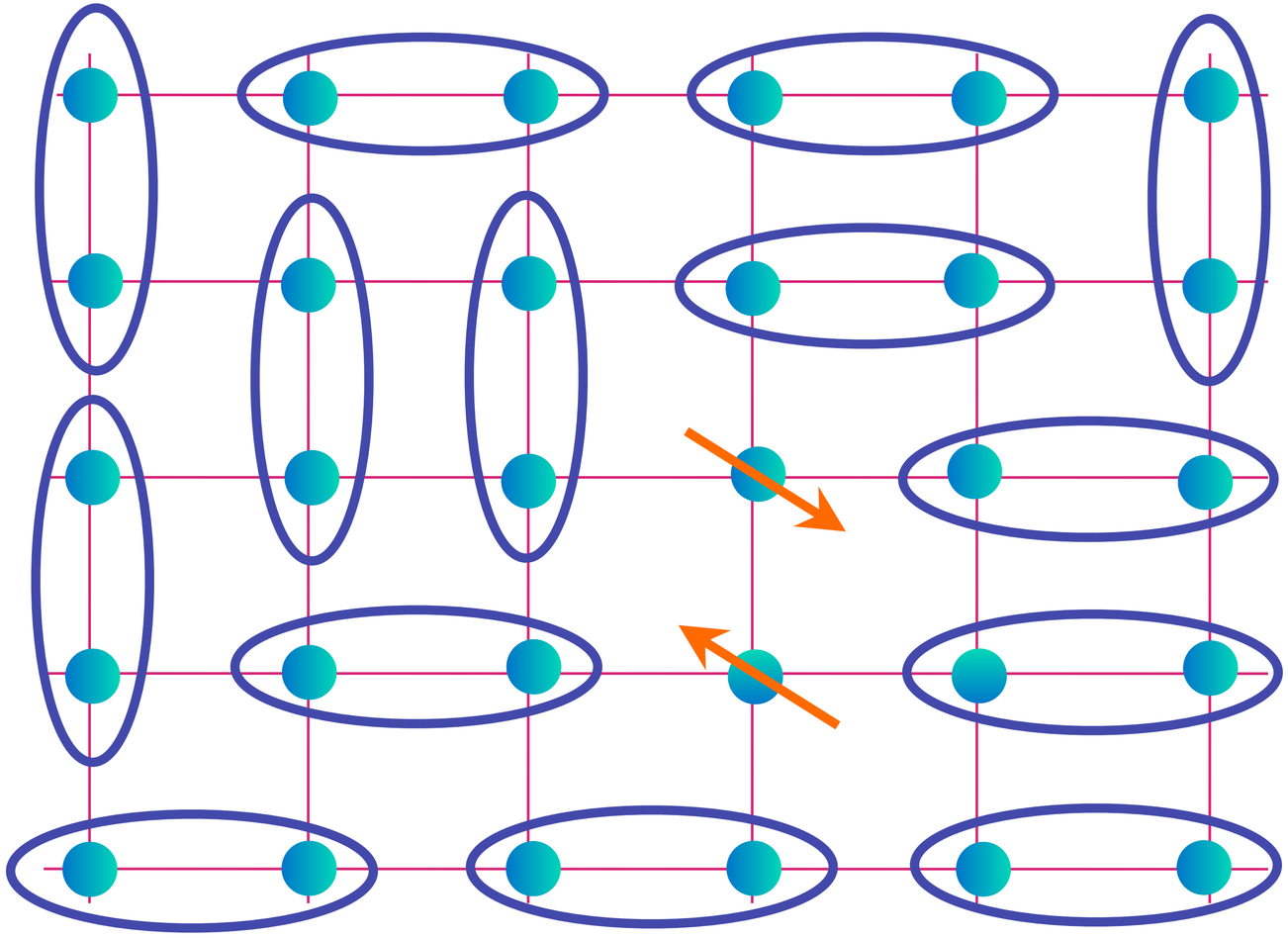

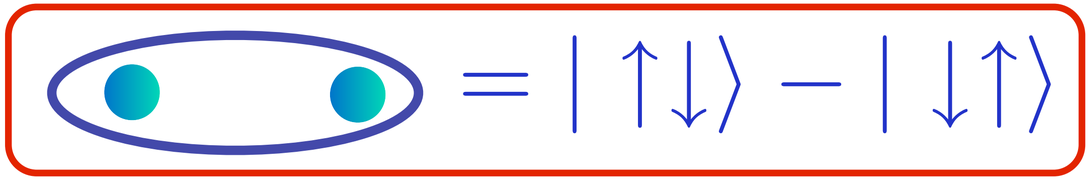

Spin liquid

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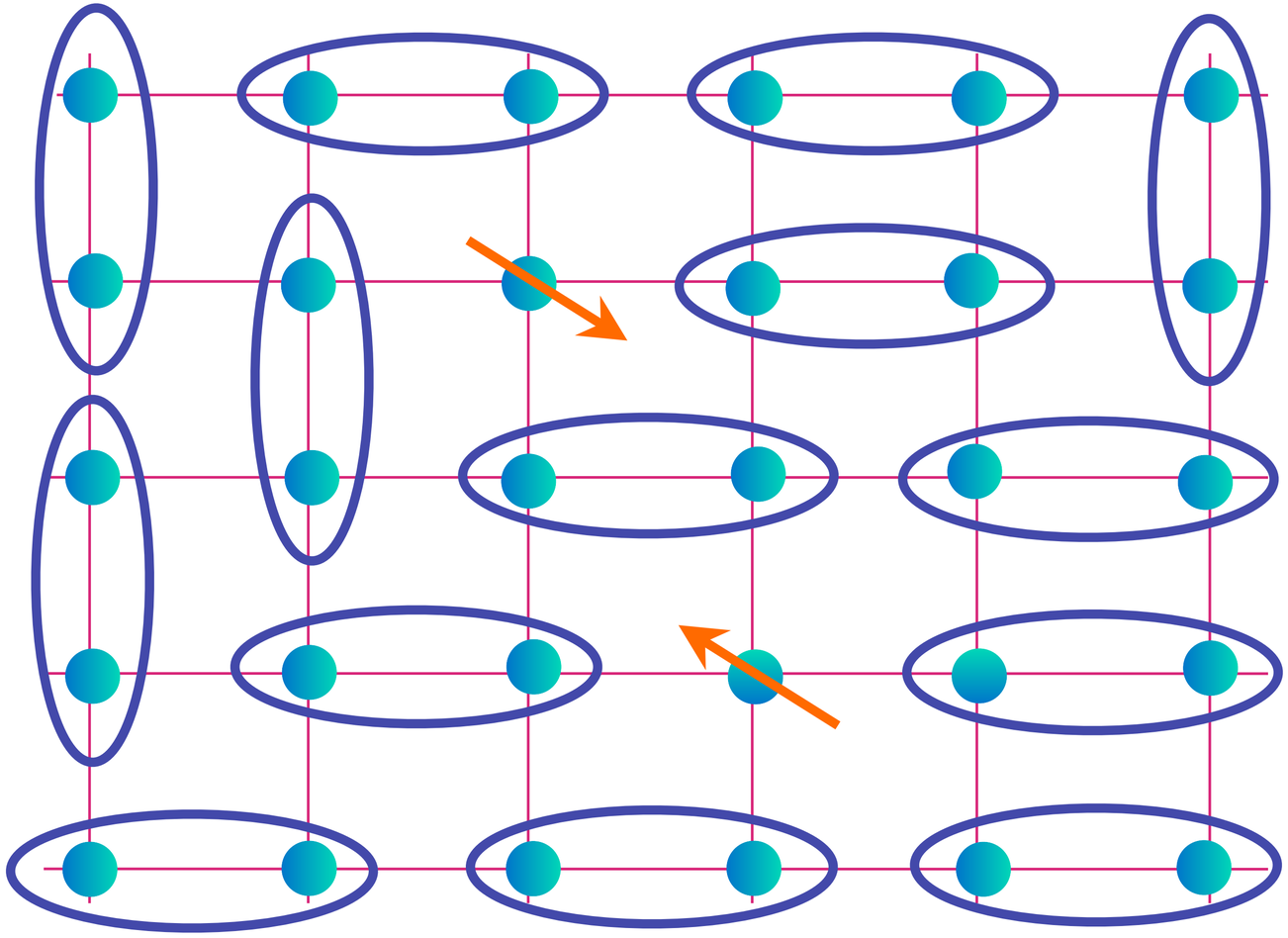

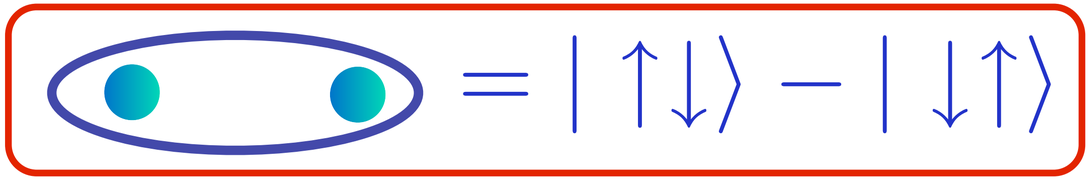

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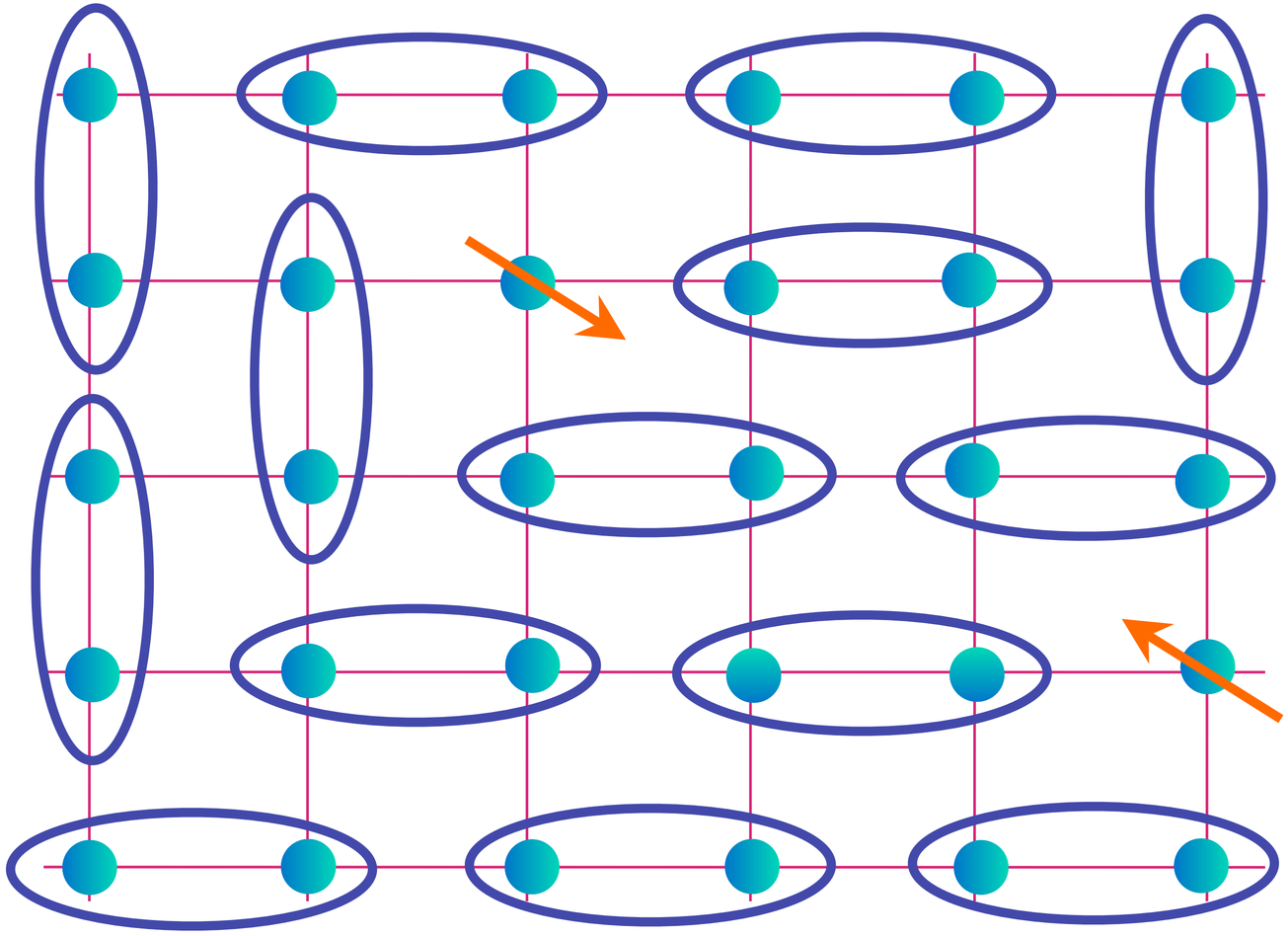

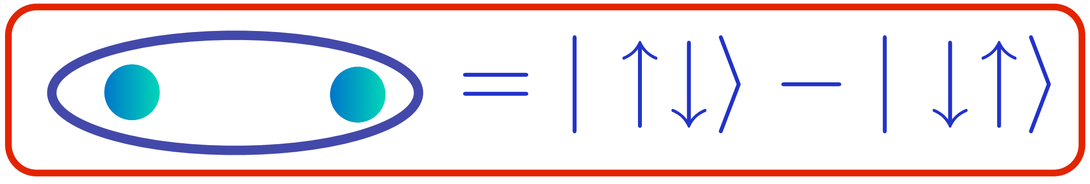

Spin liquid

Fractionalized spinon excitations with spin S=1/2 and charge 0.

G. Baskaran, Z. Zou, P.W. Anderson, *Solid State Comm.* **63**, 973 (1987)

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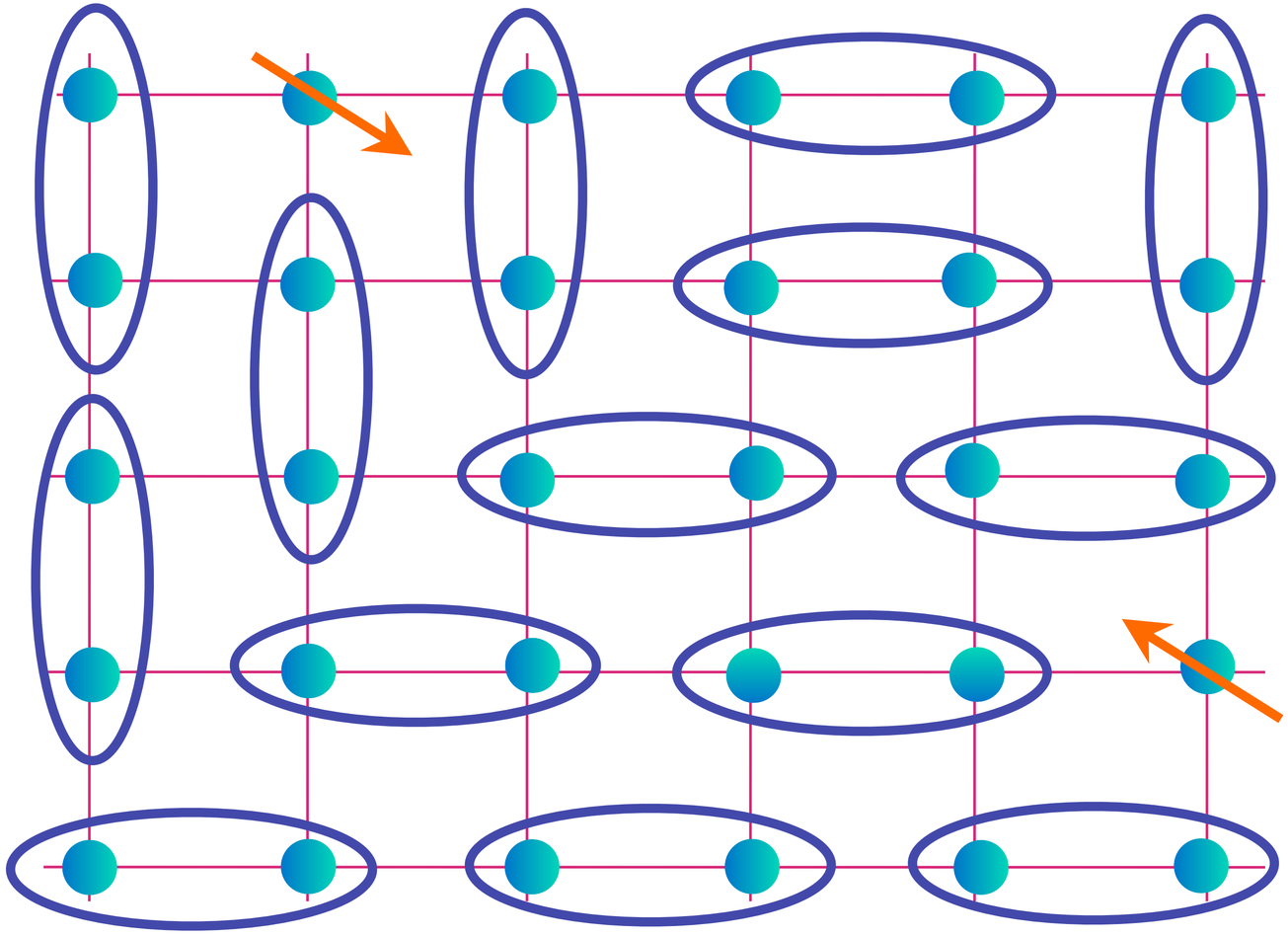

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Holons

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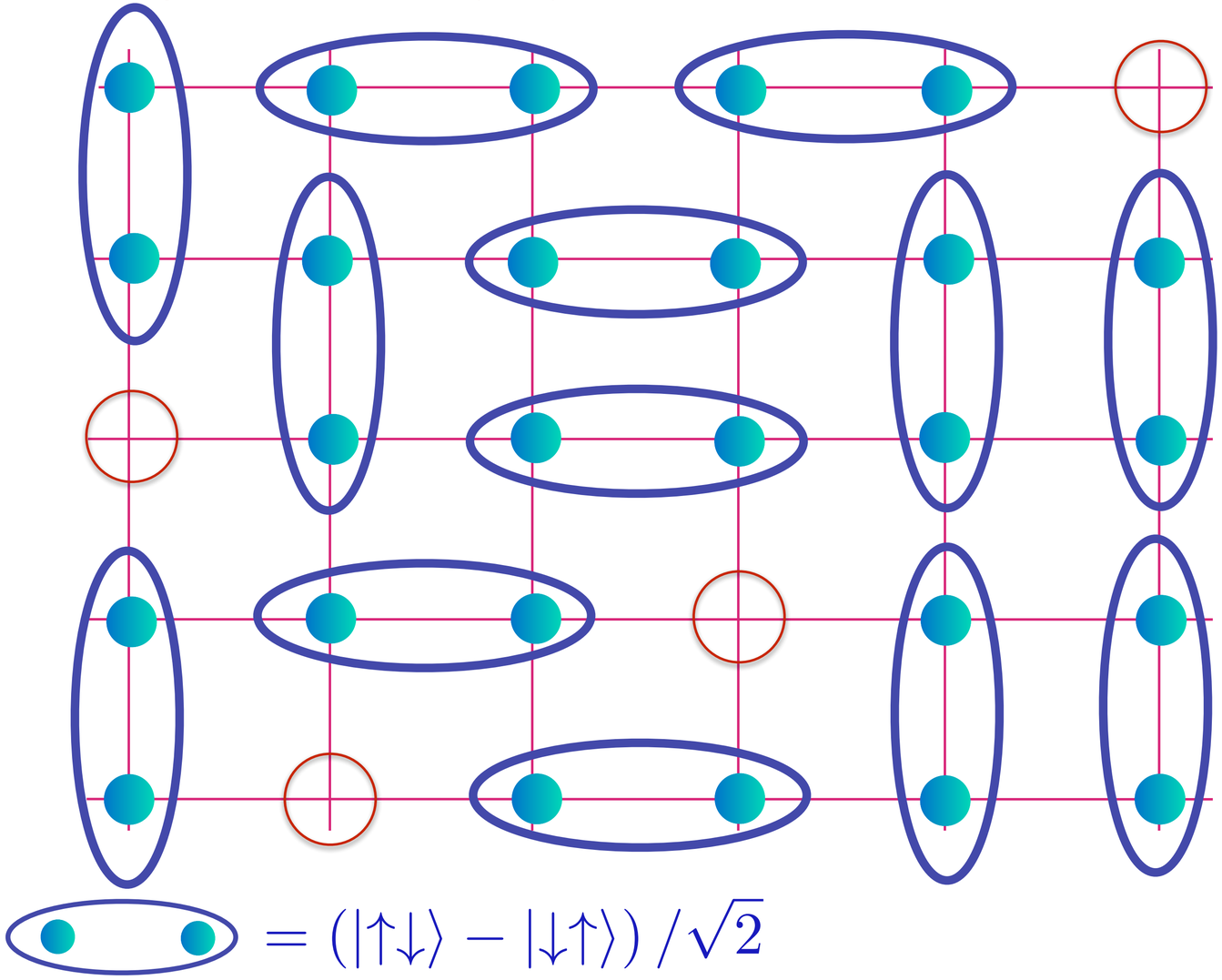

$$= \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)/\sqrt{2}$$

Spin liquid

Fractionalized holon excitations with spin S=0 and charge +e.

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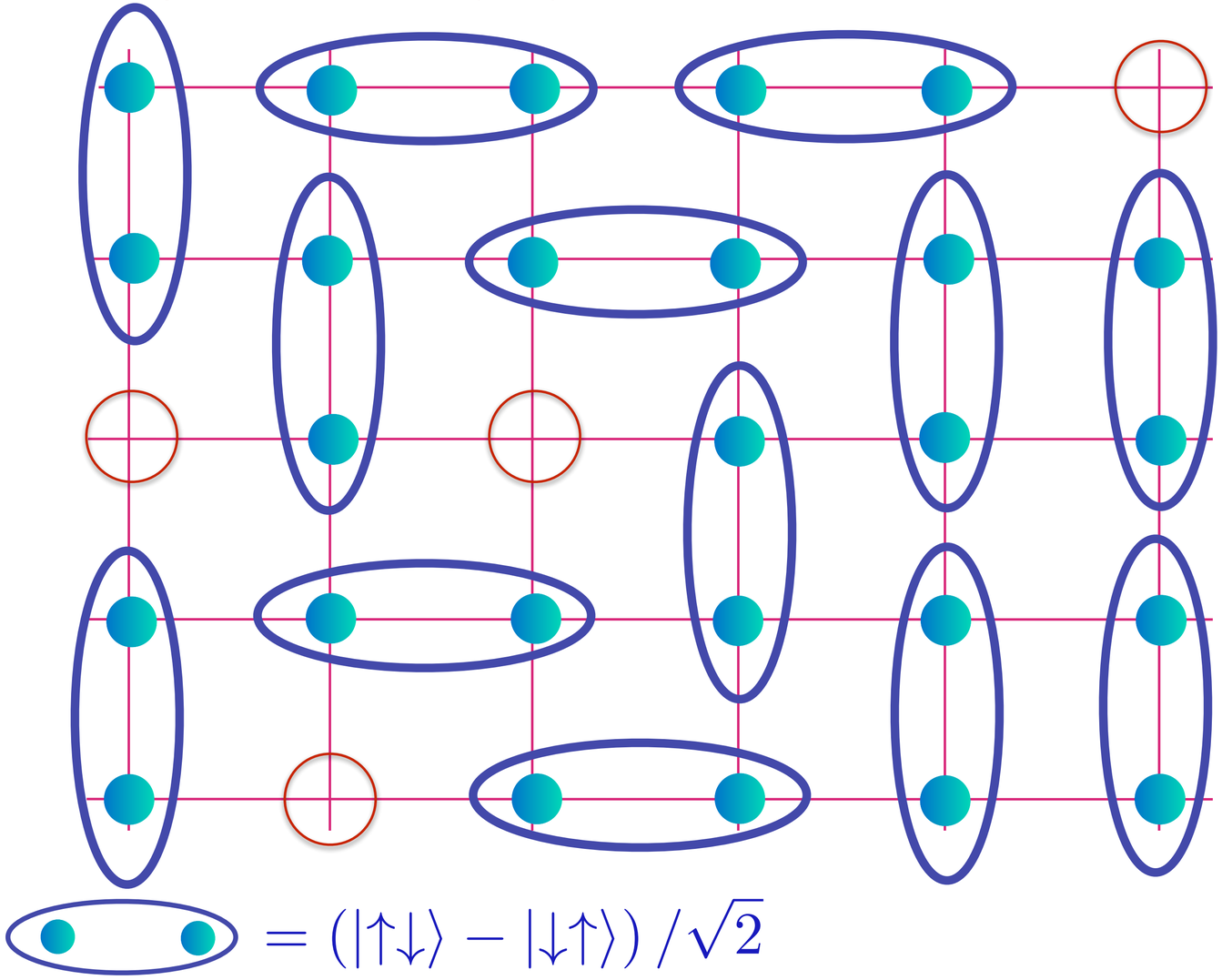

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Spin liquid

Fractionalized holon excitations with spin S=0 and charge +e.

Holon metal

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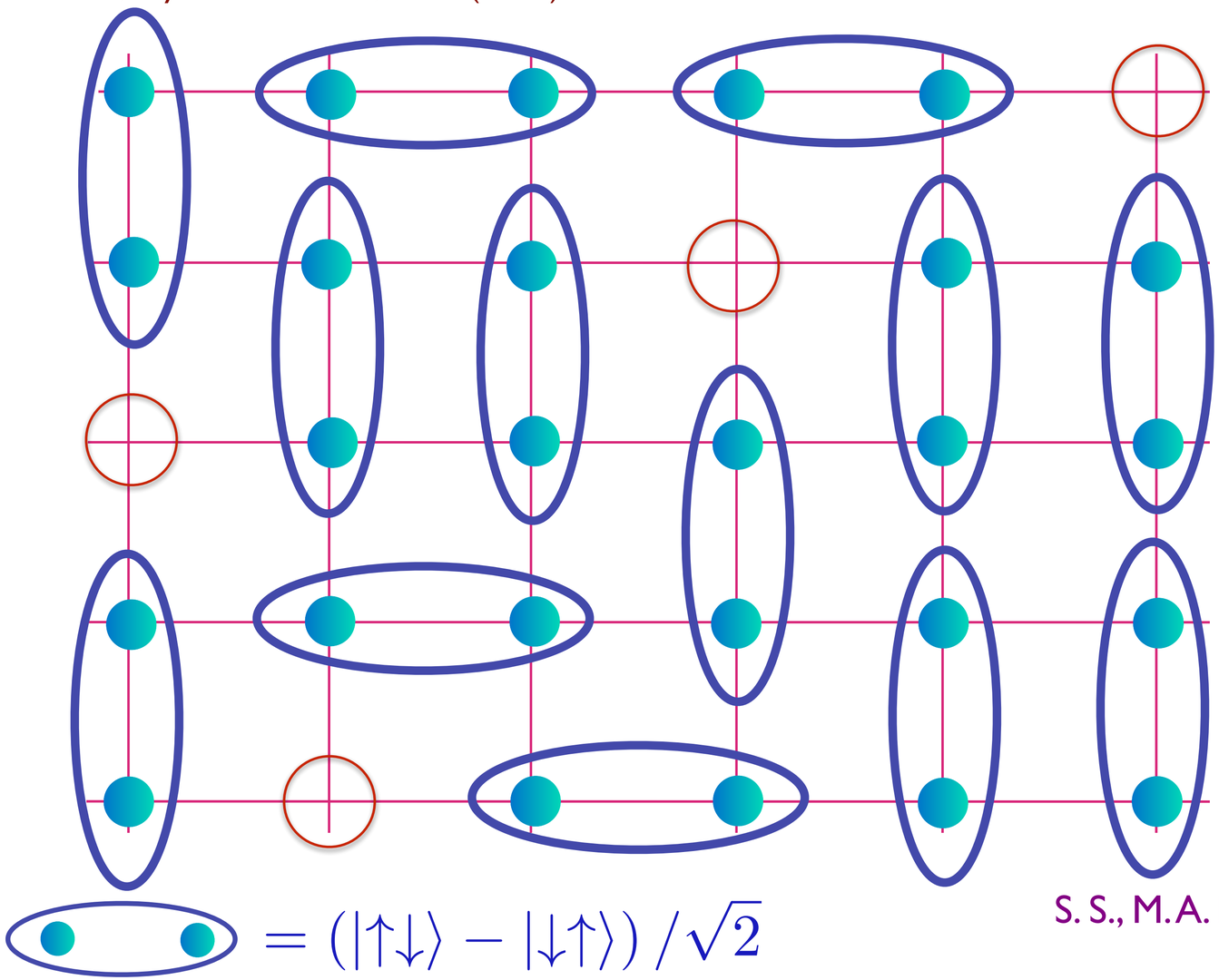

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If each holon is a fermion, we obtain a Fermi surface of holons of size p

S. S., M.A. Metlitski, Y. Qi, and C. Xu, PRB **80**, 155129 (2009)
M. S. Scheurer, S. Chatterjee, Wei Wu, M. Ferrero, A. Georges, and S. S., PNAS **115**, E3665 (2018)
Pietro M. Bonetti and Walter Metzner, PRB **106**, 205152 (2022)

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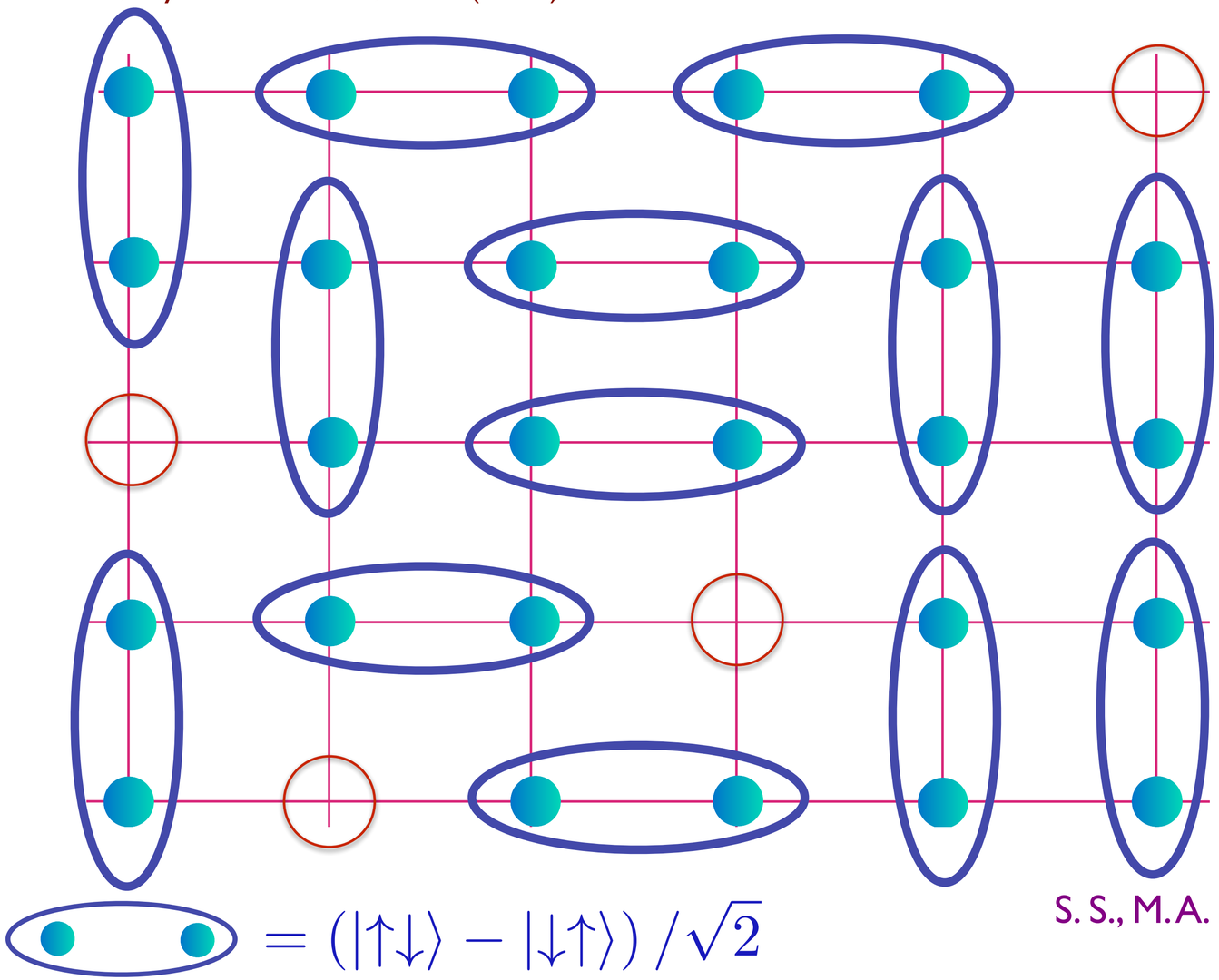

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FL* in a ***one-band*** model

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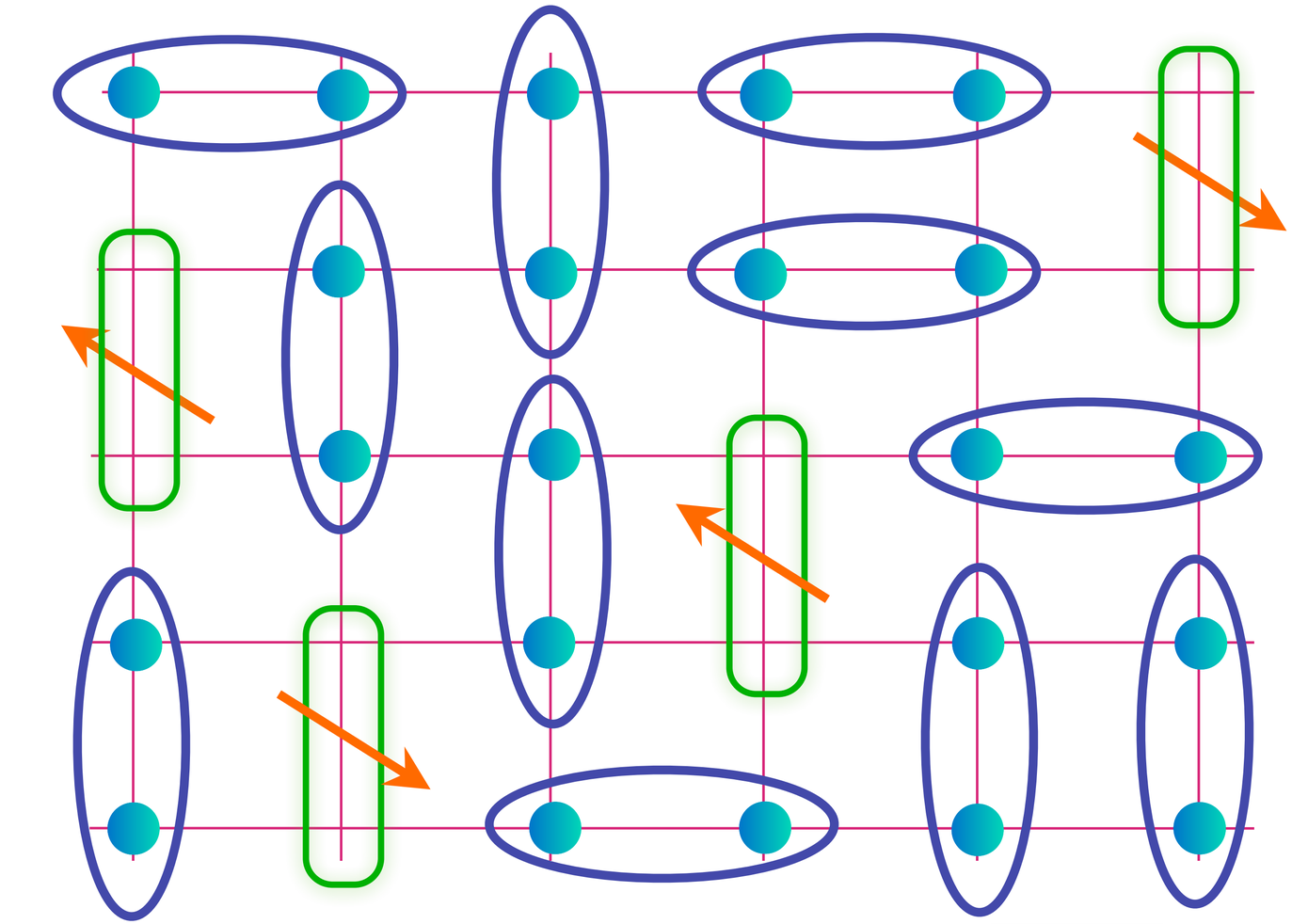

Metal with electron-like quasiparticles on a Fermi surface of size p, and emergent gauge fields

Spinon-holon bound state

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

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

E. G. Moon and S. Sachdev, *Phys. Rev. B* **83**, 224508 (2011); M. Punk, A. Allais, and S. Sachdev, *Proc. Nat. Acad. Sci.* **112**, 9552 (2015)

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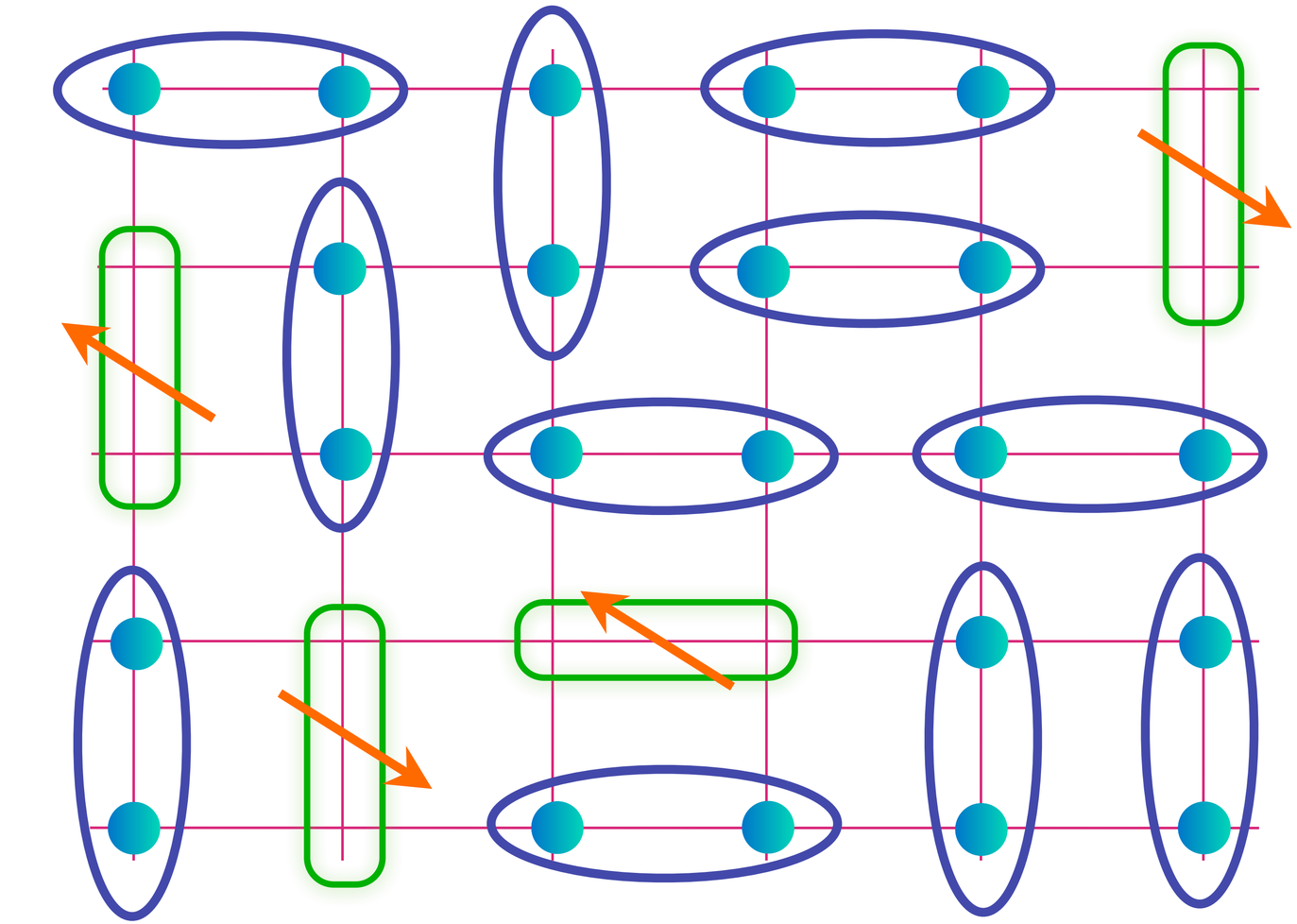

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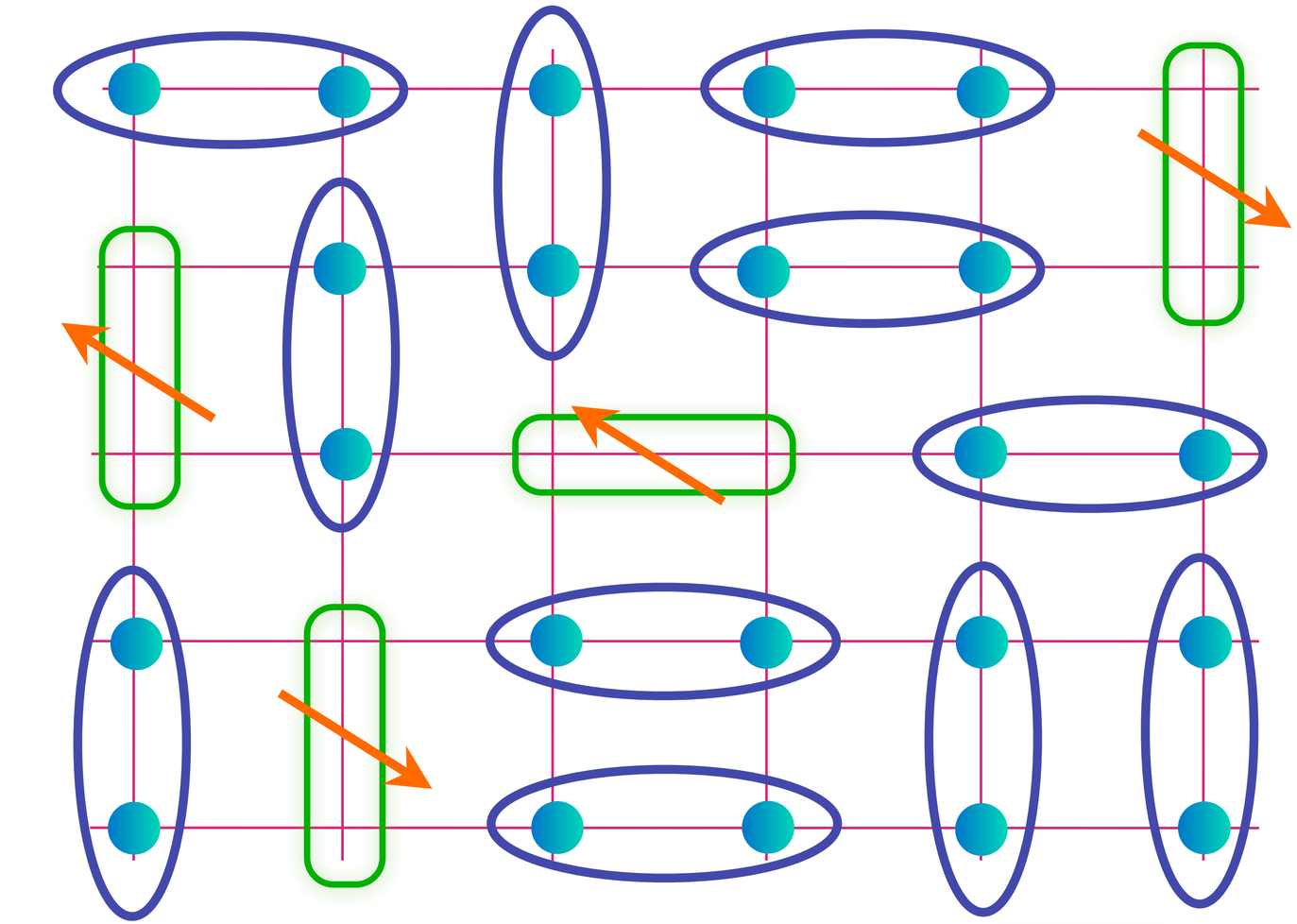

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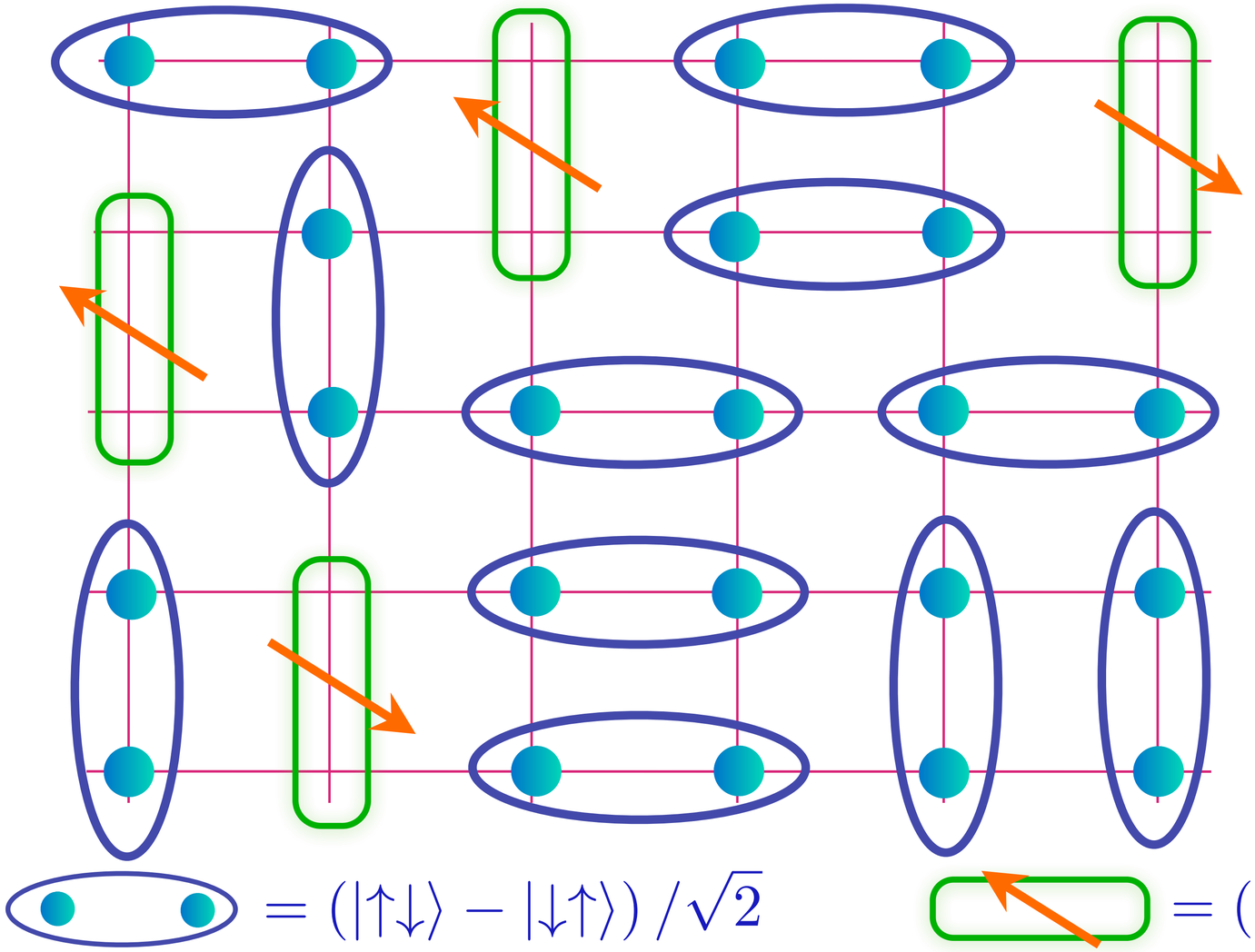

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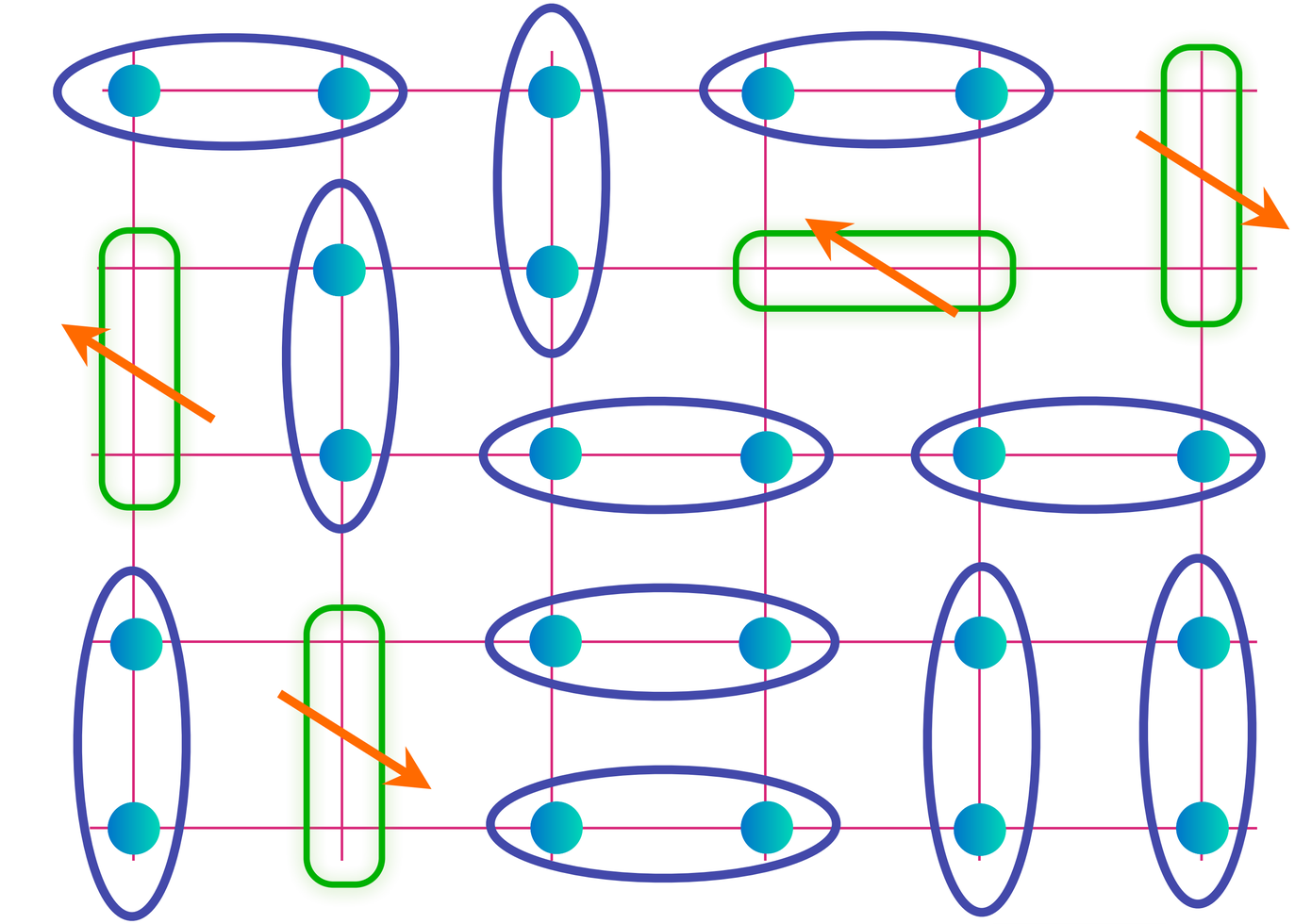

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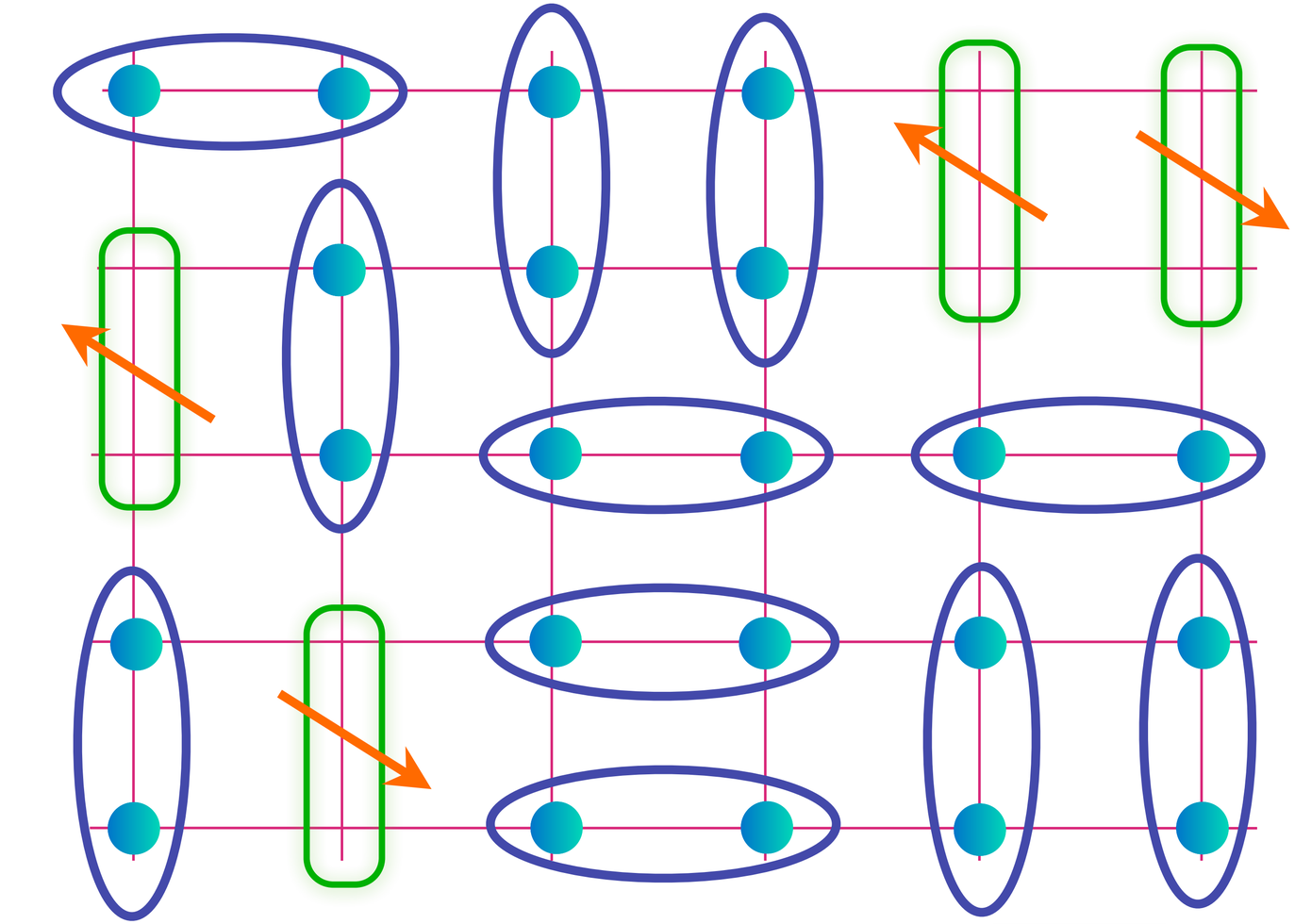

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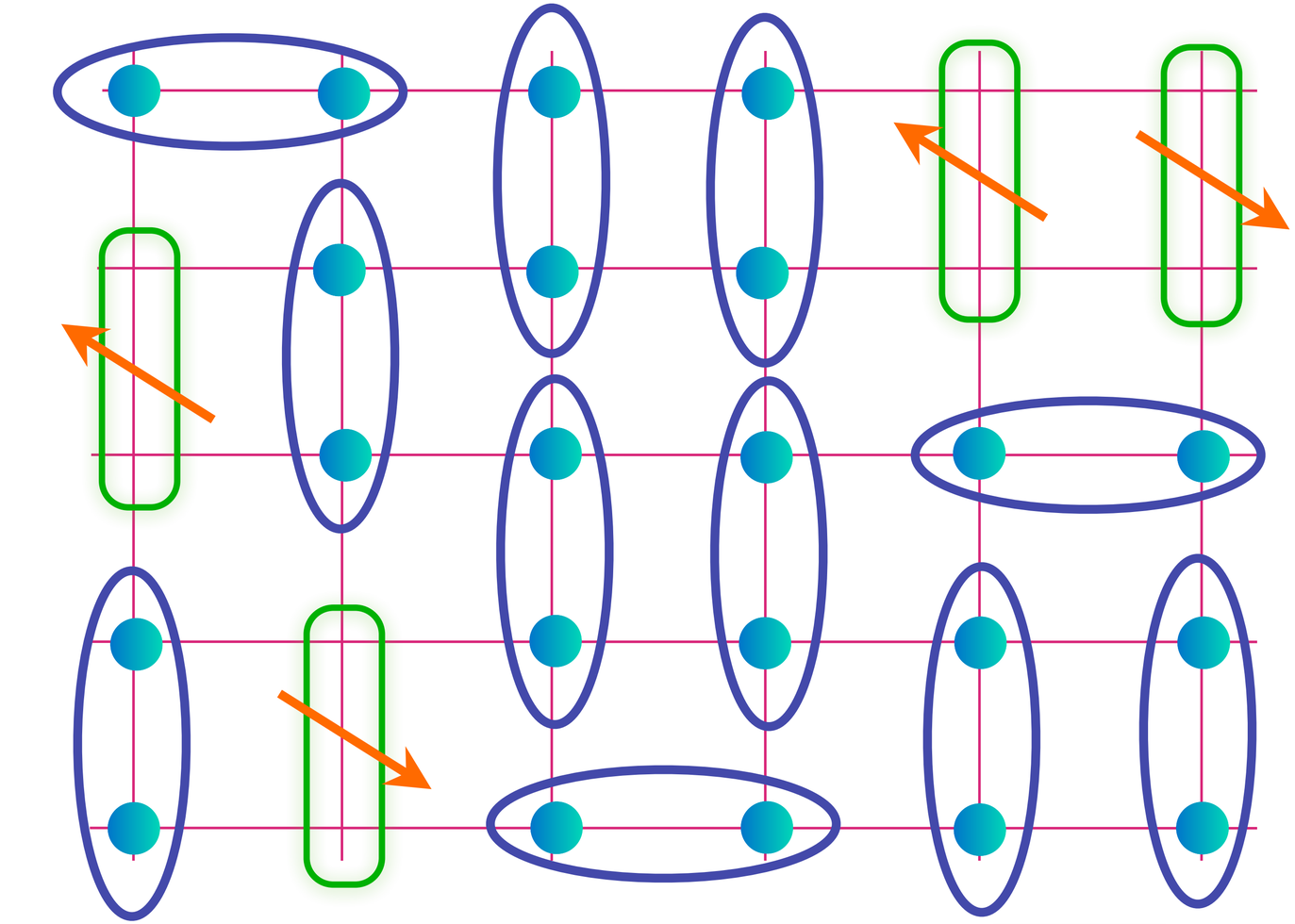

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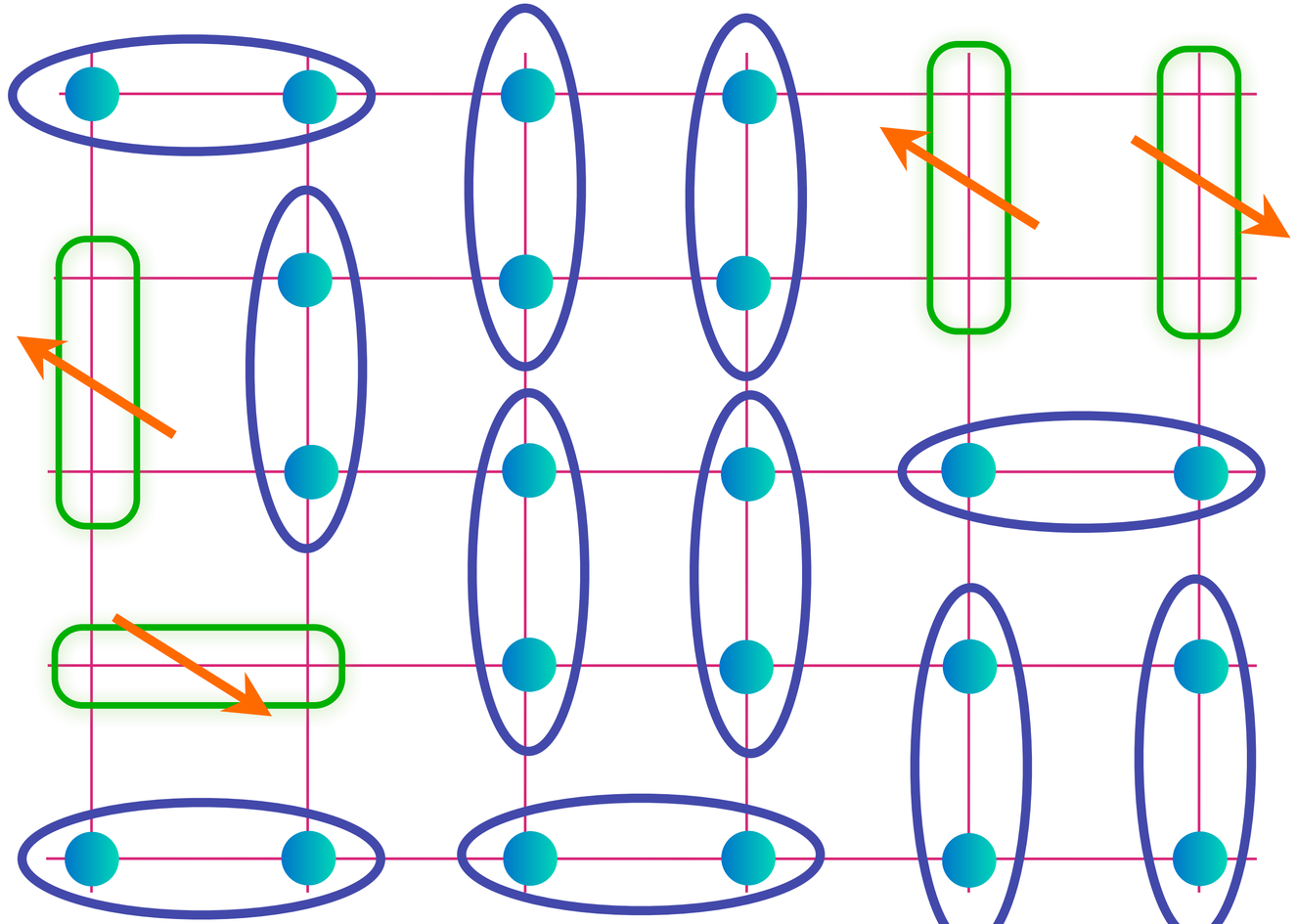

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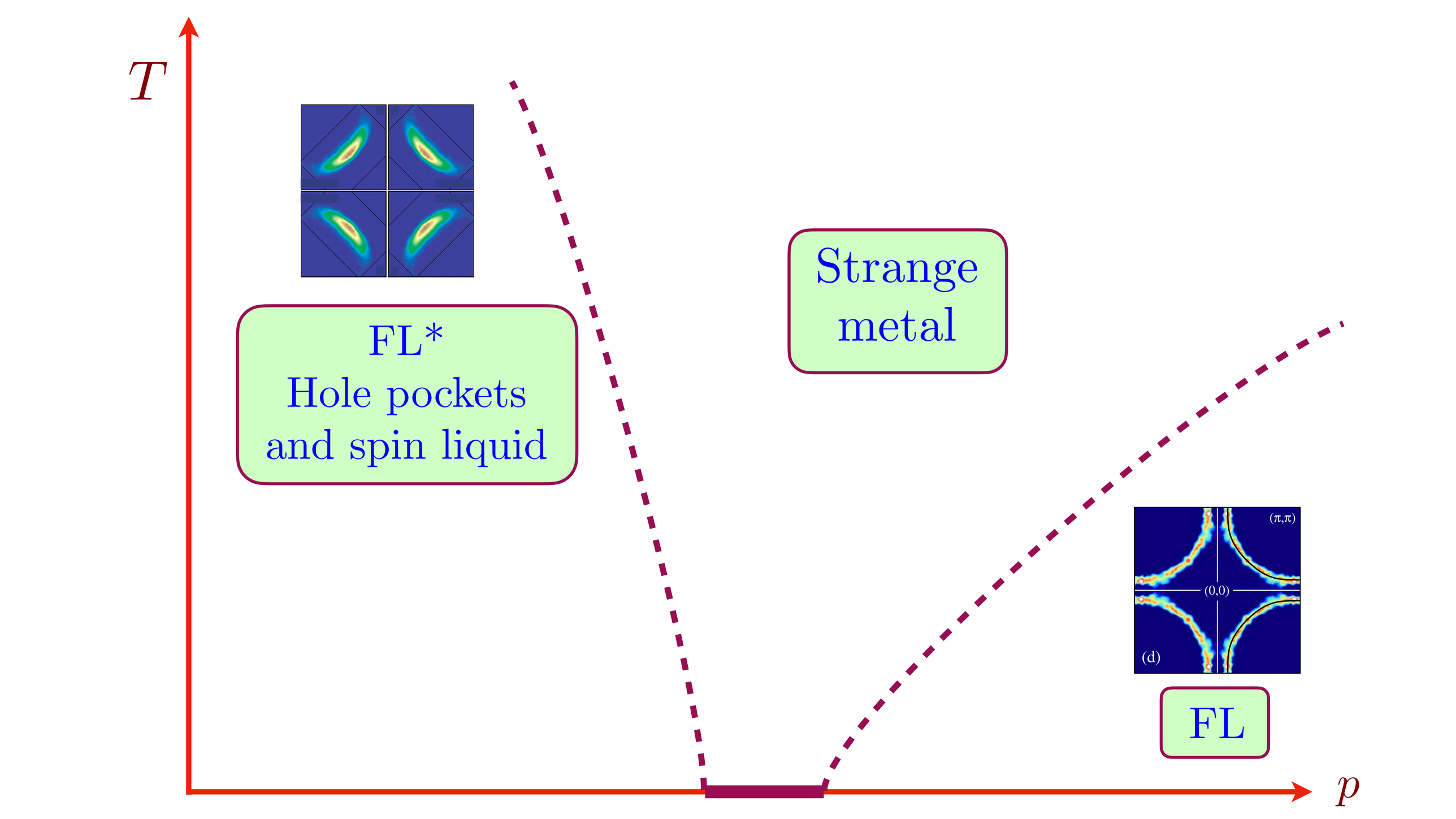
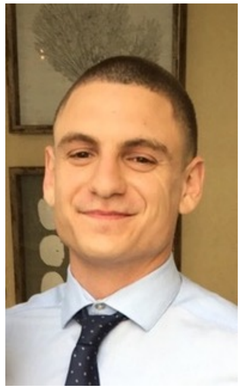
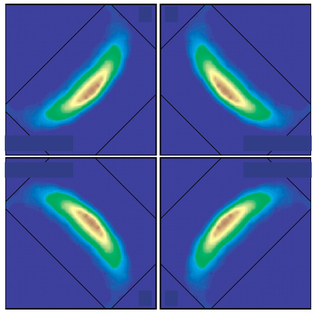
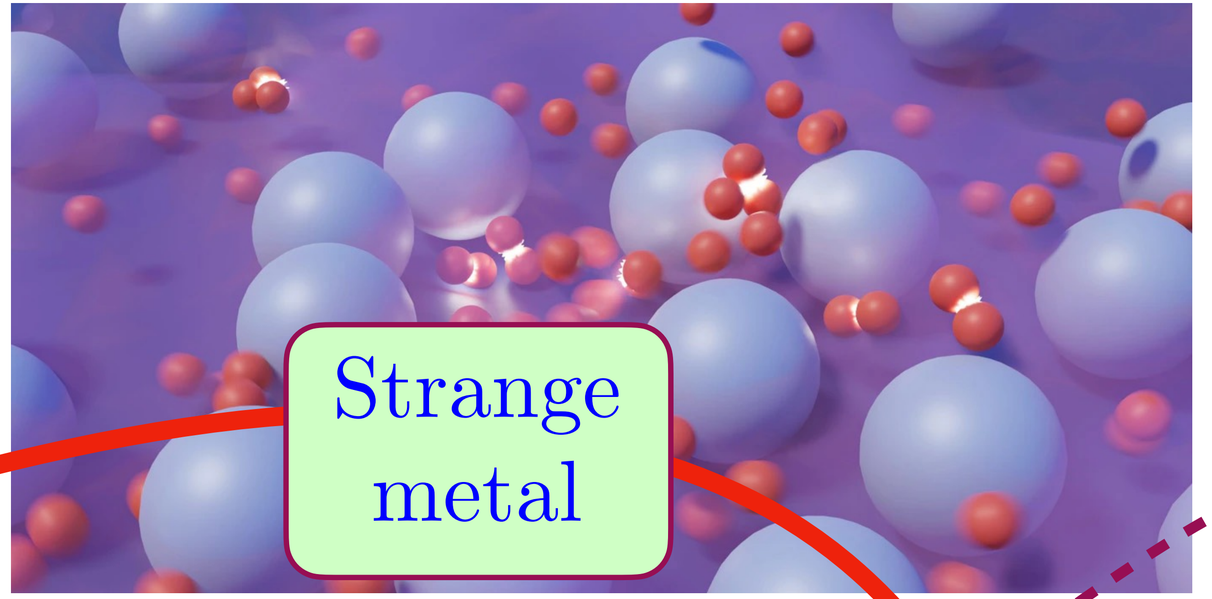

T
p
FL*
Hole pockets
and spin liquid
Strange
metal
FL
(π,π)
(0,0)
(d)



T

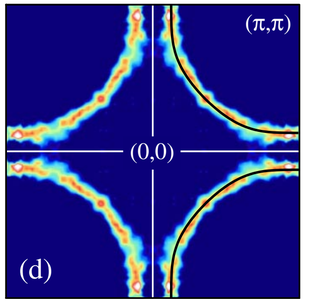


FL*
Hole pockets
and spin liquid



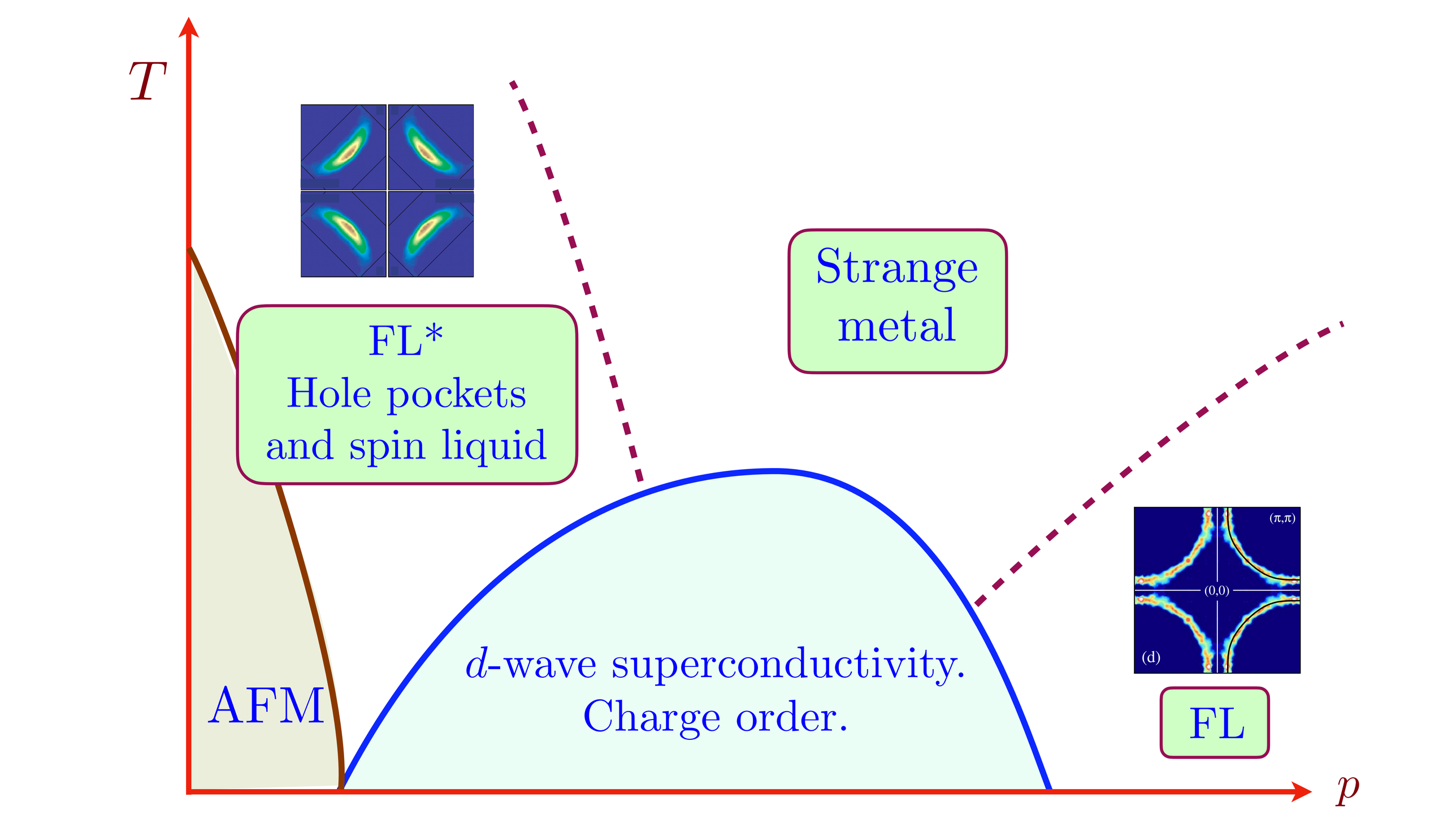
Strange
metal

Patel,
Haoyu
Guo,
Esterlis,
Sachdev,
Science
381, 790
(2023)



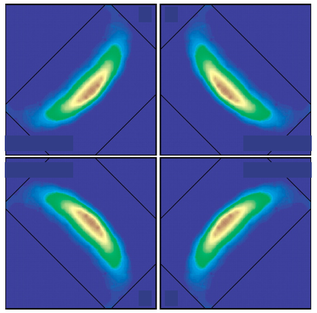
FL

p


T
FL*
Hole pockets
and spin liquid
Strange
metal
AFM
d-wave superconductivity.
Charge order.
(π,π)
(0,0)
(d)
FL
p

The onset of conventional order is a *confinement transition* for the gauge theory describing the fractionalized excitations of the FL* spin liquid

T



Strange metal

FL*
Hole pockets and spin liquid

AFM

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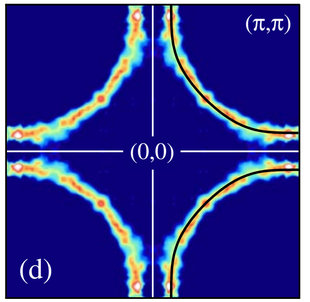
Charge order.

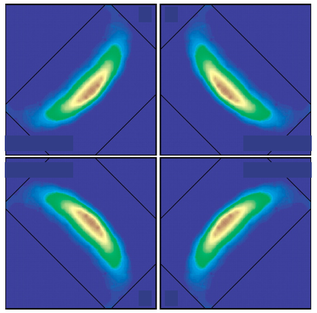


FL

p

- Variational wavefunction for FL* in a single-band model?

T

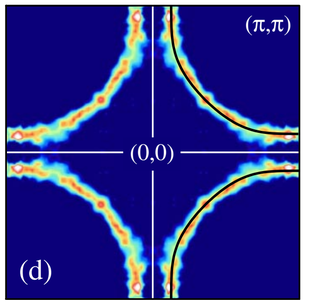


FL*
Hole pockets
and spin liquid

Strange
metal

AFM

d-wave superconductivity.
Charge order.

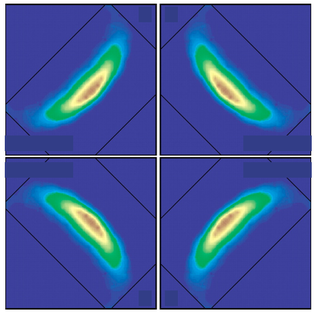


FL

p

- Variational wavefunction for FL* in a single-band model?
- Which spin liquid?

T



FL*
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and spin liquid

Strange
metal

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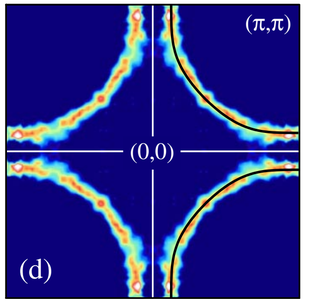
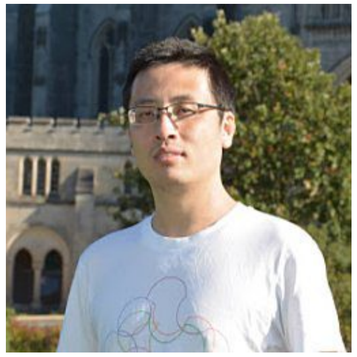


FL

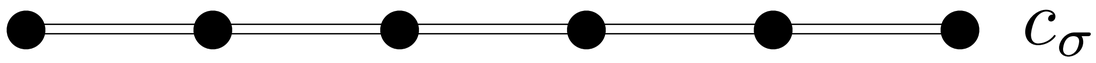
p

Ancilla theory of FL* in a single-band model



Ya-Hui Zhang

Ancilla theory of the Hubbard model



Hubbard model of hole density 1+p

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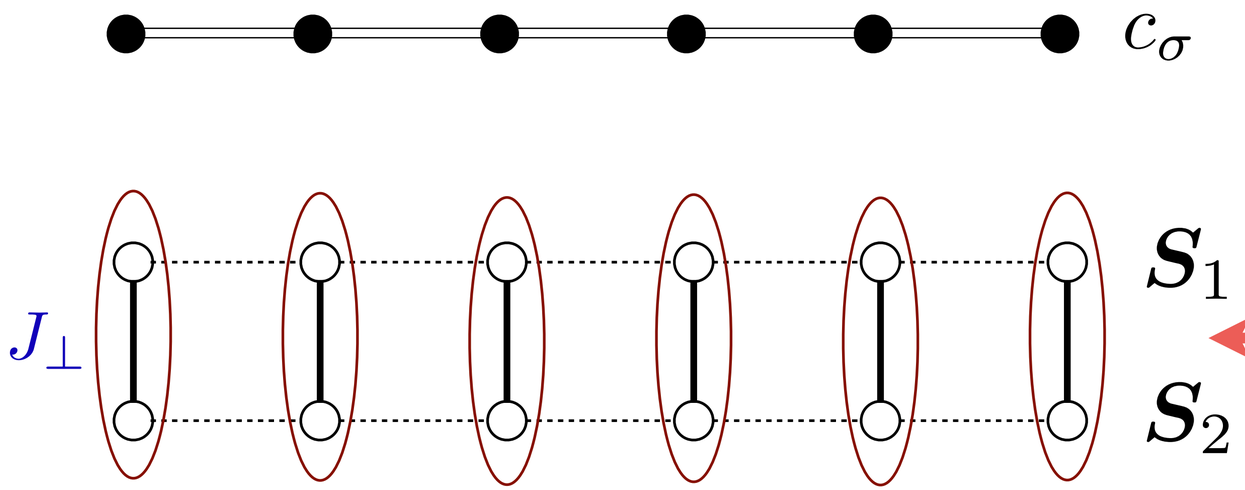
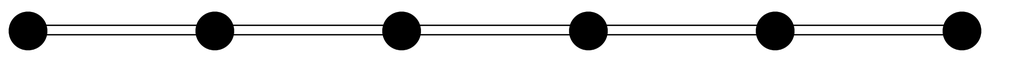


Hubbard model of hole density 1+p

Ancilla qubits in a "trivial" gapped insulator

$$\mathcal{H}_{\text{Hubbard}} + \mathcal{H}_{\text{trivial insulator}}$$

Ancilla theory of the Hubbard model



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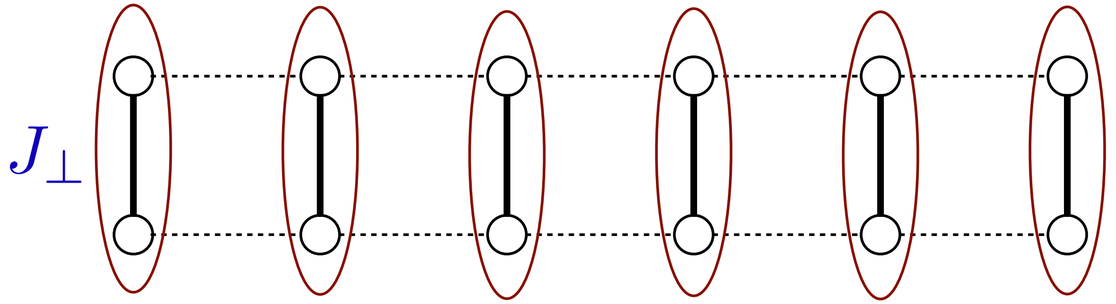
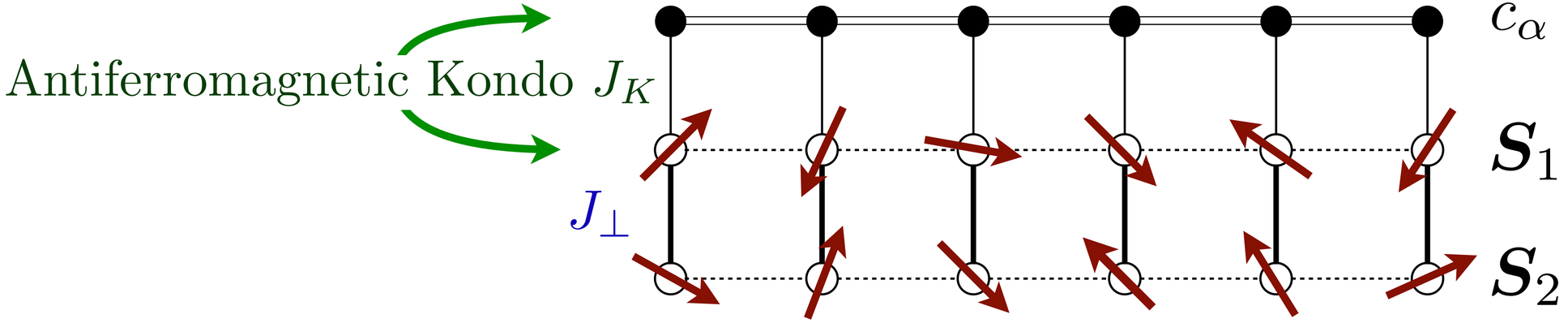


Ancilla qubits in a "trivial" gapped insulator

$$U\left(\mathcal{H}_{\text{Hubbard}} + \mathcal{H}_{\text{trivial insulator}}\right) U^{-1} = \mathcal{H}_{\text{ancilla}}$$



Free holes of density 1+p

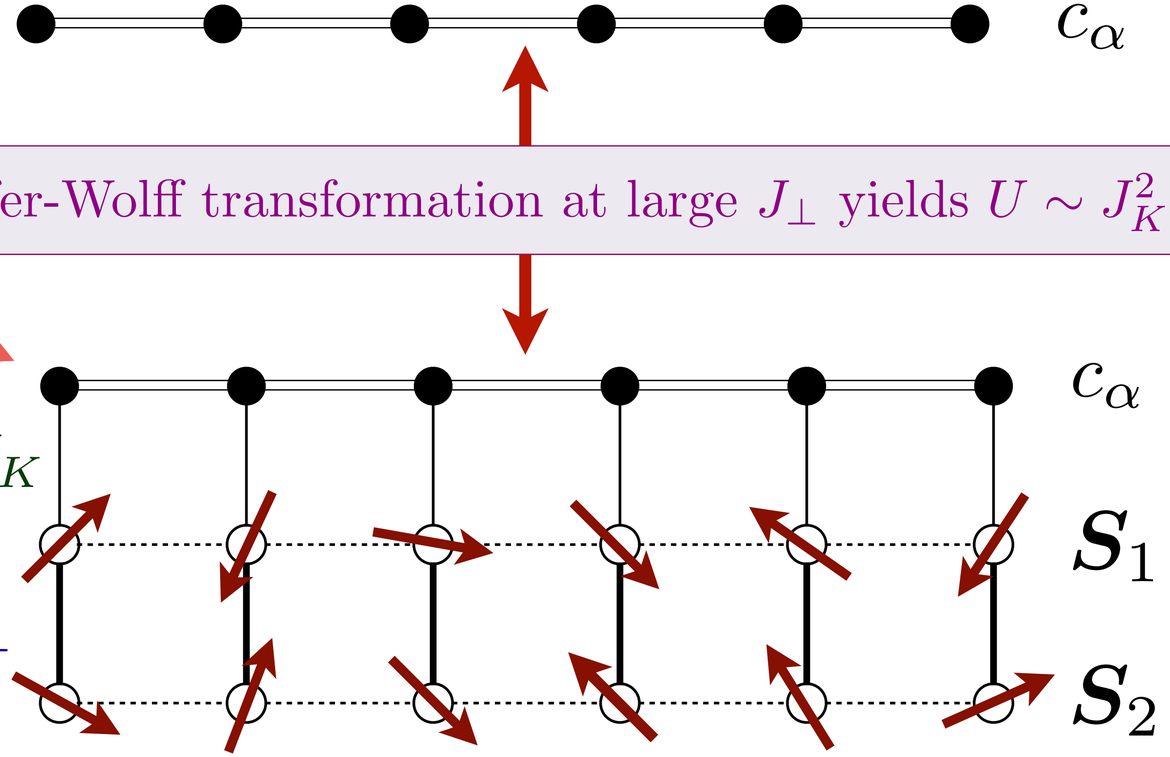
Ancilla theory of the Hubbard model

Ya-Hui Zhang and S. Sachdev,
Phys. Rev. Res. **2**, 023172 (2020)

Hubbard model of hole density 1+p

Free holes of density 1+p

Schrieffer-Wolff transformation at large $J_\perp$ yields $U \sim J_K^2/J_\perp$



Antiferromagnetic Kondo J_K

Ancilla qubits

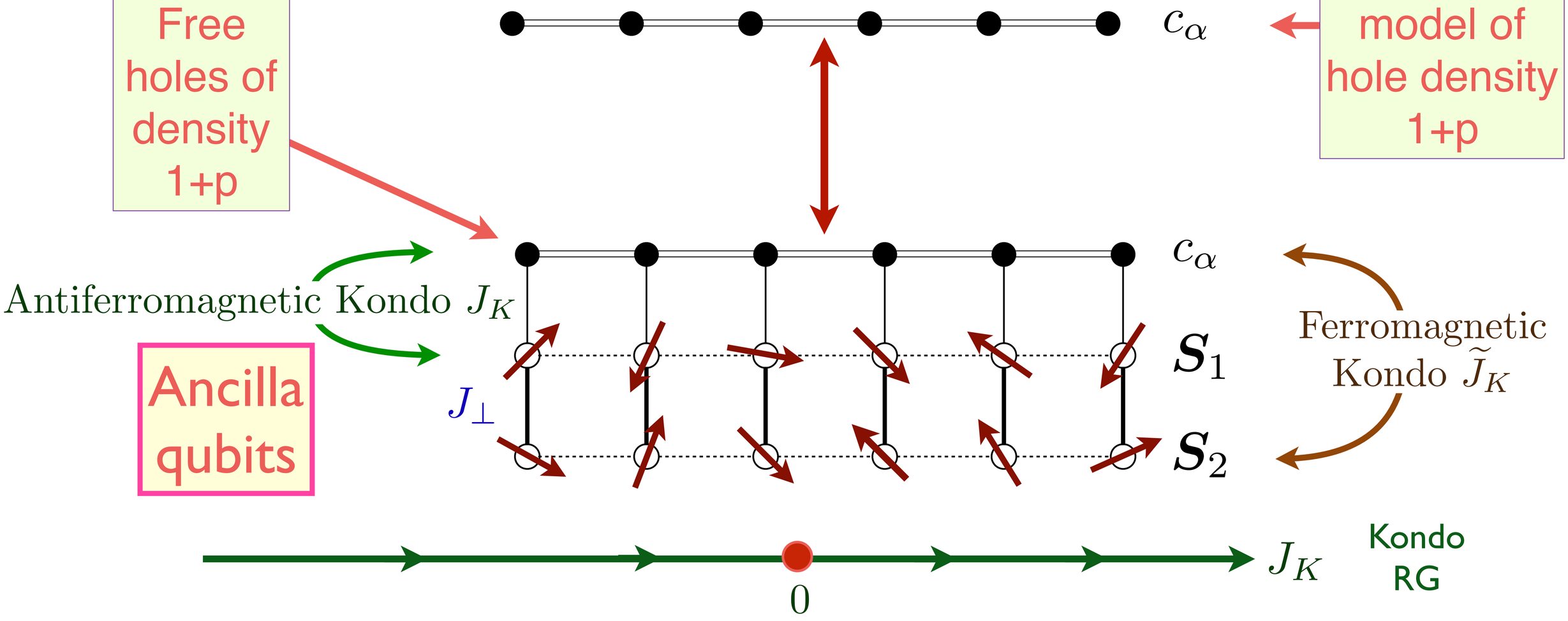
$$\mathcal{H}_{\text{ancilla}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} + J_K \sum_i c^\dagger_{i\alpha} \frac{\boldsymbol{\sigma}_{\alpha\alpha'}}{2} c_{i\alpha'} \cdot \boldsymbol{S}_{1i} + J_\perp \sum_i \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{2i}$$

Ancilla theory of the Hubbard model

Ya-Hui Zhang and S. Sachdev,
Phys. Rev. Res. **2**, 023172 (2020)

Free holes of density 1+p

Hubbard model of hole density 1+p



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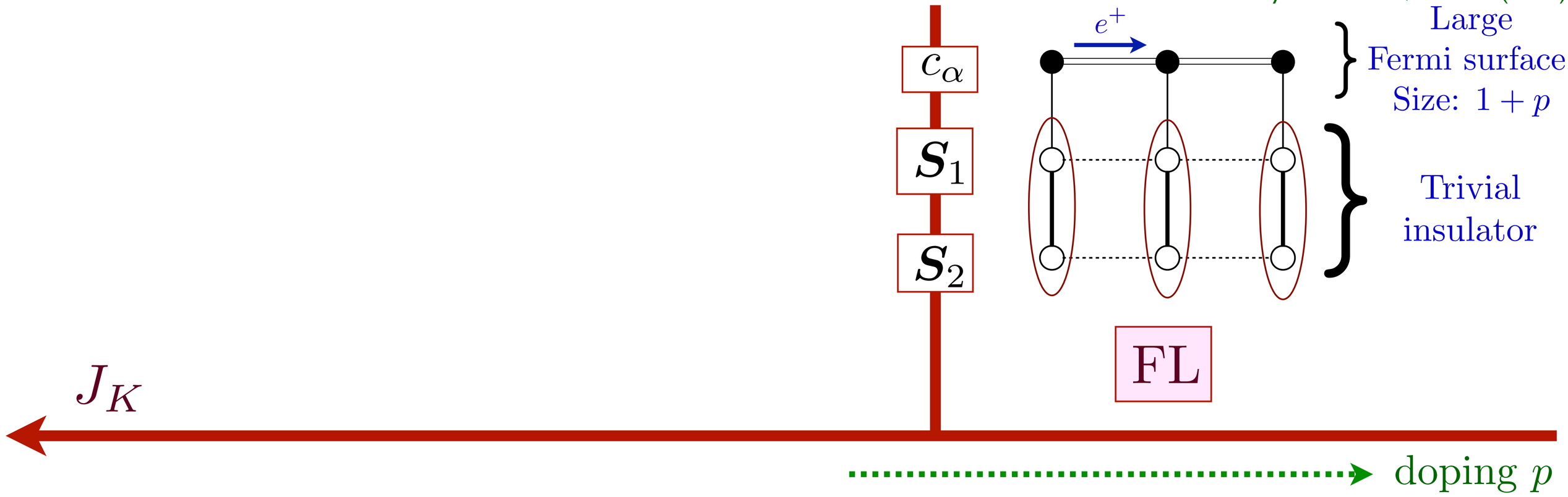


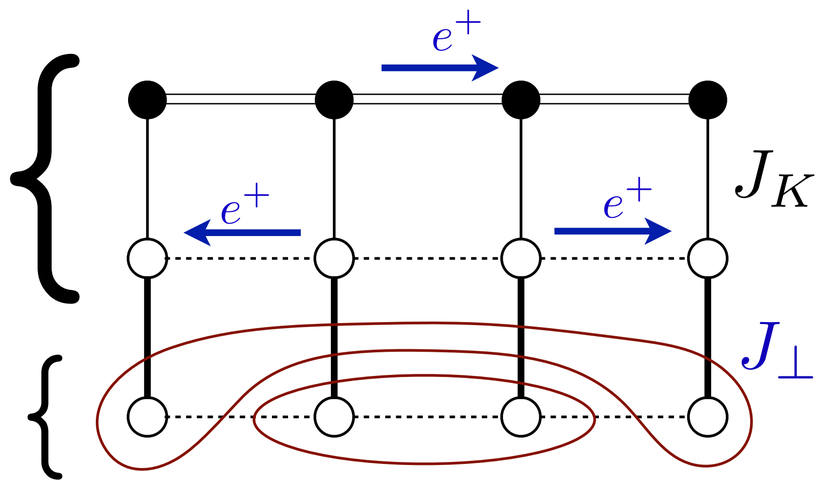
Ya-Hui Zhang

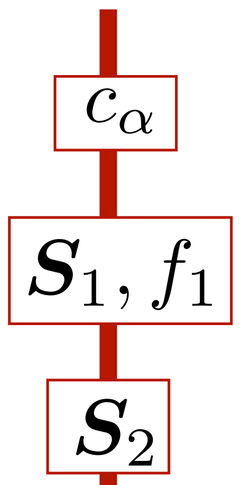
Ancilla theory of the Hubbard model

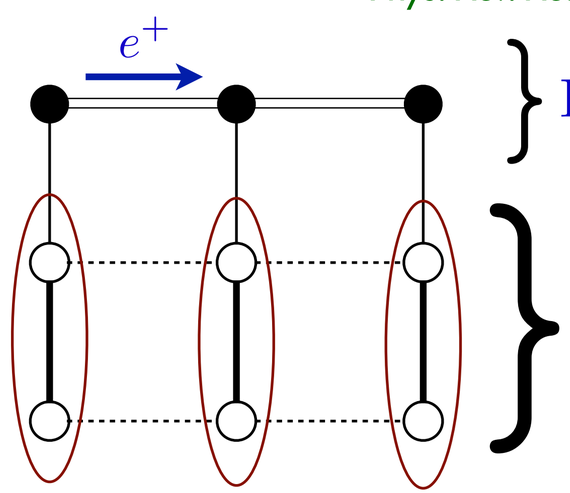
Ya-Hui Zhang and S. Sachdev,
Phys. Rev. Res. **2**, 023172 (2020)

Kondo lattice
heavy Fermi liquid.
Size $1 + p + 1$
$= p \pmod 2$.
Small Fermi surface!

Spin liquid







Large
Fermi surface.
Size: $1 + p$

Trivial
insulator

FL*

FL

J_K

doping p

Pseudogap metal =
Kondo Lattice Heavy
Fermi Liquid
$\oplus$
Spin Liquid

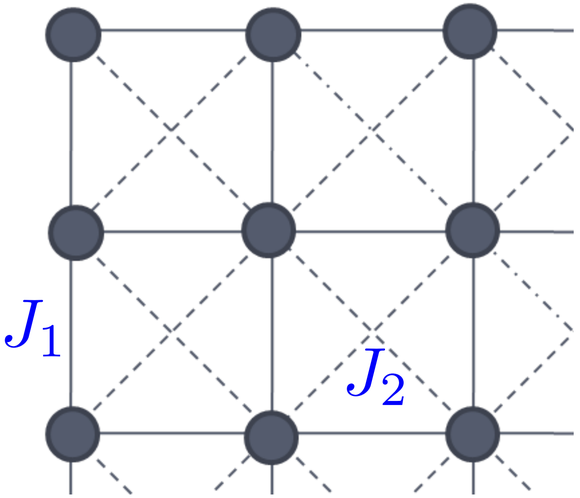
$|\mathrm{FL}*\rangle = [\text{Projection onto rung singlets of } \boldsymbol{S}_1, \boldsymbol{S}_2]$
$\bowtie |\text{Slater determinant of } (c, f_1)\rangle$
$\otimes |\text{Spin liquid of } \boldsymbol{S}_2\rangle$

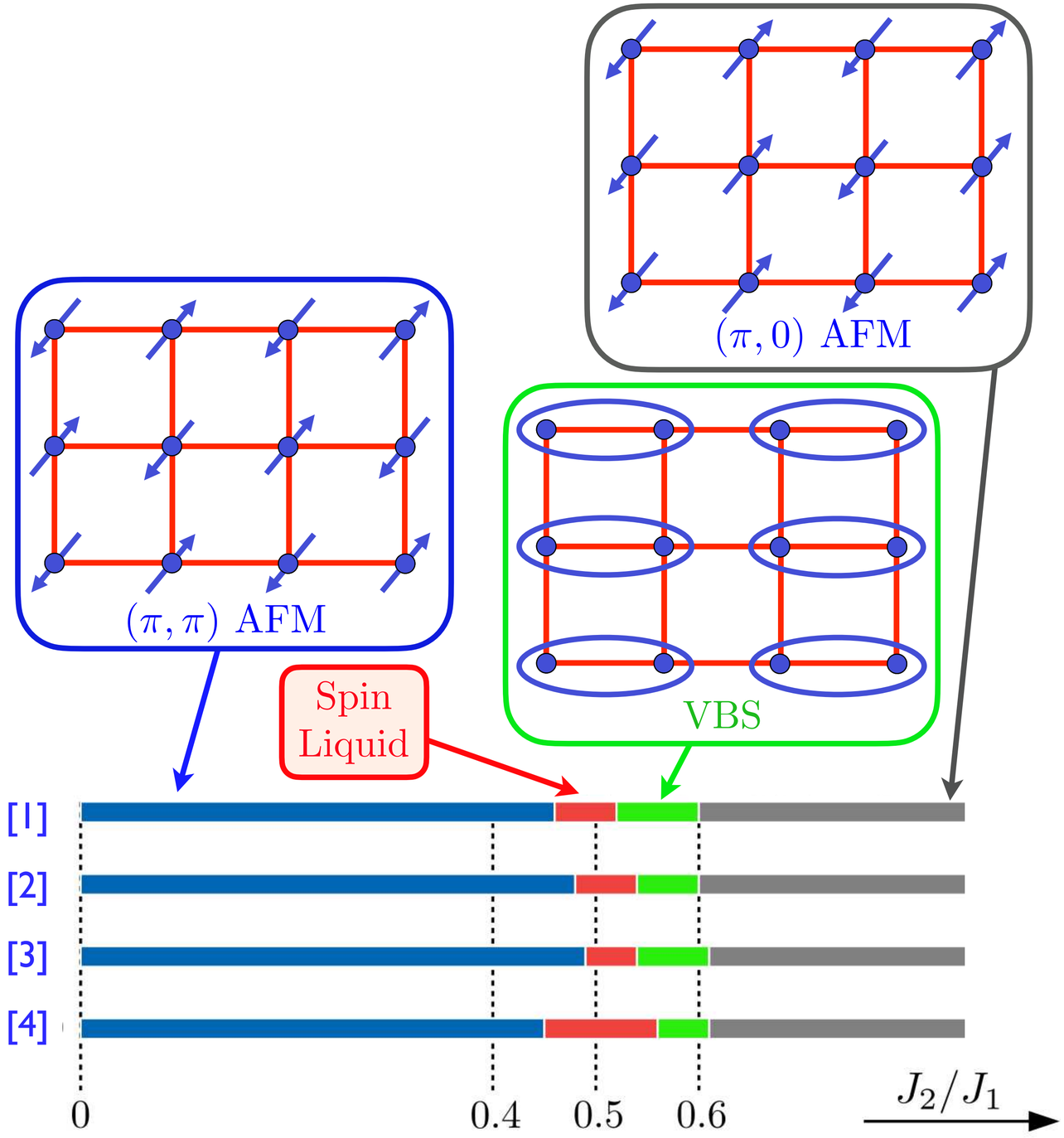
Ya-Hui
Zhang

Replacement for "vanilla" Gutzwiller-projected Fermi liquid in the underdoped regime

The CP^1/π-flux spin liquid

$$H = J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$





1. L. Wang and A. W. Sandvik, *Phys. Rev. Lett.* **121**, 107202 (2018)
2. F. Ferrari and F. Becca, *Phys. Rev. B* **102**, 014417 (2020)
3. Y. Nomura and M. Imada, *Phys. Rev. X* **11**, 031034 (2021)
4. W.-Y. Liu, S.-S. Gong, Y.-B. Li, D. Poilblanc, W.-Q. Chen, and Z.-C. Gu, *Science Bulletin* **67,** 1034 (2022)

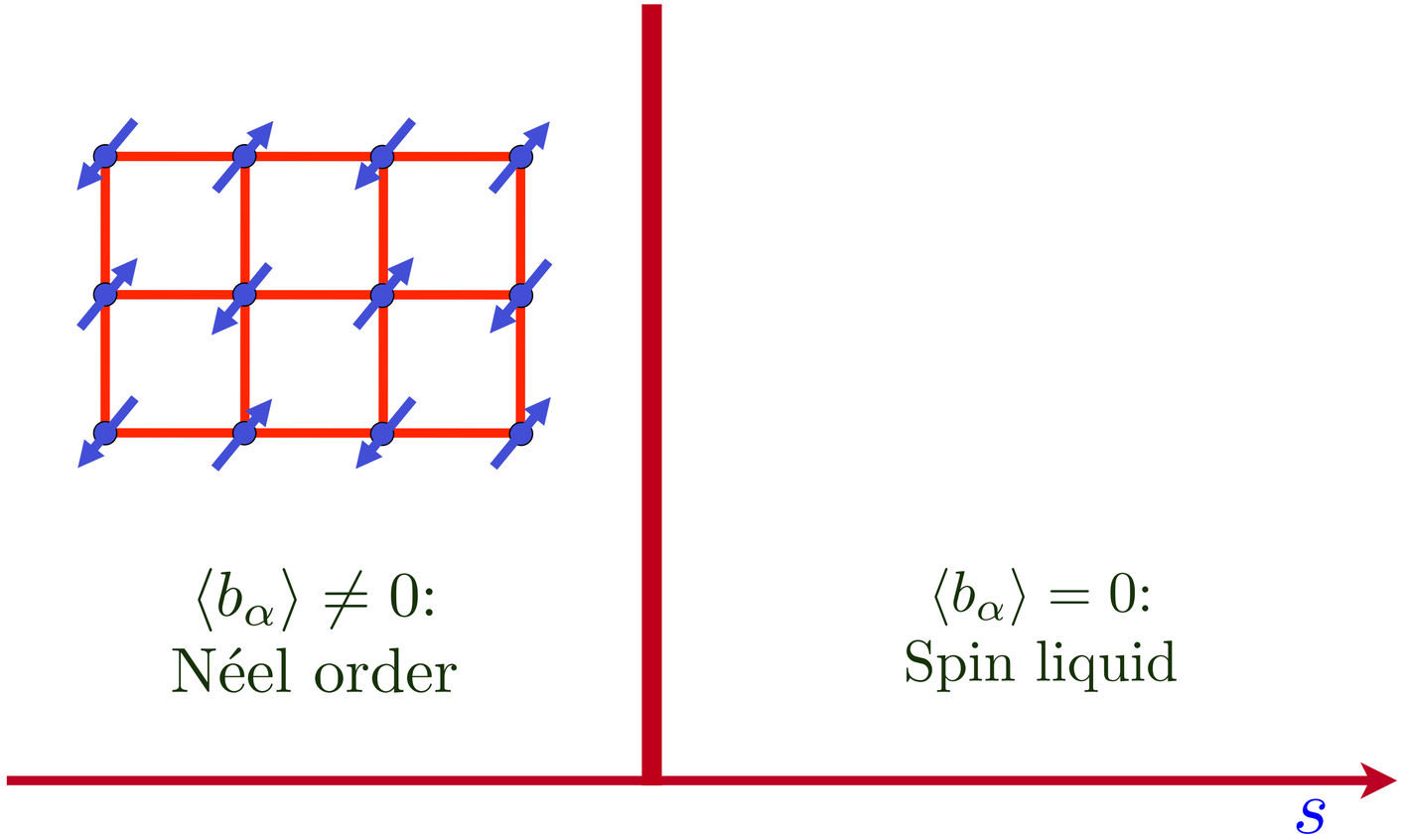
Insulating $S=1/2$ antiferromagnet

$$H = \sum_{i<j} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

Schwinger bosons

$$\boldsymbol{S}_i = \frac{1}{2} b^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} b_{i\beta} \,, \qquad \sum_{\alpha=\uparrow,\downarrow} b^\dagger_{i\alpha} b_{i\alpha} = 1$$

Mean-field spin liquid
with gapped bosonic spinons.



D.P. Arovas and A. Auerbach, *Phys. Rev. B* **38**, 316 (1988)

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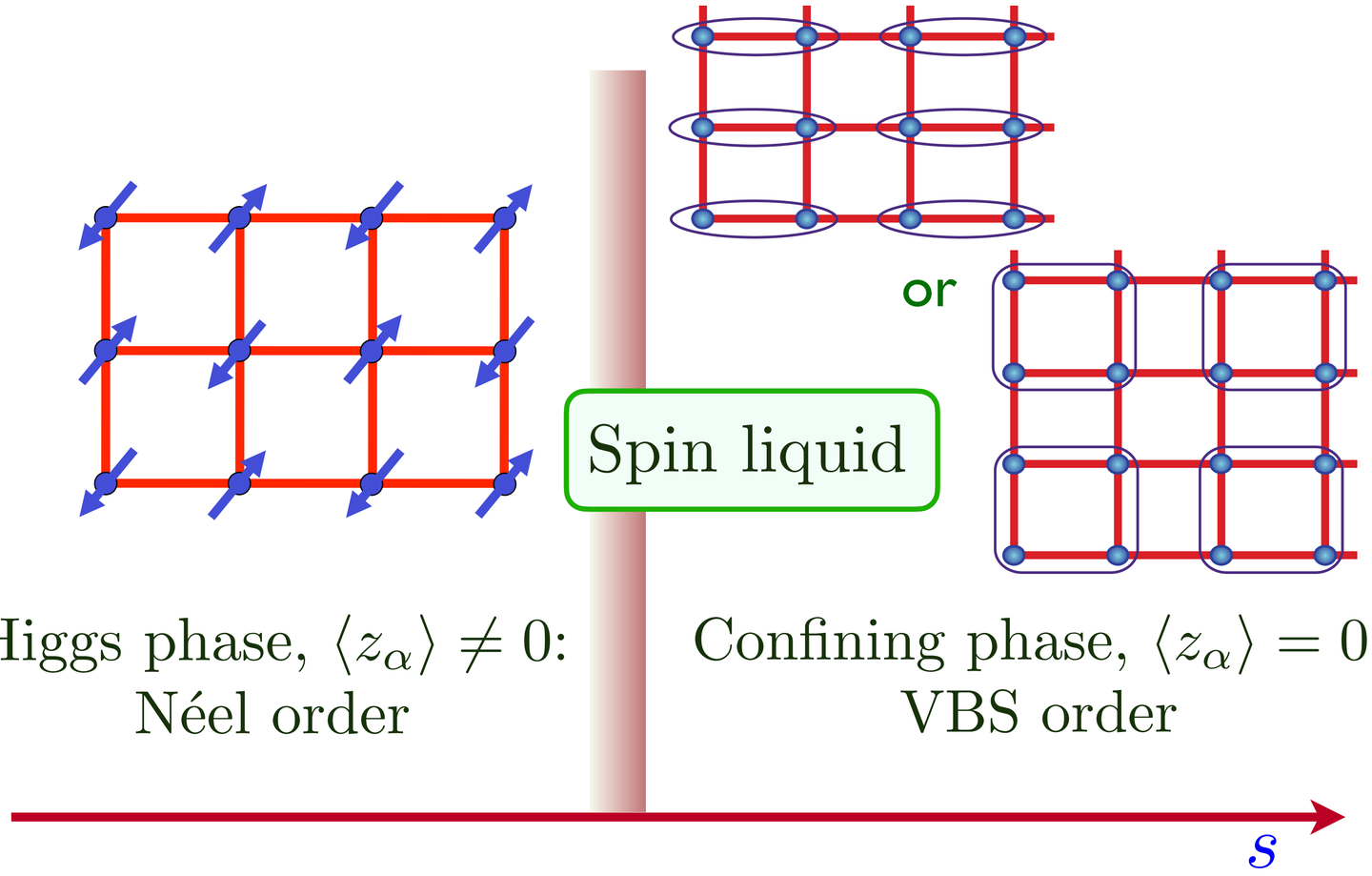

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Mean-field spin liquid
with gapped bosonic spinons.

Low energy $\mathbb{CP}^1$ U(1) gauge theory

$$z_\alpha \sim b_{A\alpha} + \varepsilon_{\alpha\beta} b_{B\beta}$$

$$\mathcal{L} = |(\partial_\mu - i a_\mu) z_\alpha|^2 + s|z_\alpha|^2 + u|z_\alpha|^4 + \mathcal{L}_{\text{monopole}}$$

N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989)

$\mathbb{CP}^1$ U(1) gauge theory

S=1/2 square lattice anti-ferromagnet

SU(2) gauge theory of $N_f = 2$ fundamental, massless, Dirac fermions.

Obtained from a saddle-point of fermionic spinons moving in π-flux.

I. Affleck and J.B. Marston, *Phys. Rev. B* **37**, 3774 (1988)

SO(5) non-linear σ-model of Néel/VBS orders with $k = 1$ WZW term

A. Tanaka and X. Hu, *Phys. Rev. Lett.* **95**, 036402 (2005); T. Senthil and M.P.A. Fisher *Phys. Rev. B* **74**, 064405 (2006); Ying Ran and X.-G. Wen, cond-mat/0609620; C. Wang, A. Nahum, M. A. Metlitski, C. Xu, and T. Senthil, *Phys. Rev. X* **7**, 031051 (2017)

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Many numerical works show that deconfined critical theory applies over a substantial length scale, but ultimately confines at the longest distances.

Anders W. Sandvik *Phys. Rev. Lett.* **98**, 227202 (2007)

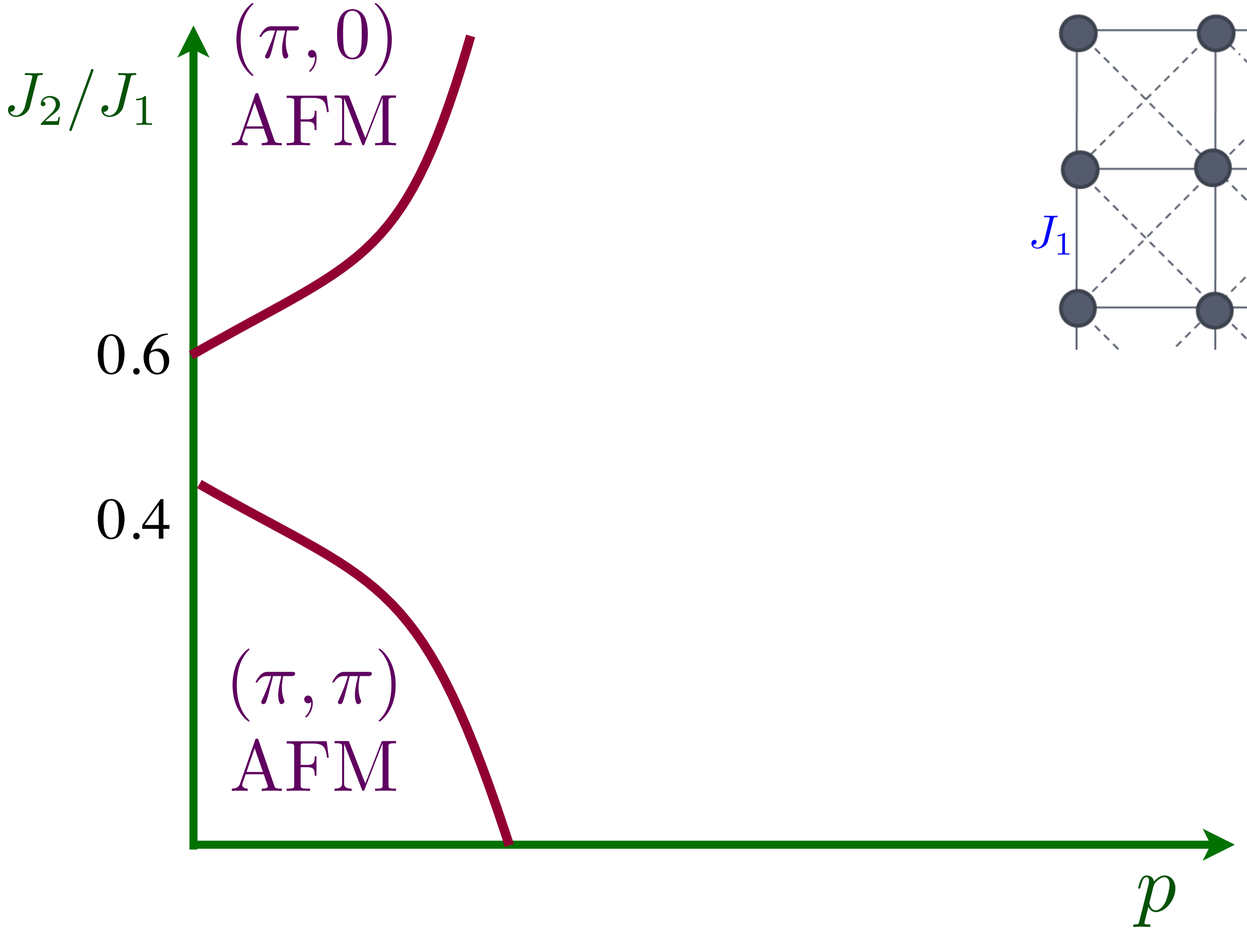
Adam Nahum, P. Serna, J. T. Chalker, M. Ortuño, and A. M. Somoza, *Phys. Rev. Lett.* **115**, 267203 (2015)

Z. Zhou, L. Hu, W. Zhu, and Yin-Chen He, arXiv:2306.16435

High Temperature Superconductivity in a Lightly Doped Quantum Spin Liquid

Hong-Chen Jiang[1,*] and Steven A. Kivelson[2]

Phys. Rev. Lett. **127**, 097002 (2021)



Superconducting valence bond fluid in lightly doped 8-leg *t-J* cylinders
Hong-Chen Jiang, Steven A. Kivelson, and Dung-Hai Lee, arXiv:2302.11633

Upon increasing the cylinder width from 4 to 8, we observed a significant strengthening of the quasi-long-range superconducting correlations, and a dramatic suppression of any "competing" charge-density-wave order. Extrapolating from the observed behavior of the width 8 cylinders, we speculate that the system has a nodeless d-wave superconducting ground-state in the 2D limit.

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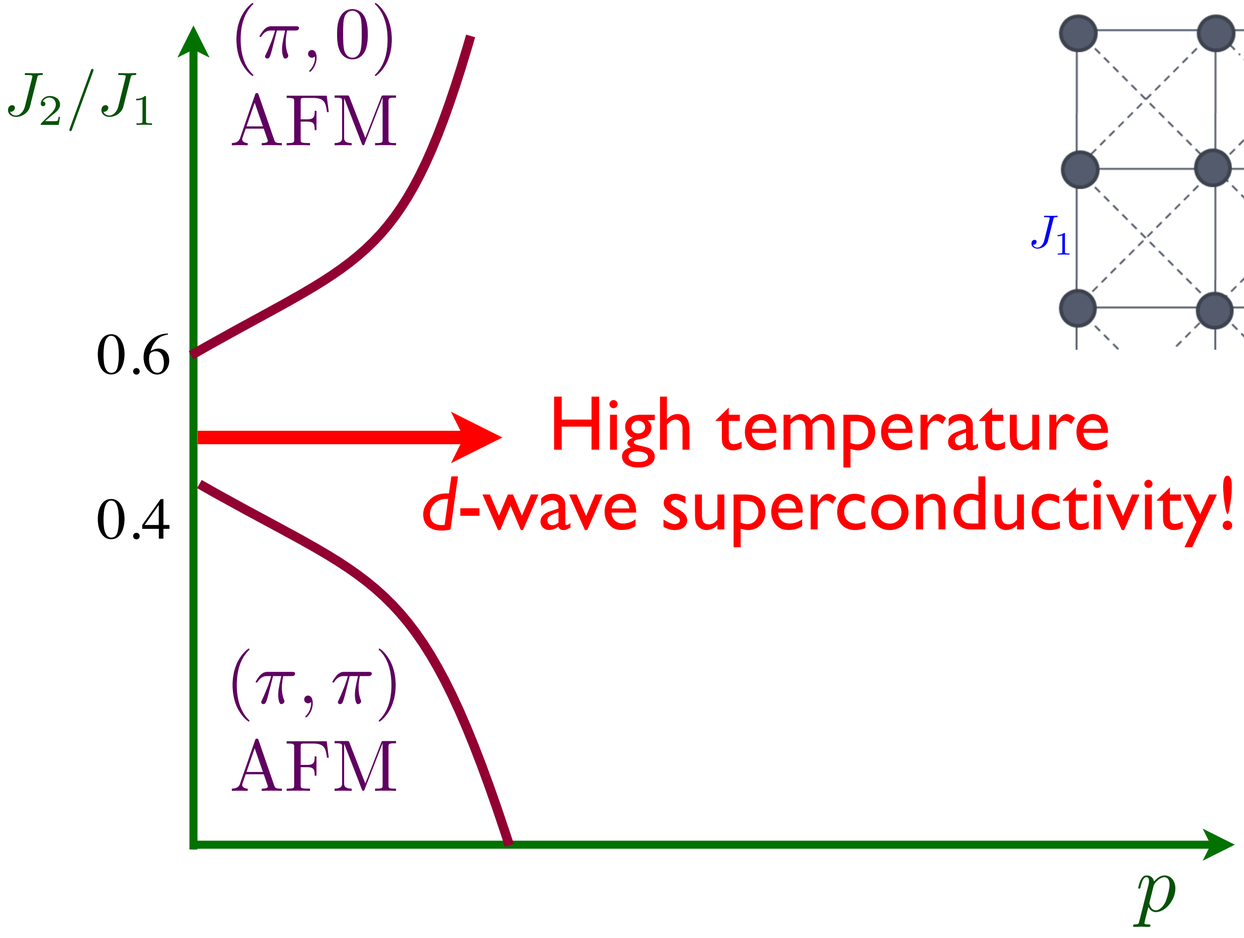

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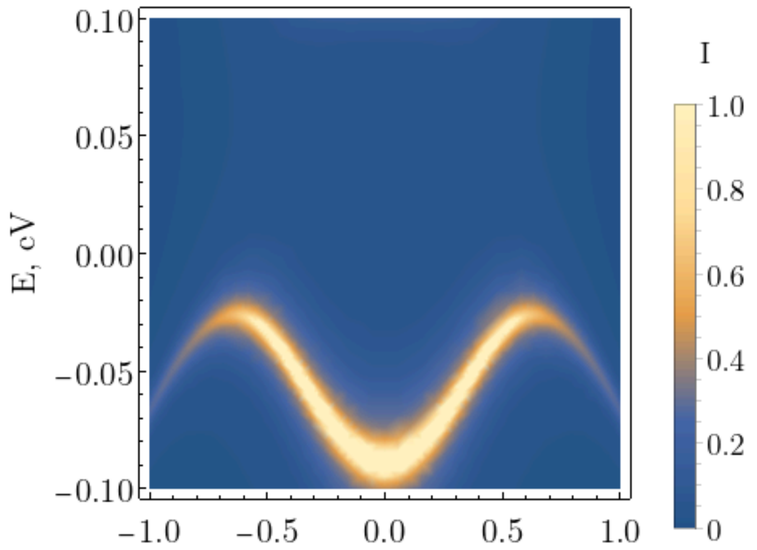
Connections to observations

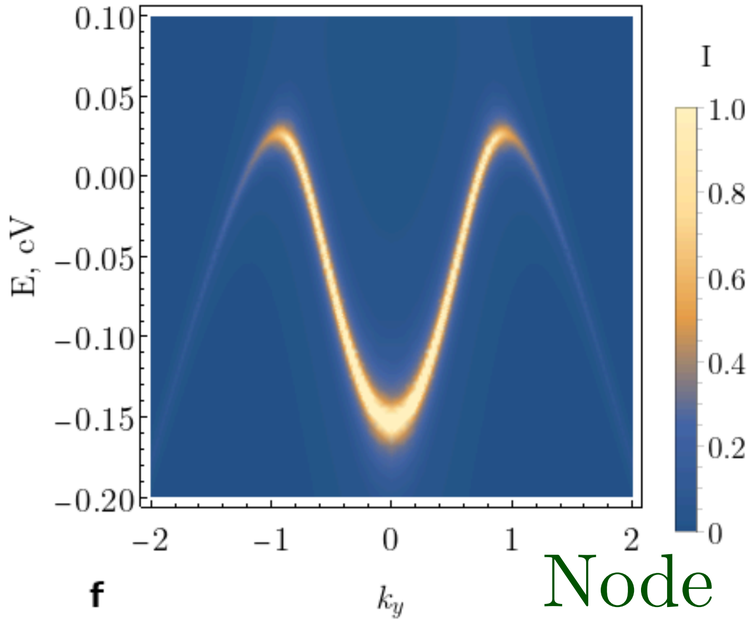
Mascot, Nikolaenko, Tikhanovskaya, Zhang, Morr, and Sachdev, *Phys. Rev. B* **105**, 075146 (2022)

FL* in a ***one-band*** model

Broadening by second ancilla layer is needed to describe MDC and EDC

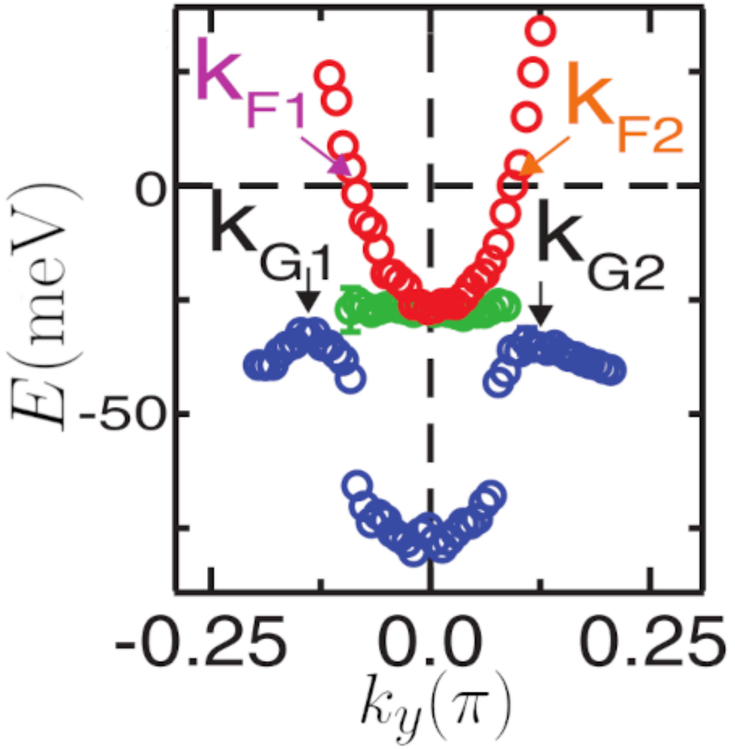


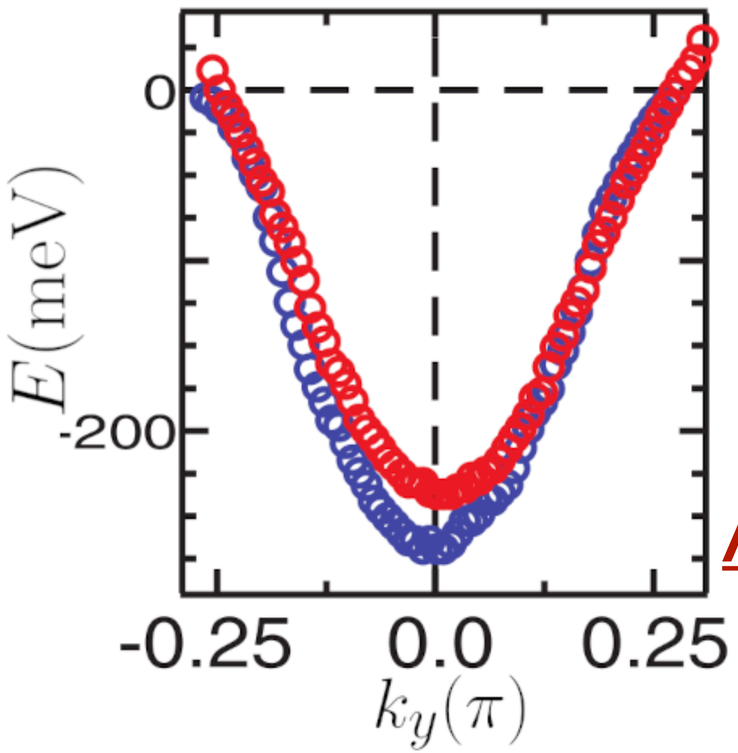
Anti-node



f

Node

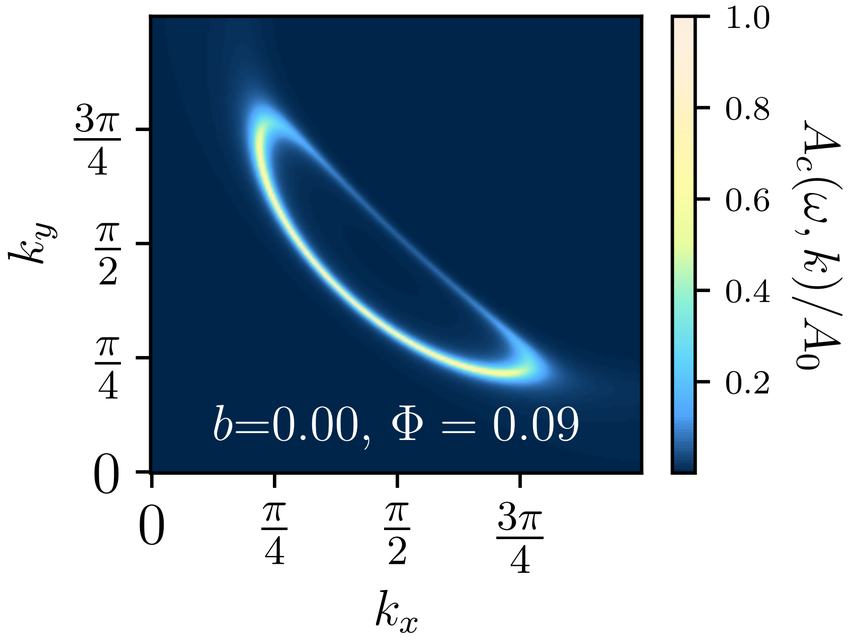




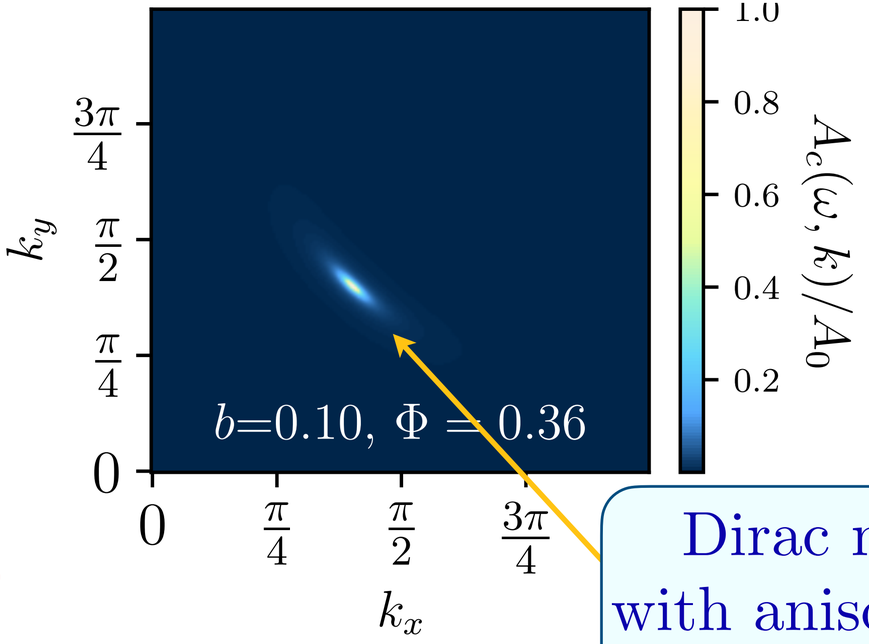
He, Hashimoto, Karapetyan, Koralek, Hinton, Testaud, Nathan, Yoshida, Yao, Tanaka, Meevasana, Moore, Lu, Mo, Ishikado, Eisaki, Hussain, Devereaux, Kivelson, Orenstein, Kapitulnik, and Shen, *Science* **331**, 1579 (2011)

ARPES on Bi2201

Electron spectral density in hole-doped cuprates



FL*



dSC

Dirac node with anisotropic velocities

d-wave superconductor obtained by condensing charge-e, SU(2) fundamental boson.

Spinons of the π-flux state annihilate the extra nodes in the d-wave superconductor.

Shubhayu Chatterjee and S. S., PRB **94**, 205117 (2016)

Maine Christos and S.Sachdev, arXiv:2308.03835

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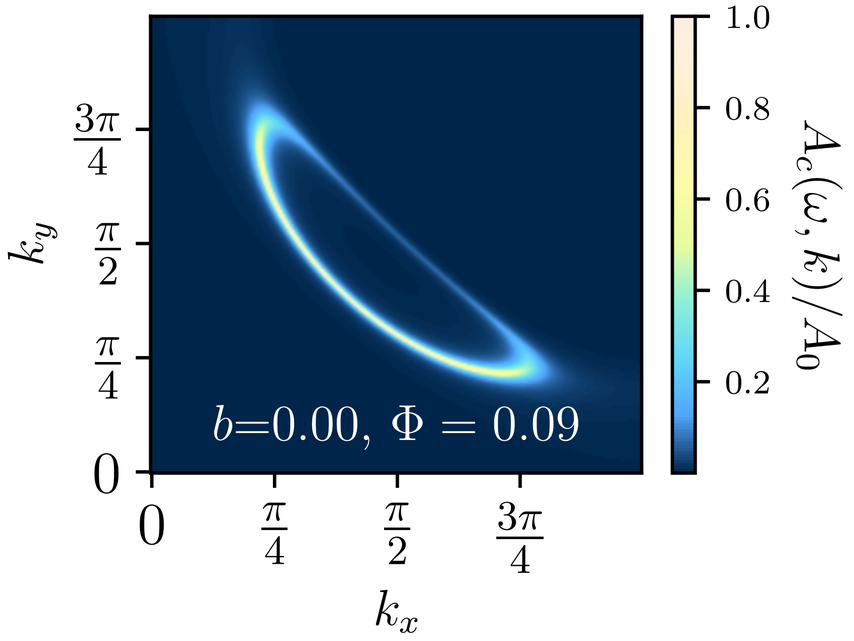

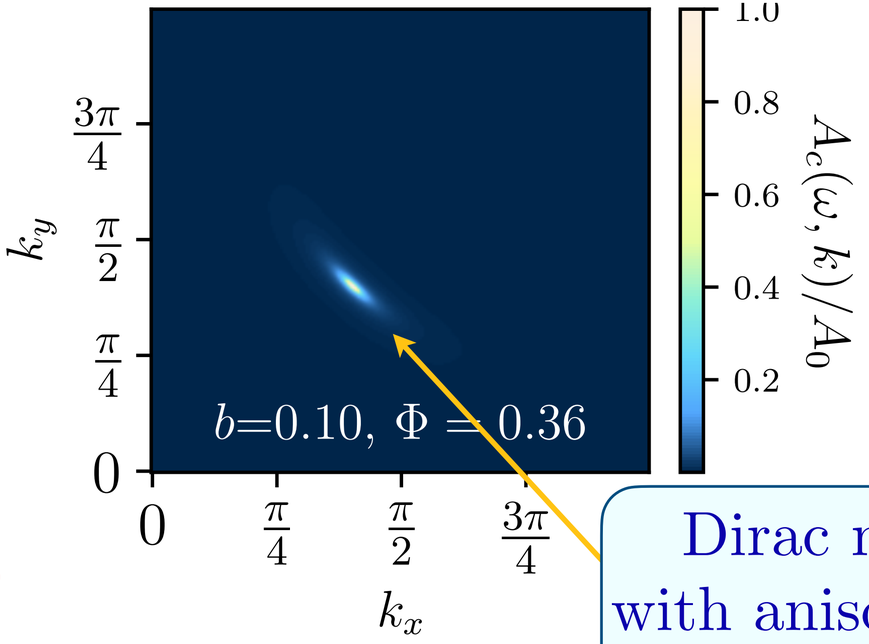

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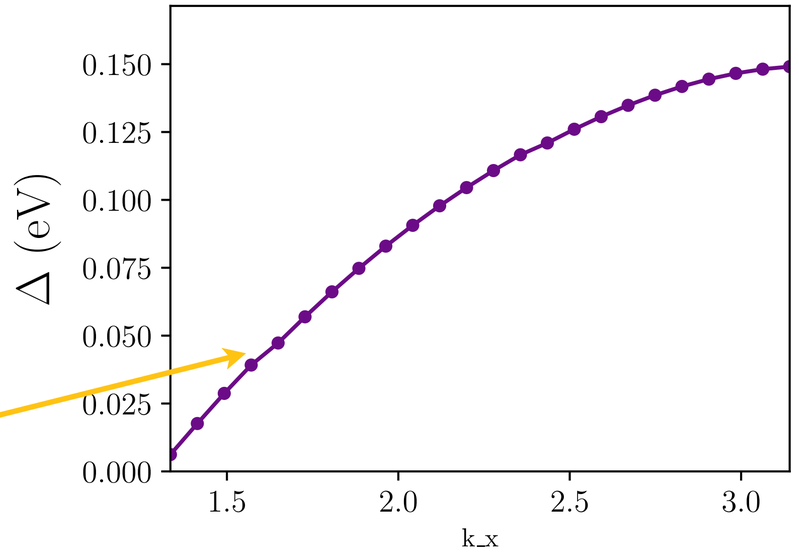
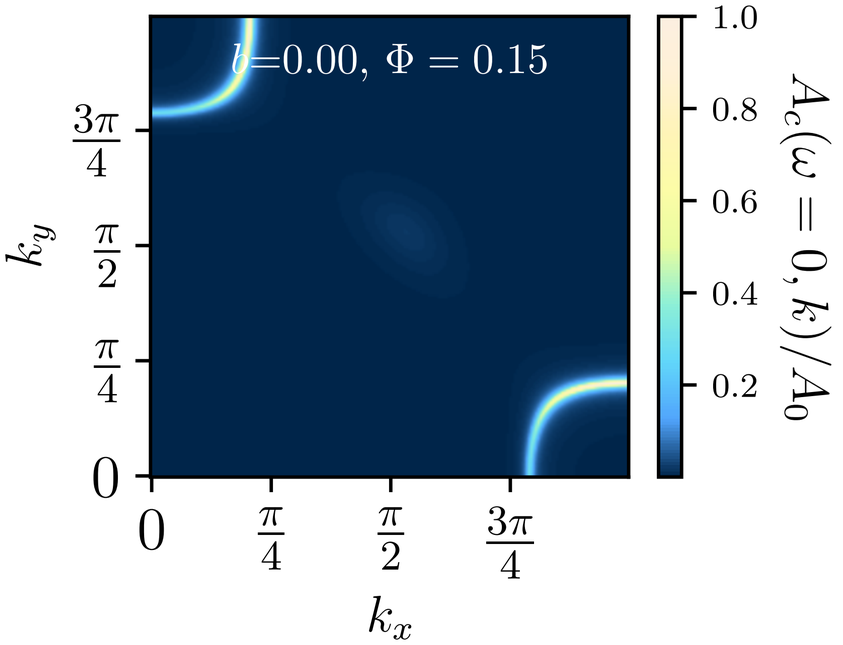
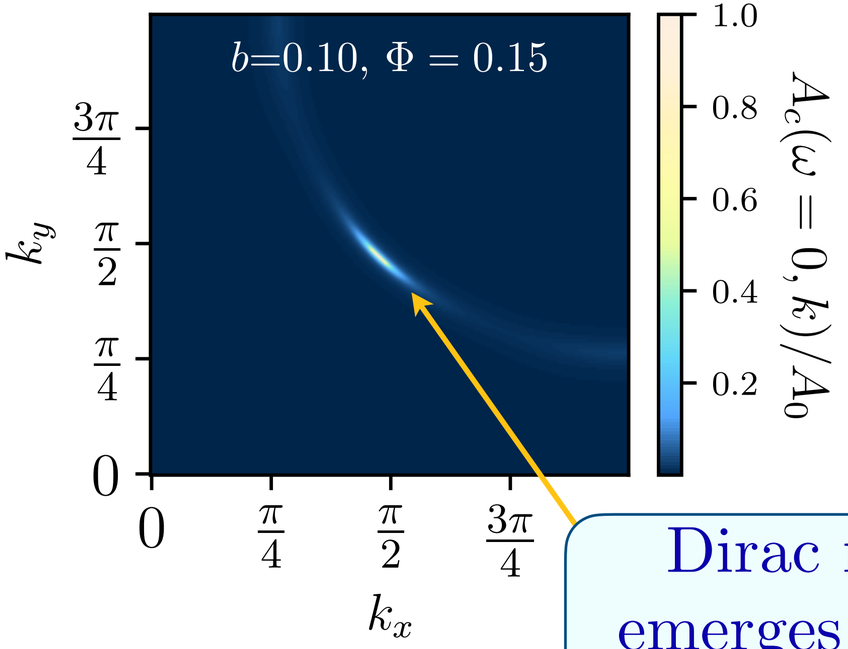


Electron spectral density in electron-doped cuprates





FL*

d-wave superconductor obtained by condensing charge-e, SU(2) fundamental boson.

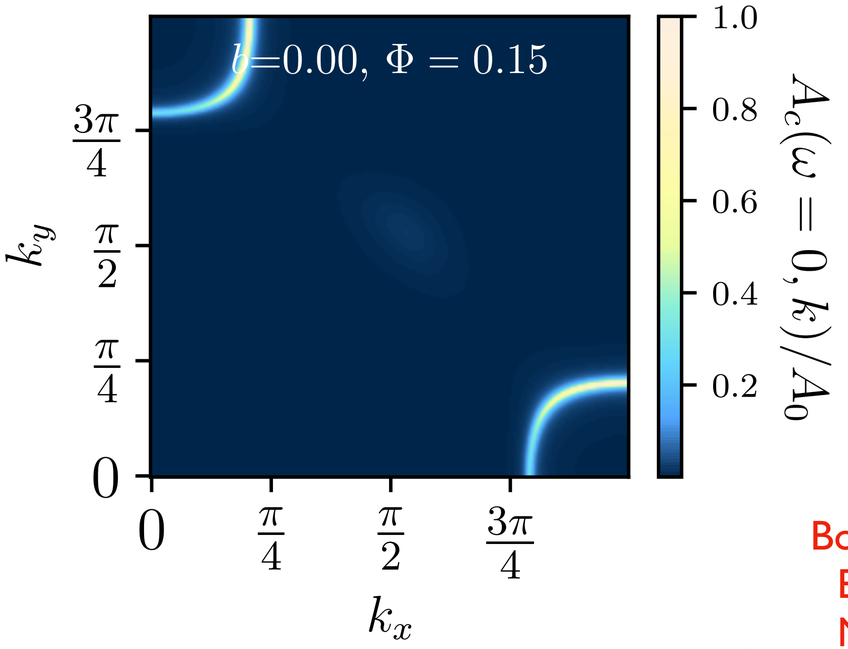
Nodes of the d-wave superconductor are remnants of the spinons of the π-flux state.

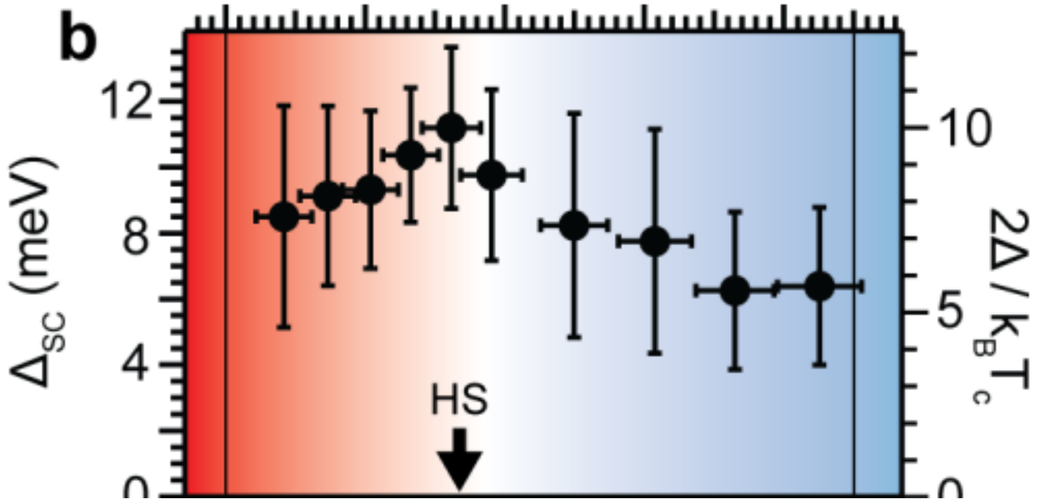
dSC

Dirac node emerges inside normal state gap

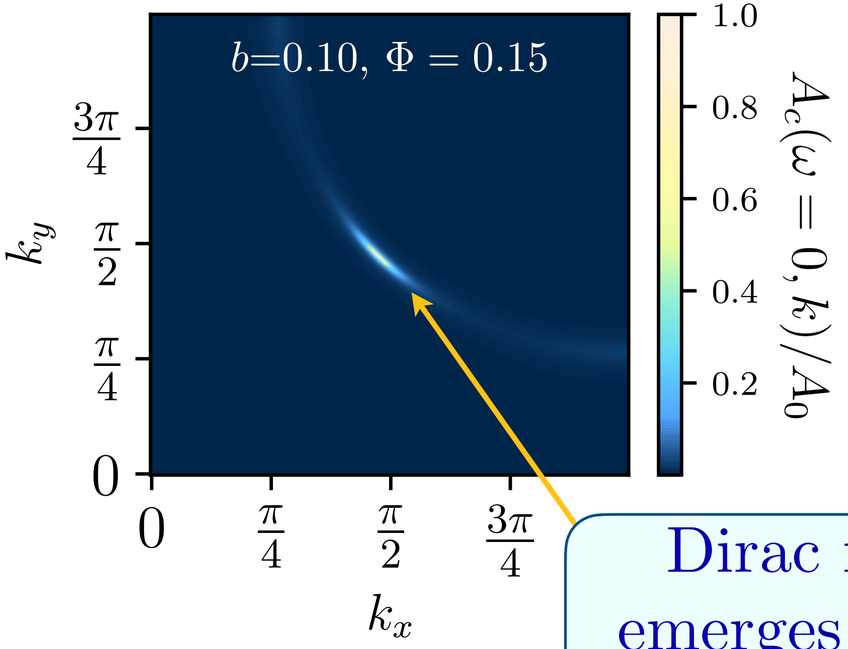
Maine Christos and S.Sachdev, arXiv:2308.03835

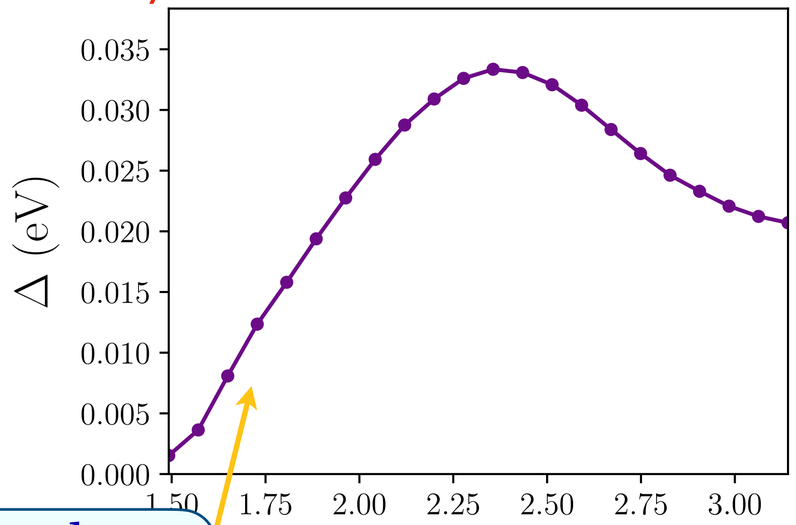
Electron spectral density in electron-doped cuprates





Bogoliubov Quasiparticle on the Gossamer Fermi Surface in Electron-Doped Cuprates, Ke-Jun Xu……Z.-X. Shen, arXiv:2308.05313; Nature Physics

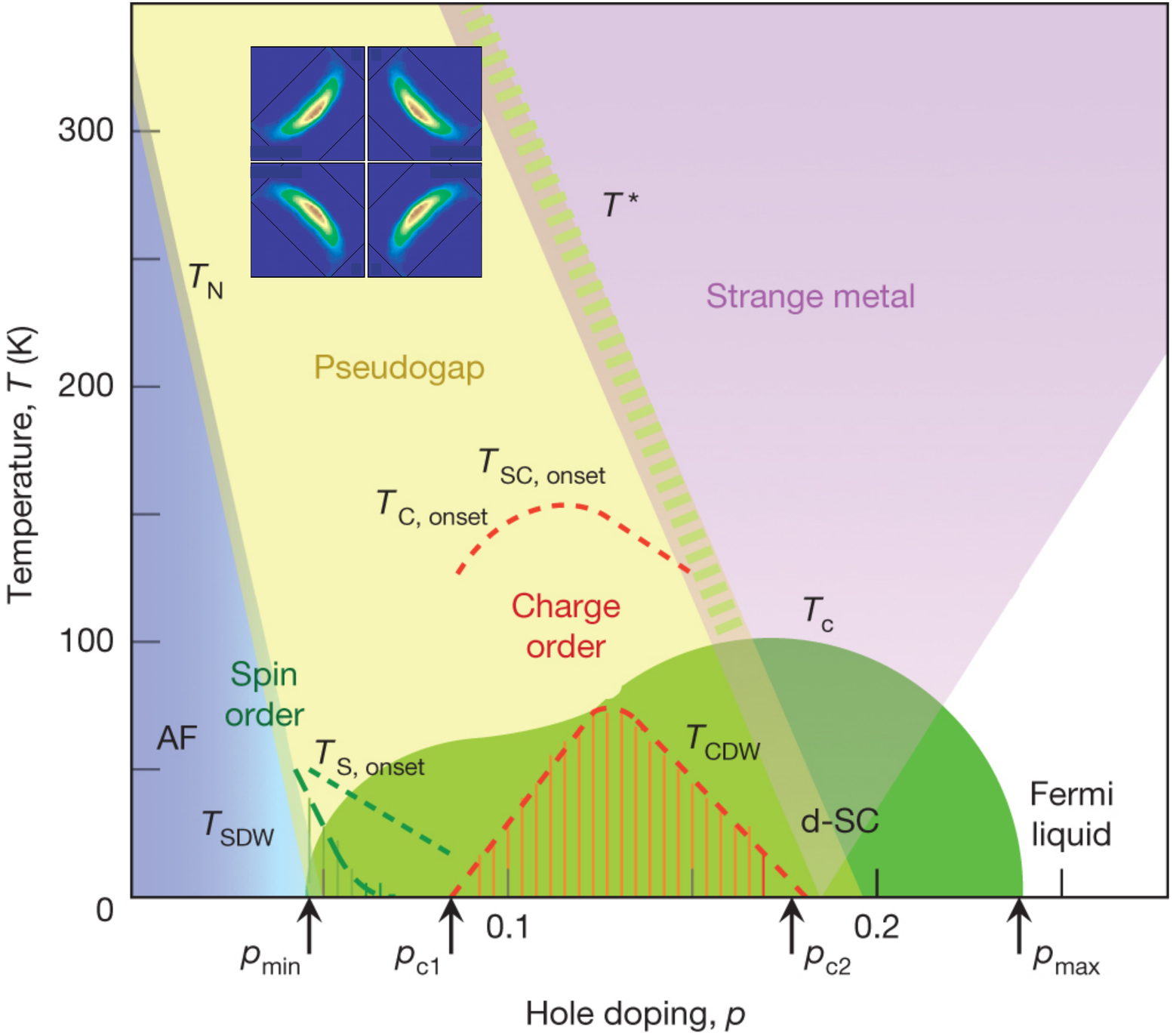




Dirac node emerges inside normal state gap

Maine Christos and S.Sachdev, arXiv:2308.03835

Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)

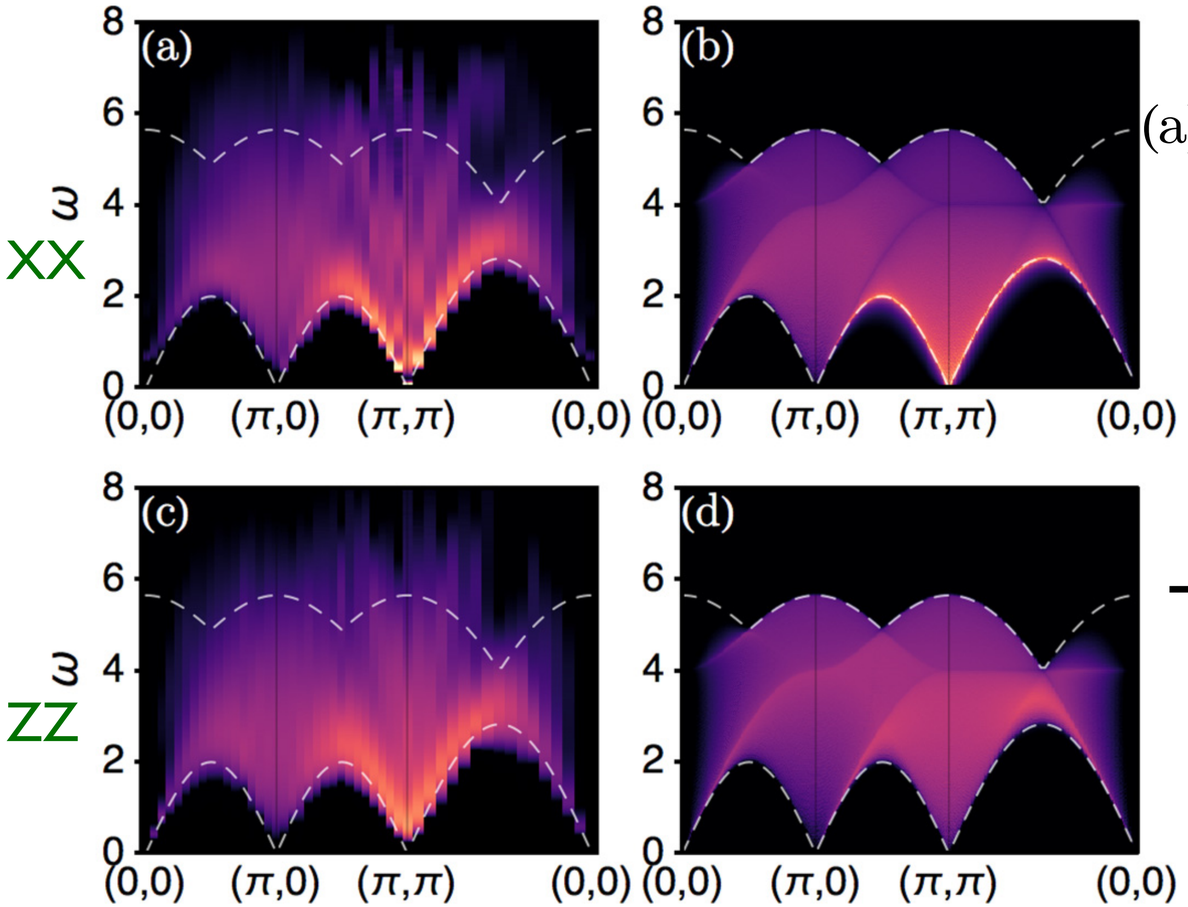


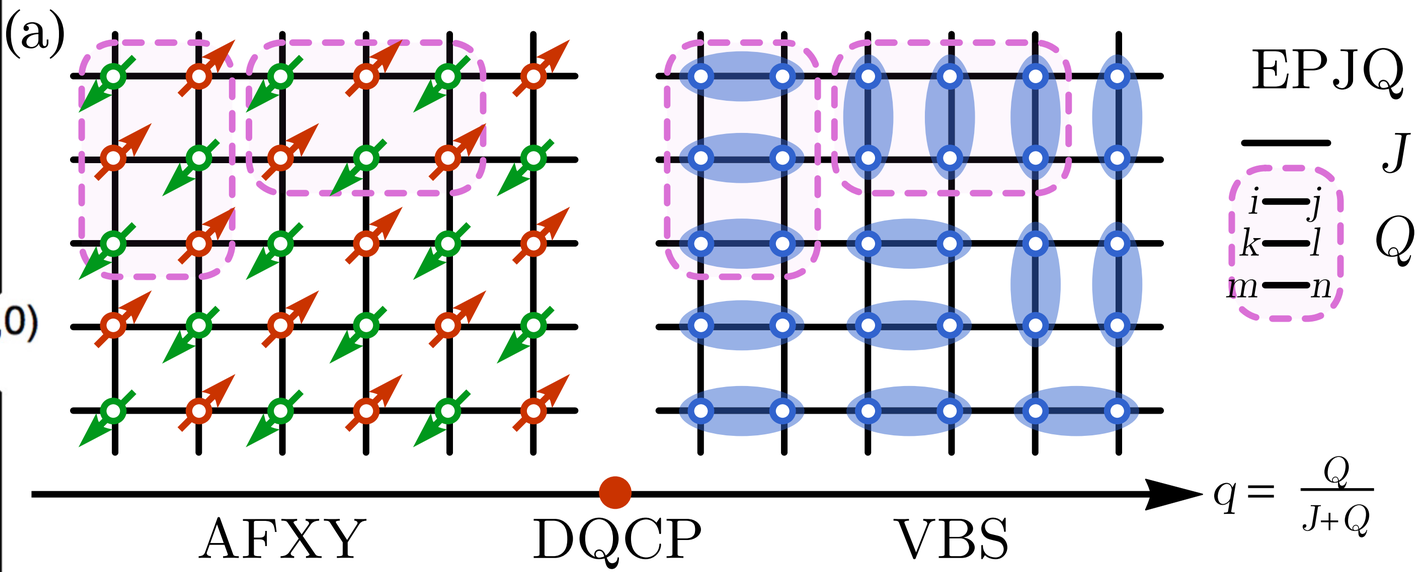
Emergent symmetry of the charge-e, SU(2) fundamental boson effective theory of the π-flux state provides a rationale for the near equality of the onset temperatures of d-wave superconductivity and charge order.

Observable by neutron scattering in pseudogap ?

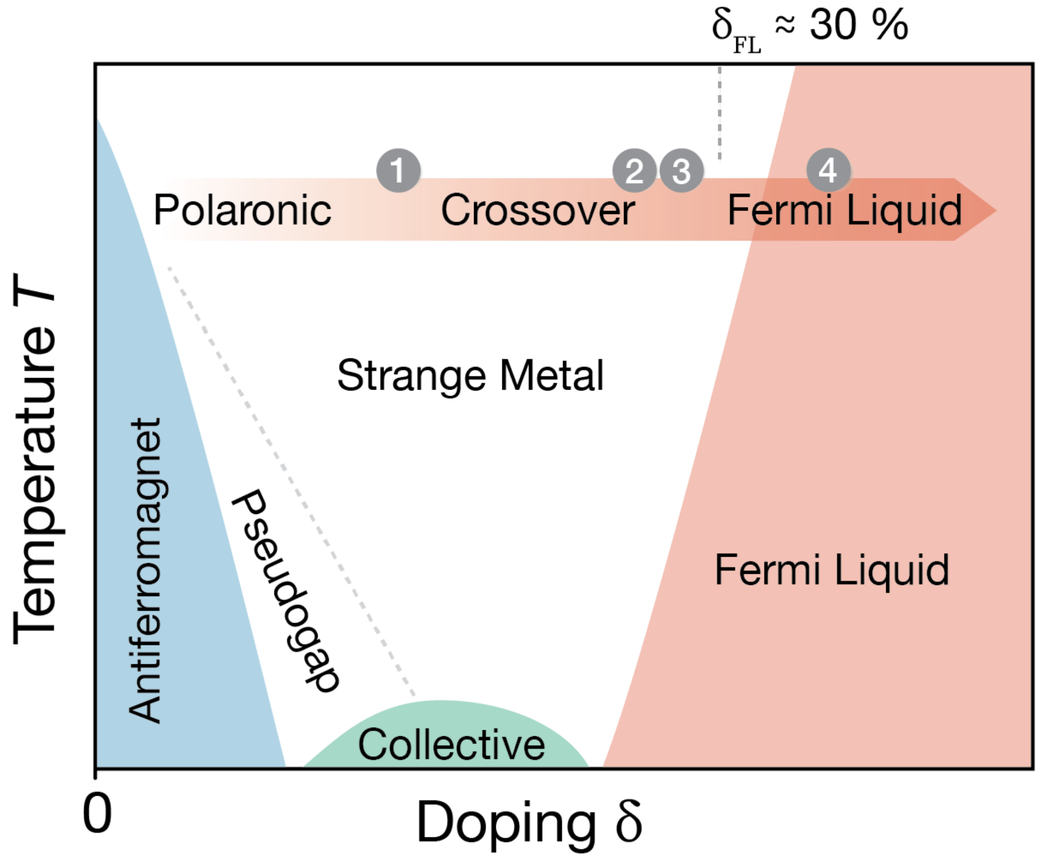
QMC

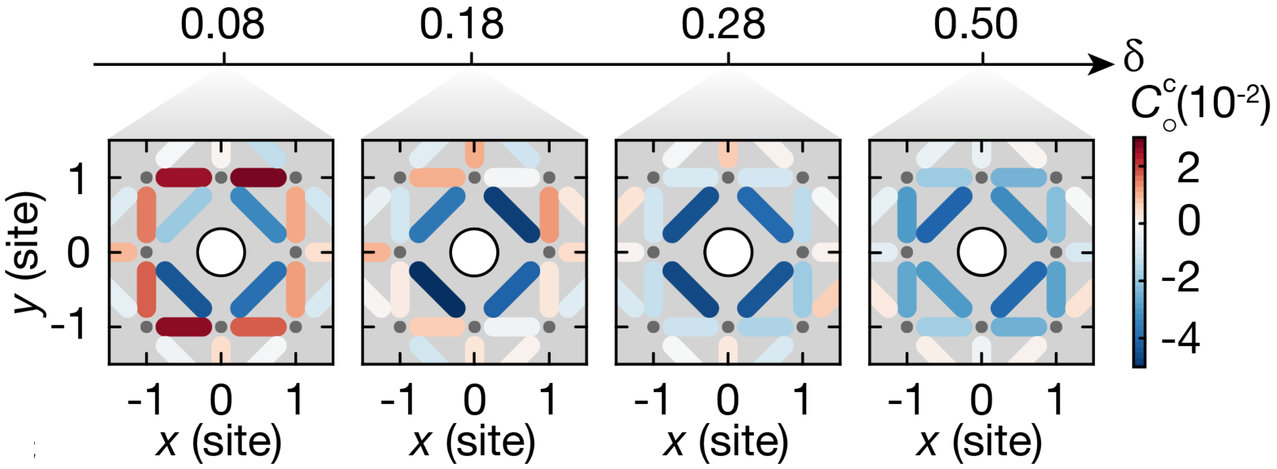
Free fermion
spinons in π-flux





Nvsen Ma, Guang-Yu Sun, Yi-Zhuang You, Cenke Xu, Ashvin Vishwanath, Anders W. Sandvik, and Zi Yang Meng,
Phys. Rev. B **98**, 174421 (2018)





Ultracold fermionic atoms in optical lattices

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

Joannis Koepsell, Dominik Bourgund, Pimonpan Sompet, Sarah Hirthe, Annabelle Bohrdt, Yao Wang, Fabian Grusdt, Eugene Demler, Guillaume Salomon, Christian Gross, Immanuel Bloch

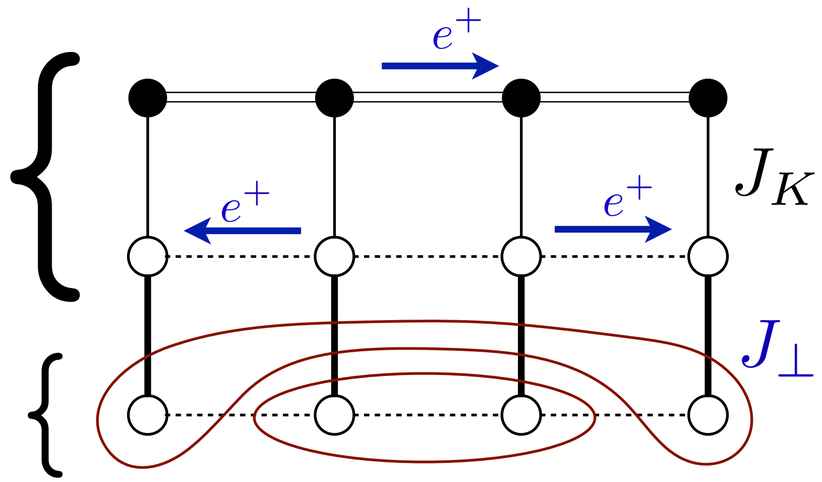
Science **374** (2021) 82

Max-Planck-Institut für Quantenoptik
Garching

Ancilla theory of the Hubbard model

Kondo lattice
heavy Fermi liquid.
Size $1 + p + 1$
$= p \pmod 2$.
Small Fermi surface!

Spin liquid



Pseudogap metal =
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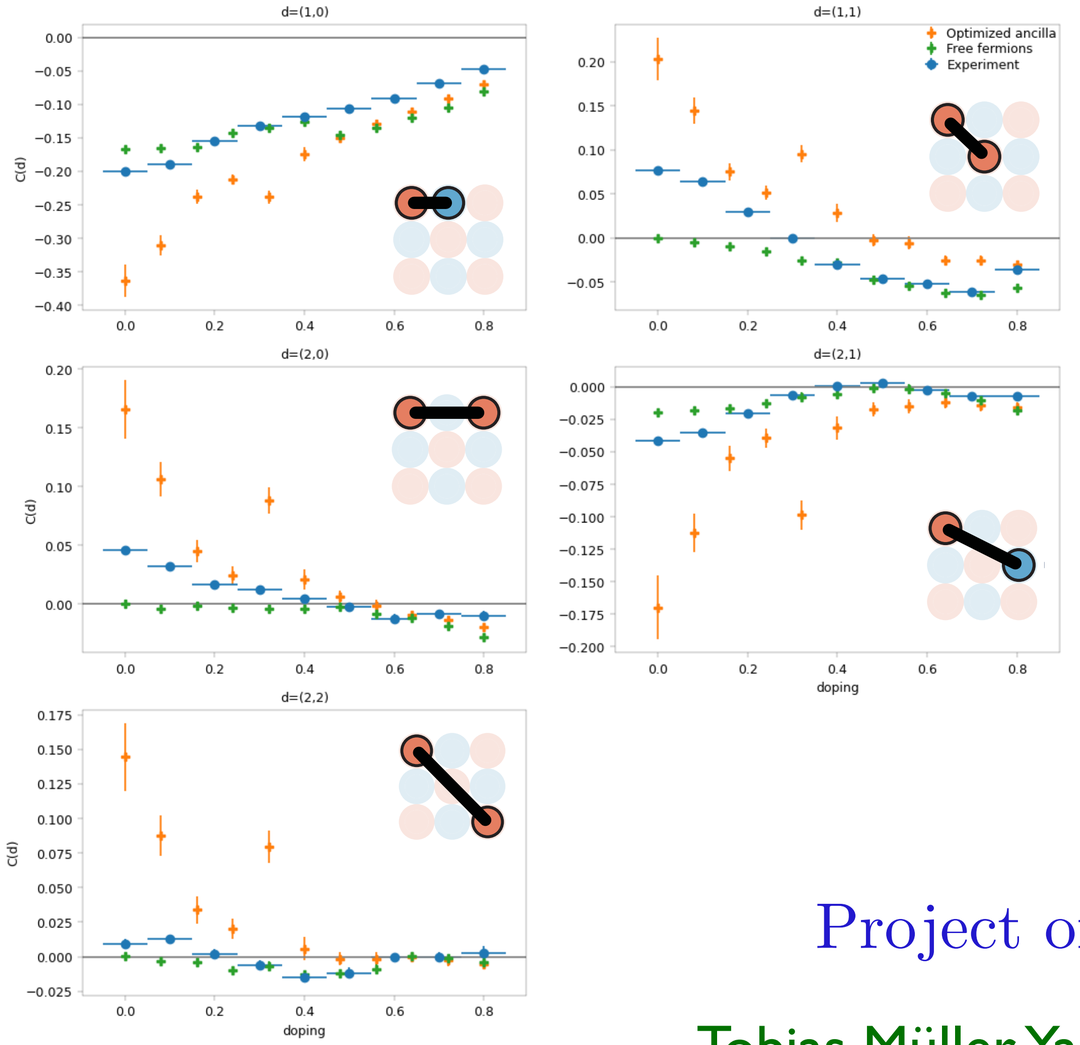
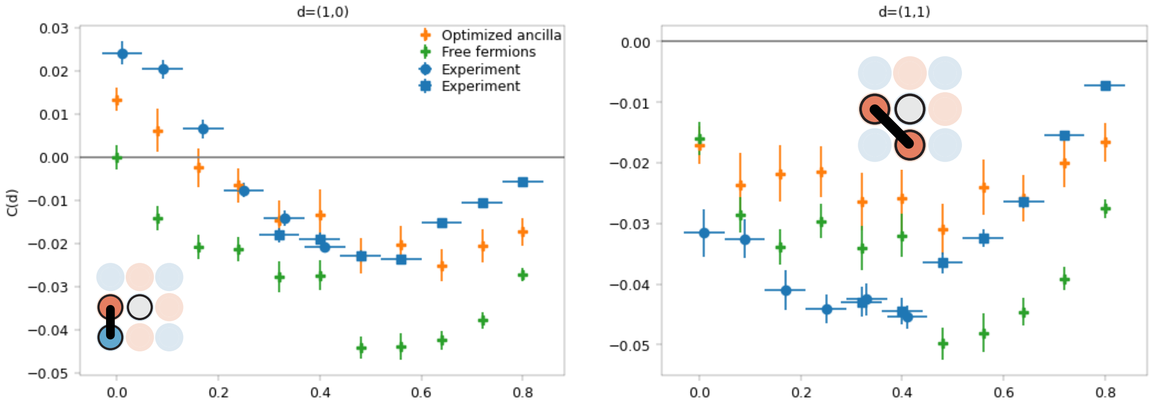
Replacement for "vanilla" Gutzwiller-projected Fermi liquid in the underdoped regime

Results for Connected Correlators: Comparison with experiment

Bare Spin-Spin Correlators



Hole-induced Spin-Spin Correlators



Preliminary data

*Test different spin-liquid ansätze for second ancilla layer

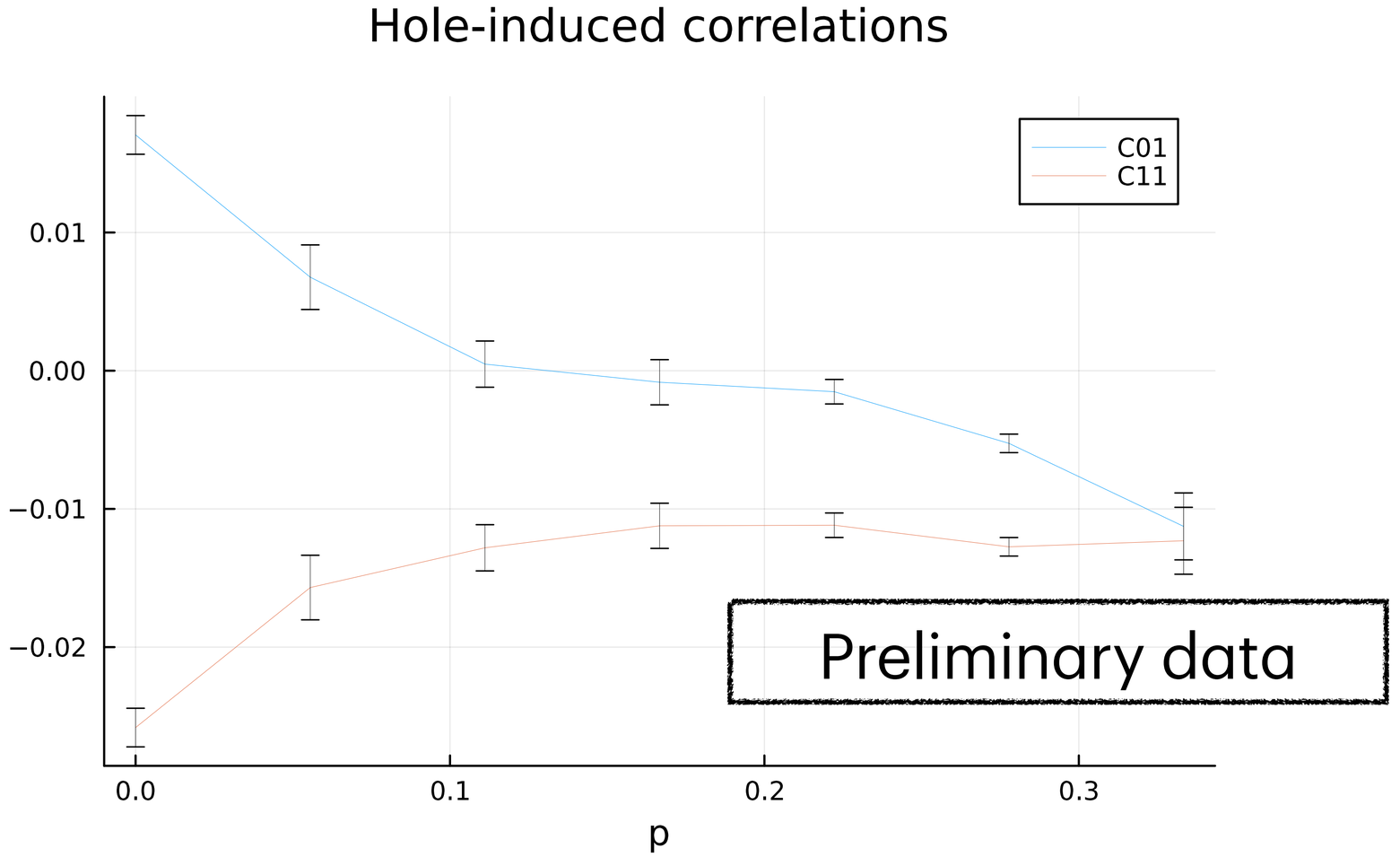
*Improve sampling of wave-functions

*Better statistics to obtain more reliable error-bars

Project only to $S_{1z} + S_{2z} = 0$

Tobias Müller, Yasir Iqbal, Ronny Thomale to appear

Ancilla theory of the Hubbard model



Project to $\boldsymbol{S}_1 + \boldsymbol{S}_2 = 0$

H. Shackleton, S.S., Shiwei Zhang, to appear

Summary

Ancilla theory of pseudogap metal with hole pockets and underlying π-flux spin liquid yields:

- Theory for Fermi arcs in hole-doped pseudogap metal.
- ADMR in pseudogap.
- Anti-nodal and nodal electronic dispersion.
- d-wave superconductor with 4 nodal points in both electron- and hole-doped cuprates.
- Near-equality of dSC and charge order onset temperatures
- Multipoint correlators measured by cold atom experiments
- Theory for strange metal in the crossover from FL* to FL