Understanding the cuprate phase diagram from a theory of the pseudogap metal

Quantum Materials With and Without Quasiparticles
KITP, Santa Barbara
October 5, 2023
Subir Sachdev

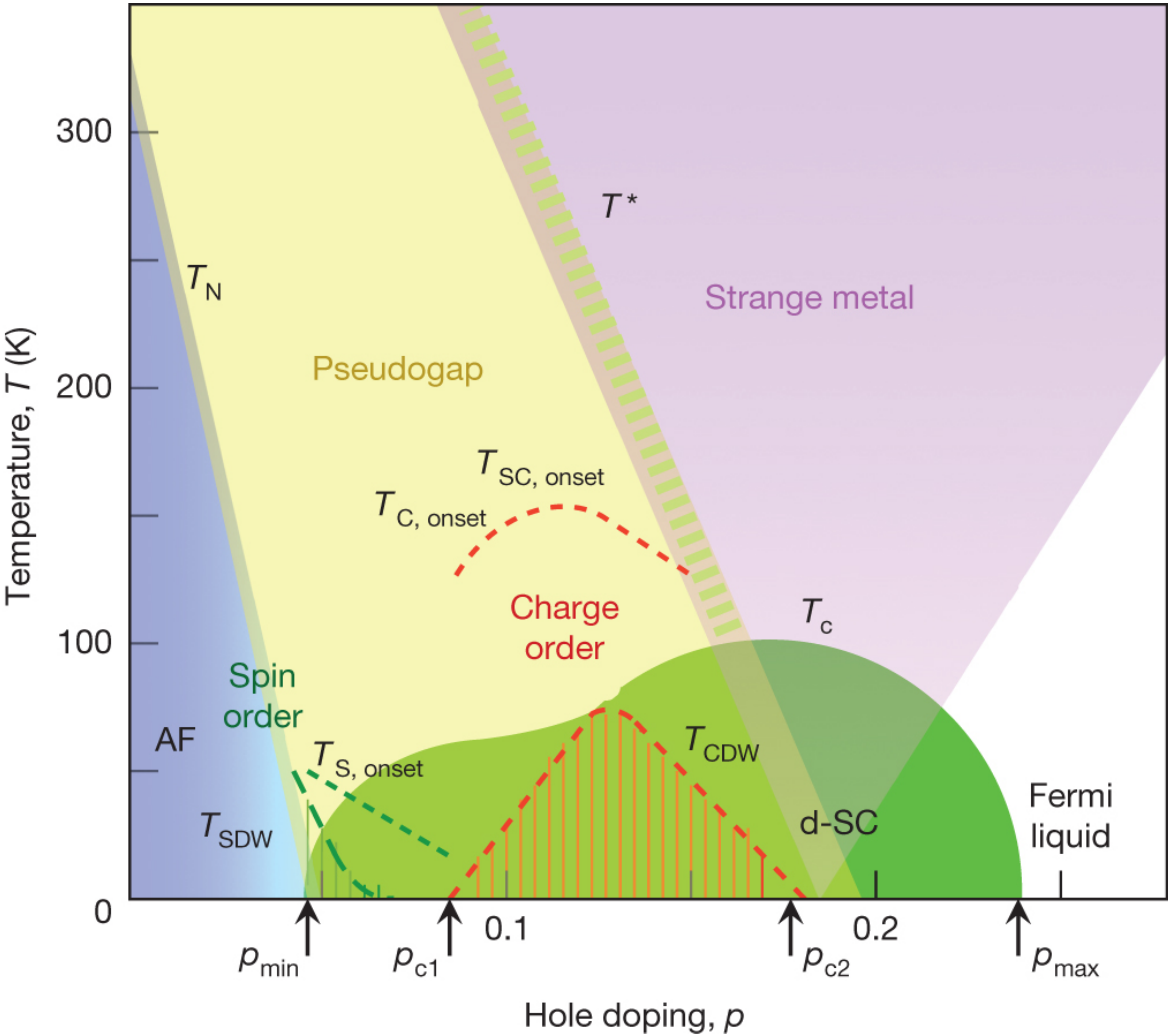
Maine Christos, Zhu-Xi Luo, Henry Shackleton, Ya-Hui Zhang, Mathias Scheurer, and S. Sachdev, *Proc. Nat. Acad. Sci.* **120**, e2302701120 (2023)

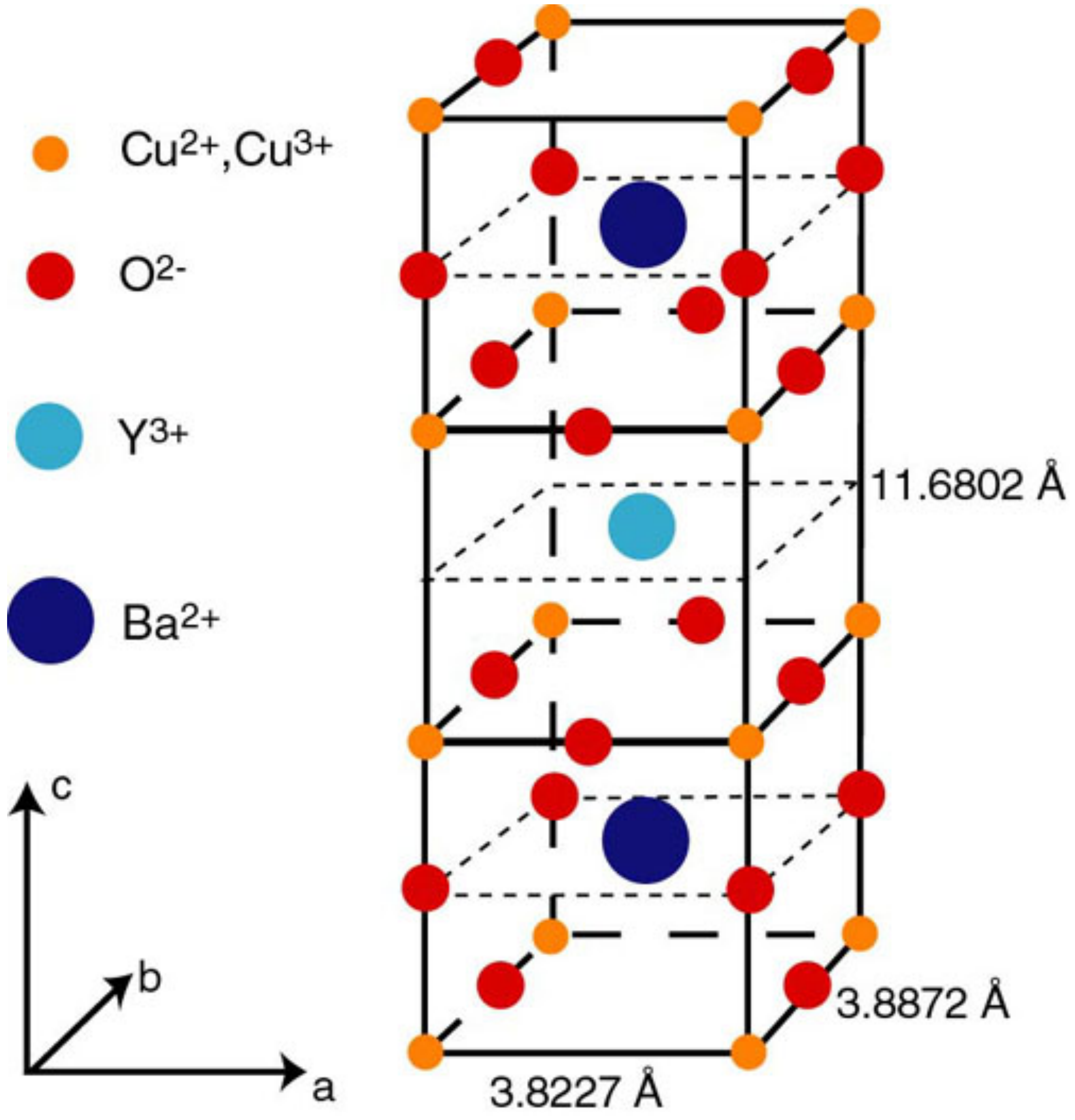
Alexander Nikolaenko, Jonas v. Milczewski, Darshan G. Joshi, and S.Sachdev, *Phys. Rev. B* **108**, 045123 (2023)

Maine Christos and S.Sachdev, arXiv:2308.03835

PHYSICS
HARVARD

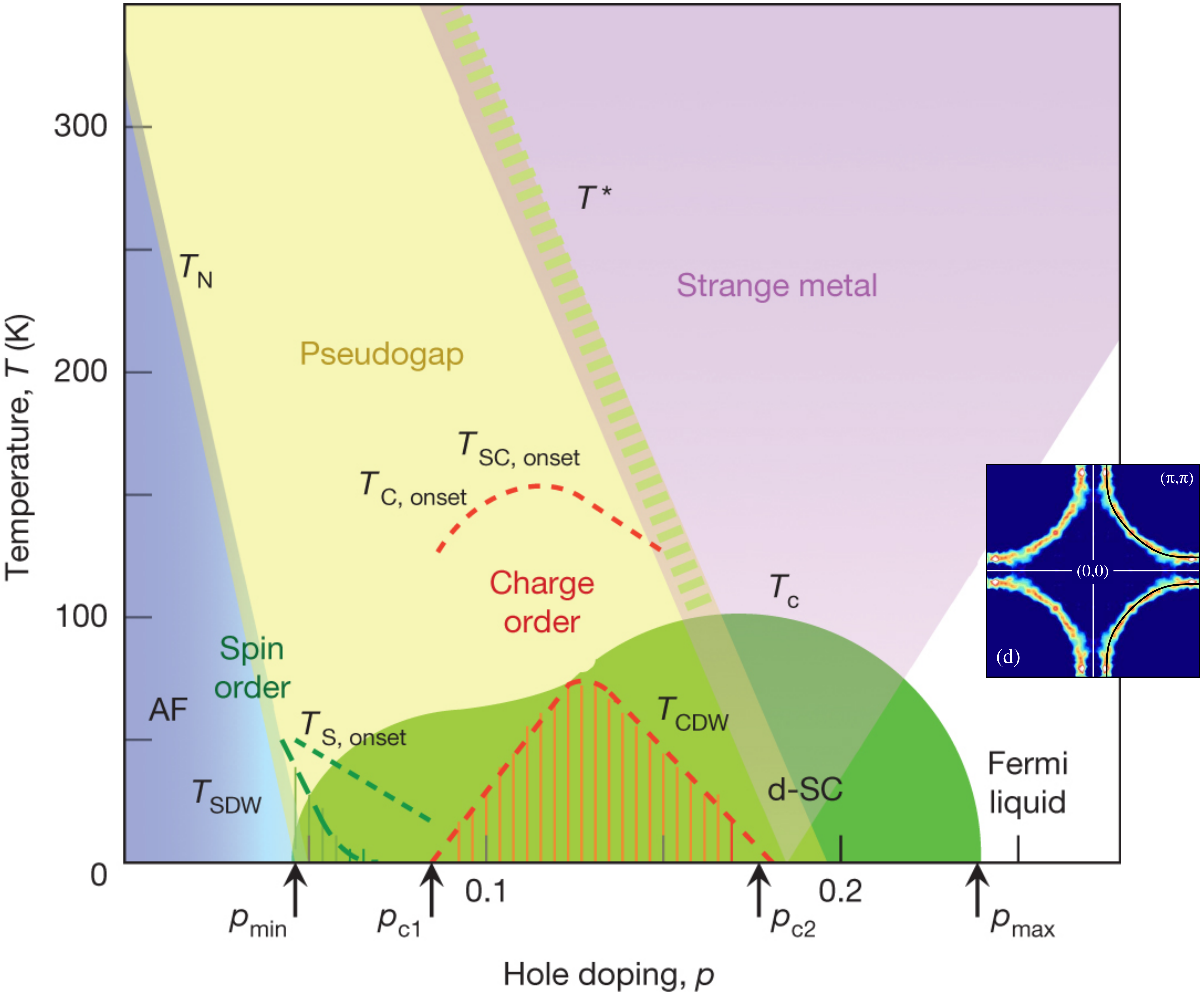
Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)





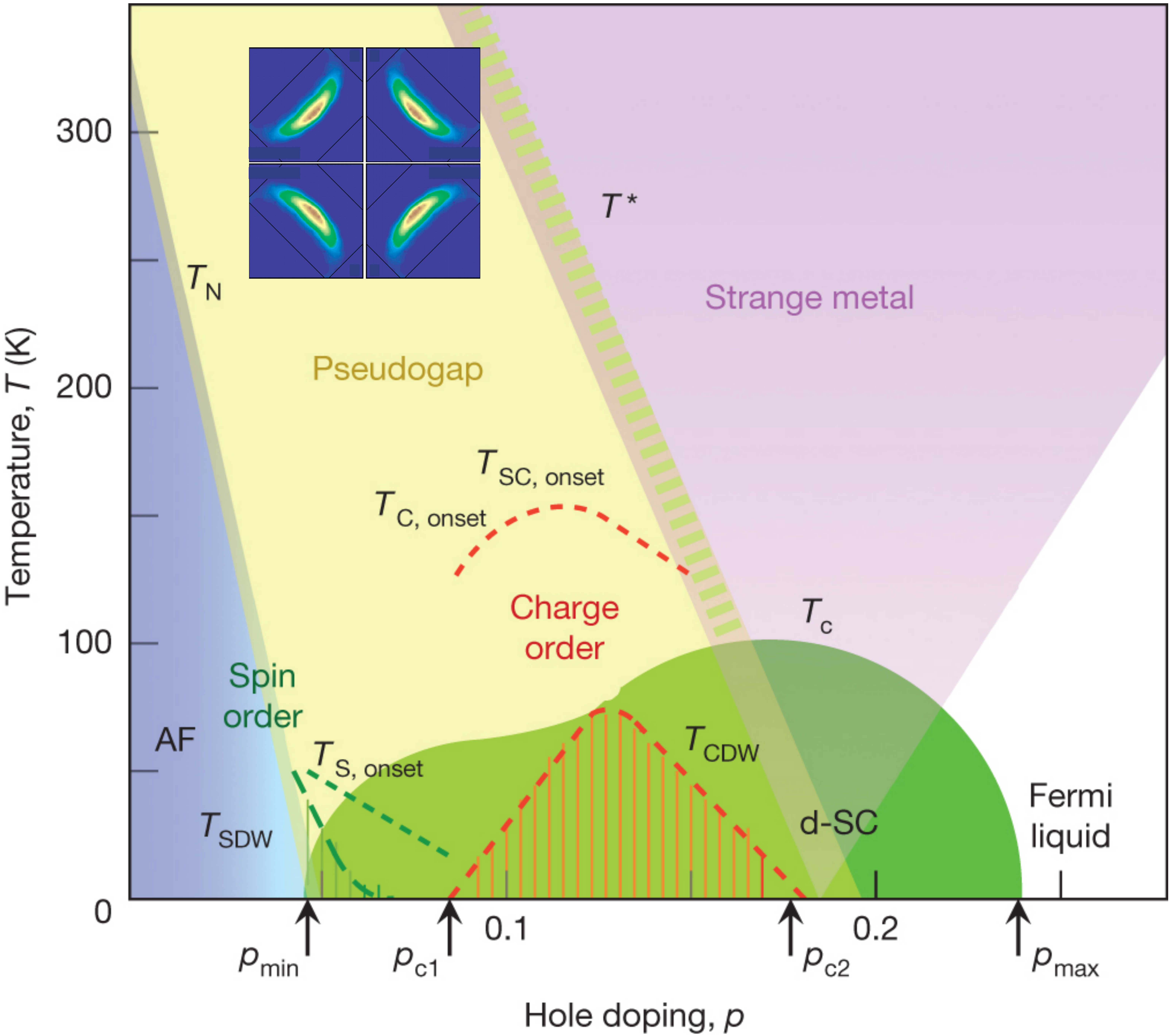
$YBa_2Cu_3O_{6+x}$

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



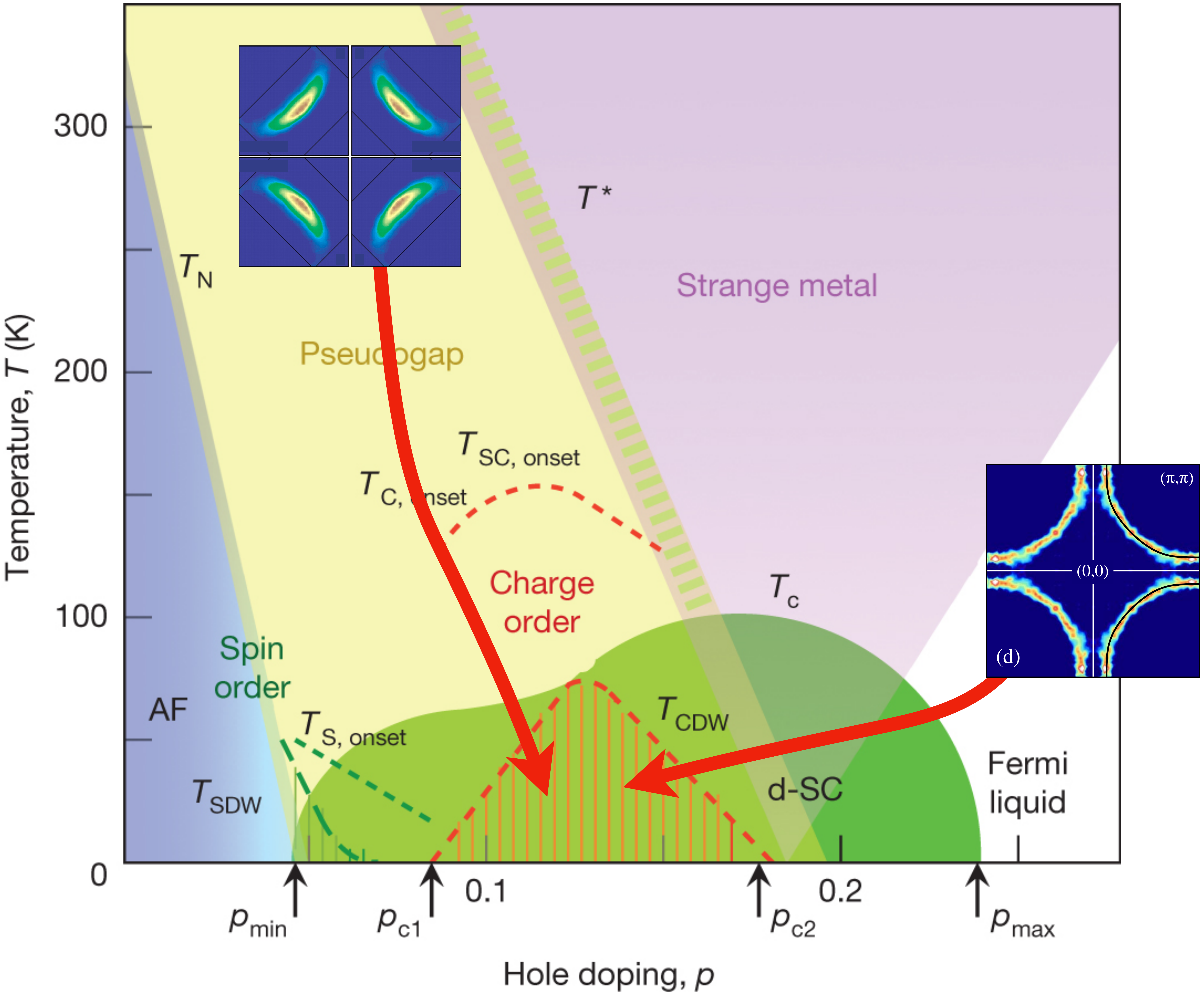
Fermi liquid
in the
overdoped metal

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



Theory for "pseudogap metal" with "Fermi arcs"?

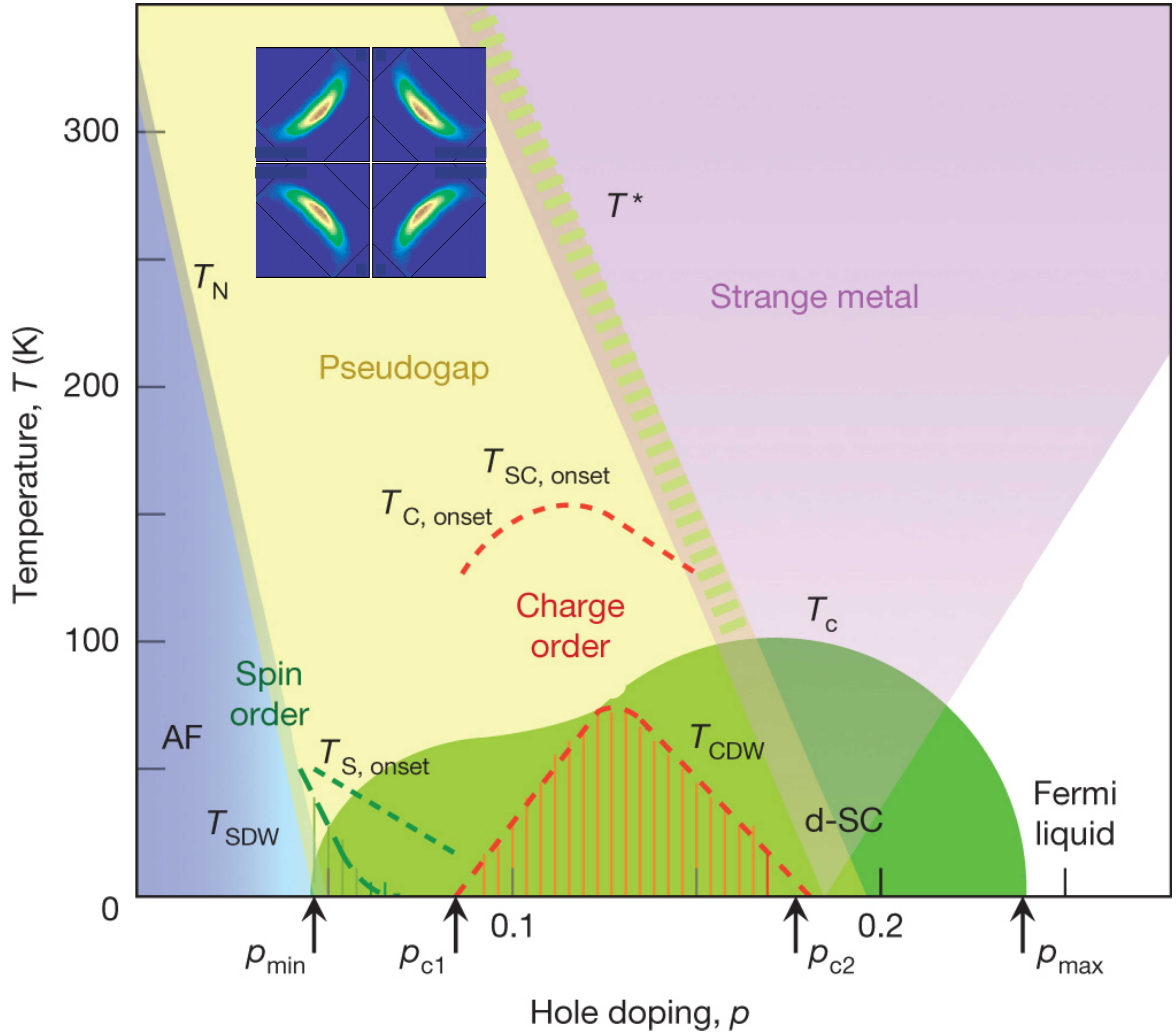
Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)

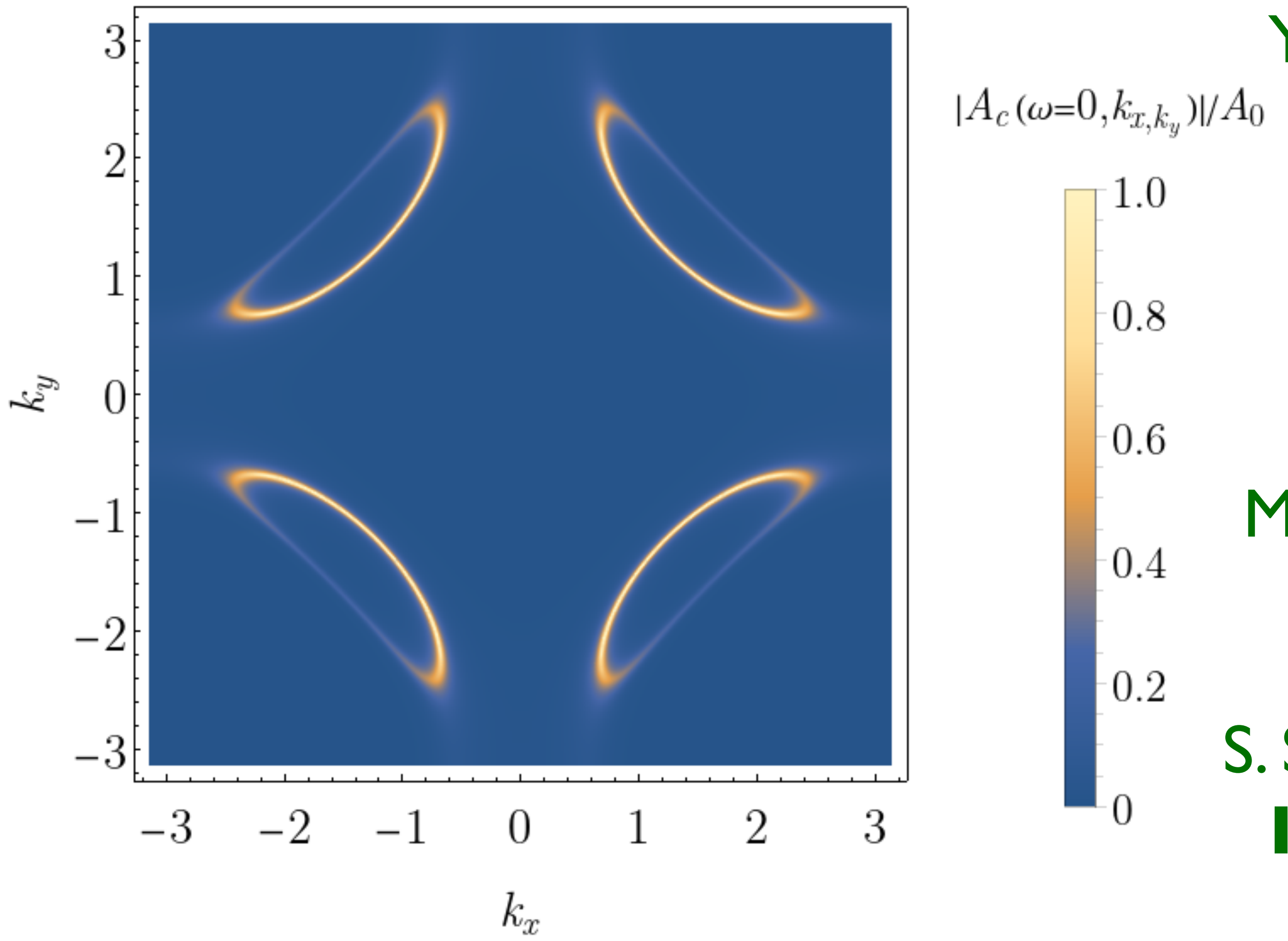


Build a theory for the phase diagram from a theory of the pseudogap metal as a 'metastable' $T = 0$ quantum phase.

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

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

Kai-Yu Yang, T. M. Rice, Fu-Chun Zhang, *Phys. Rev. B* **73**, 174501 (2006).
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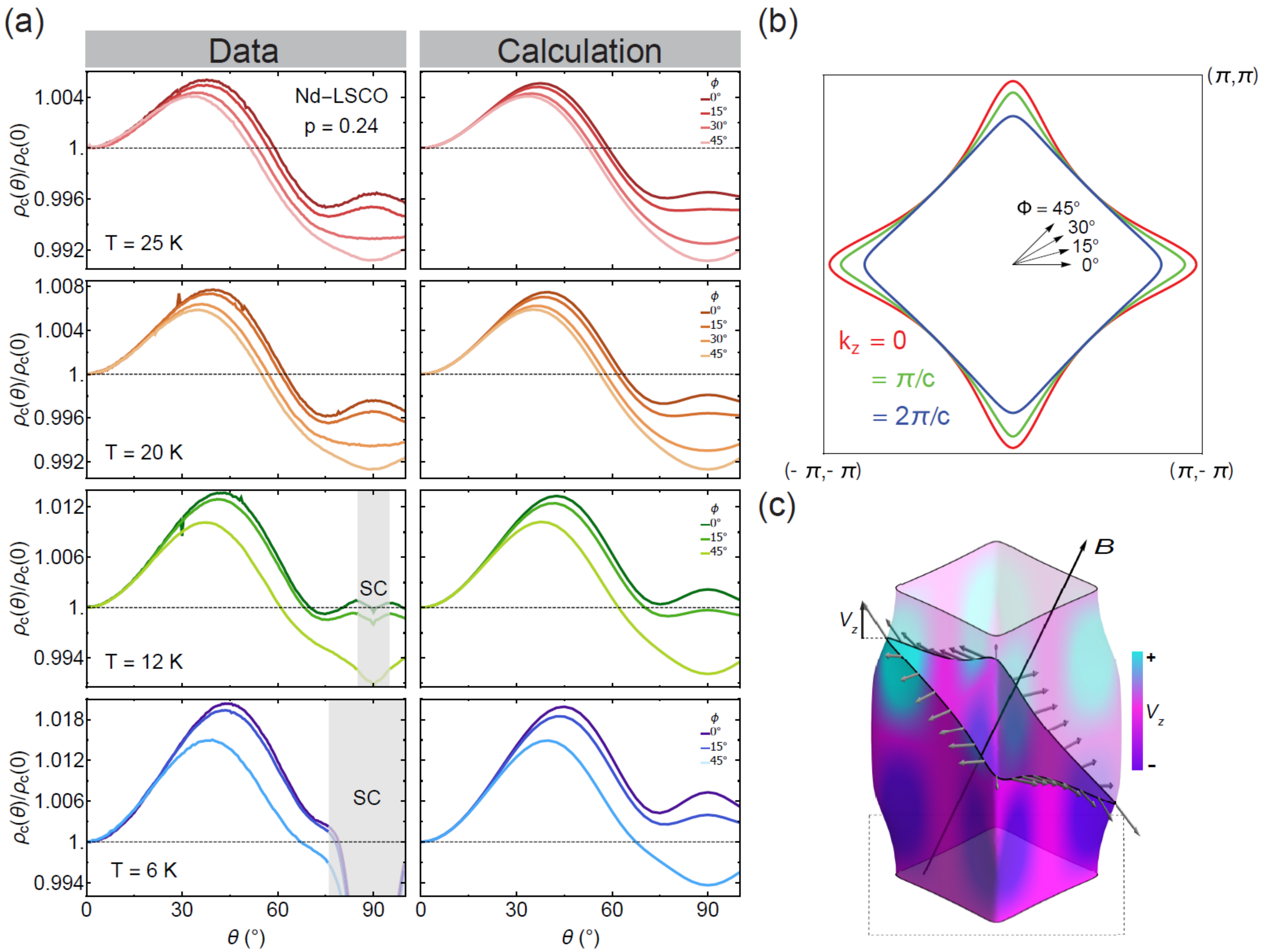
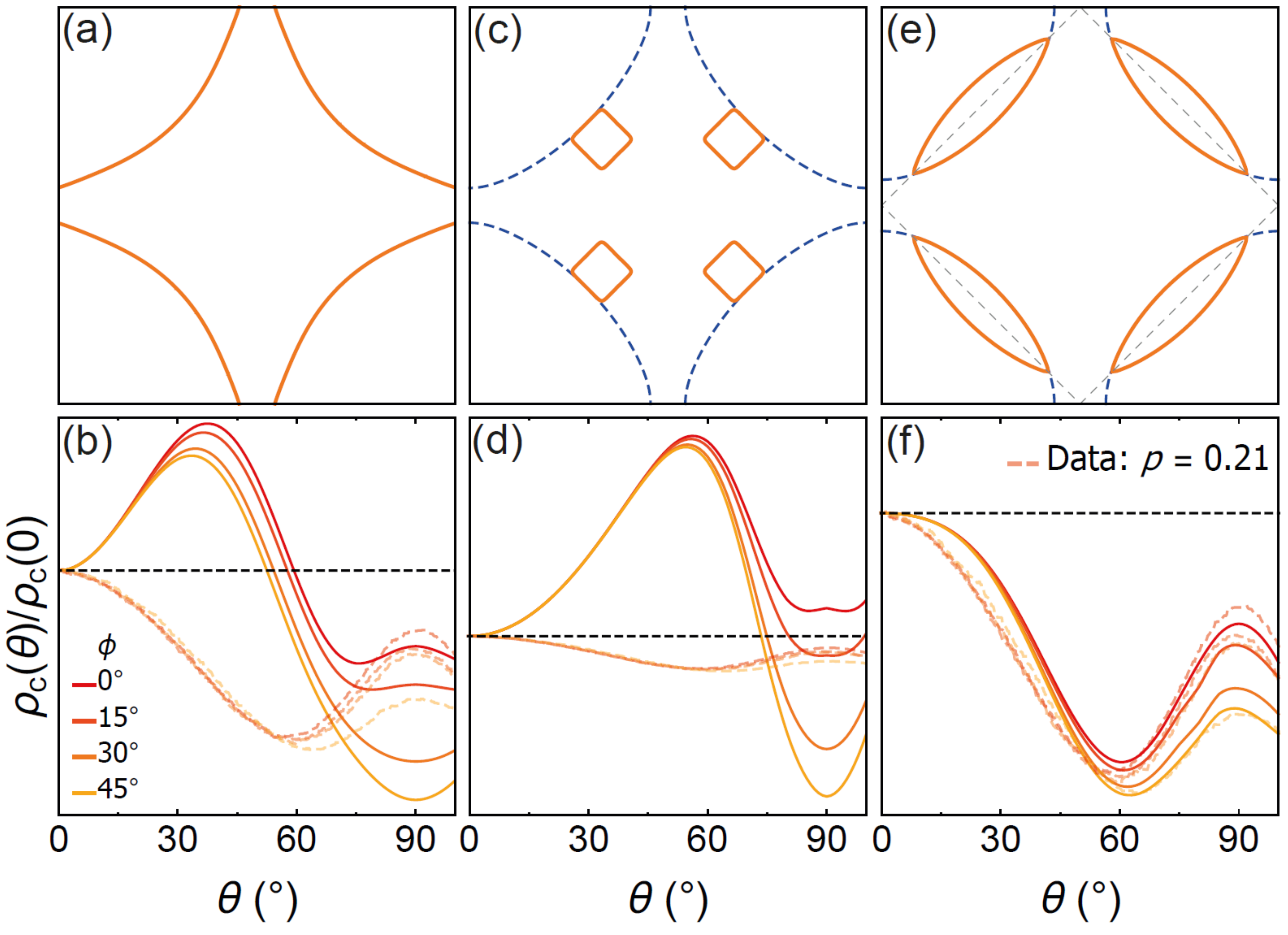
N. Wagner….A. Georges, G. Sangiovanni, arXiv:2301.05588
Jinchao Zhao, Gabriele La Nave, Philip Phillips, arXiv:2304.04787.

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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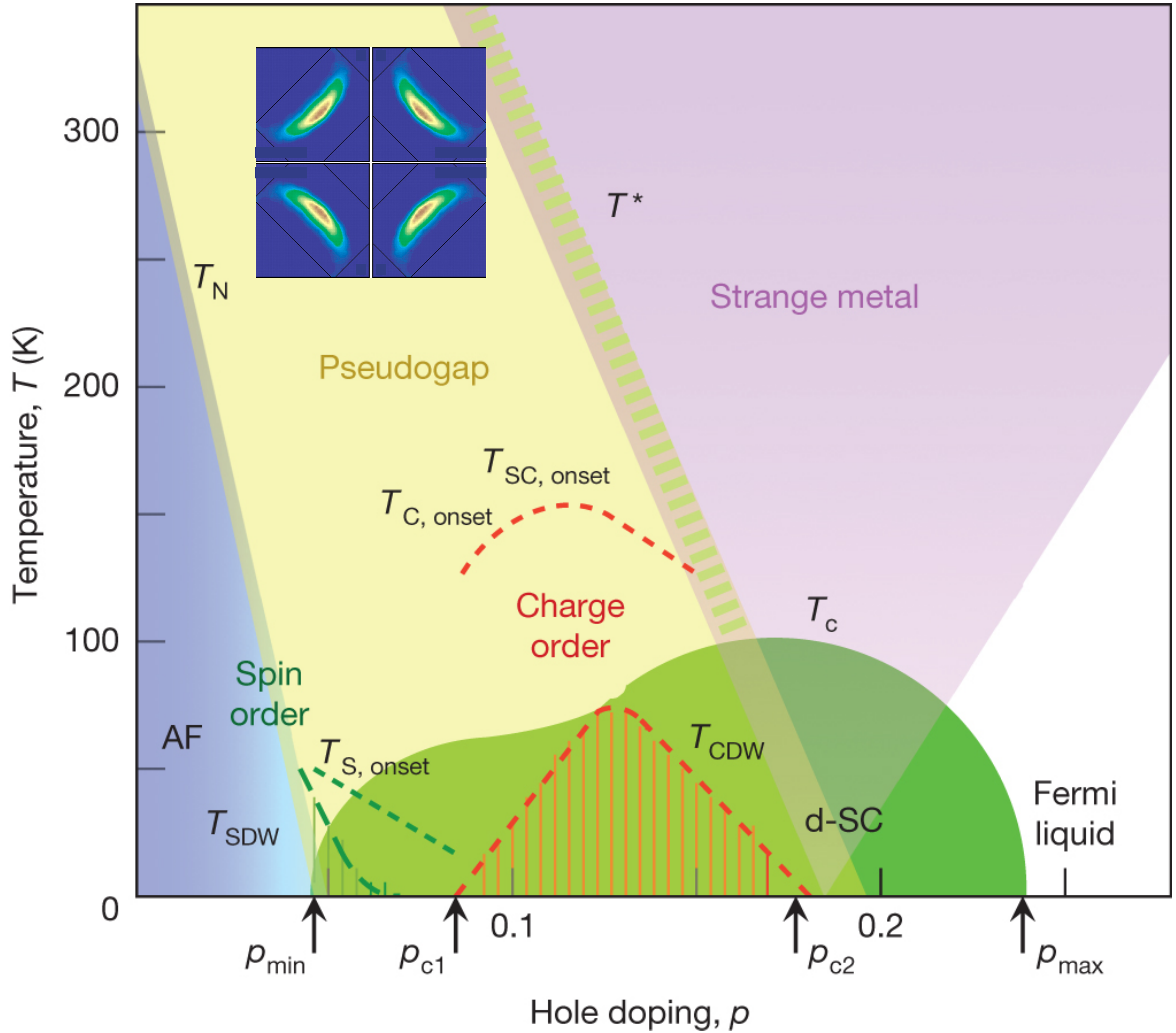

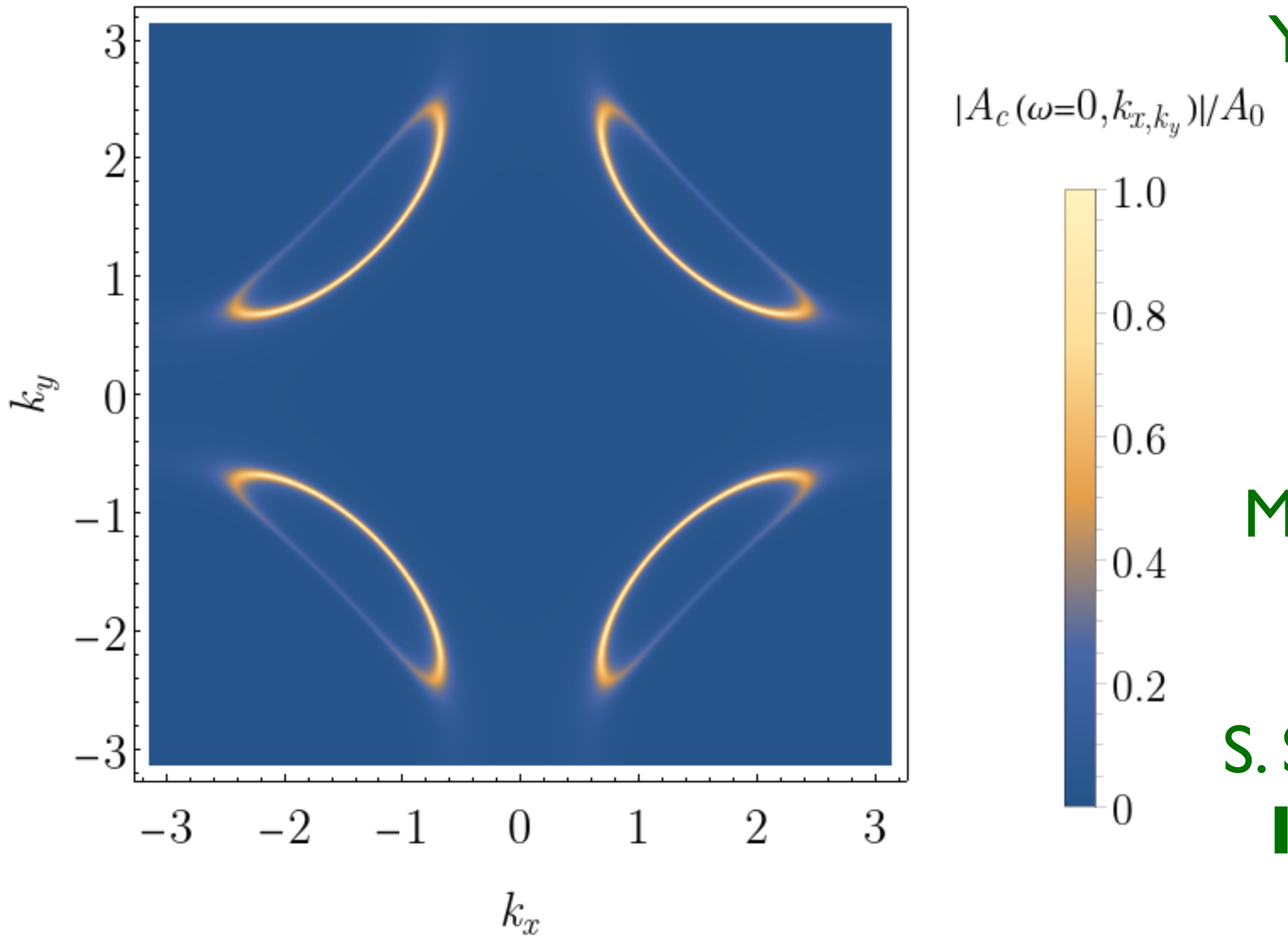

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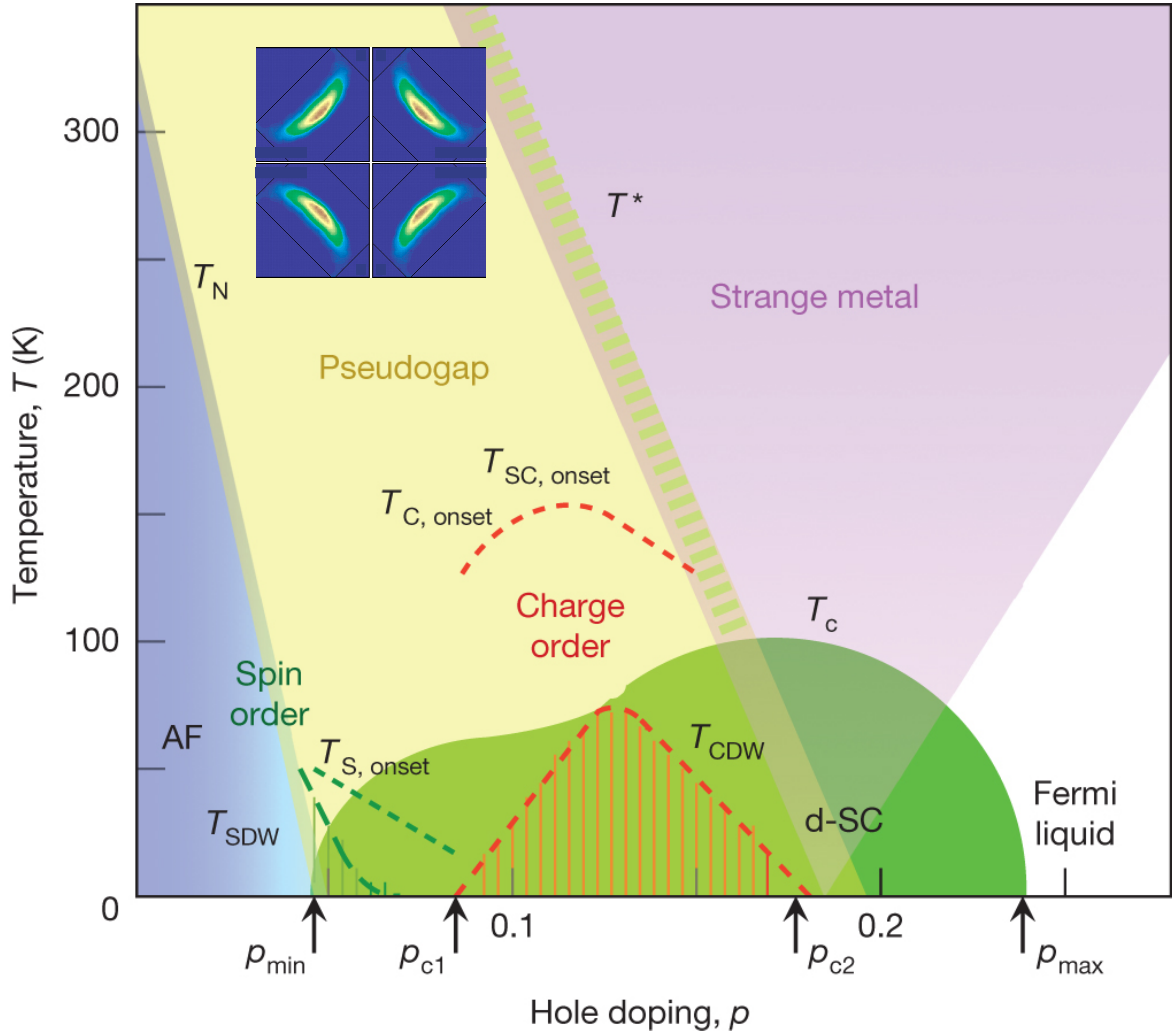

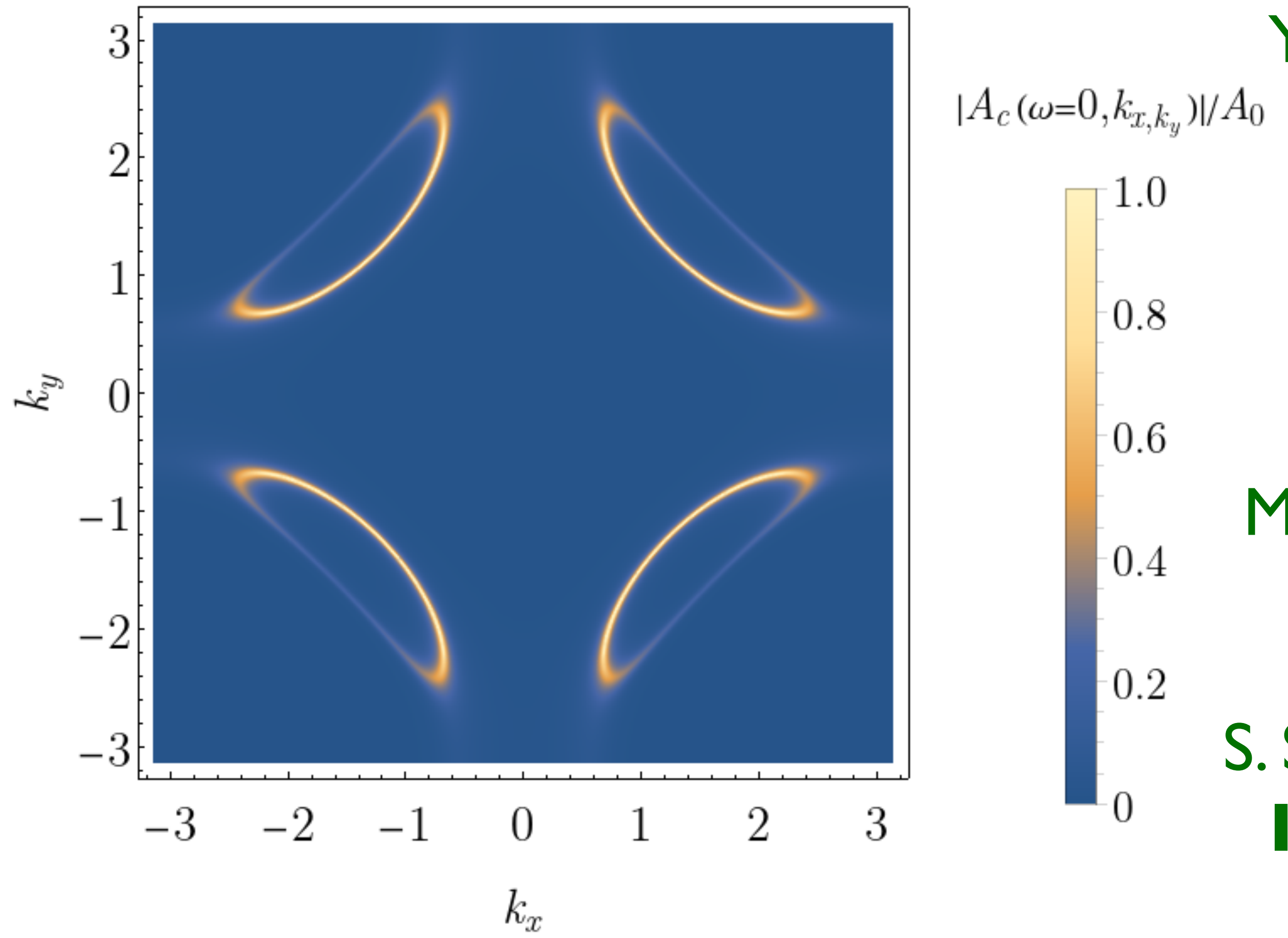

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Green function zeros….

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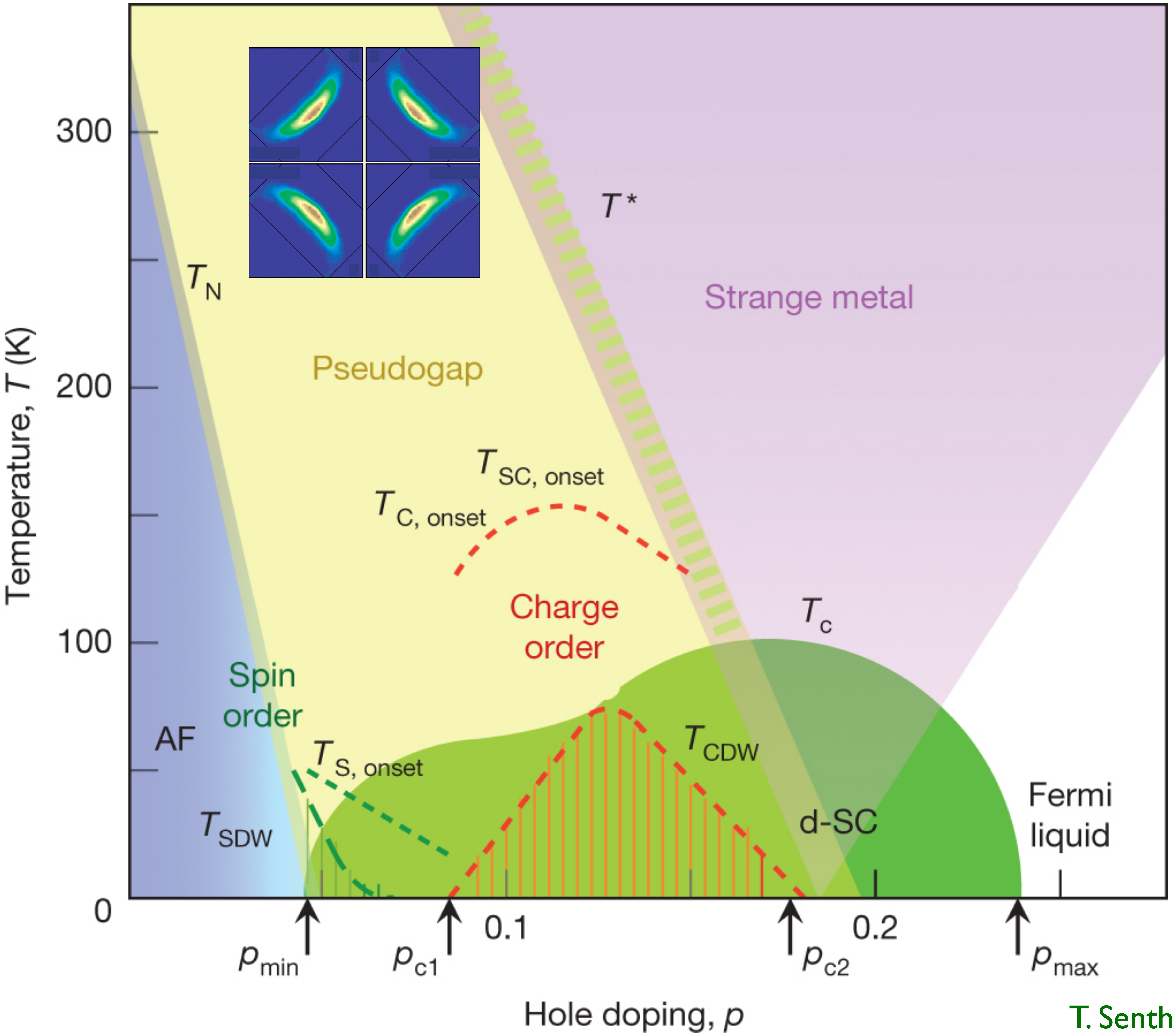

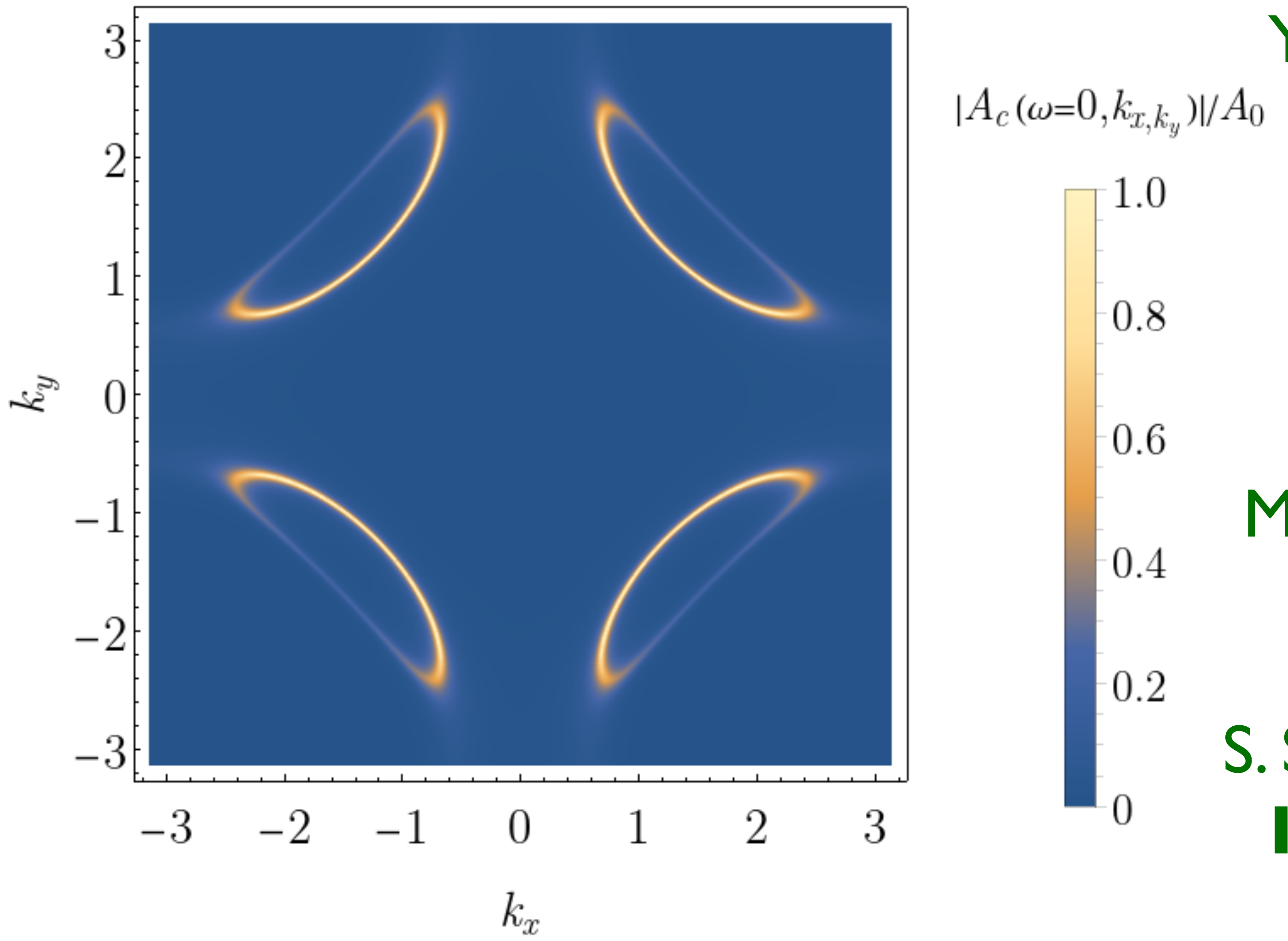

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$+$

'spectator' square lattice spin liquid *at half-filling.*

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

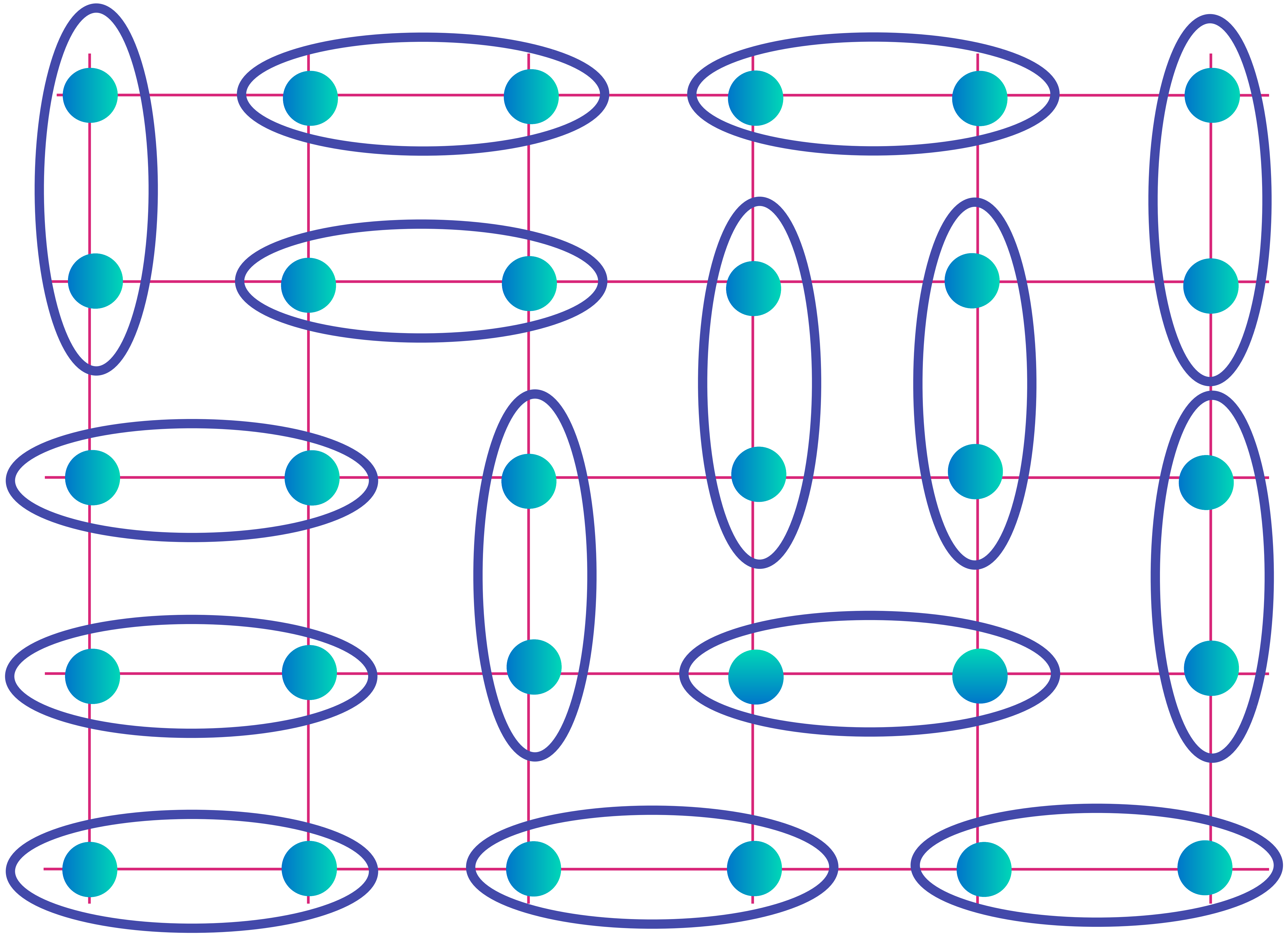
T. Senthil, M. Vojta, and S. Sachdev , *Phys. Rev. B* **69**, 035111 (2004)

From FL*
to
a cuprate phase diagram

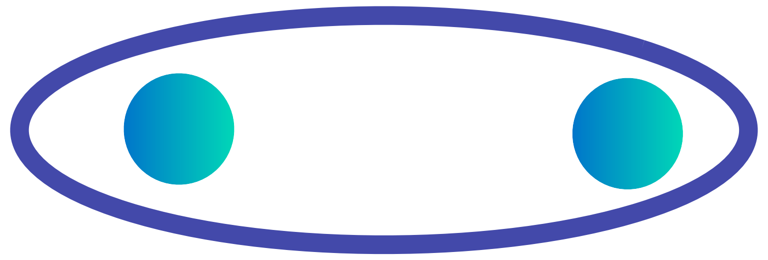
The dance of electrons on Cu atoms in YBCO

P.W. Anderson (1973)

Spin liquid



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



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

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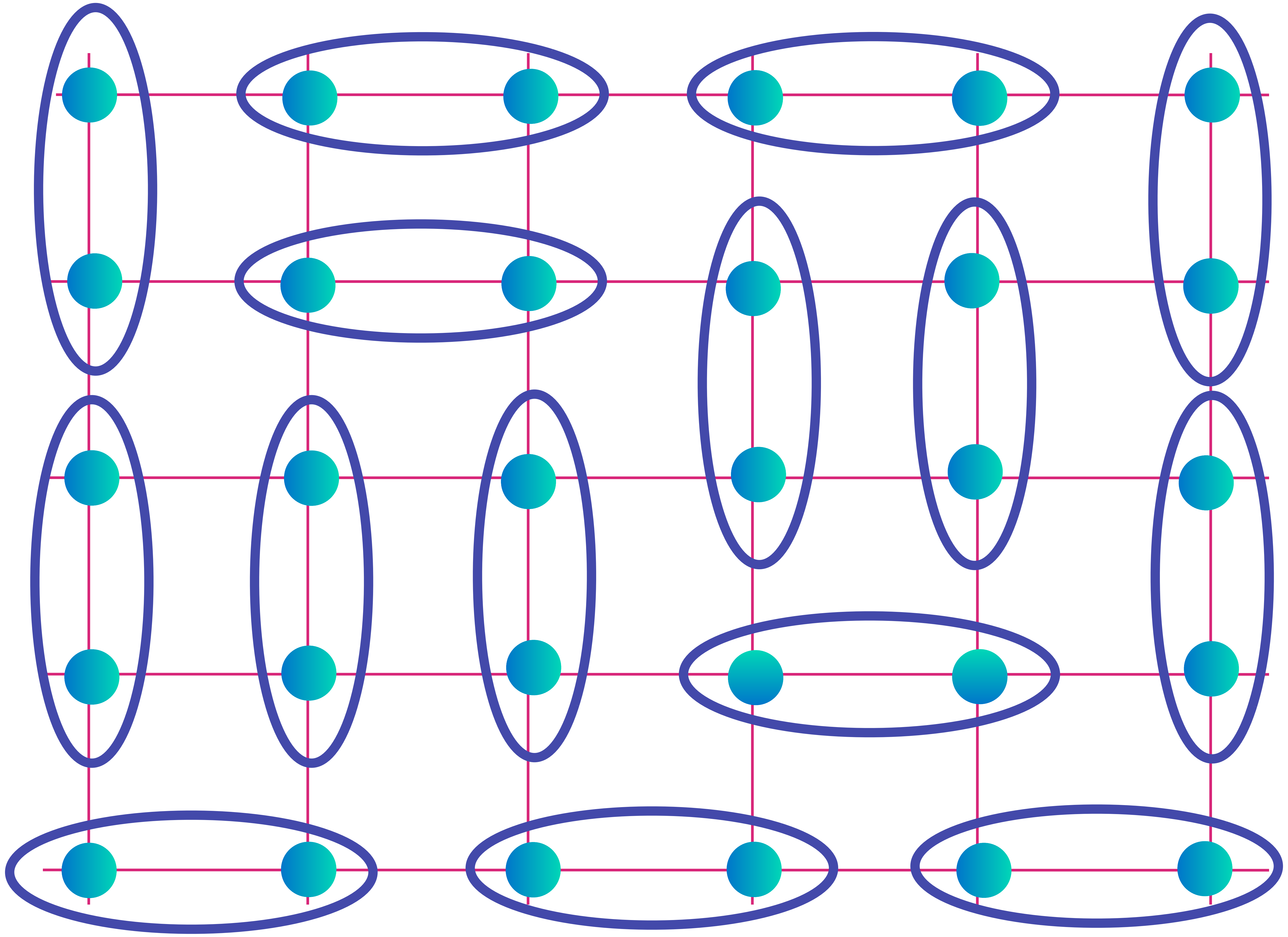

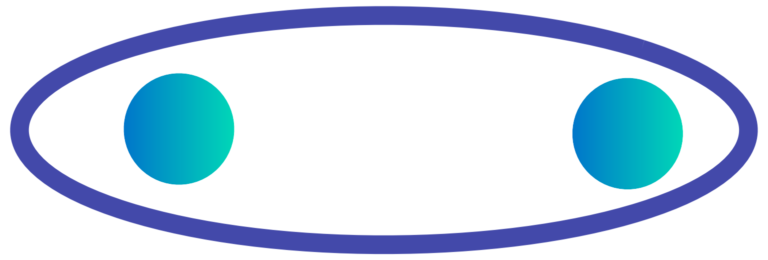 $= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

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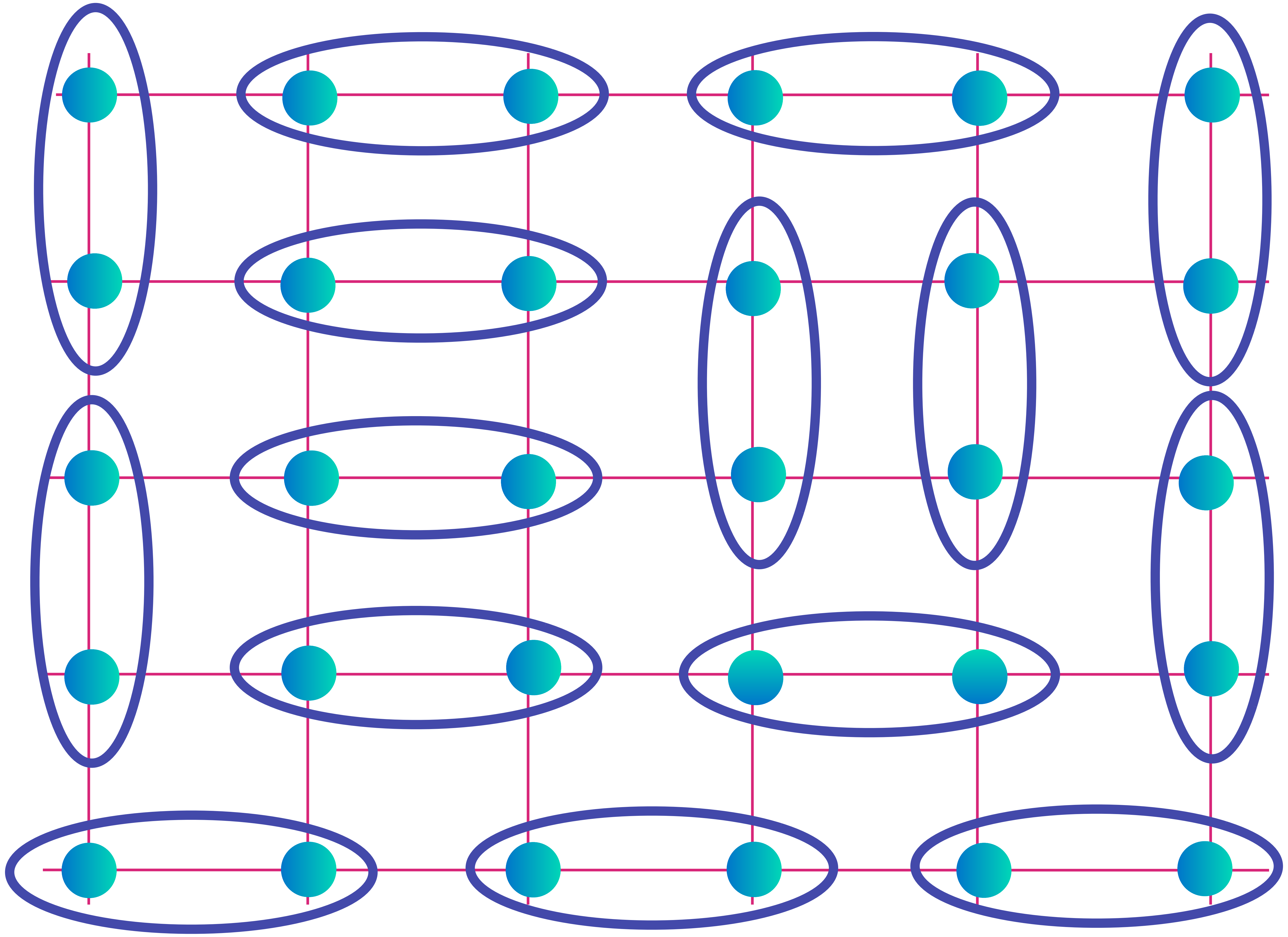

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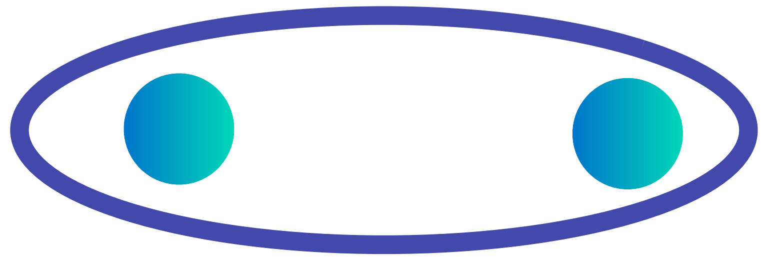

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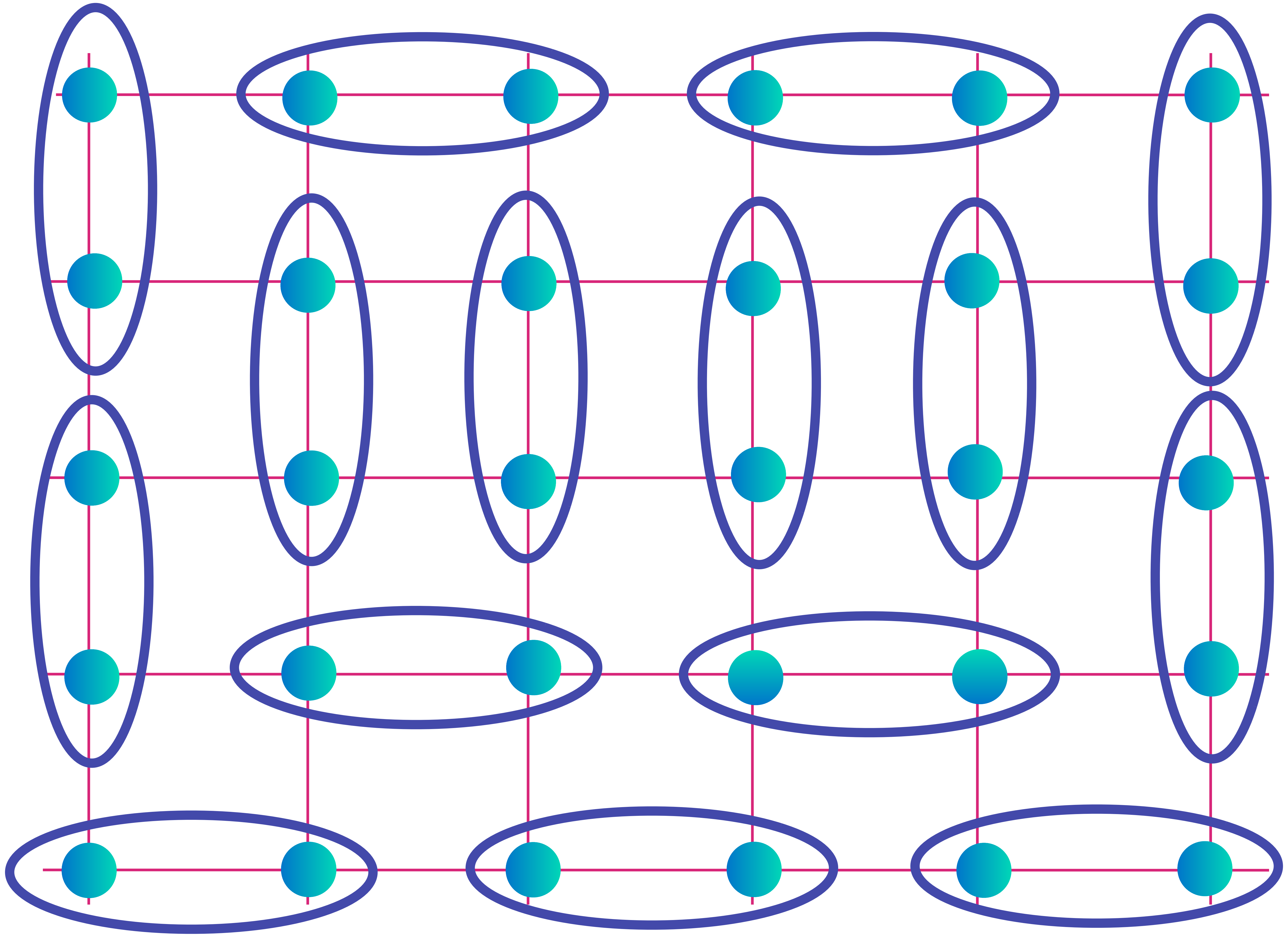

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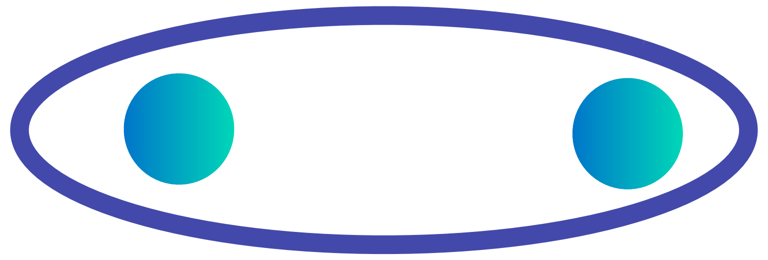

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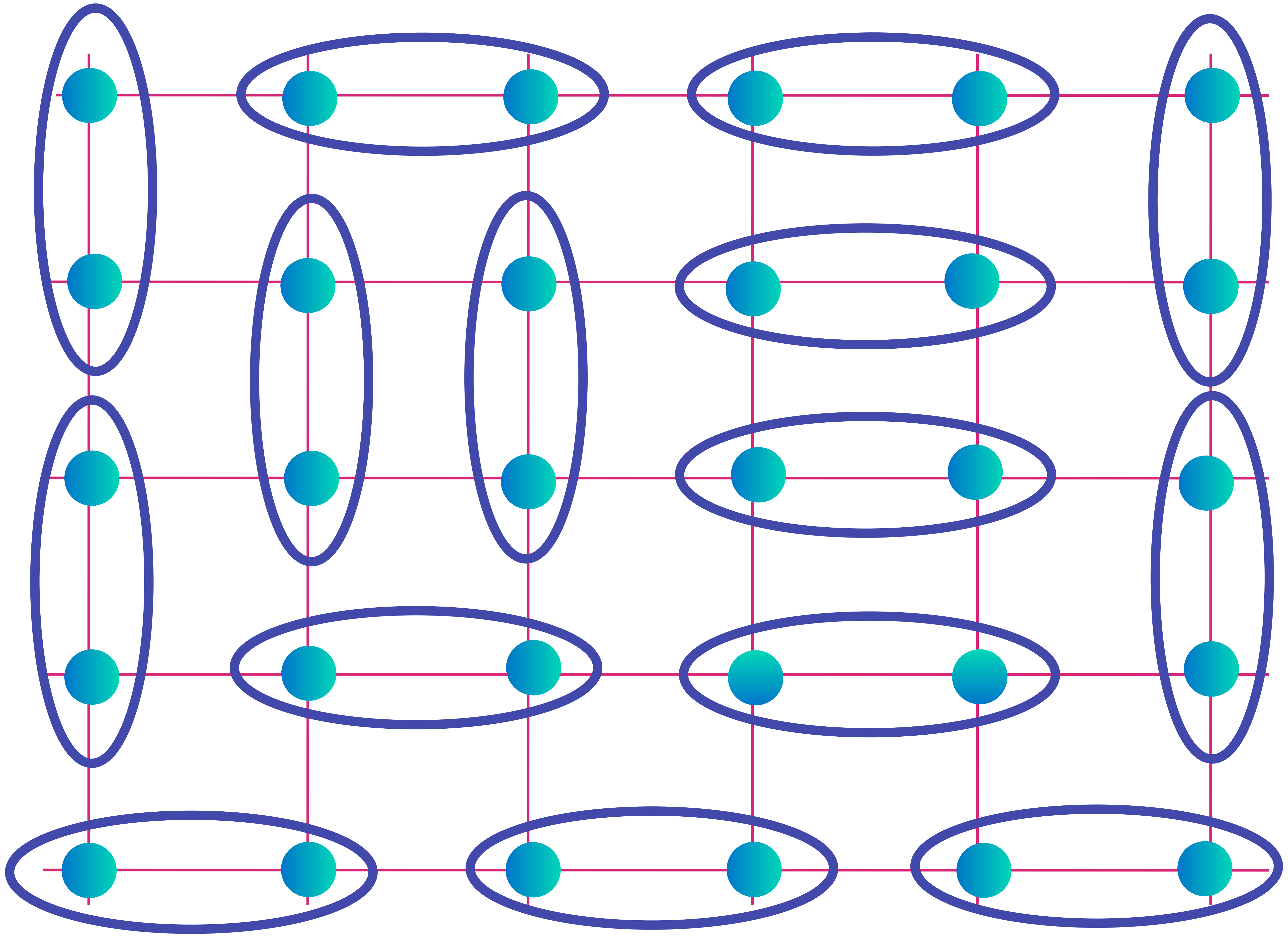

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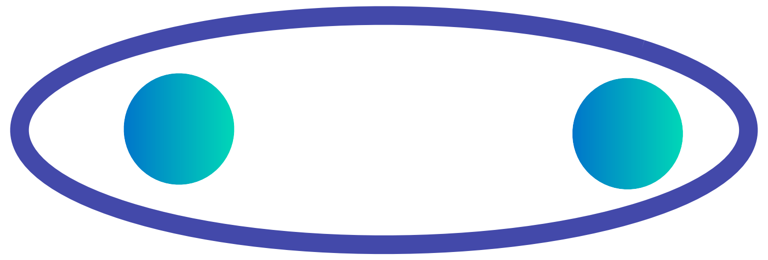

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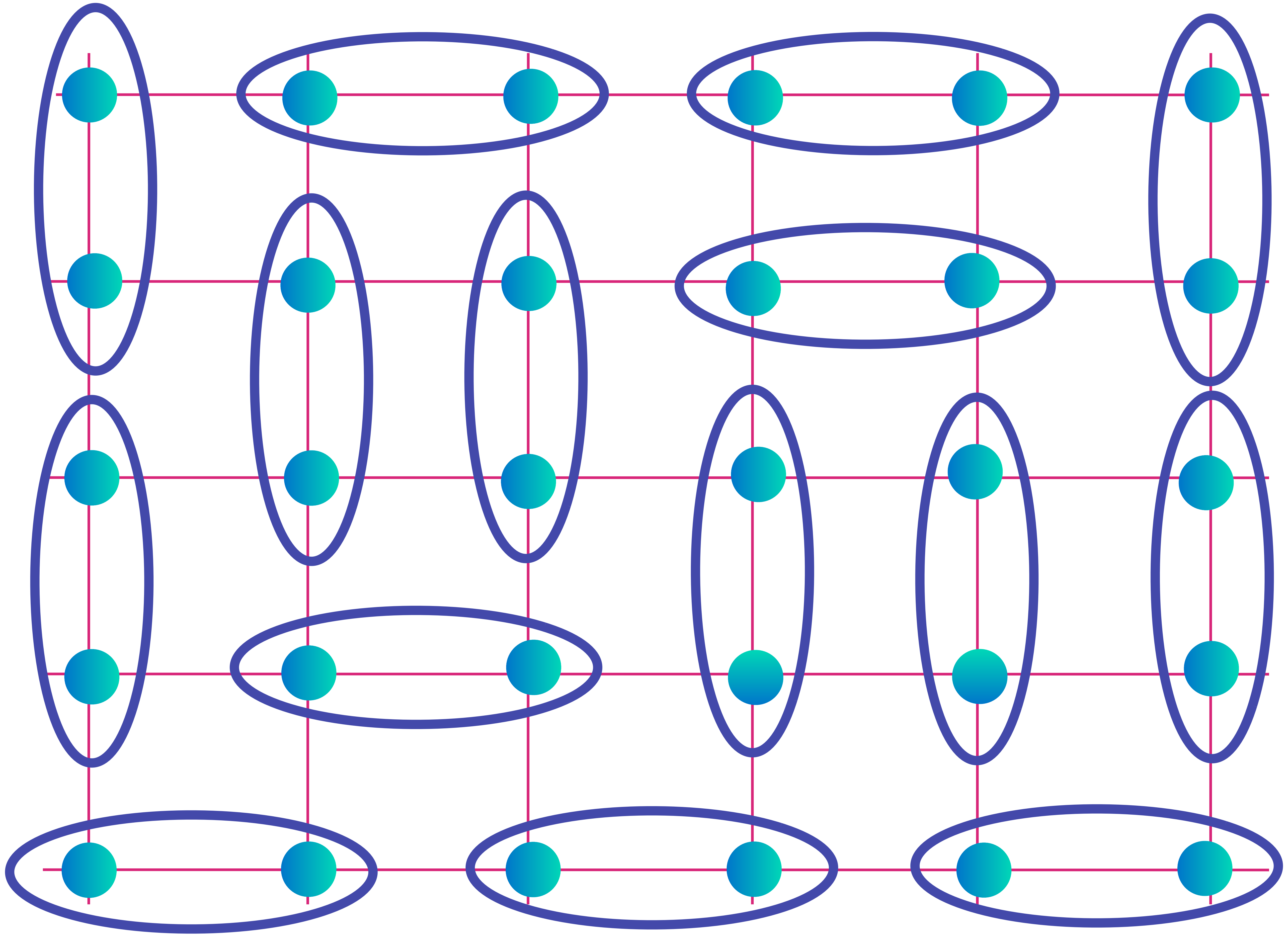

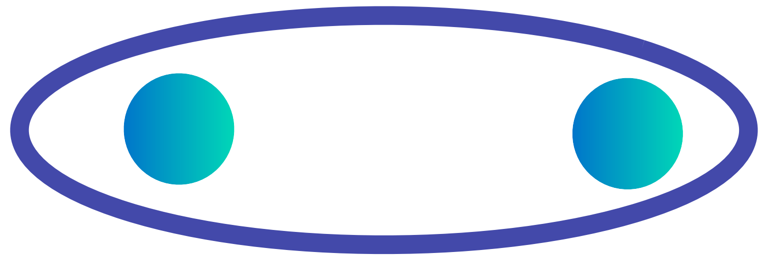

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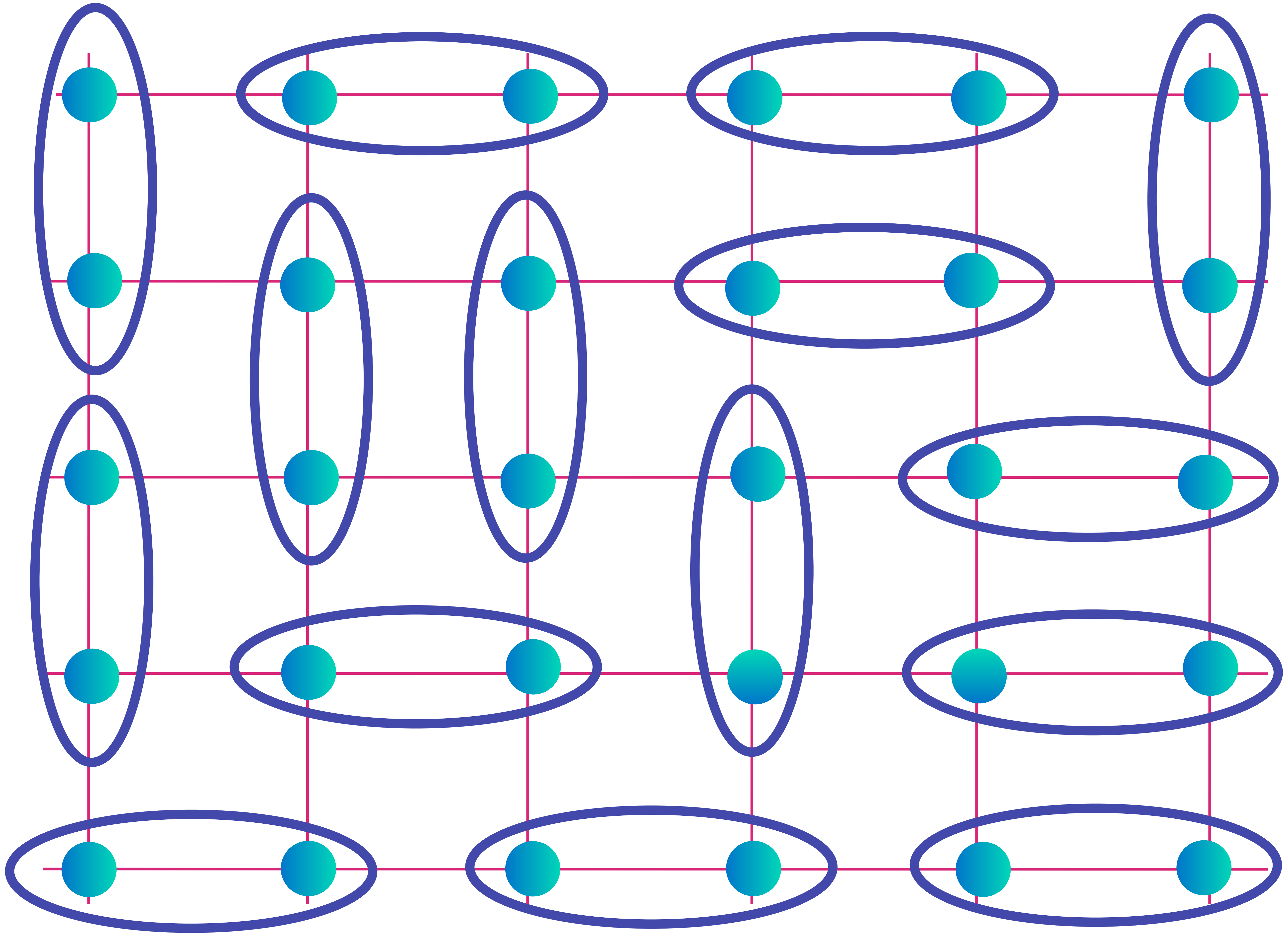

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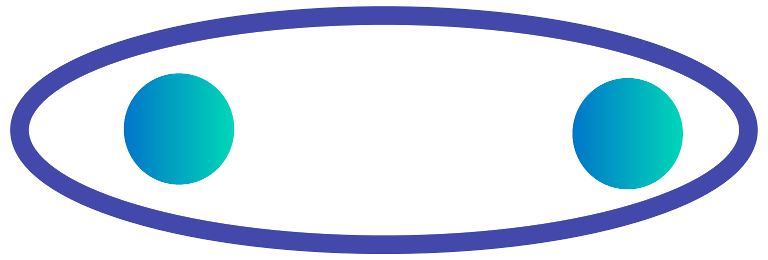

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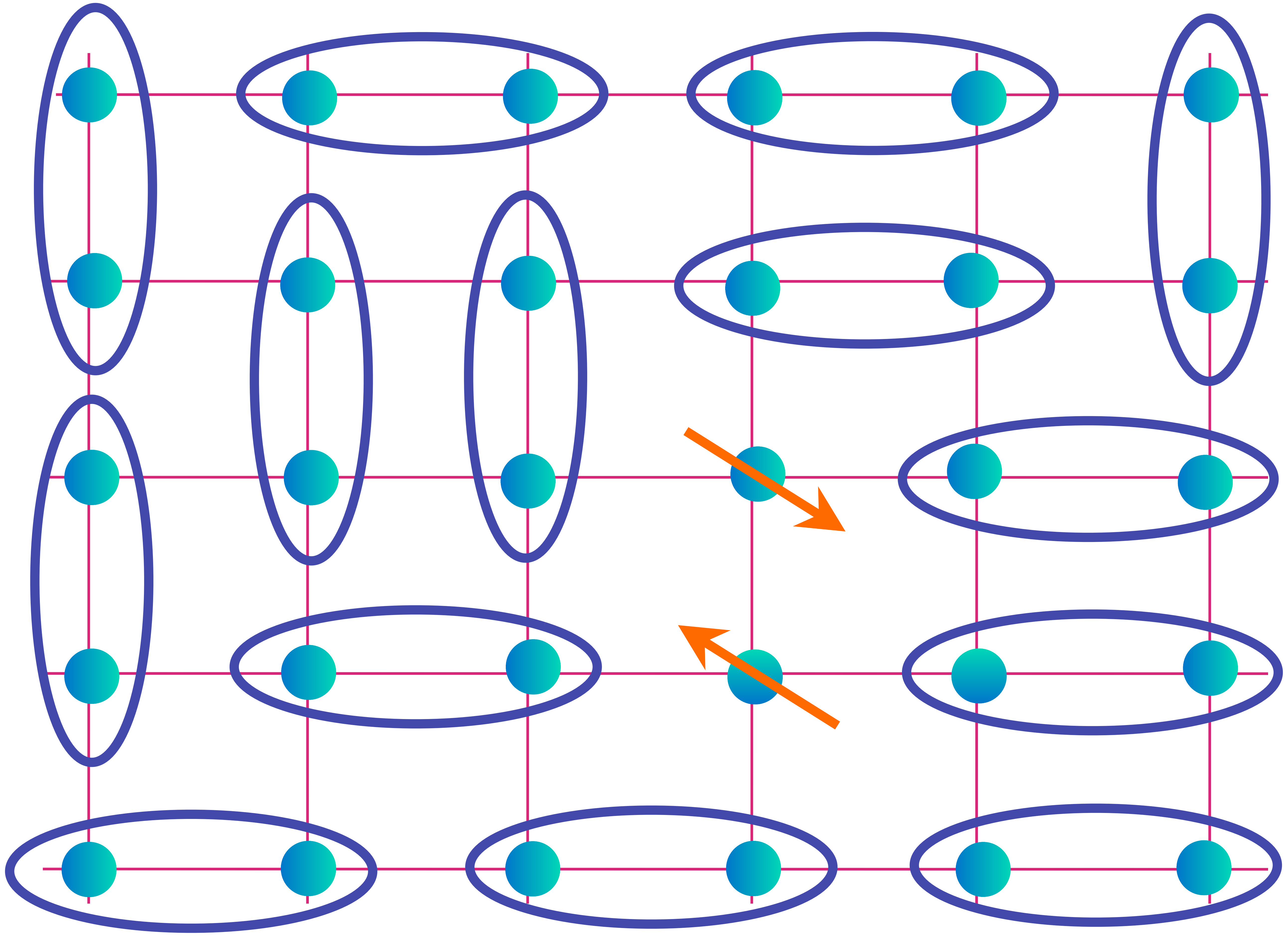
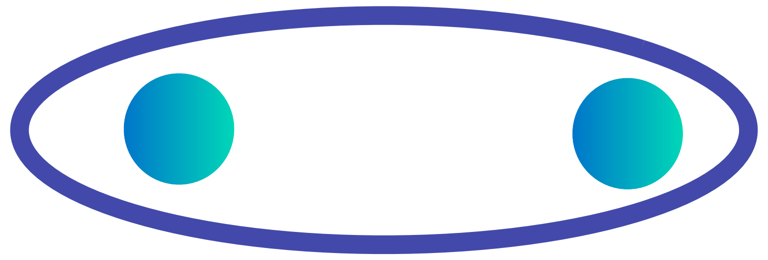


Spin liquid

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



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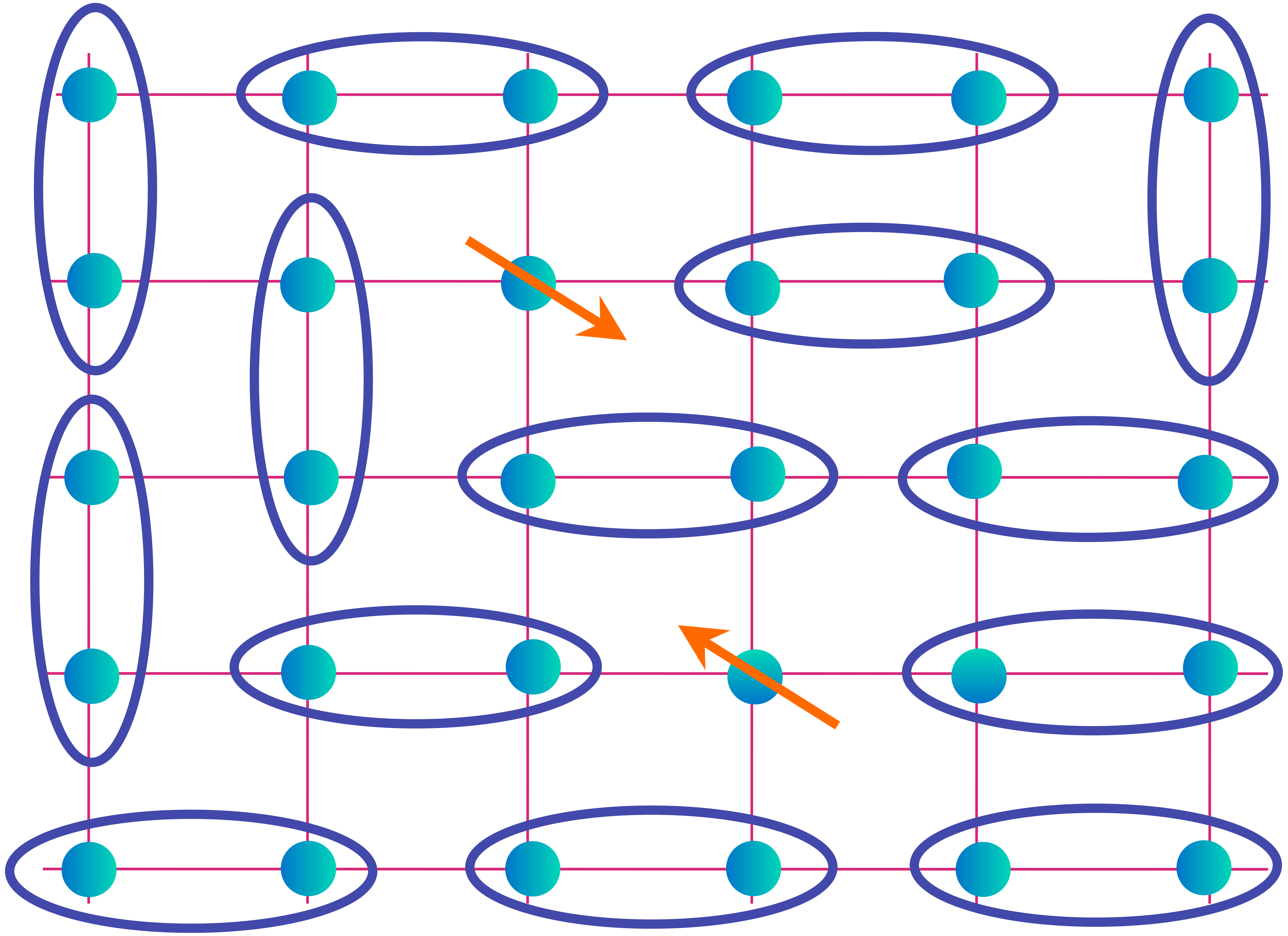

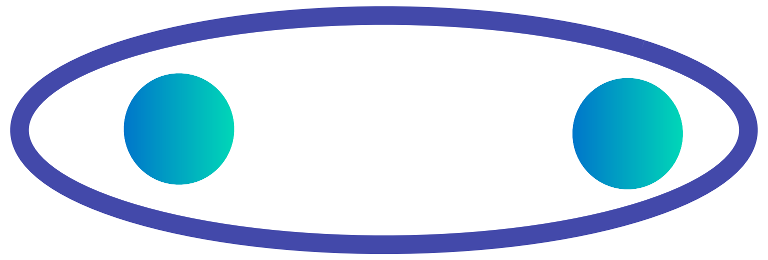 $= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

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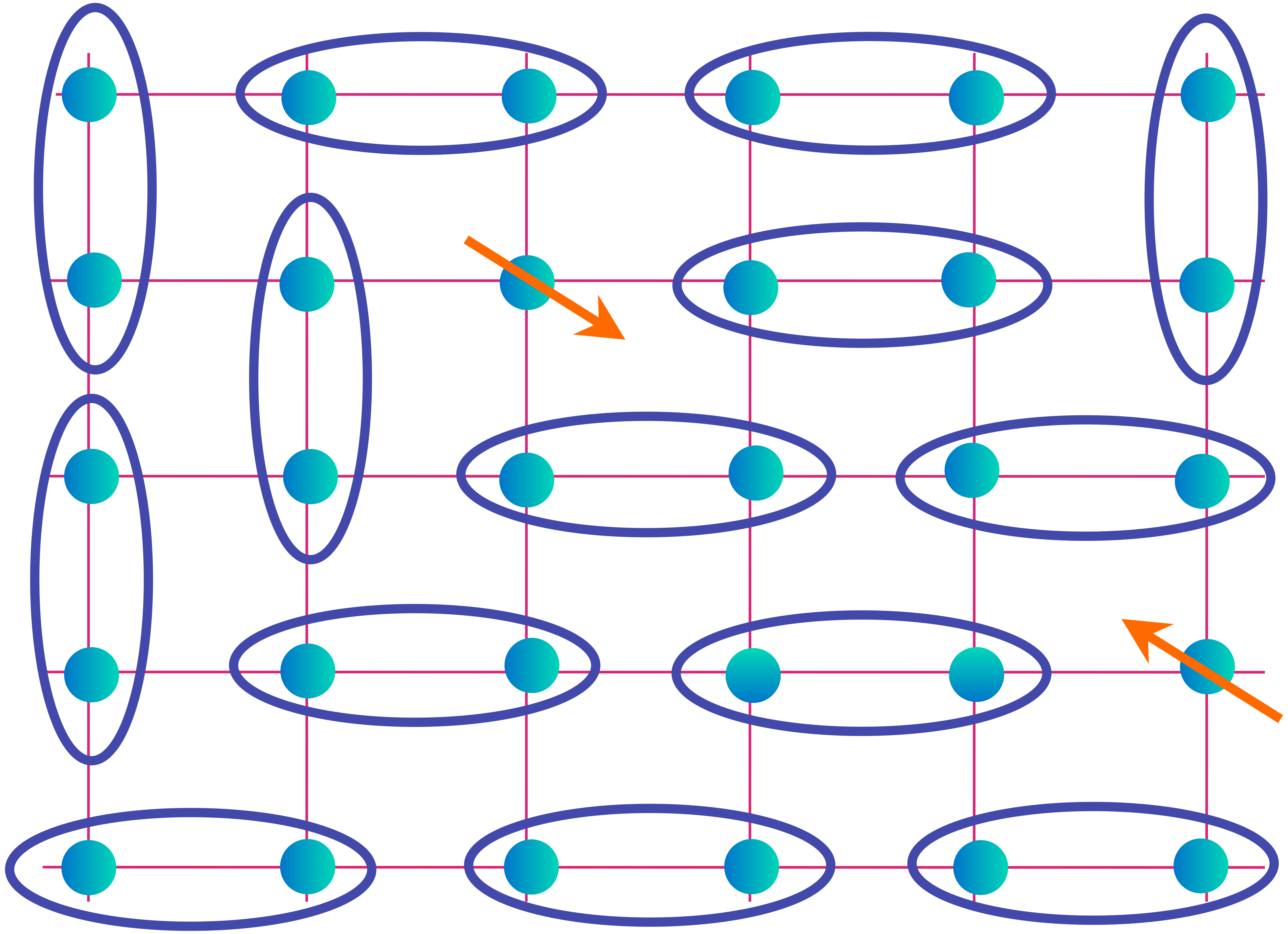

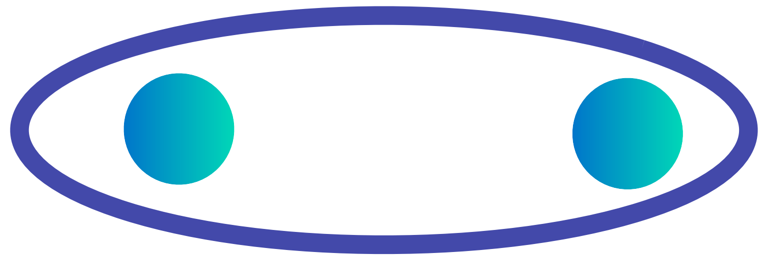
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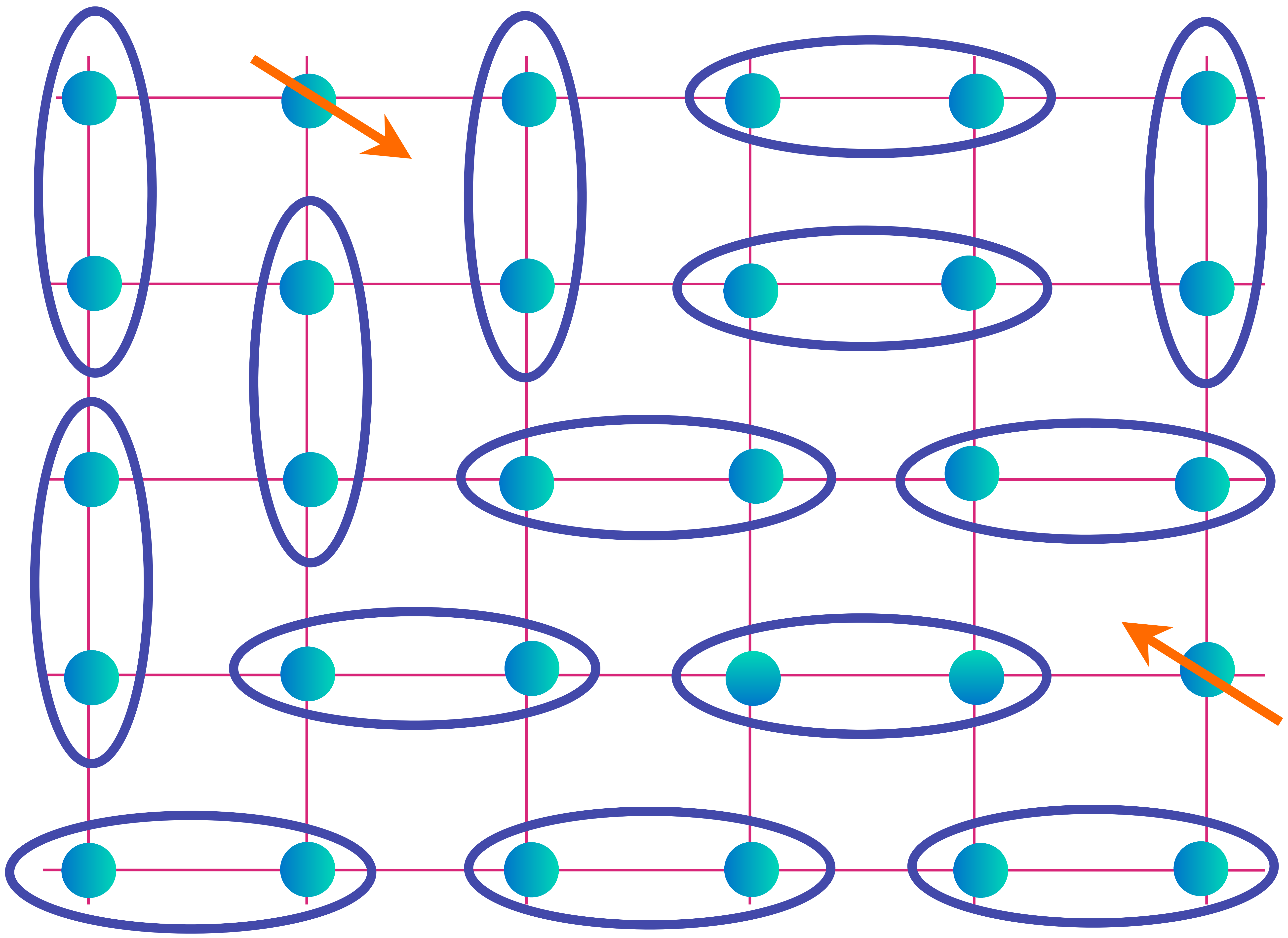

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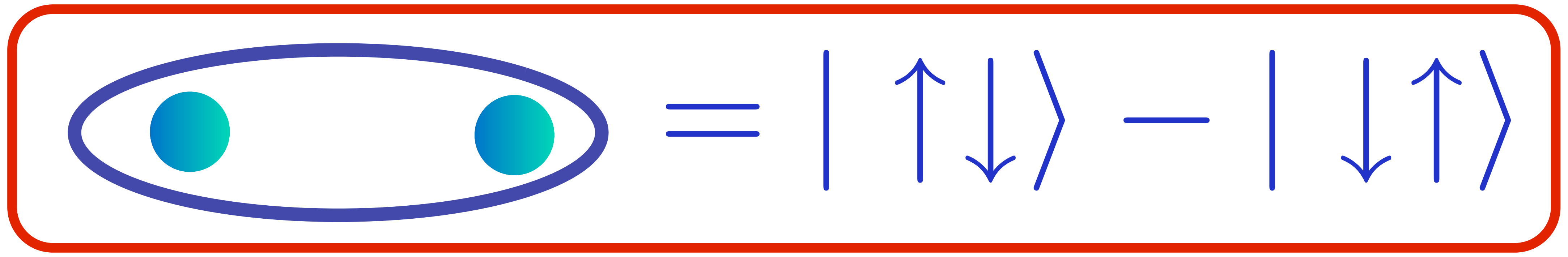

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Holons

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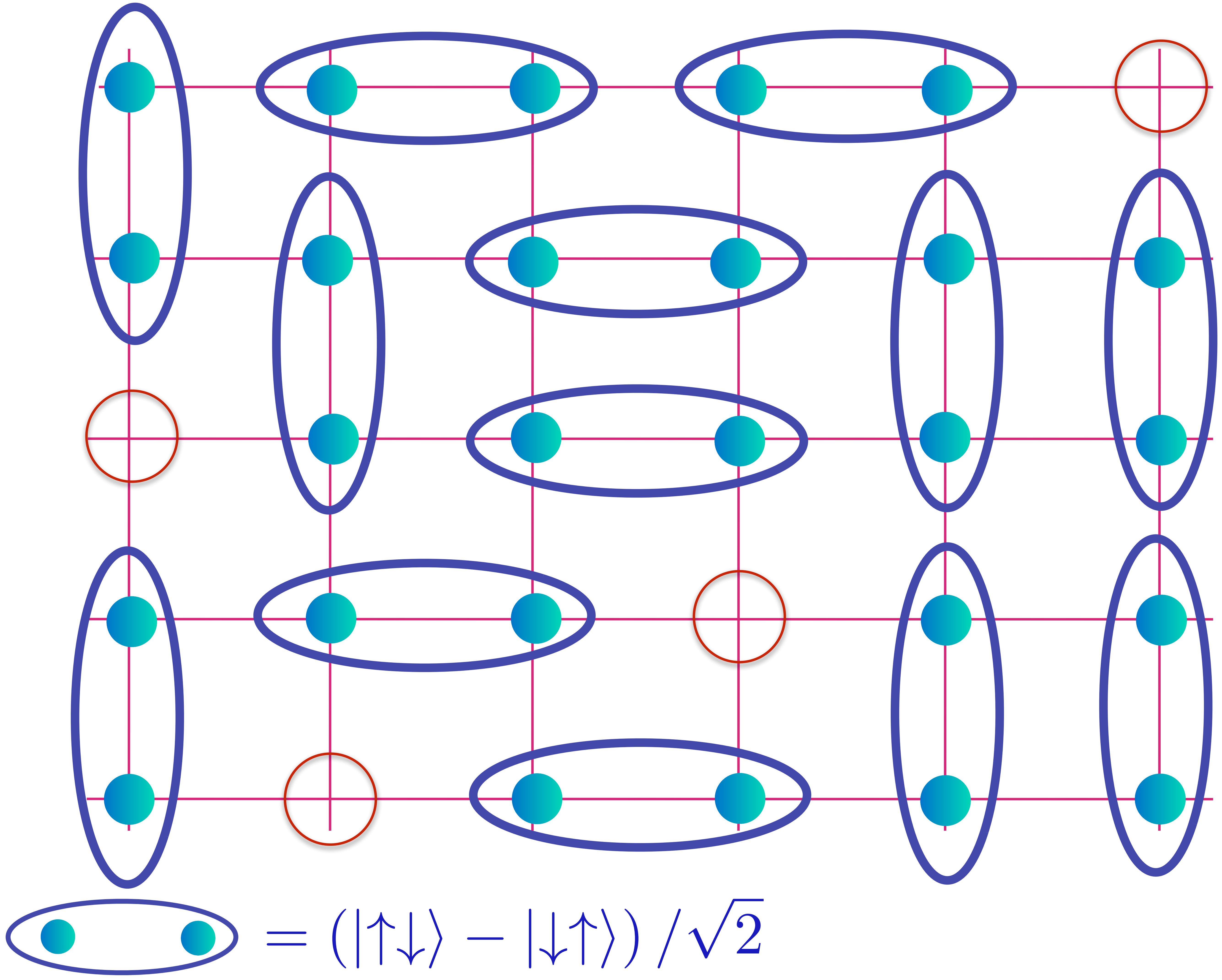


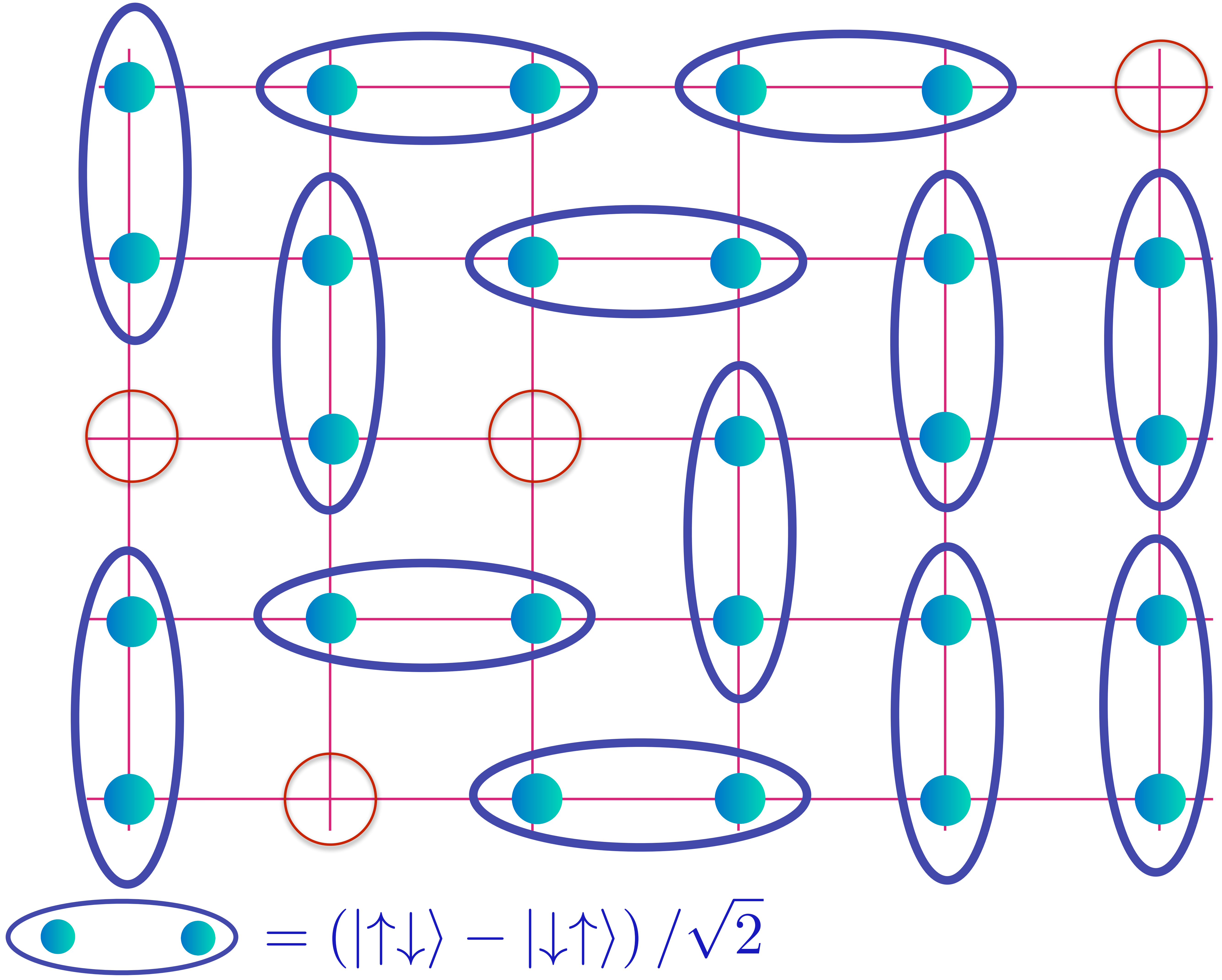
$$= \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)/\sqrt{2}$$

Spin liquid

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

Holons

G. Baskaran, Z. Zou, P.W. Anderson, *Solid State Comm.* **63**, 973 (1987)
S.A. Kivelson, D.S. Rokhsar and J.P. Sethna, *Phys. Rev. B* **35**, 8865 (1987)
D. Rokhsar and S.A. Kivelson, *Phys. Rev. Lett.* **61**, 2376 (1988)



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

Spin liquid

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

~~Holon metal~~

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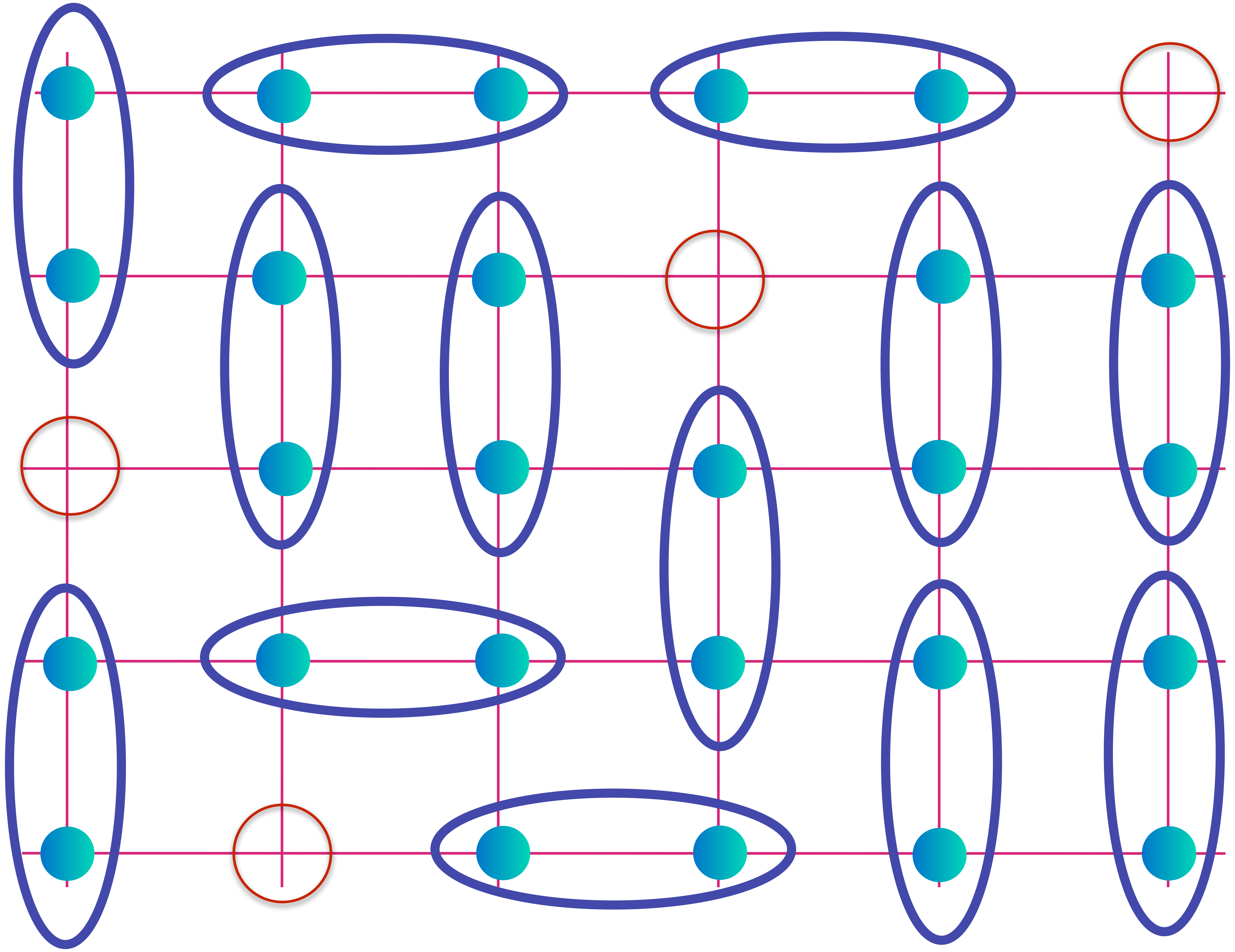

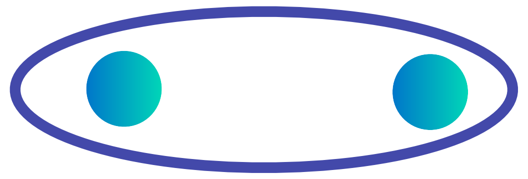

$= \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)/\sqrt{2}$

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

Cannot explain pseudogap metal

~~Holon metal~~

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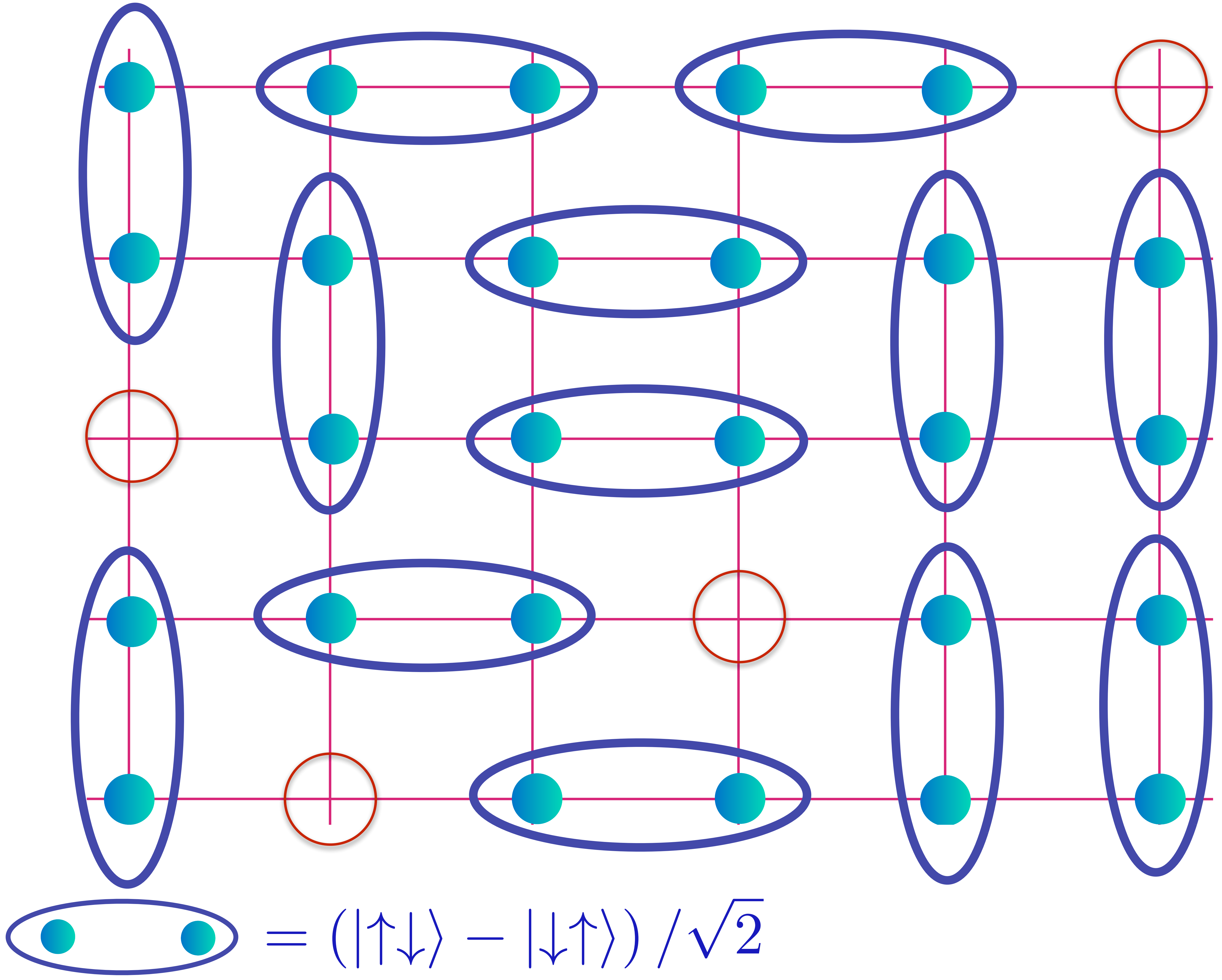

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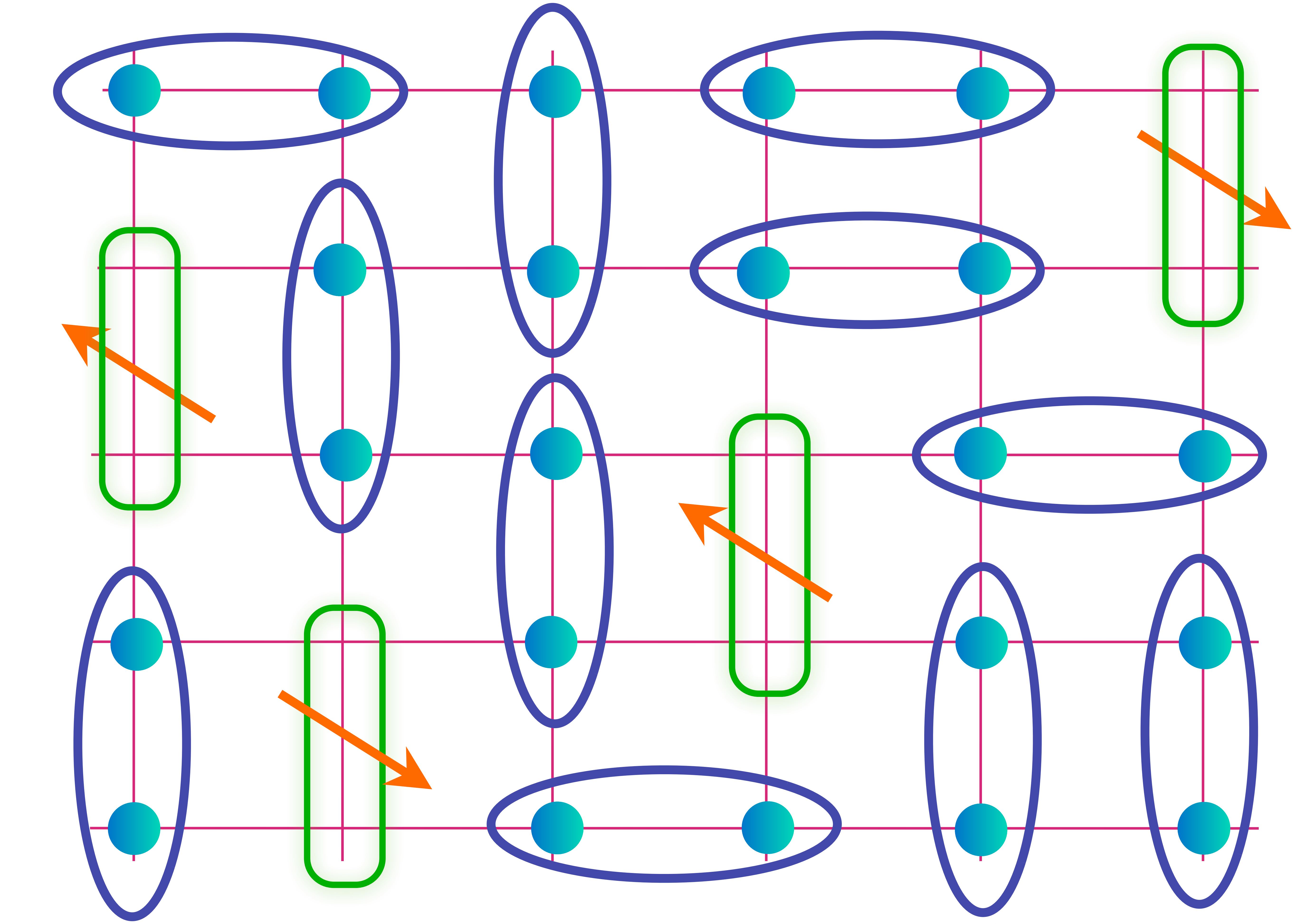
Cannot explain pseudogap metal

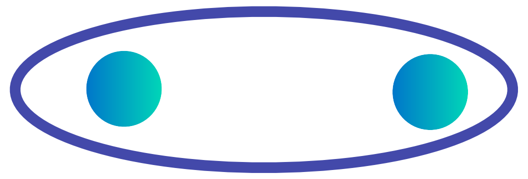
FL* in a ***one-band*** model

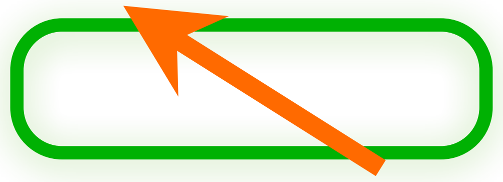
S. Sachdev *Phys. Rev. B* **49**, 6770 (1994); X.-G. Wen and P.A. Lee *Phys. Rev. Lett.* **76**, 503 (1996)
R. K. Kaul, A. Kolezhuk, M. Levin, S. Sachdev, and T. Senthil, *Phys. Rev. B* **75**, 235122 (2007)



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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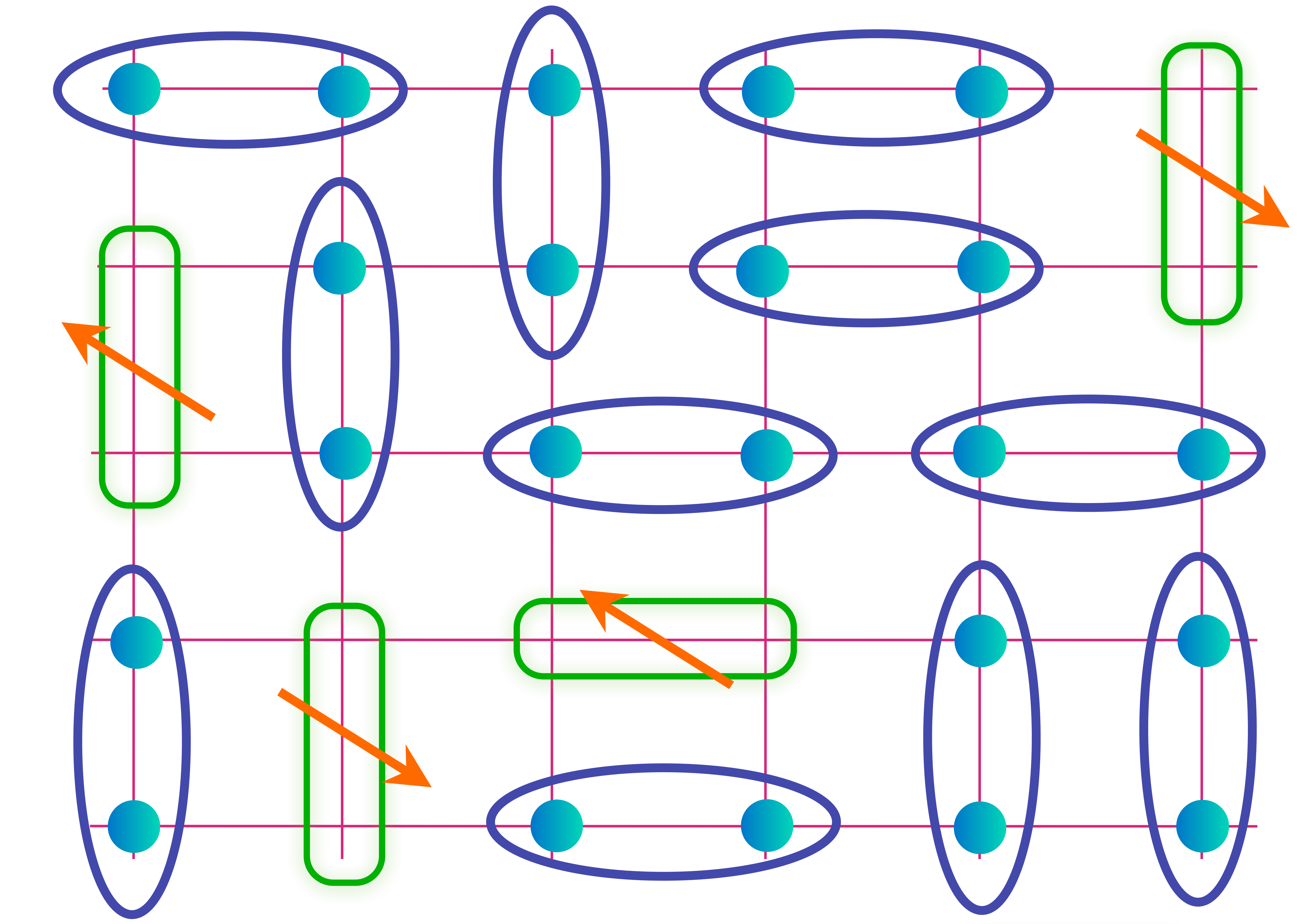

Metal with electron-like quasiparticles on a Fermi surface of size p, and emergent gauge fields

Spinon-holon bound state

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

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

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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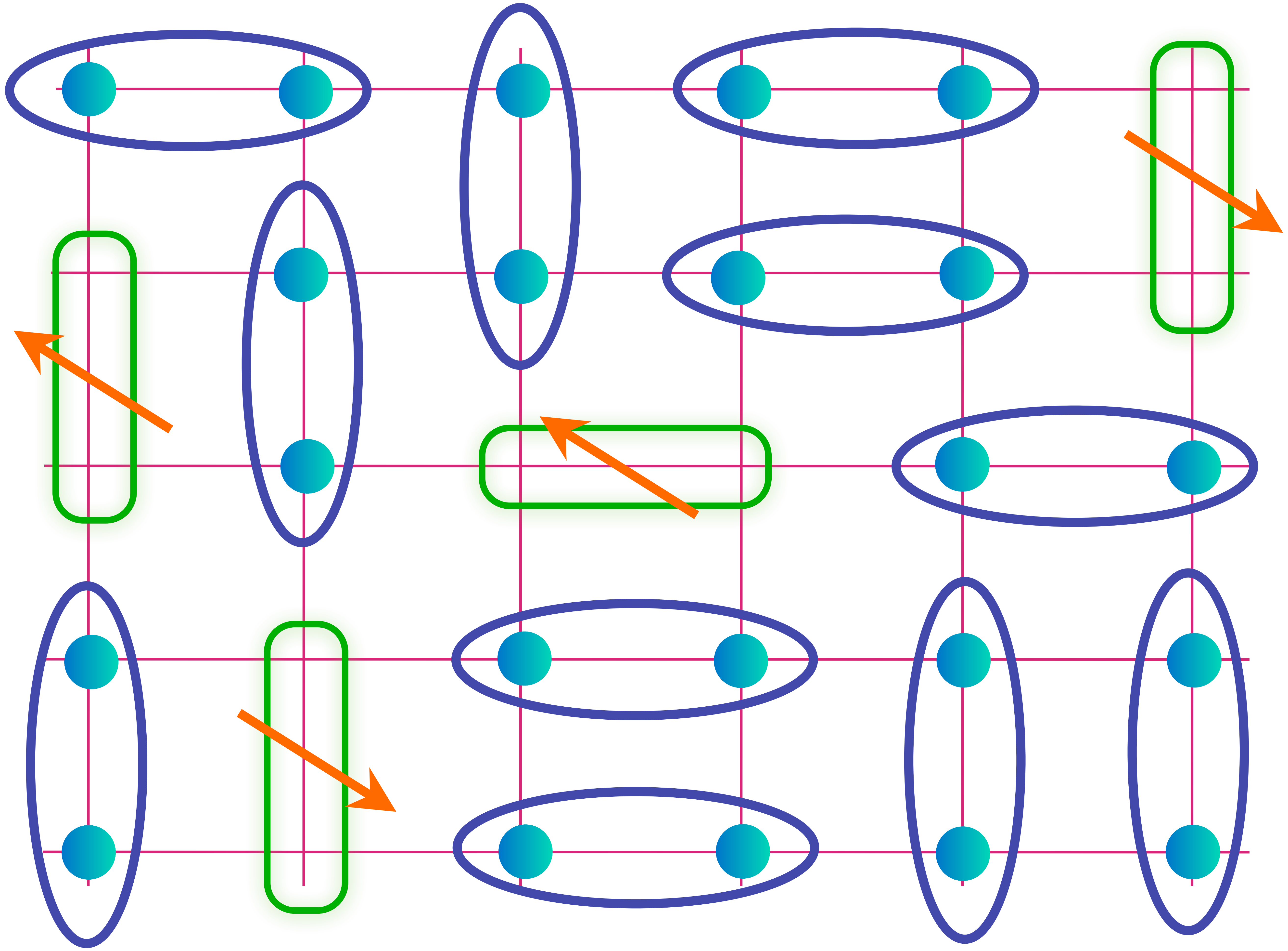

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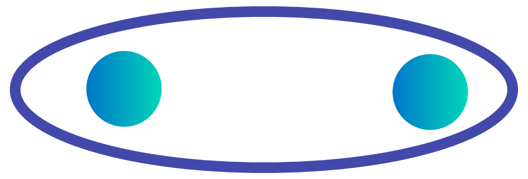
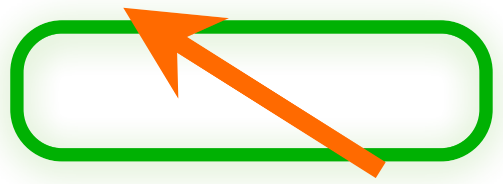
 $= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$

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

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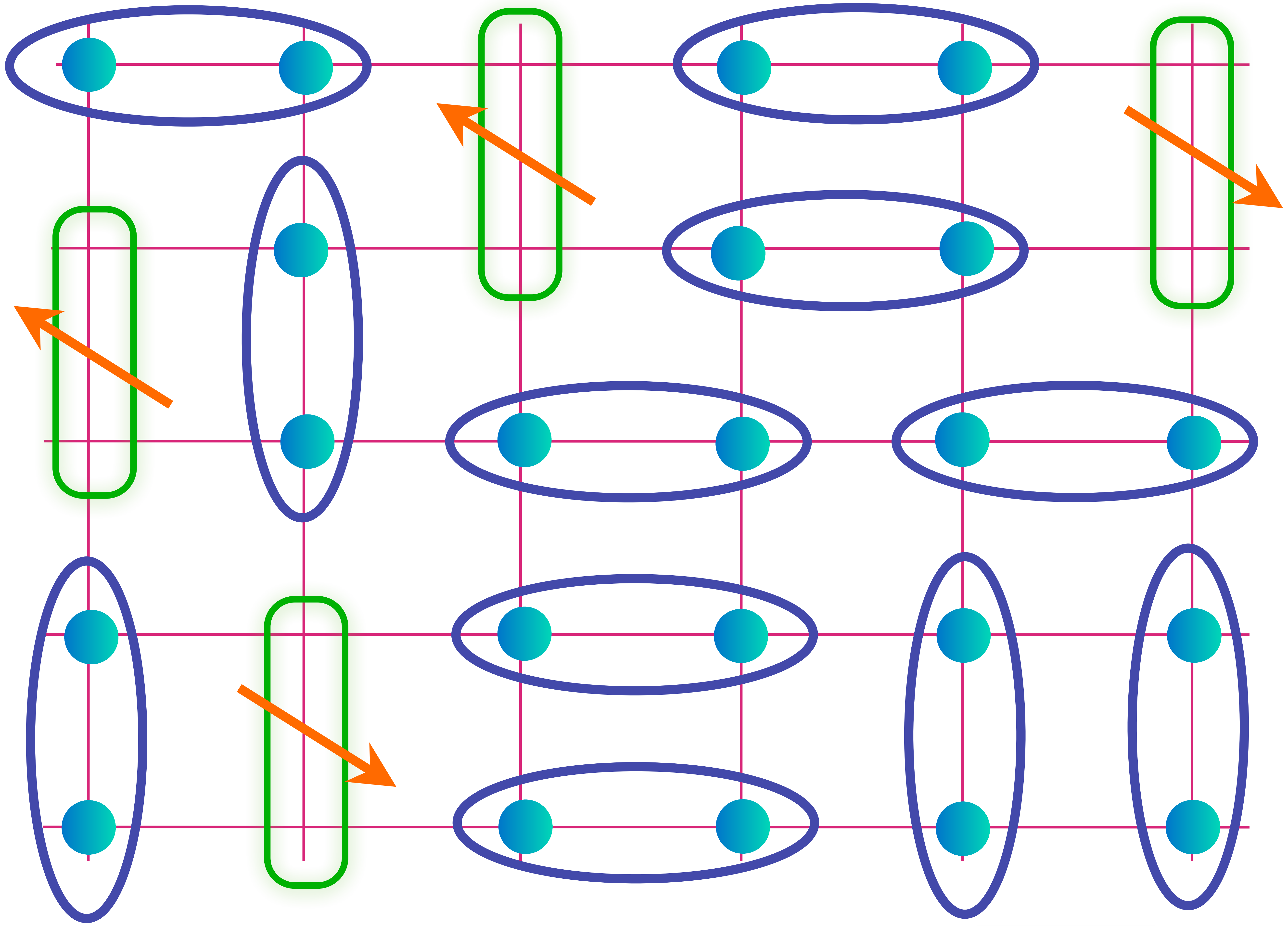

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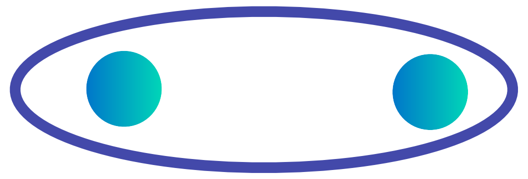
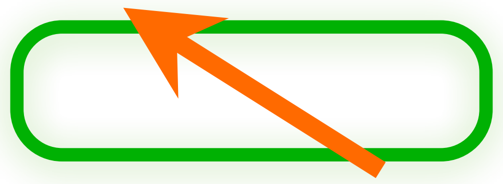
 $= \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)/\sqrt{2}$

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

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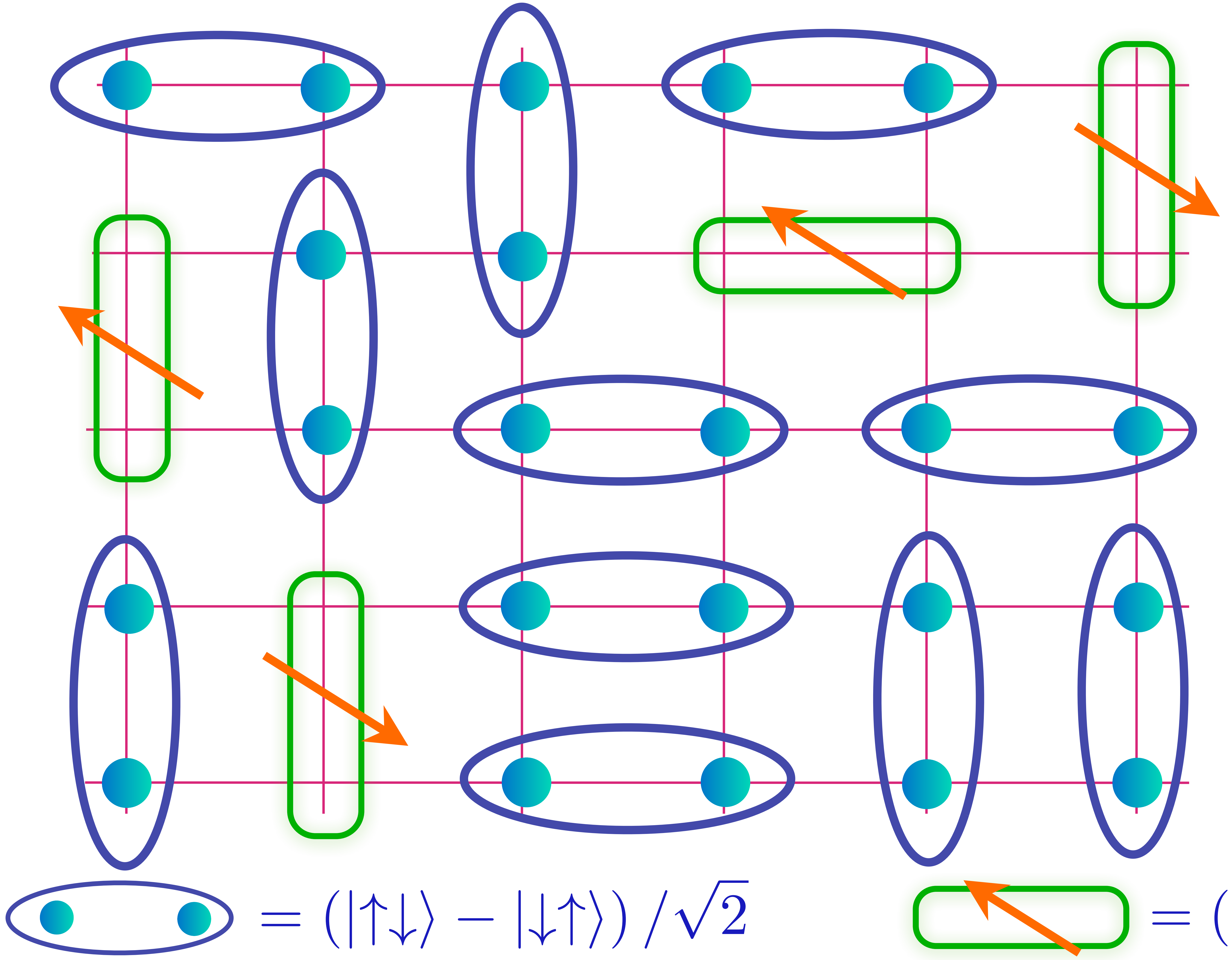

Metal with electron-like quasiparticles on a Fermi surface of size p, and emergent gauge fields

Spinon-holon bound state

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

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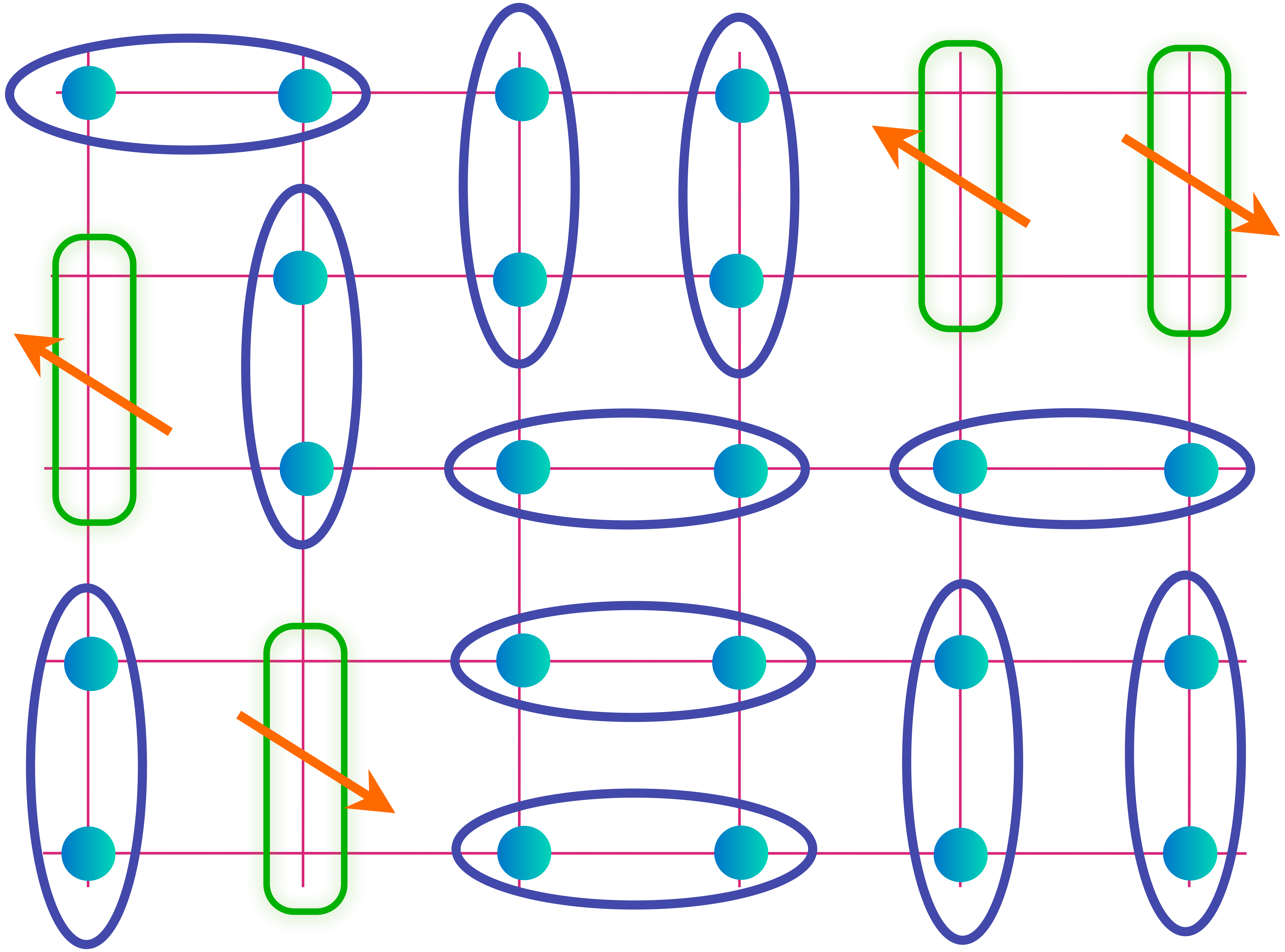

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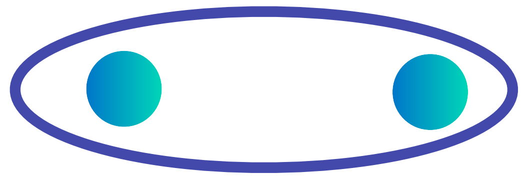

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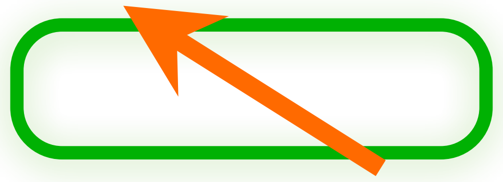

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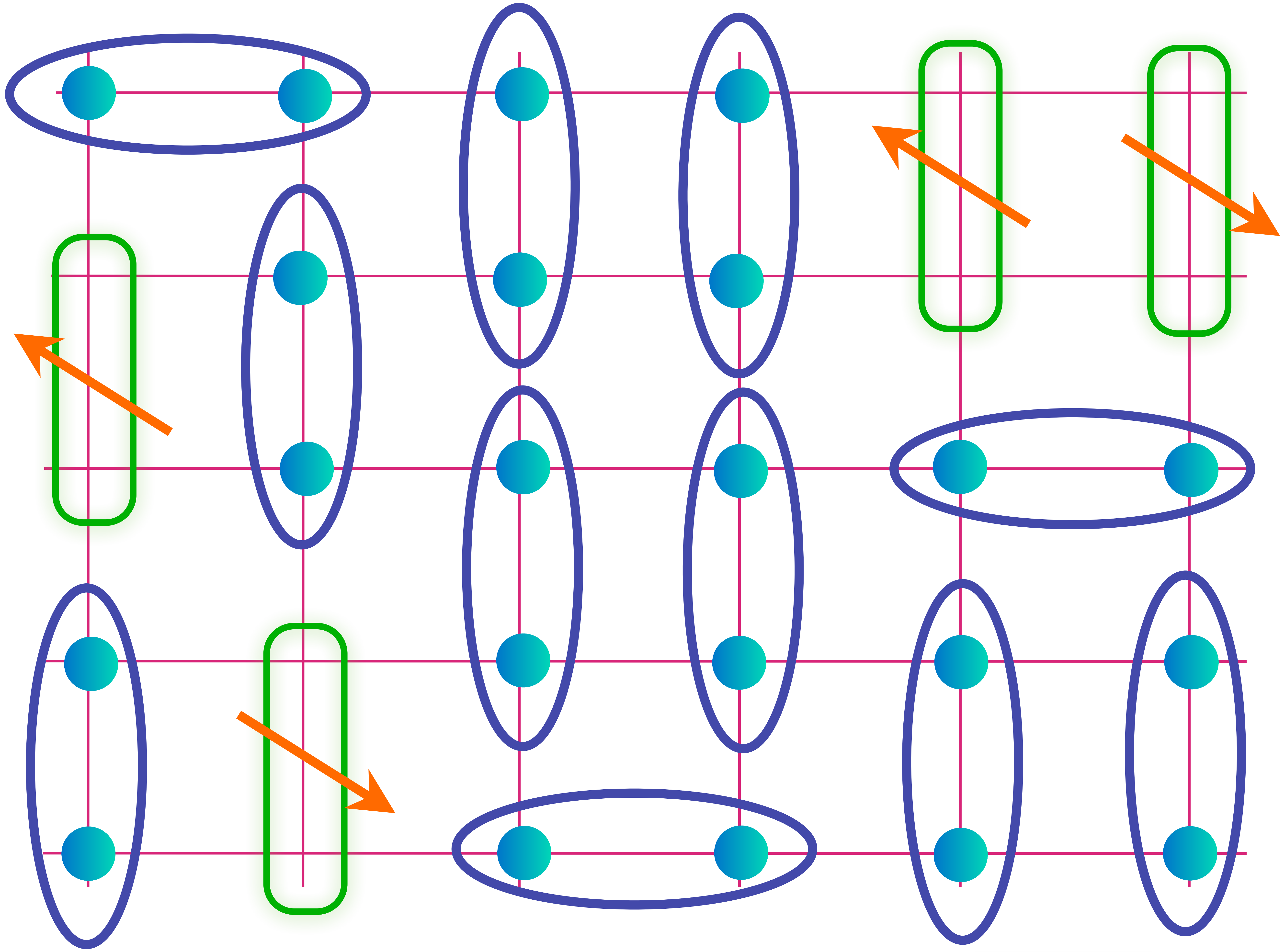

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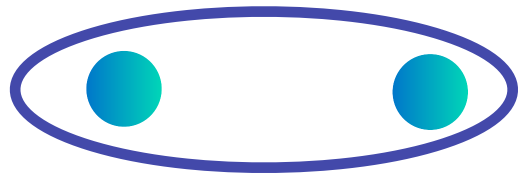
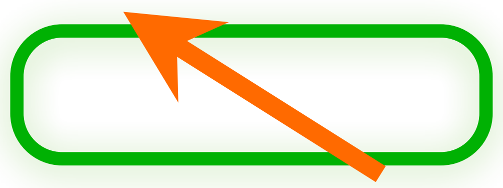
 $= \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)/\sqrt{2}$

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

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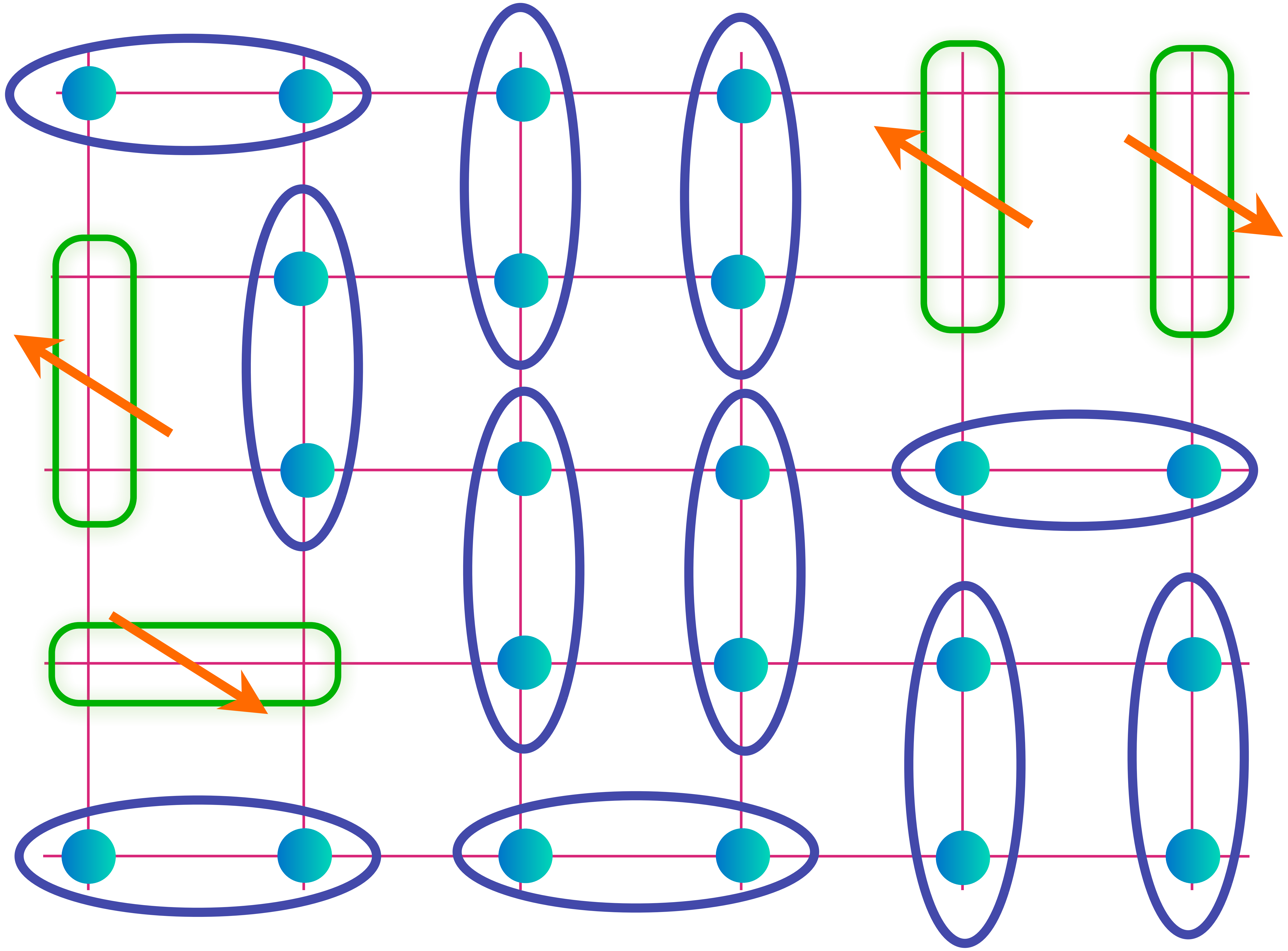

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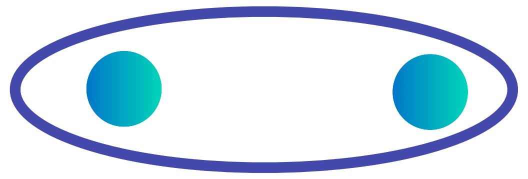
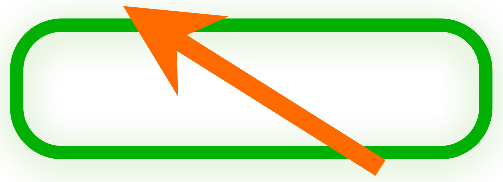
 $= \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) / \sqrt{2}$

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

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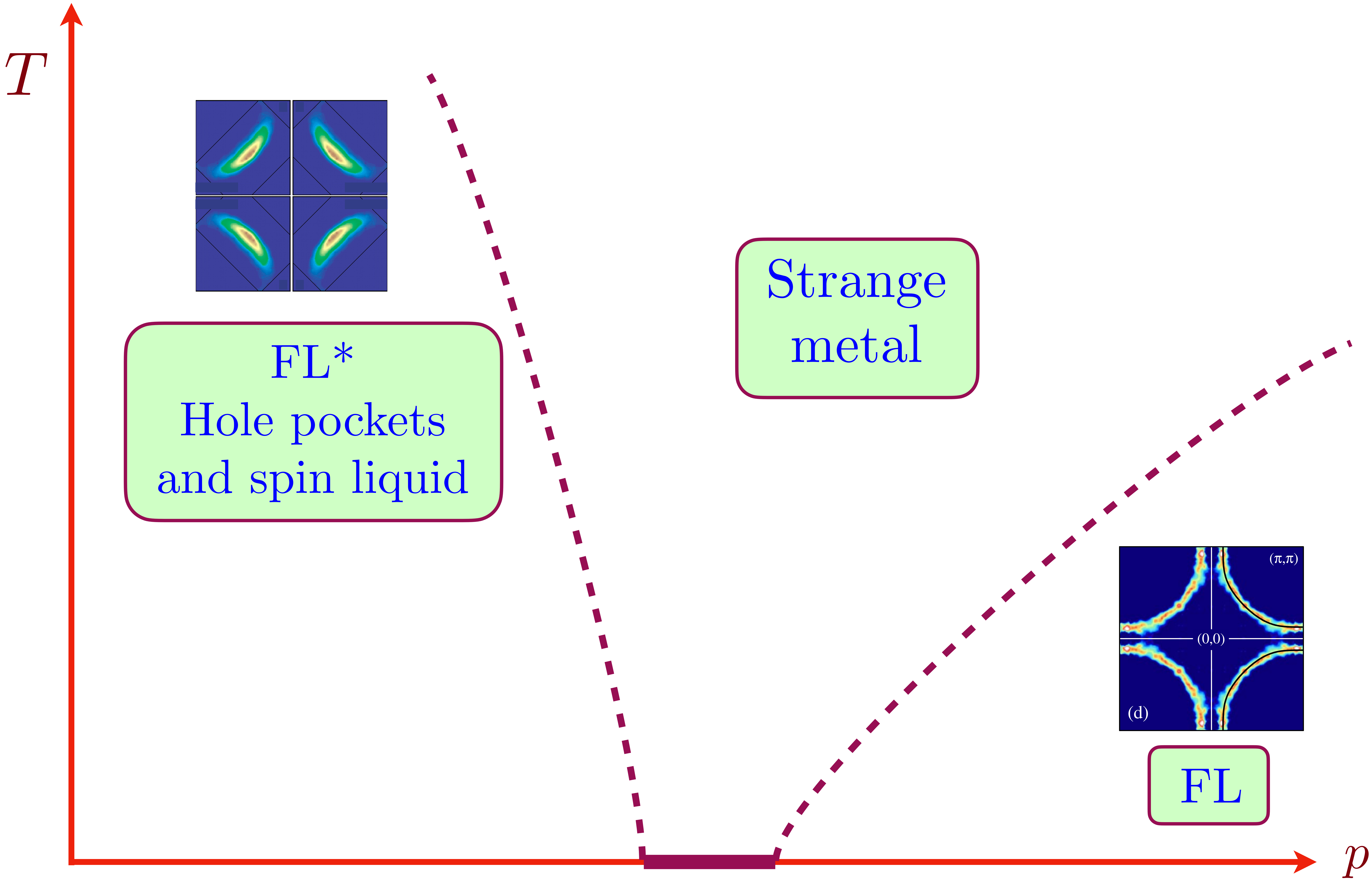
T
FL*
Hole pockets
and spin liquid
Strange
metal
(π,π)
(0,0)
(d)
FL
p

T
FL*
Hole pockets
and spin liquid
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(d)
FL
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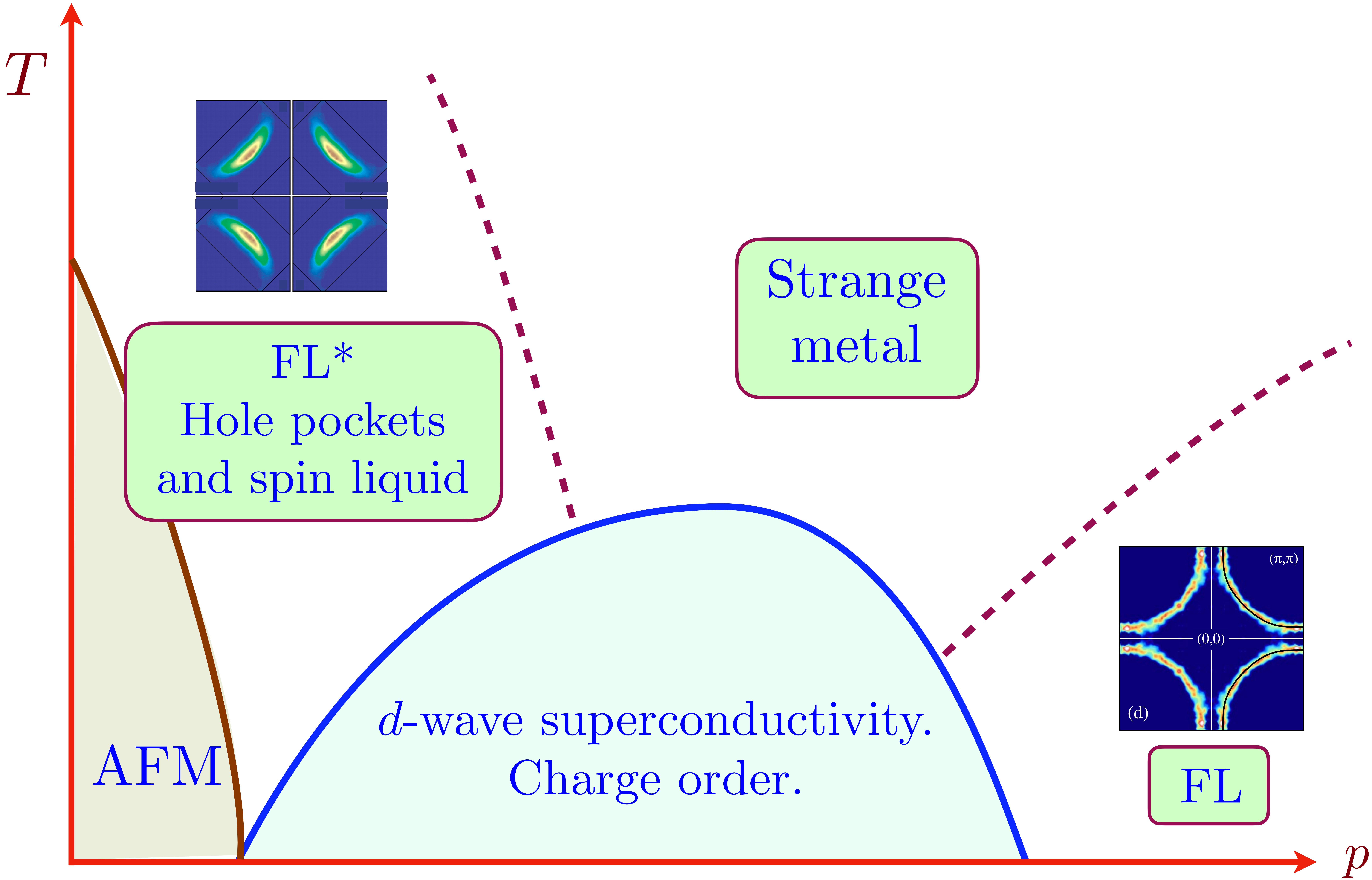
Patel,
Haoyu
Guo,
Esterlis,
Sachdev,
Science
381, 790
(2023)



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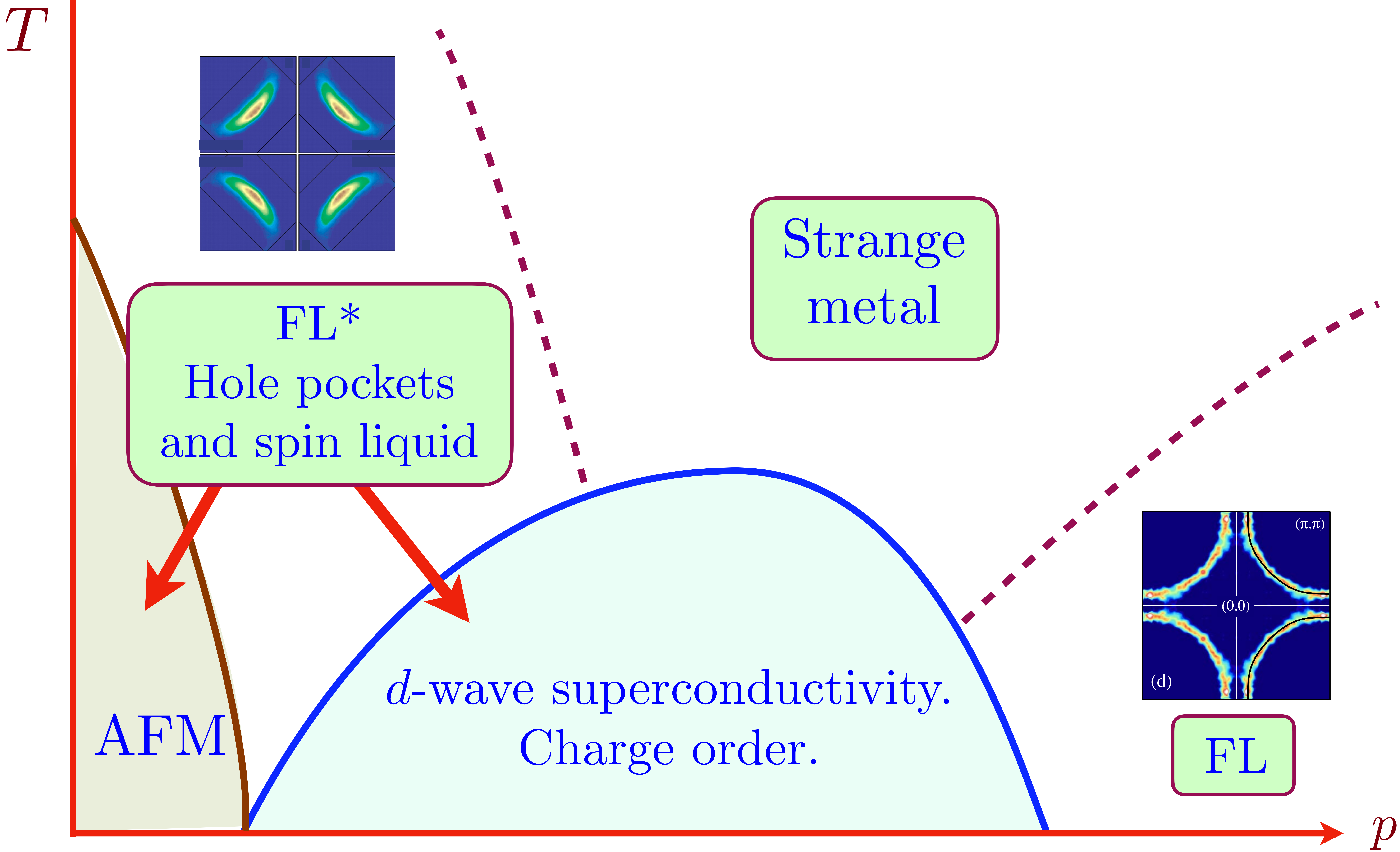
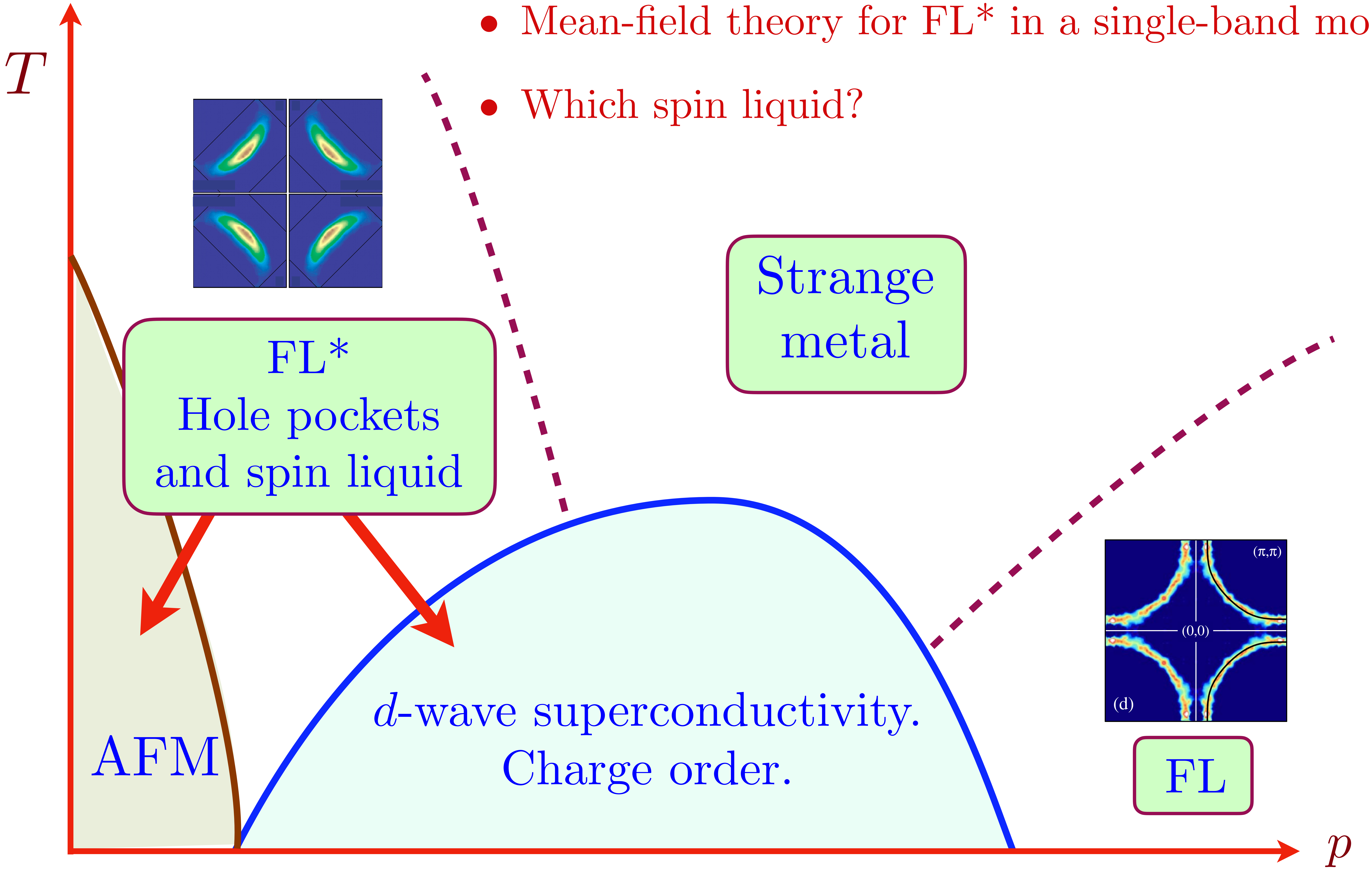
(d)
FL
p

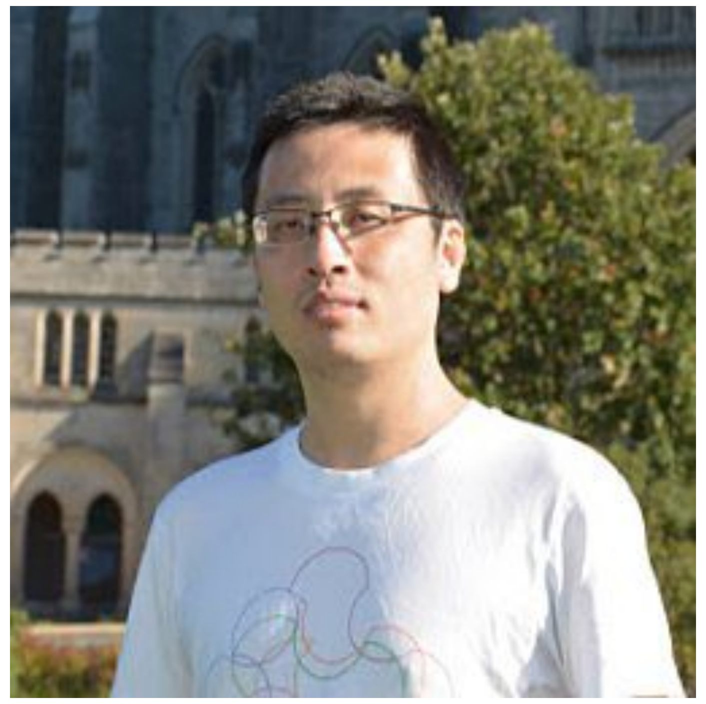
• Mean-field theory for FL* in a single-band model?



- Mean-field theory for FL* in a single-band model?
- Which spin liquid?



Ancilla theory of FL* in a single-band model



Ya-Hui Zhang

Paramagnon theory of the Hubbard model

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

We use the operator equation (valid on each site i):

$$U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) = -\frac{2U}{3}\boldsymbol{S}^2 + \frac{U}{4}$$

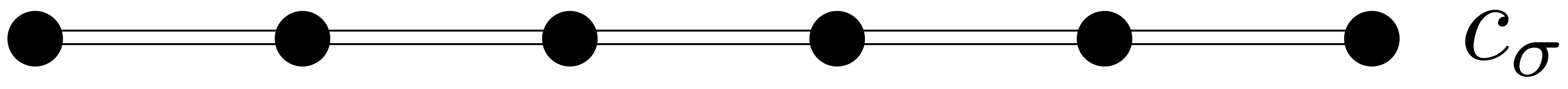
Then we decouple the interaction via

$$\exp\left(\frac{2U}{3}\sum_i \int d\tau \boldsymbol{S}_i^2\right) = \int \mathcal{D}\boldsymbol{\Phi}_i(\tau) \exp\left(-\sum_i \int d\tau \left[\frac{3}{8U}\boldsymbol{\Phi}_i^2 - \boldsymbol{\Phi}_i \cdot c_{i\sigma}^\dagger \frac{\boldsymbol{\tau}_{\sigma\sigma'}}{2} c_{i\sigma'}\right]\right)$$

This yields the 'Scalapino-Pines-Chubukov-Schmalian...' theory for a 'paramagnon quantum rotor' $\boldsymbol{\Phi}_i$ coupled to otherwise free fermions $c_{i\sigma}$.

$\boldsymbol{\Phi}_i$ is the creation/annihilation operator for charge 0, spin $S = 1$ particle.

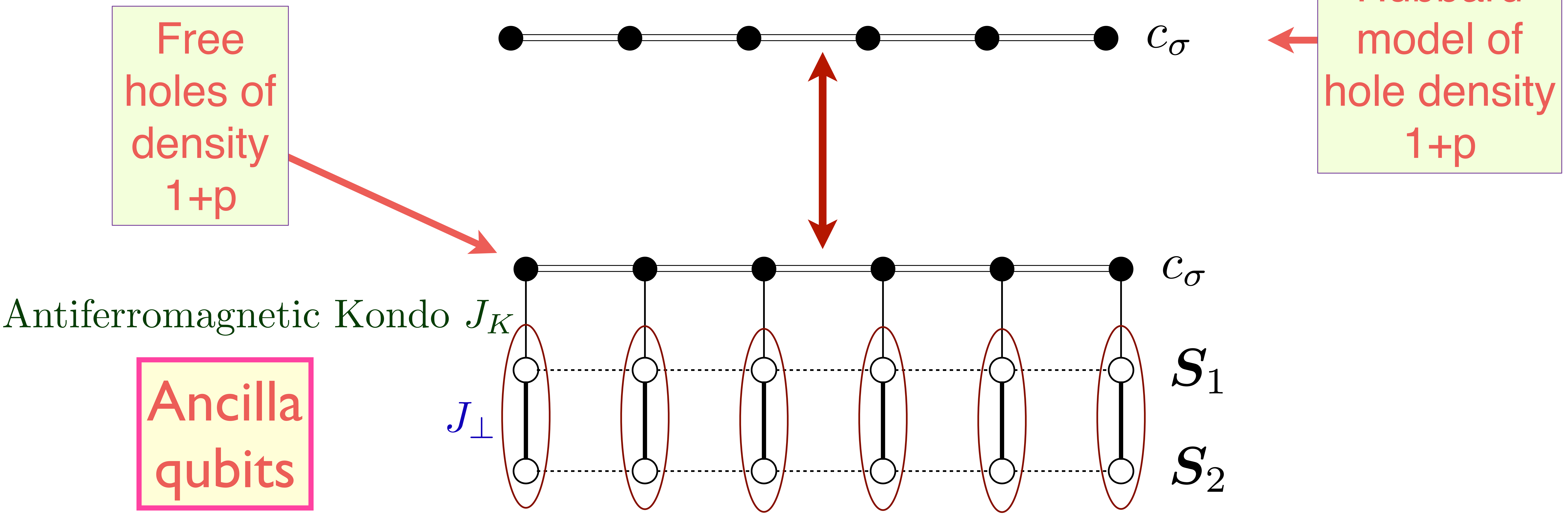
Ancilla theory of the Hubbard model



Hubbard model of hole density 1+p

Ancilla theory of the Hubbard model

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



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

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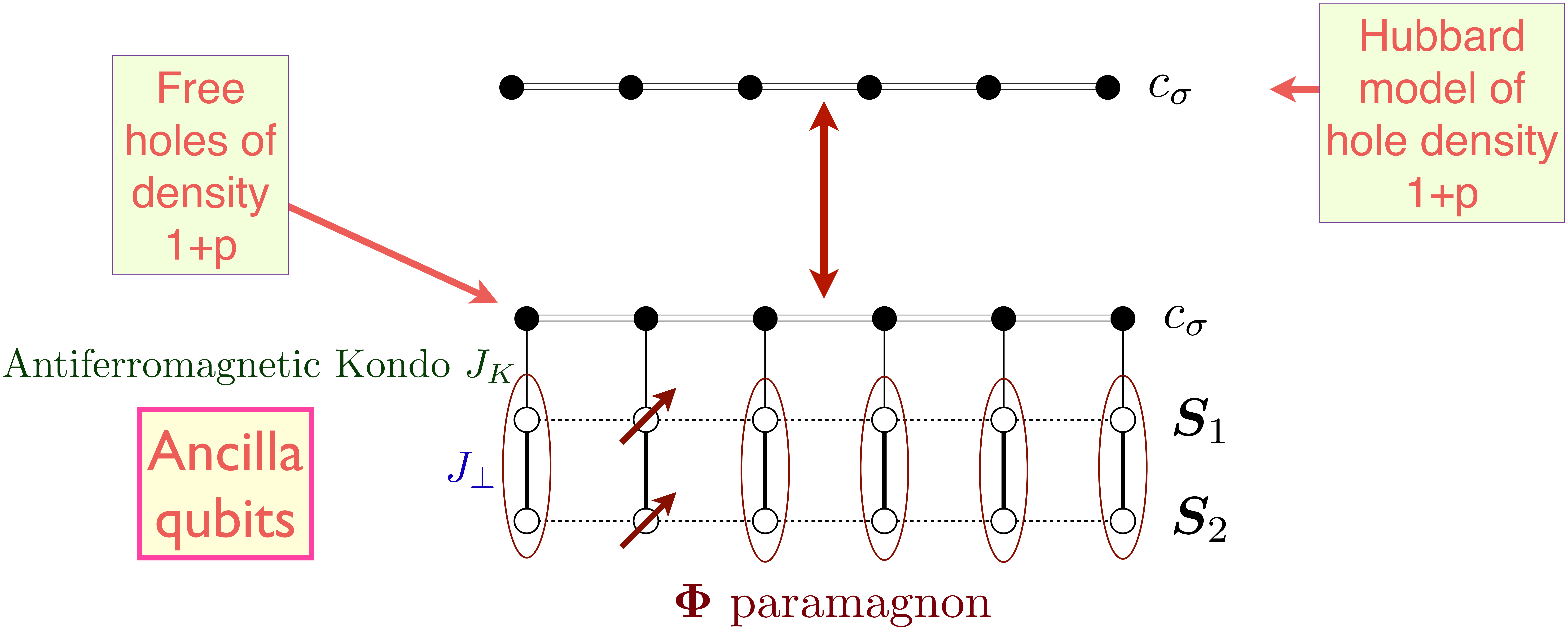

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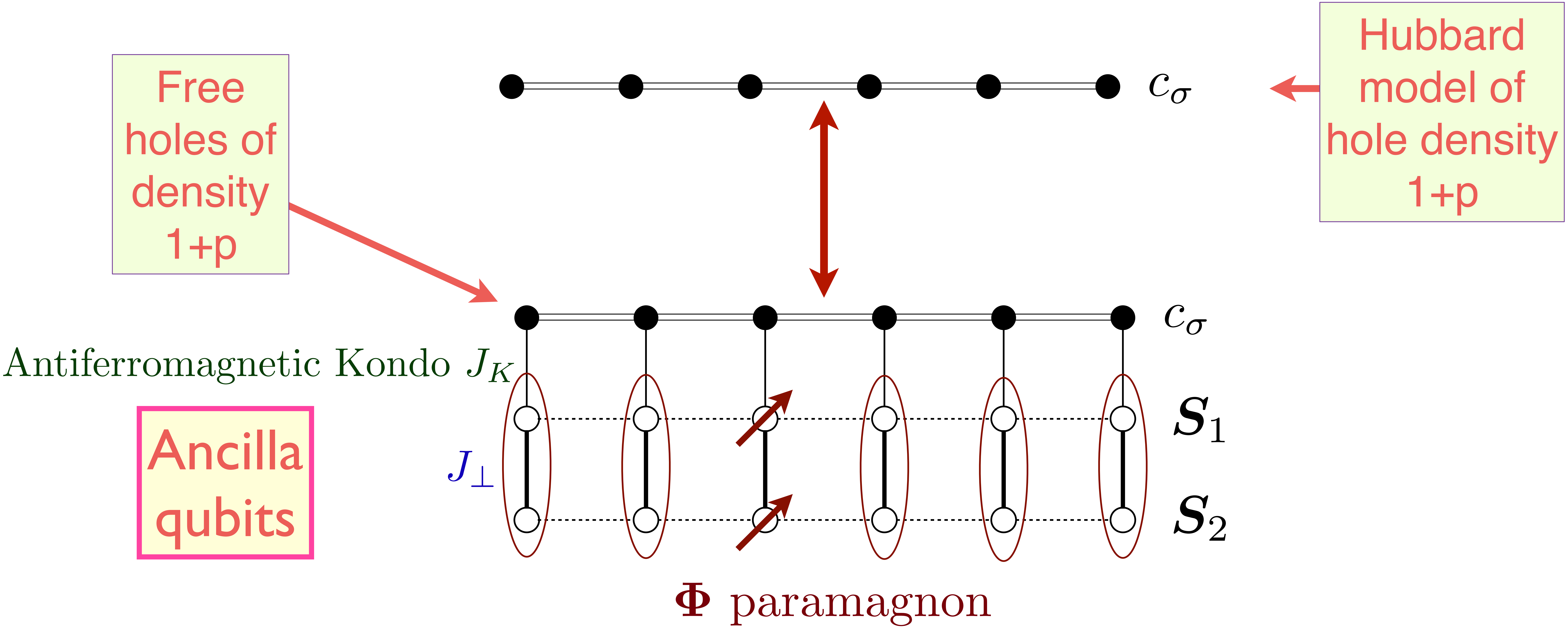

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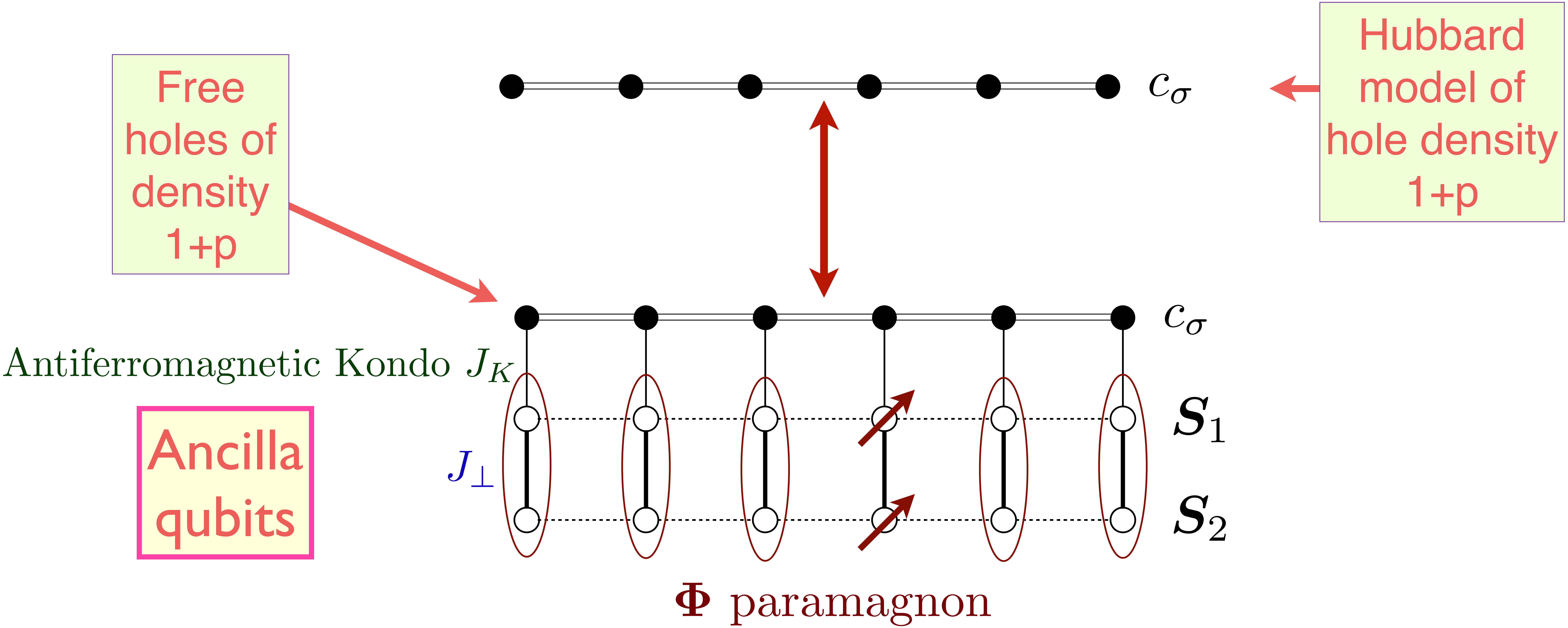

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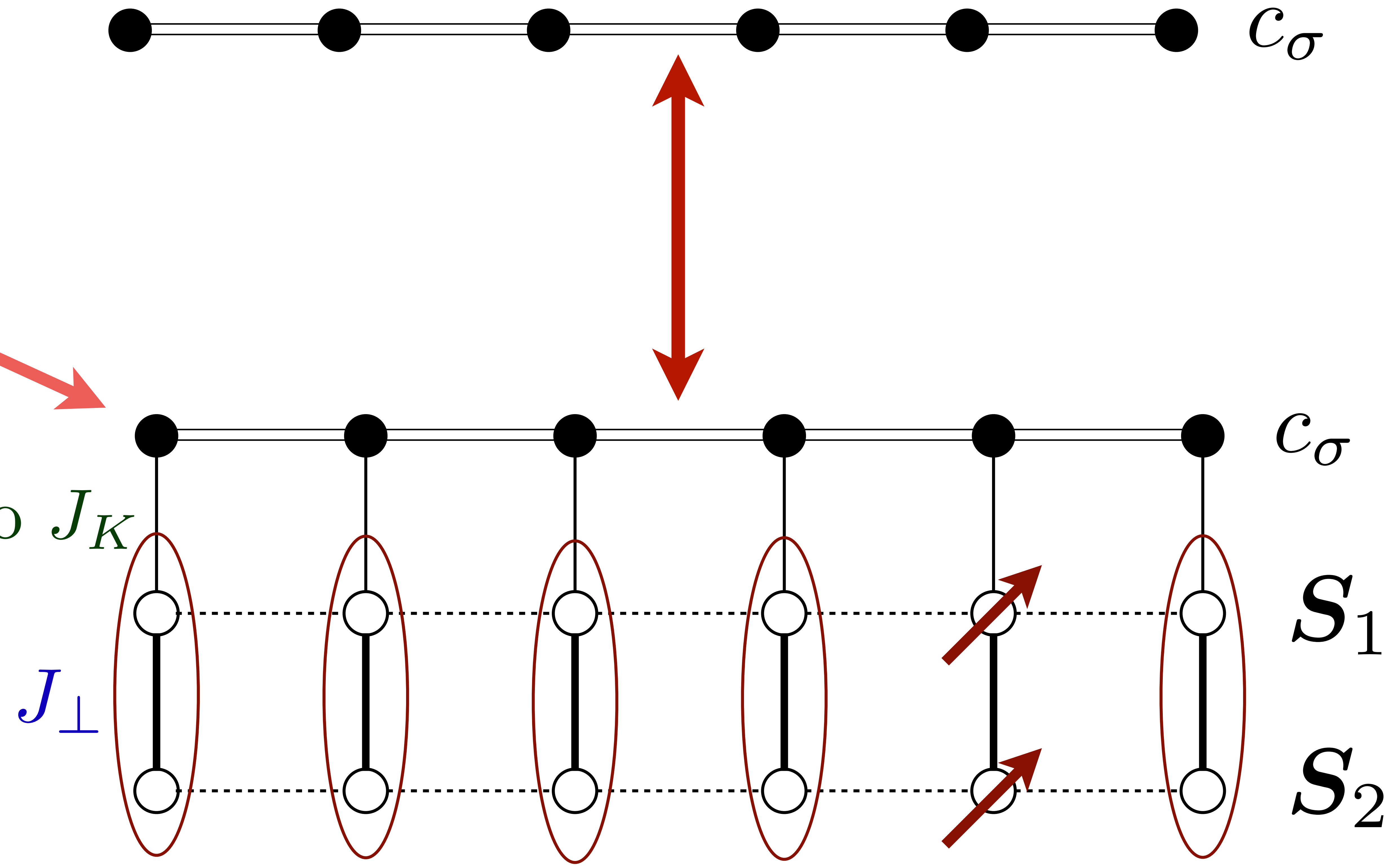
Free holes of density 1+p

Hubbard model of hole density 1+p



Antiferromagnetic Kondo J_K

Ancilla qubits

$\boldsymbol{\Phi}$ paramagnon

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

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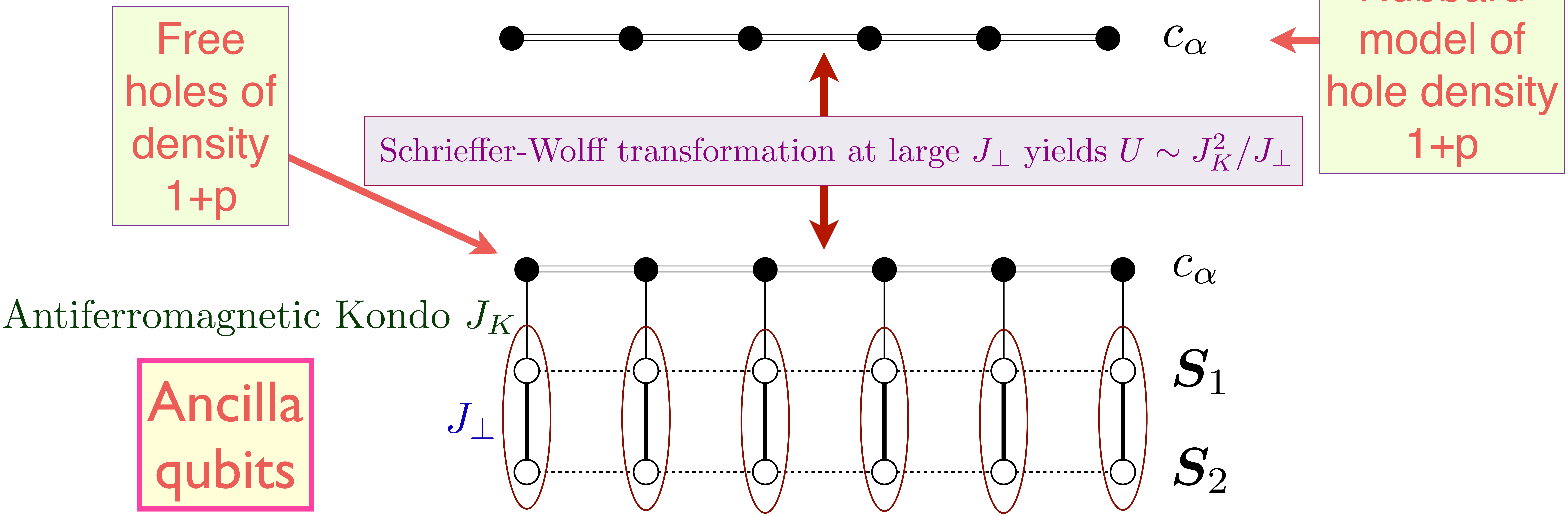

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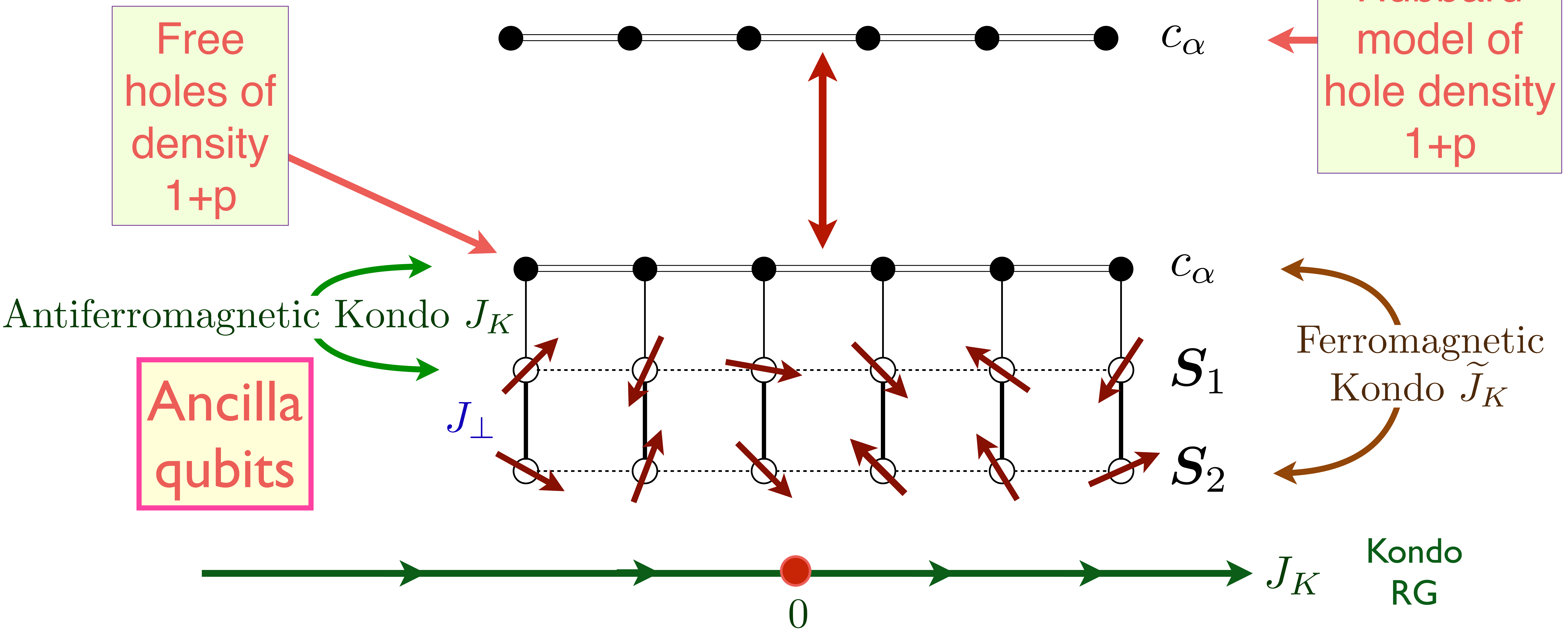
Ya-Hui Zhang and S. Sachdev, *Phys. Rev. Res.* **2**, 023172 (2020)

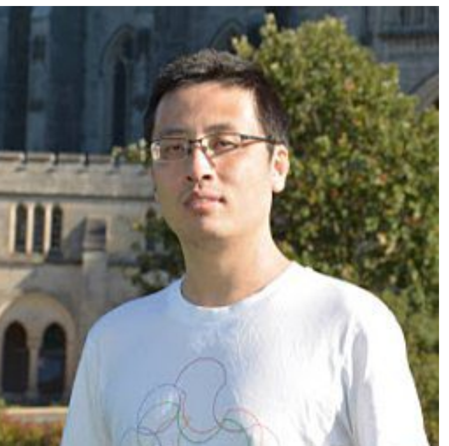


$$\mathcal{H}_{\text{ancilla}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\alpha} c_{\mathbf{p}\alpha} + J_K \sum_i c^\dagger_{i\alpha} \frac{\boldsymbol{\sigma}_{\alpha\alpha'}}{2} c_{i\alpha'} \cdot \boldsymbol{S}_{1i} + J_\perp \sum_i \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{2i}$$

Ancilla theory of the Hubbard model

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

Ya-Hui
Zhang



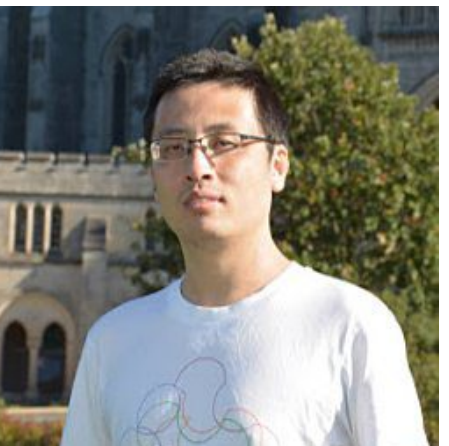
Ancilla theory of the Hubbard model

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

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

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

Ya-Hui Zhang



Ancilla theory of the Hubbard model

Henry Shackleton

To appear: numerical results from this variational wavefunction

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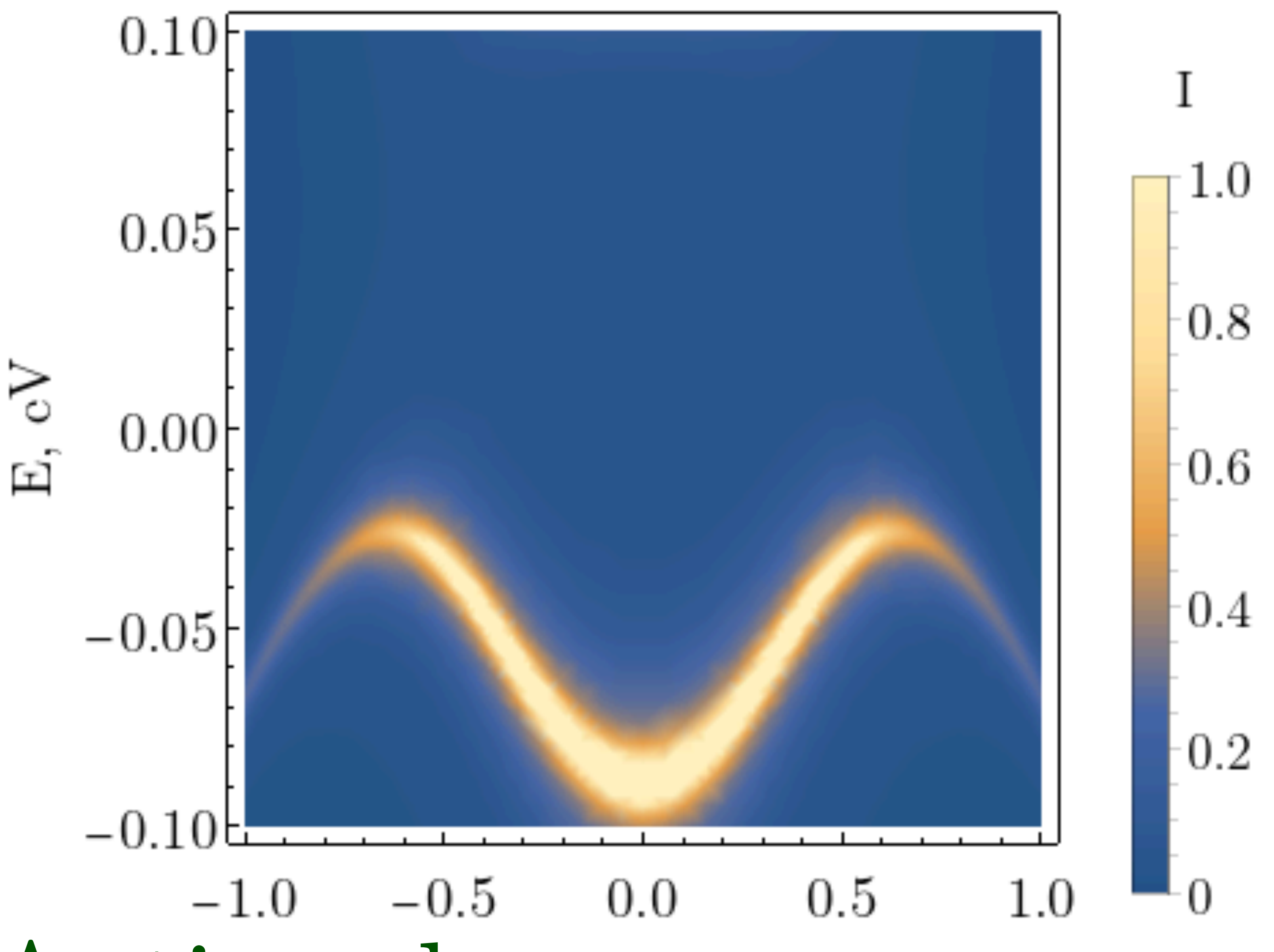
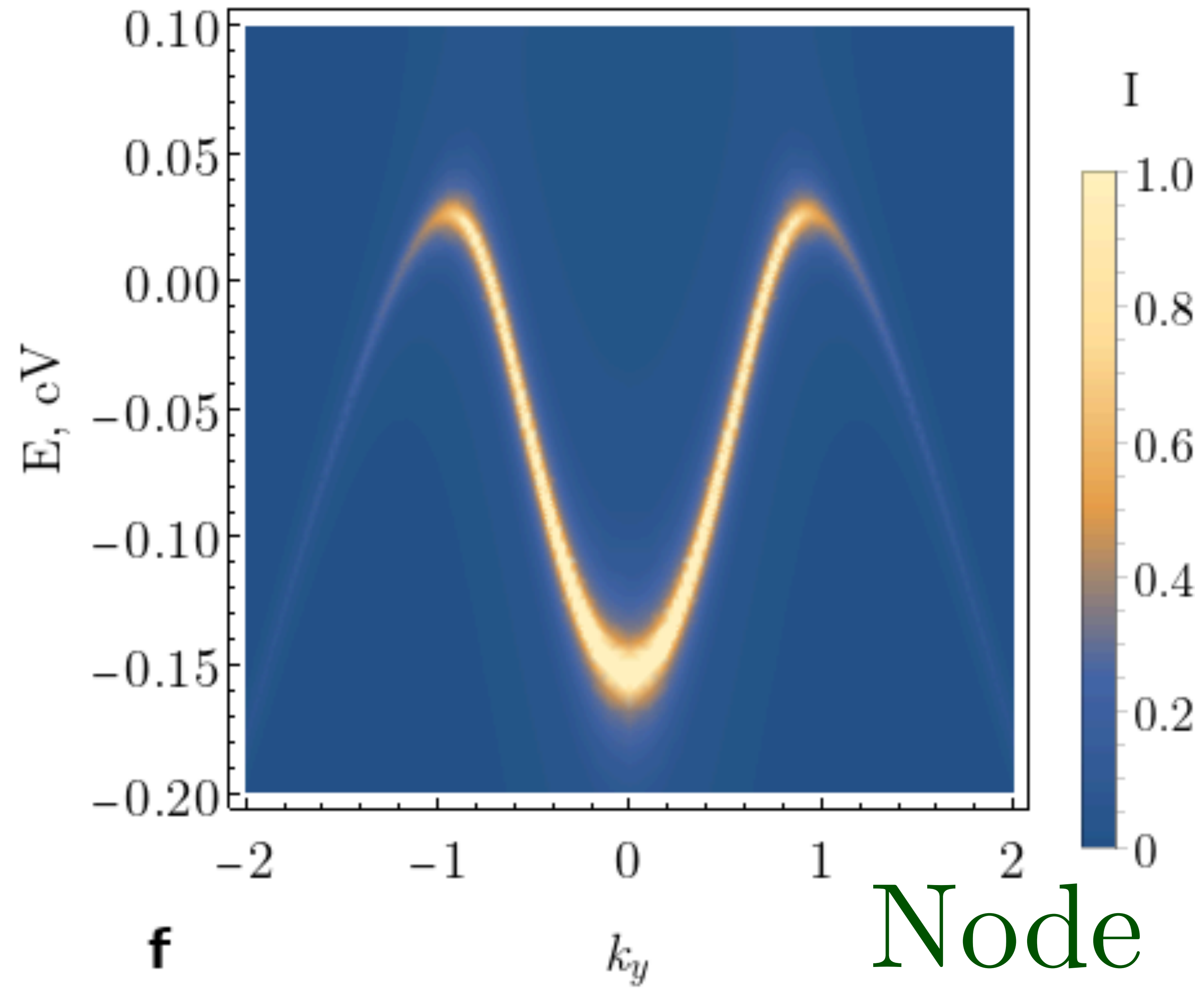
Mascot, Nikolaenko, Tikhanovskaya, Zhang, Morr, and Sachdev, *Phys. Rev. B* **105**, 075146 (2022)

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

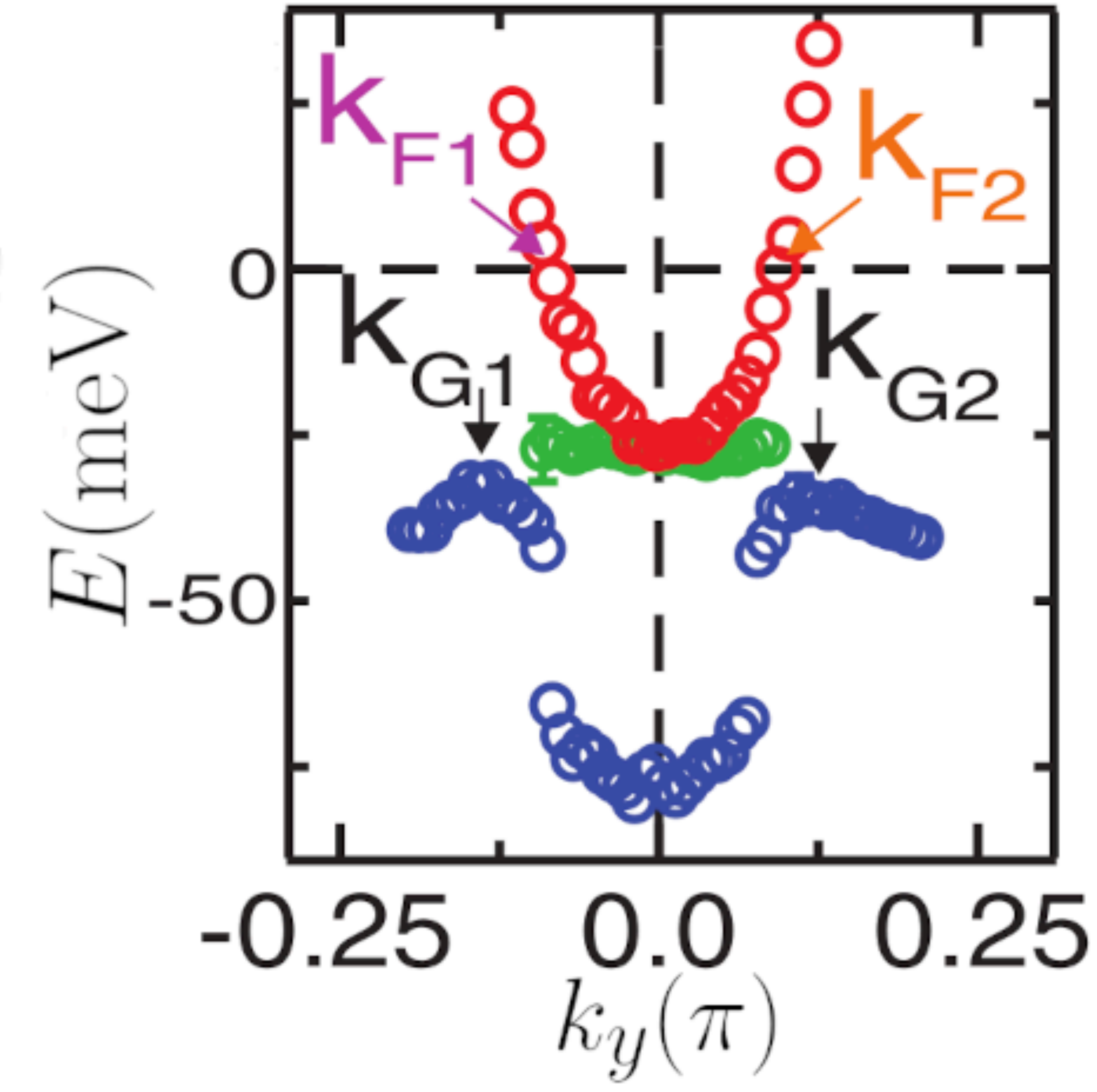


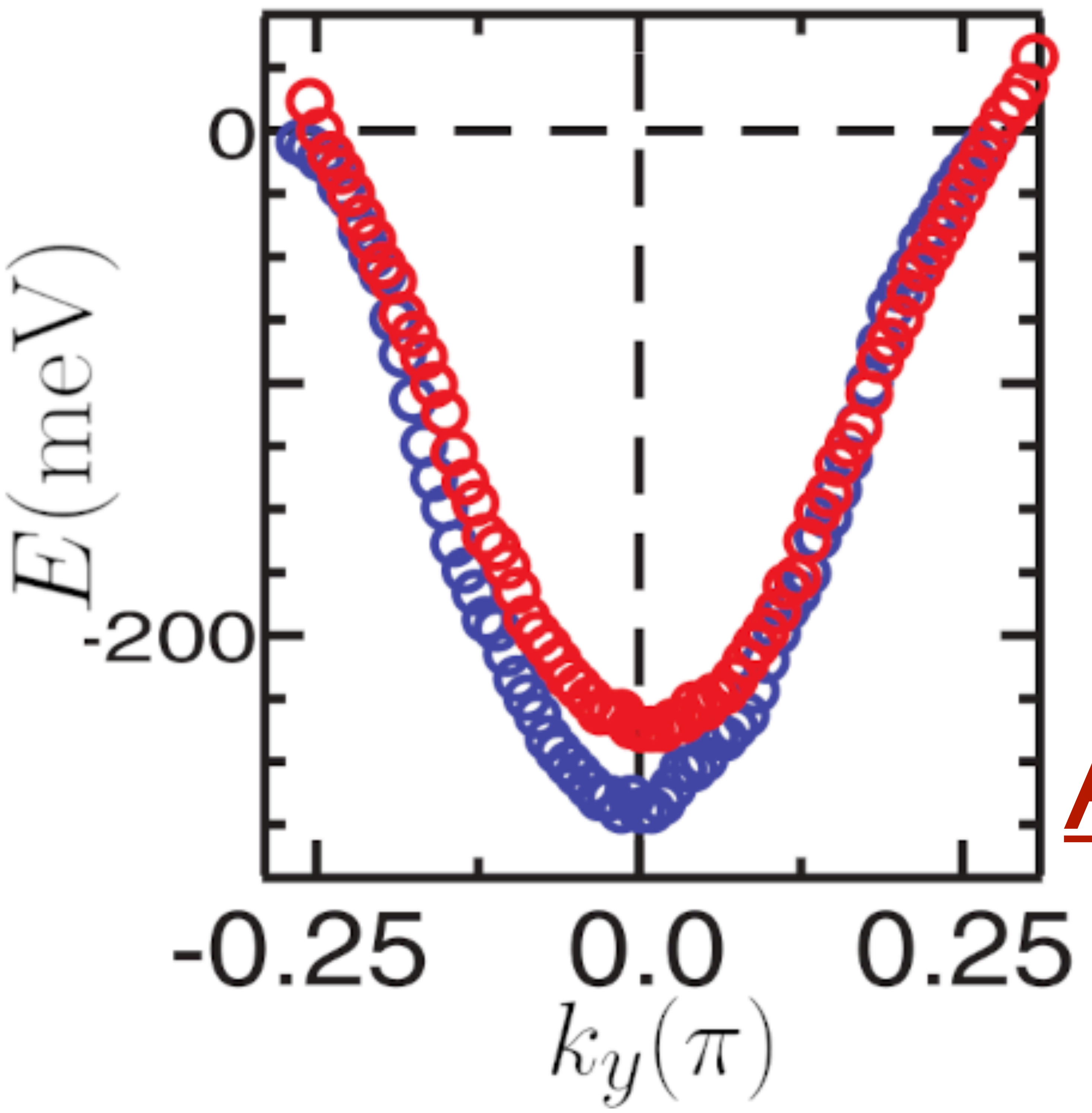
Anti-node



Node

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



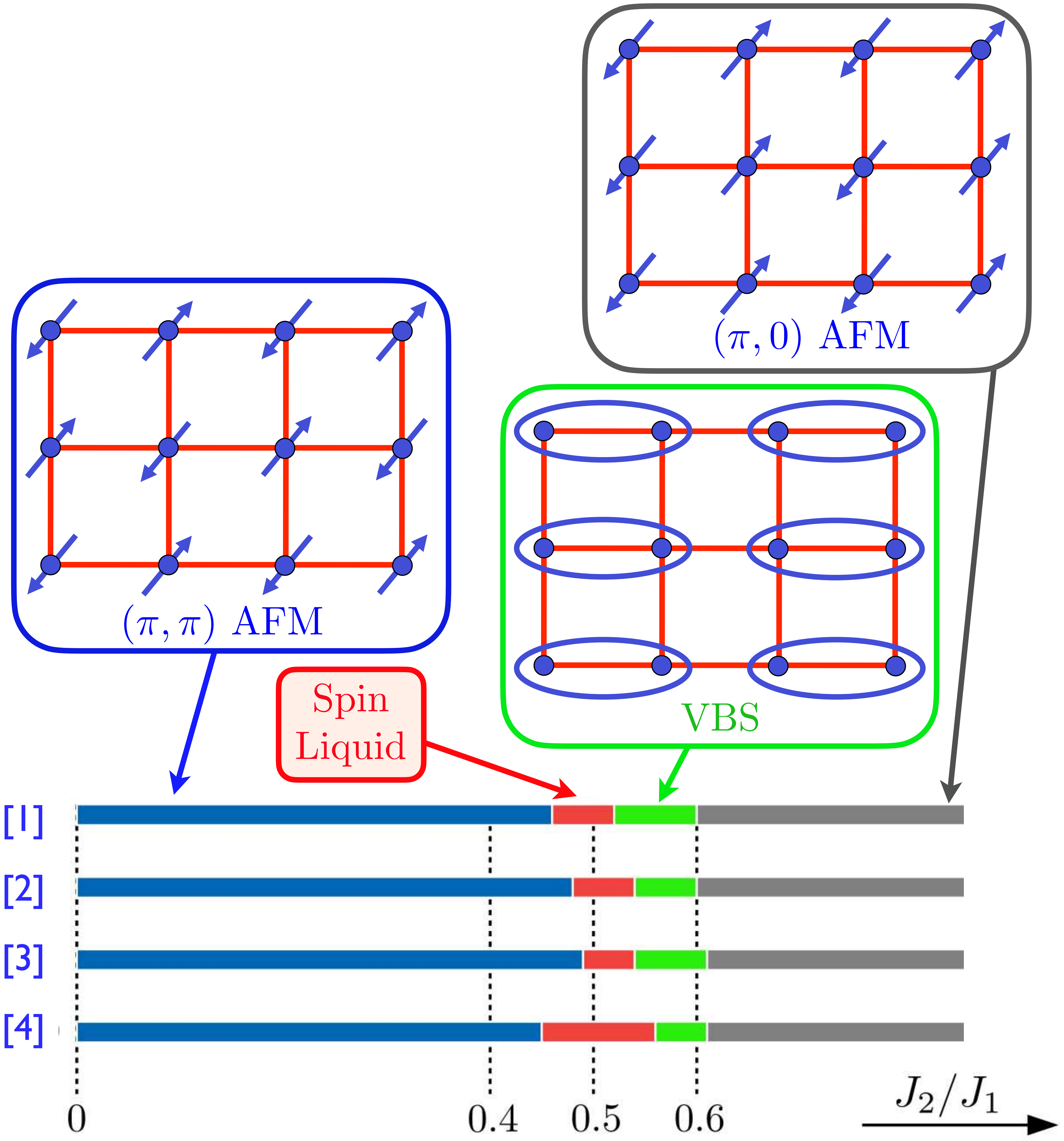


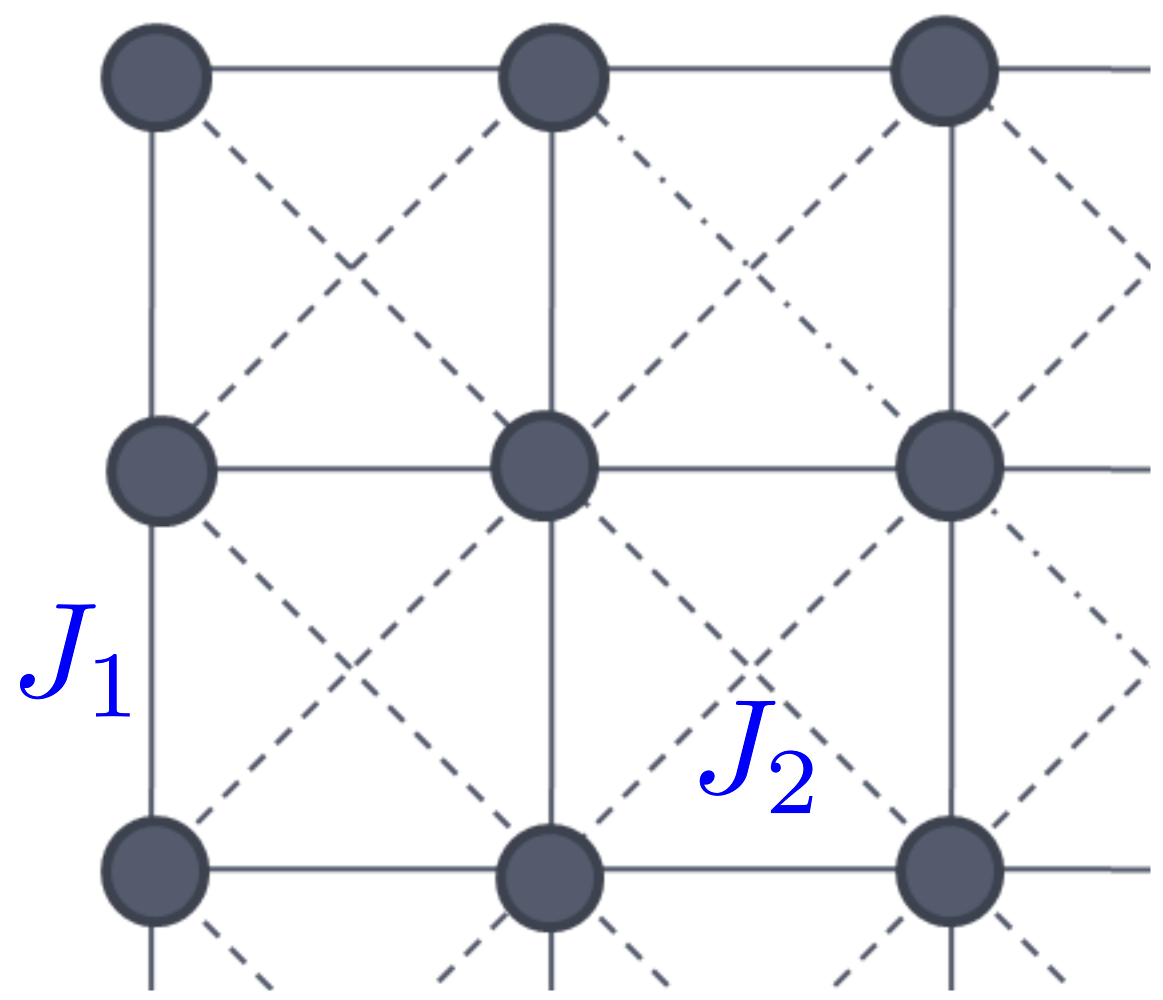
He, Hashimoto, Karapetyan, Koralek, Hinton, Testaud, Nathan, Yoshida, Yao, Tanaka, Meevasana, Moore, Lu, Mo, Ishikado, Eisaki, Hussain, Devereaux, Kivelson, Orenstein, Kapitulnik, and Shen, *Science* **331**, 1579 (2011)

ARPES on Bi2201

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)

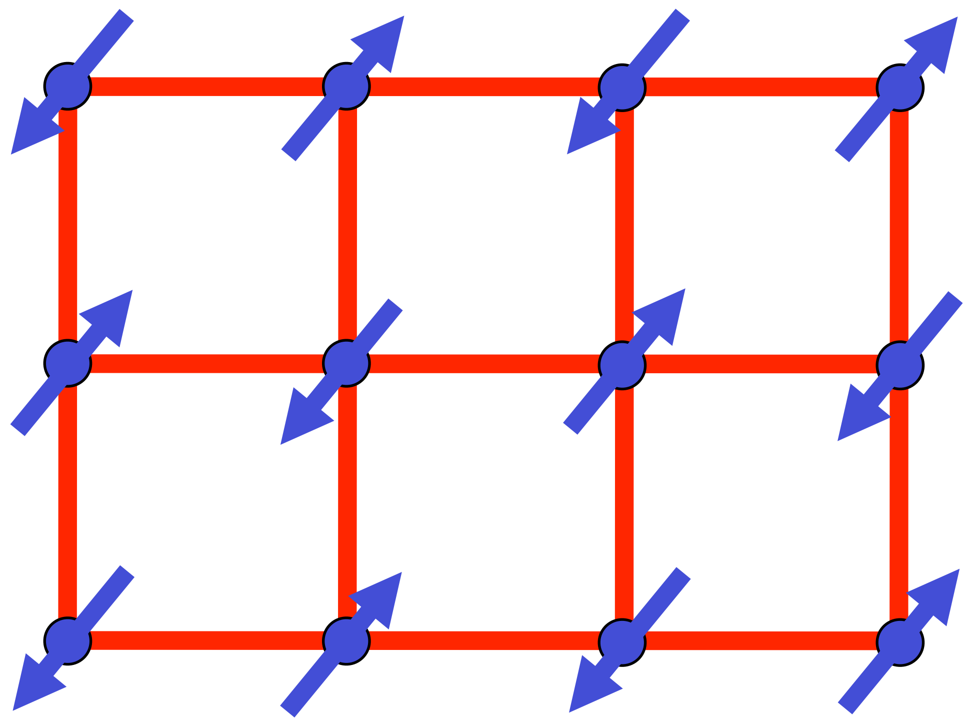
Insulating S=1/2 antiferromagnet

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

Schwinger bosons

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

Mean-field spin liquid
with gapped bosonic spinons.



$\langle b_\alpha \rangle \neq 0$:
Néel order

$\langle b_\alpha \rangle = 0$:
Spin liquid

s

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

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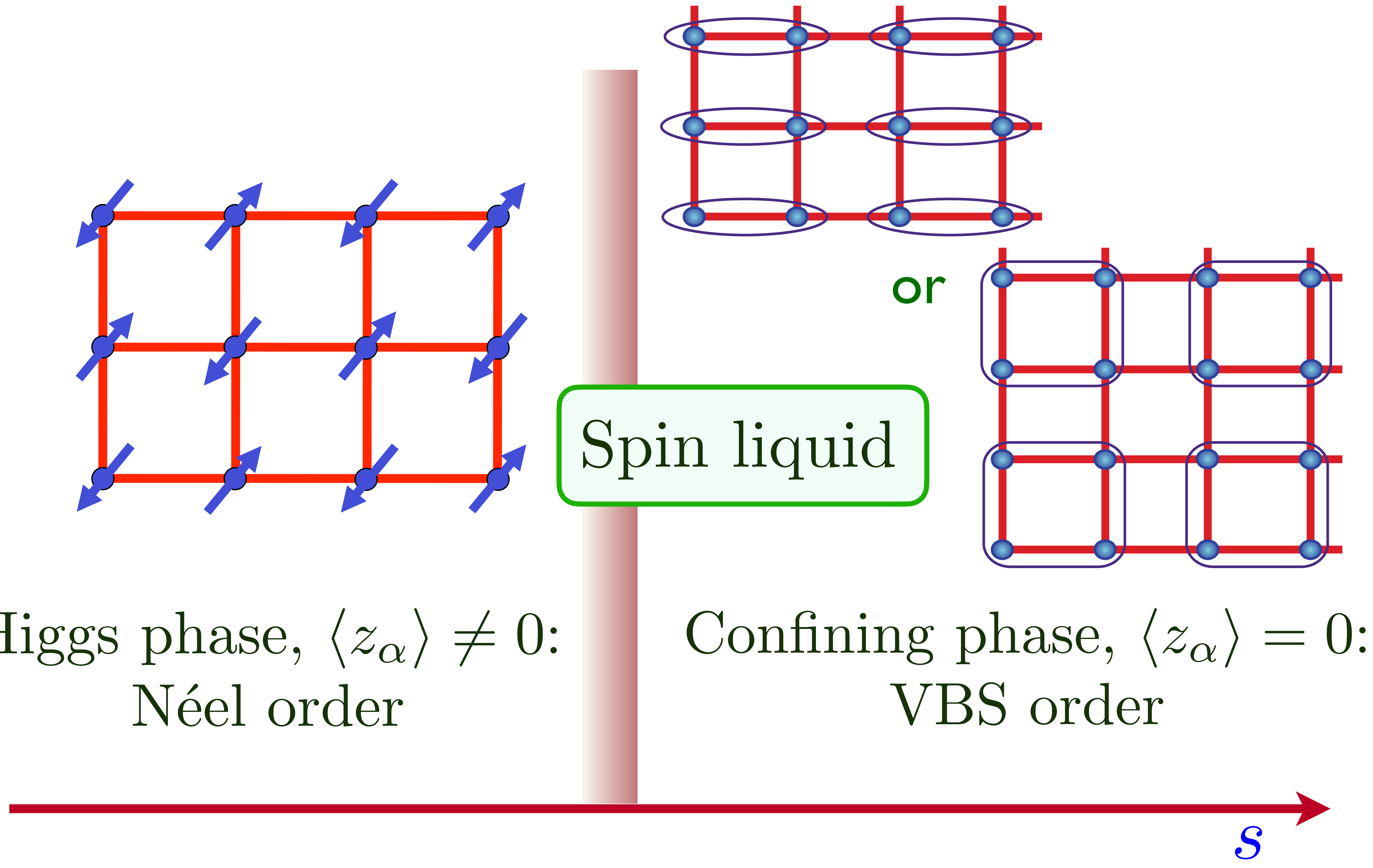

Low energy $\mathbb{CP}^1$ U(1) gauge theory

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

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

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

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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)

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

S=1/2 square lattice anti-ferromagnet

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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)

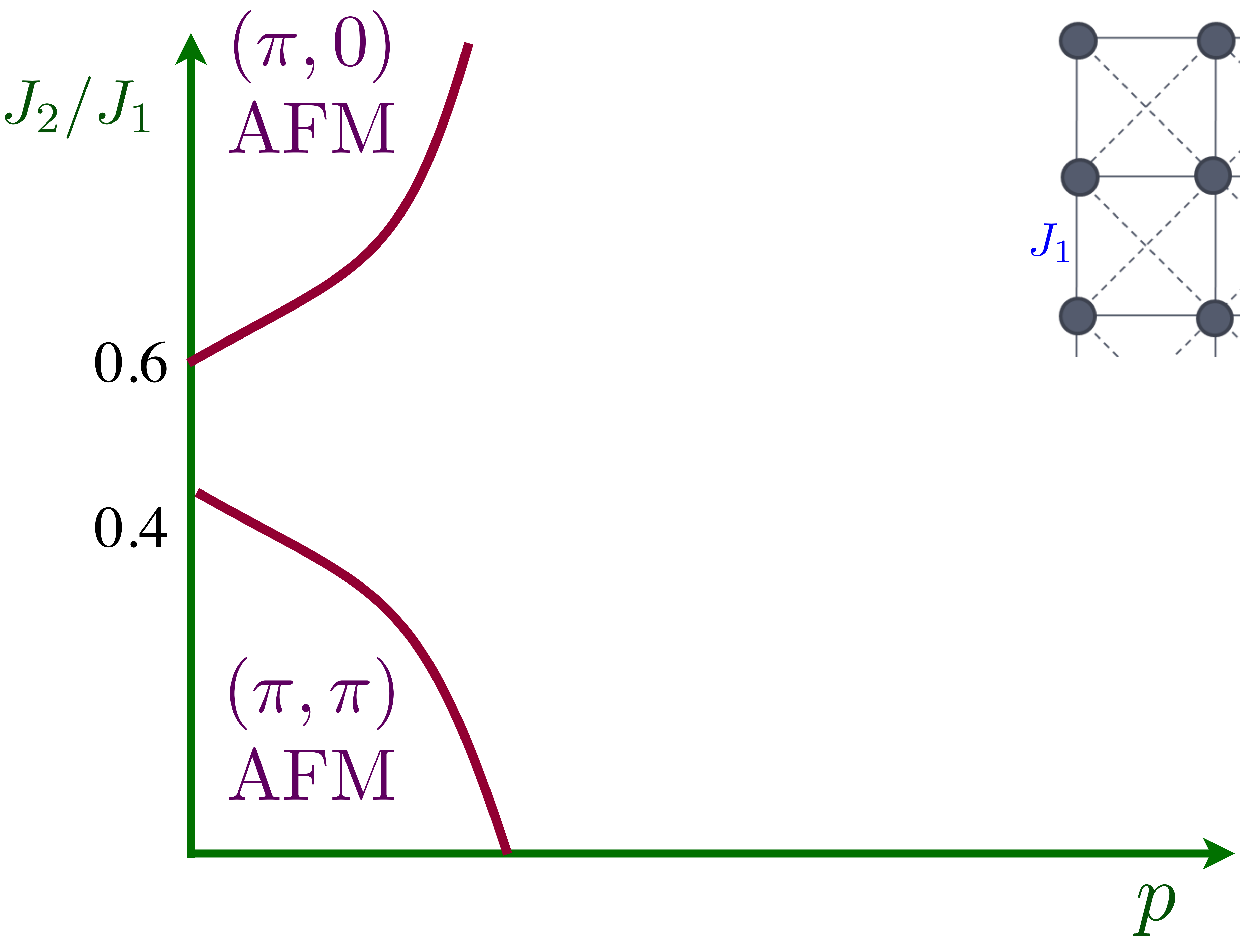
Adam Nahum, P. Serna, J. T. Chalker, M. Ortuño, and A. M. Somoza, *Phys. Rev. Lett.* **115**, 267203 (2015)

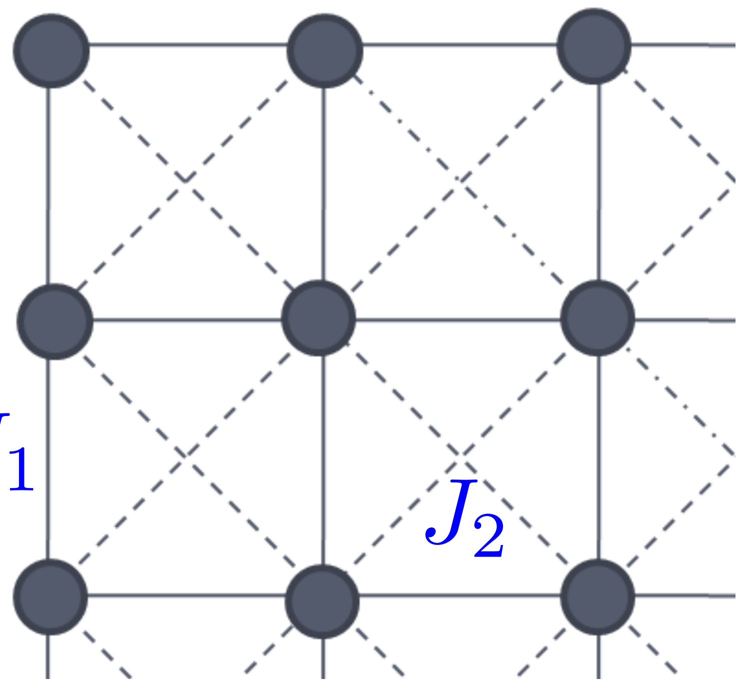
Z. Zhou, L. Hu, W. Zhu, and Yin-Chen He, arXiv:2306.16435

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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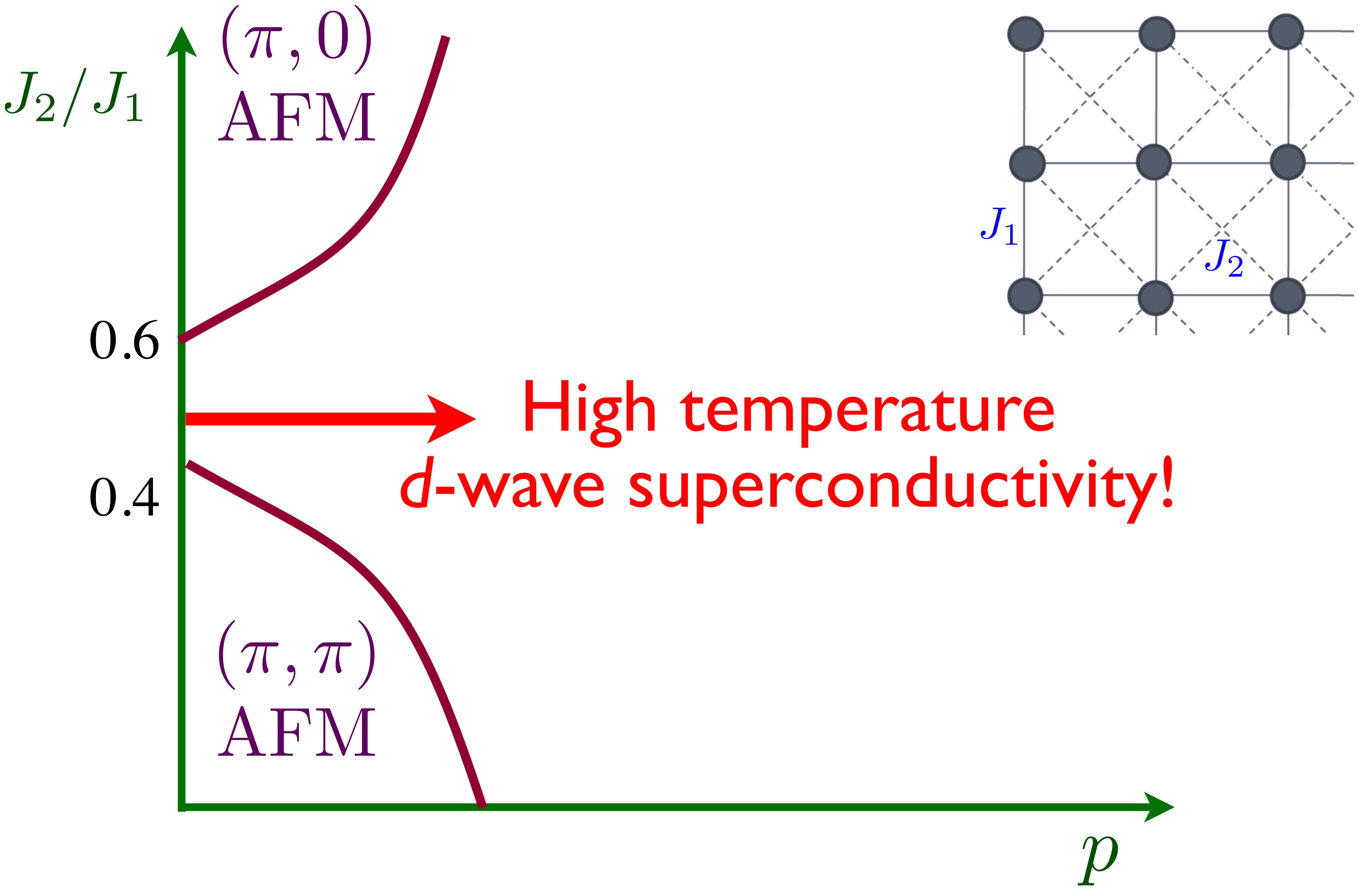

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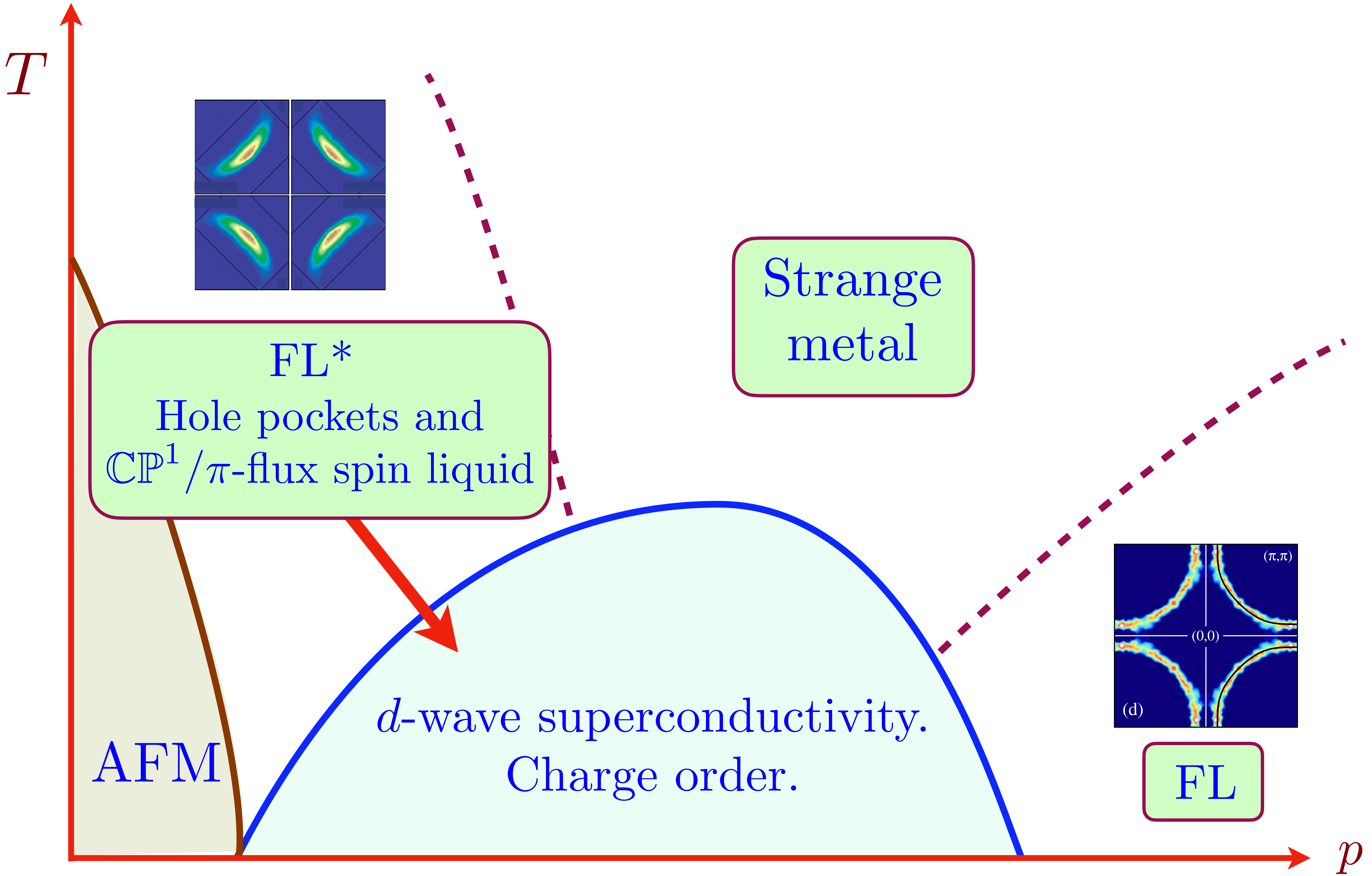
From CP^1/π-flux FL*

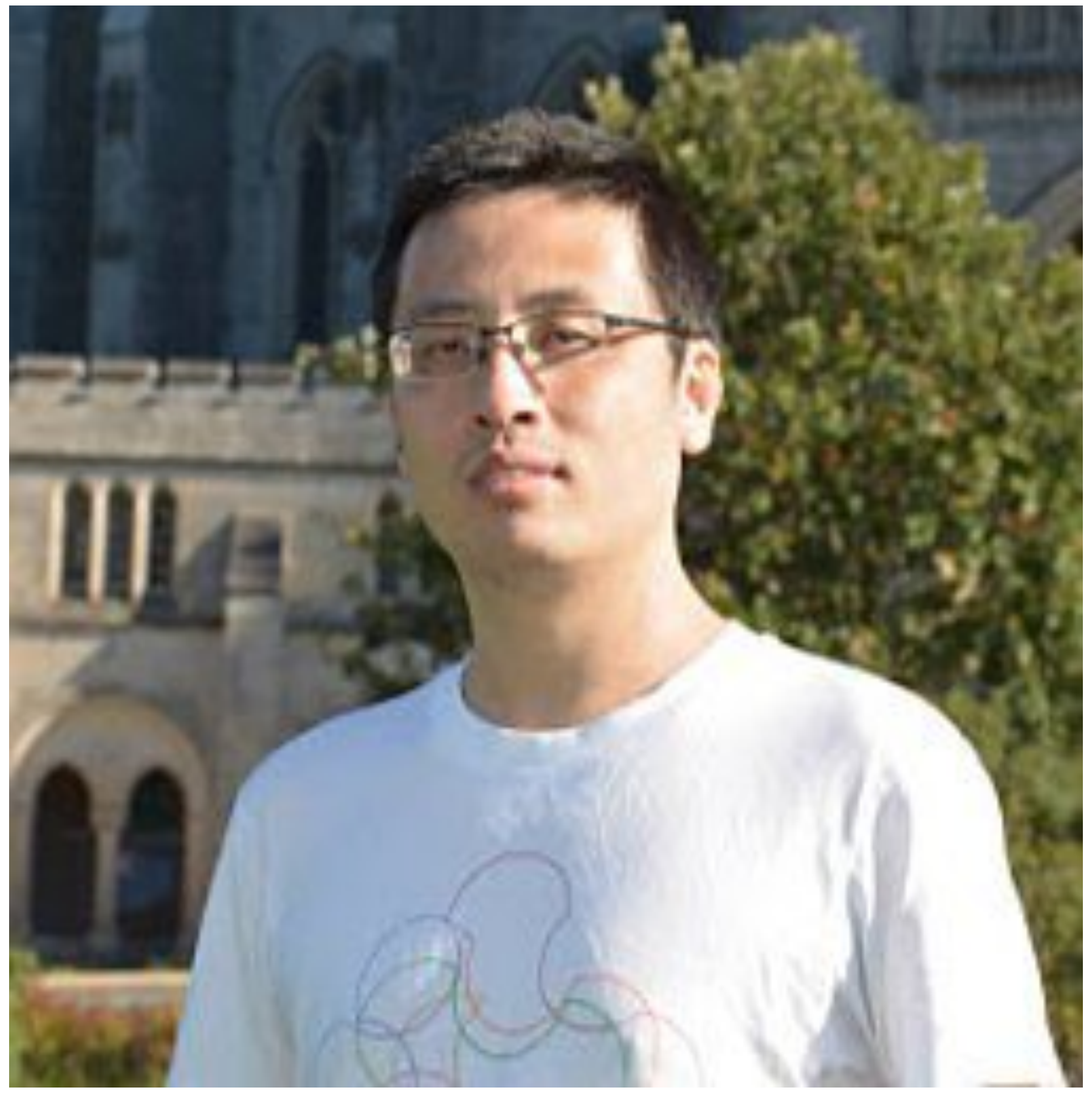
to

d-wave superconductivity

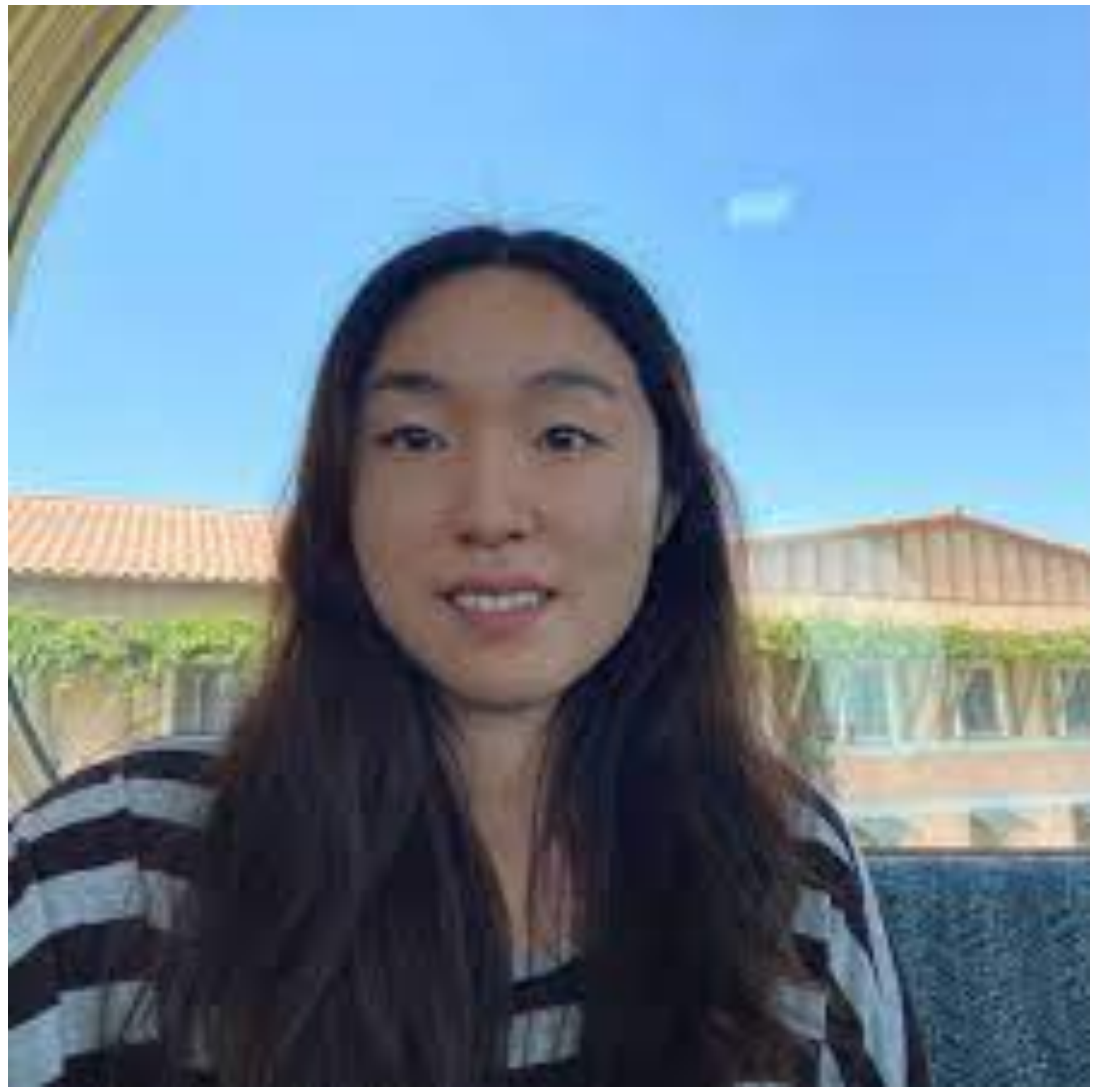


T
FL*
Hole pockets and
$\mathbb{CP}^1/\pi$-flux spin liquid
Strange
metal
(π,π)
(0,0)
(d)
AFM
d-wave superconductivity.
Charge order.
FL
p

Maine Christos



Ya-Hui Zhang



Zhu-Xi Luo

Mathias Scheurer

Henry Shackleton

Ancilla theory of the Hubbard model

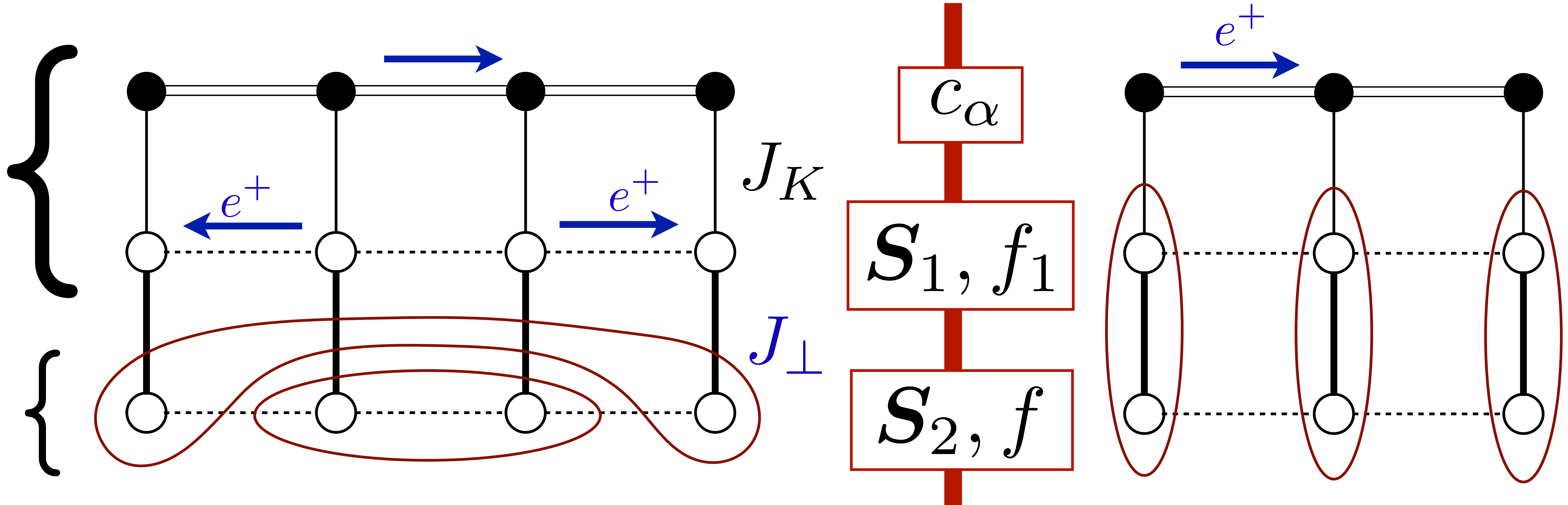
Ancilla theory of the Hubbard model

Higgs field Φ drives FL*-strange metal-FL

Ancilla theory of the Hubbard model

Higgs field 1
$\Phi \sim c_\alpha^\dagger f_{1\alpha}$
$\langle \Phi \rangle \neq 0$

π-flux spin liquid of f_α with $\mathrm{SU}(2)_N$ gauge field



FL*

FL

Higgs field 2
Charge e, $\mathrm{SU}(2)_N$ fundamental

$$B \sim \begin{pmatrix} f_{1\alpha}^\dagger f_\alpha \\ \varepsilon_{\alpha\beta} f_{1\alpha}^\dagger f_\beta^\dagger \end{pmatrix}$$

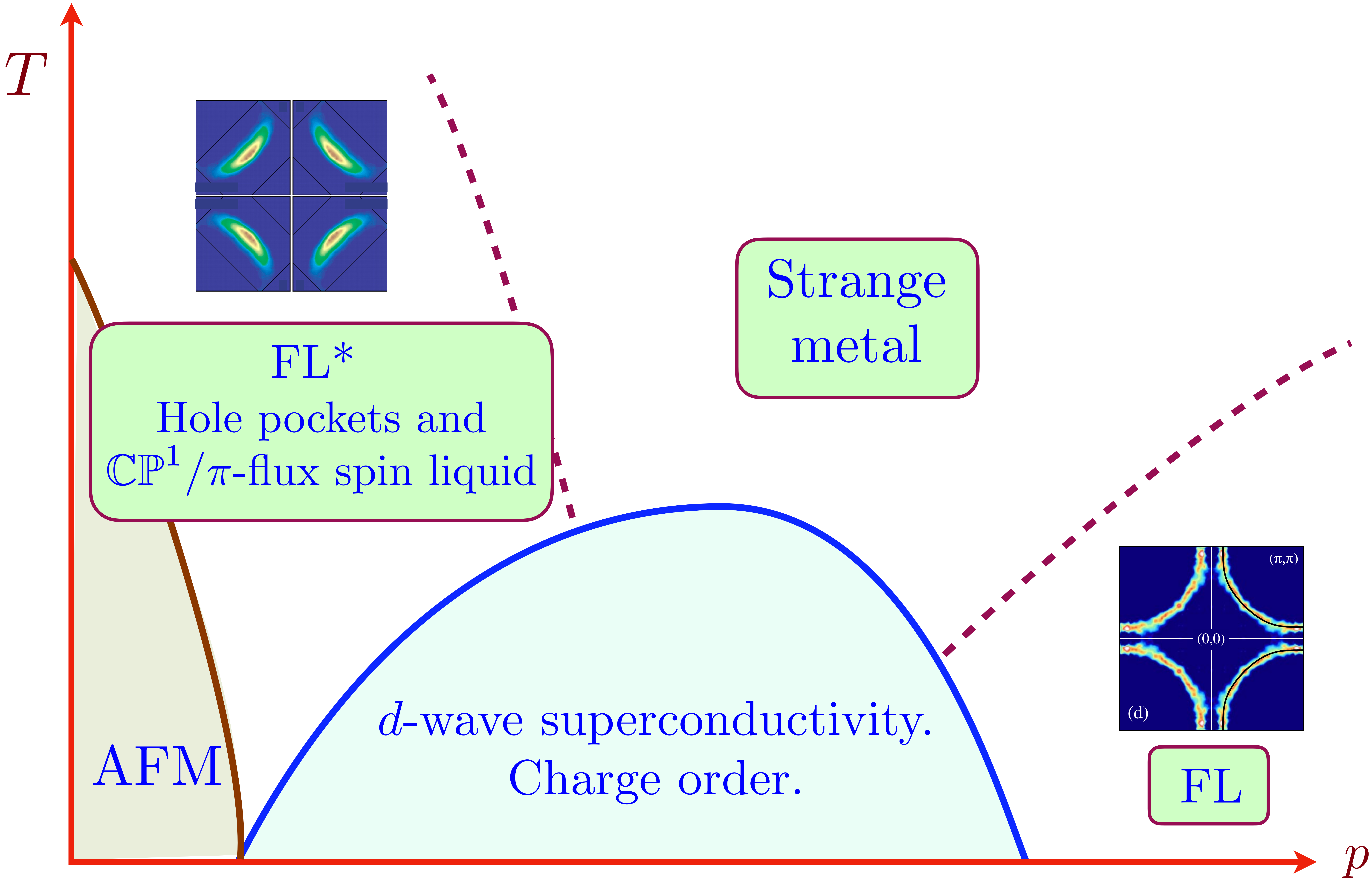
J_K

doping p

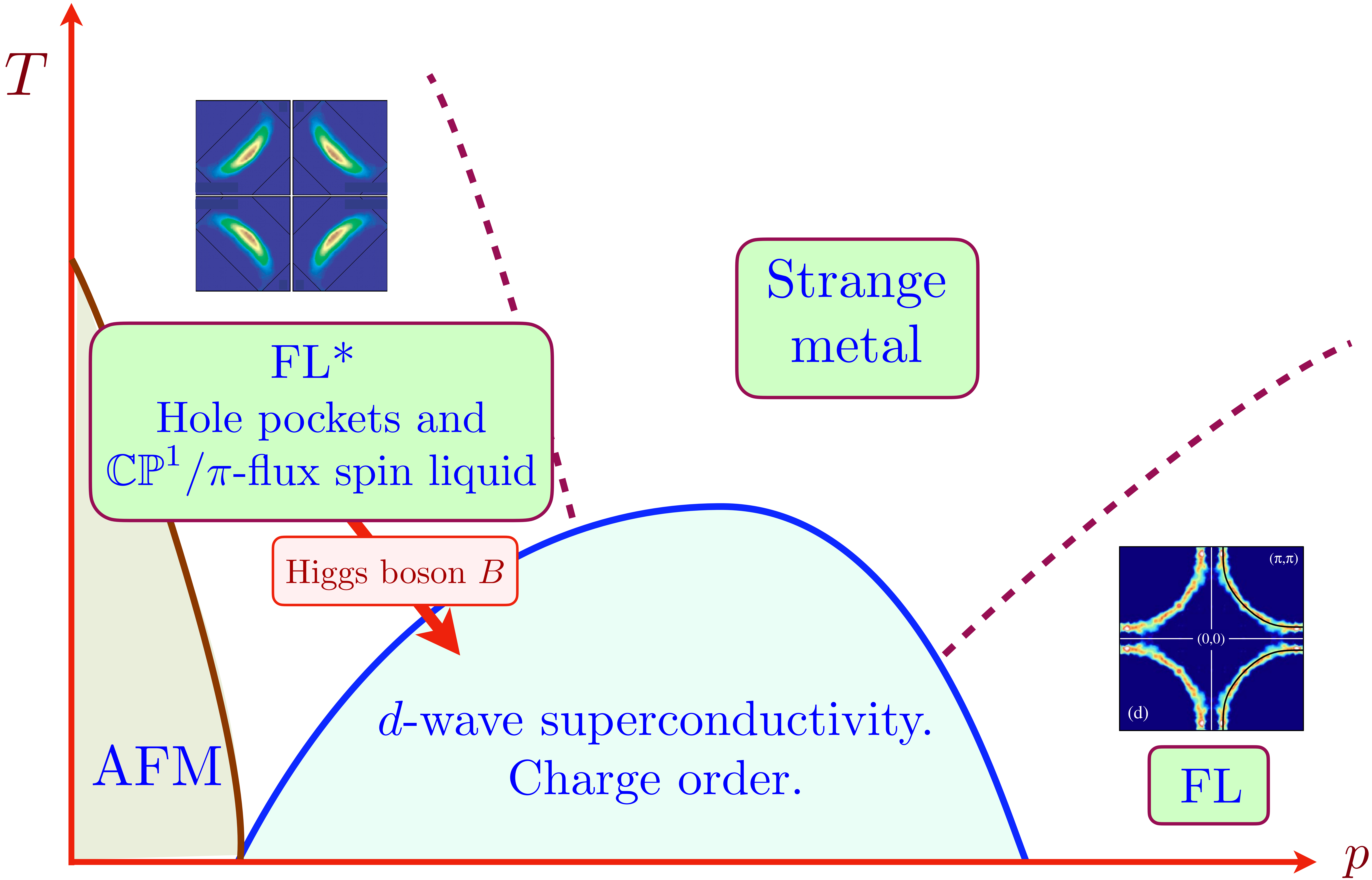
B has same quantum numbers as boson in X.-G. Wen and P.A. Lee, *Phys. Rev. Lett.* **76**, 503 (1996)

Ancilla theory of the Hubbard model

Higgs field B drives FL*-dSC/CDW



T
FL*
Hole pockets and
$\mathbb{CP}^1/\pi$-flux spin liquid
Strange
metal
d-wave superconductivity.
Charge order.
AFM
(π,π)
(0,0)
(d)
FL
p



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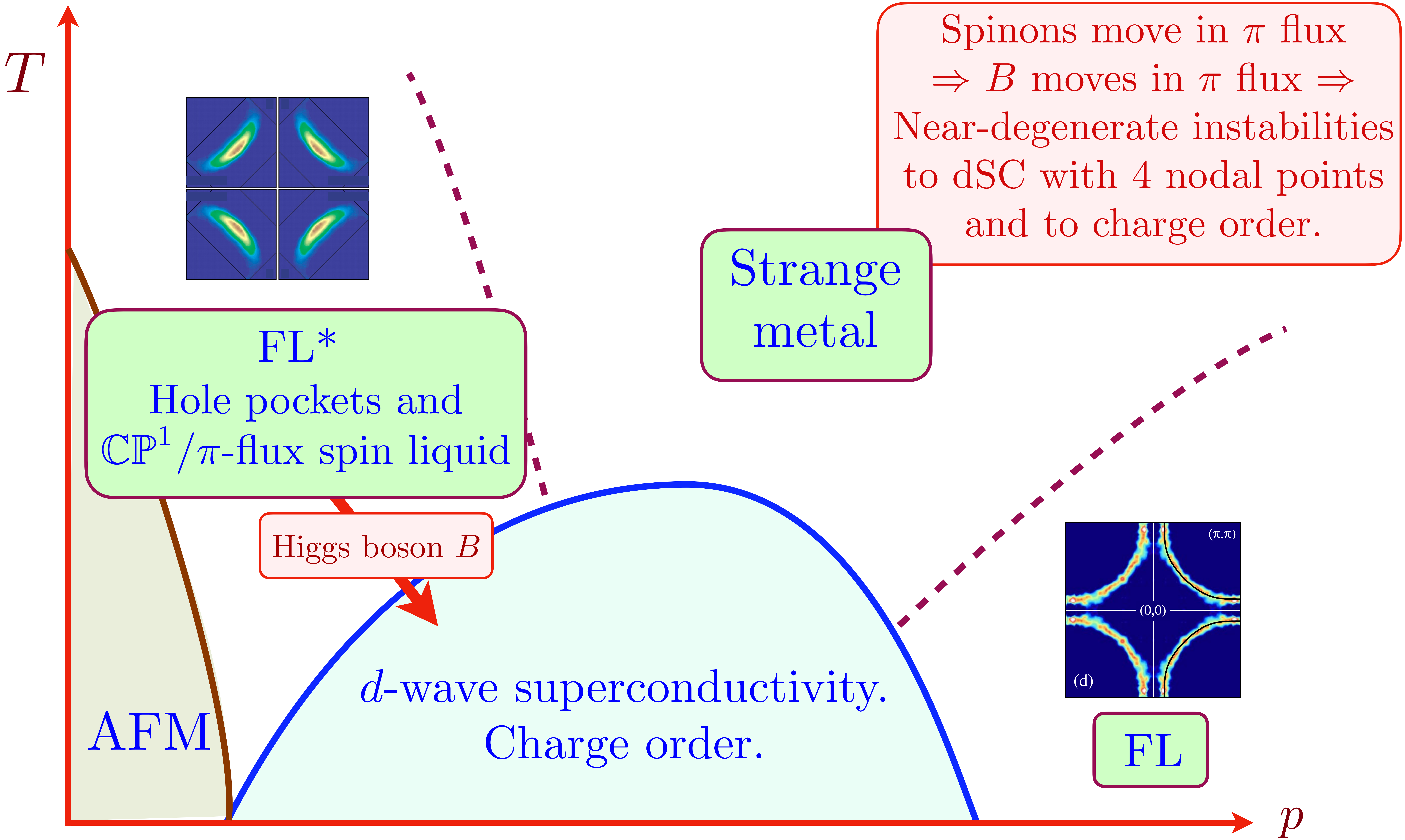

Spinons move in π flux $\Rightarrow$ B moves in π flux $\Rightarrow$ Near-degenerate instabilities to dSC with 4 nodal points and to charge order.
T
Strange metal
FL*
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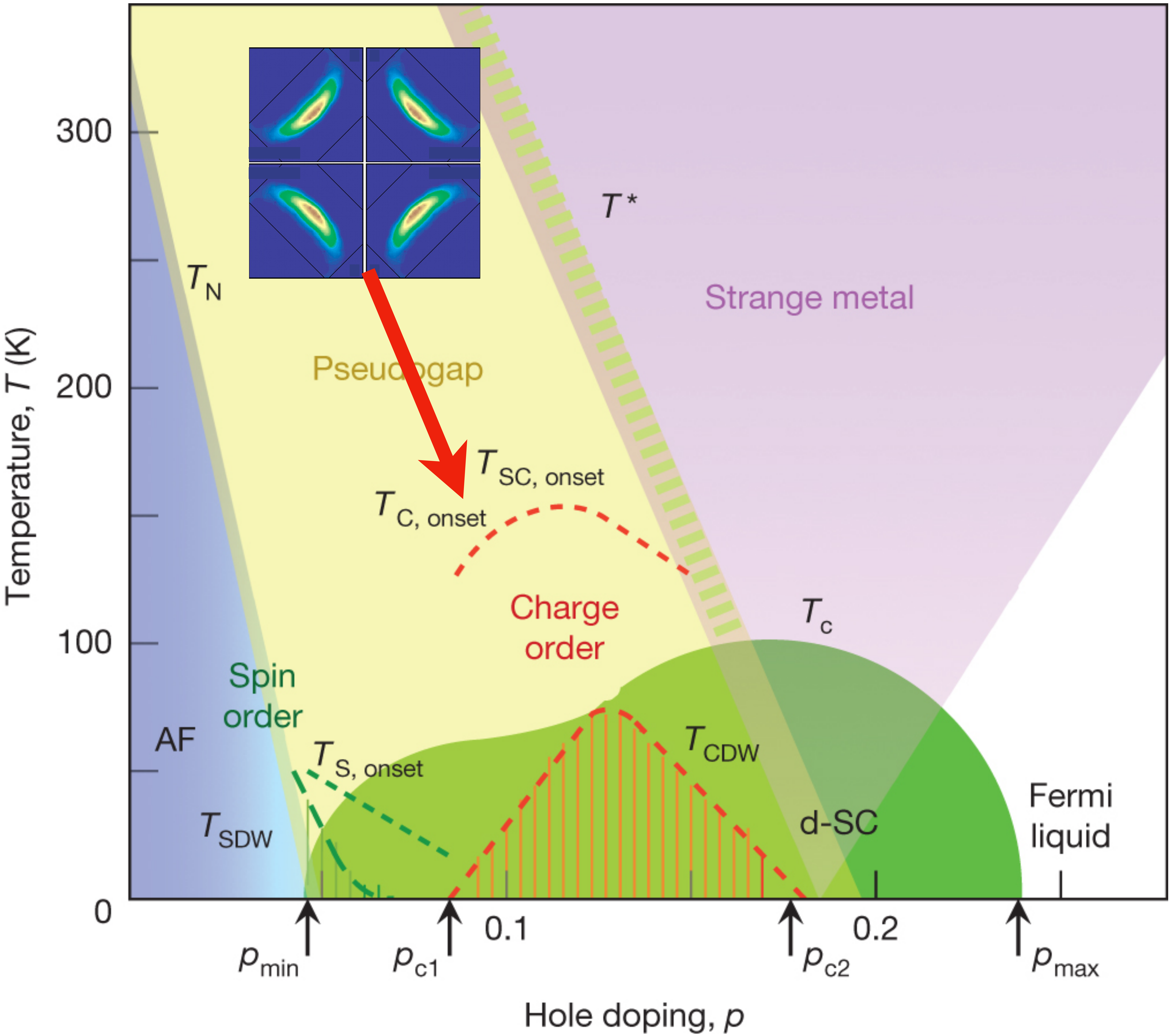
Keimer, Kivelson, Norman, Uchida, and Zaanen, *Nature* **518**, 179 (2015)



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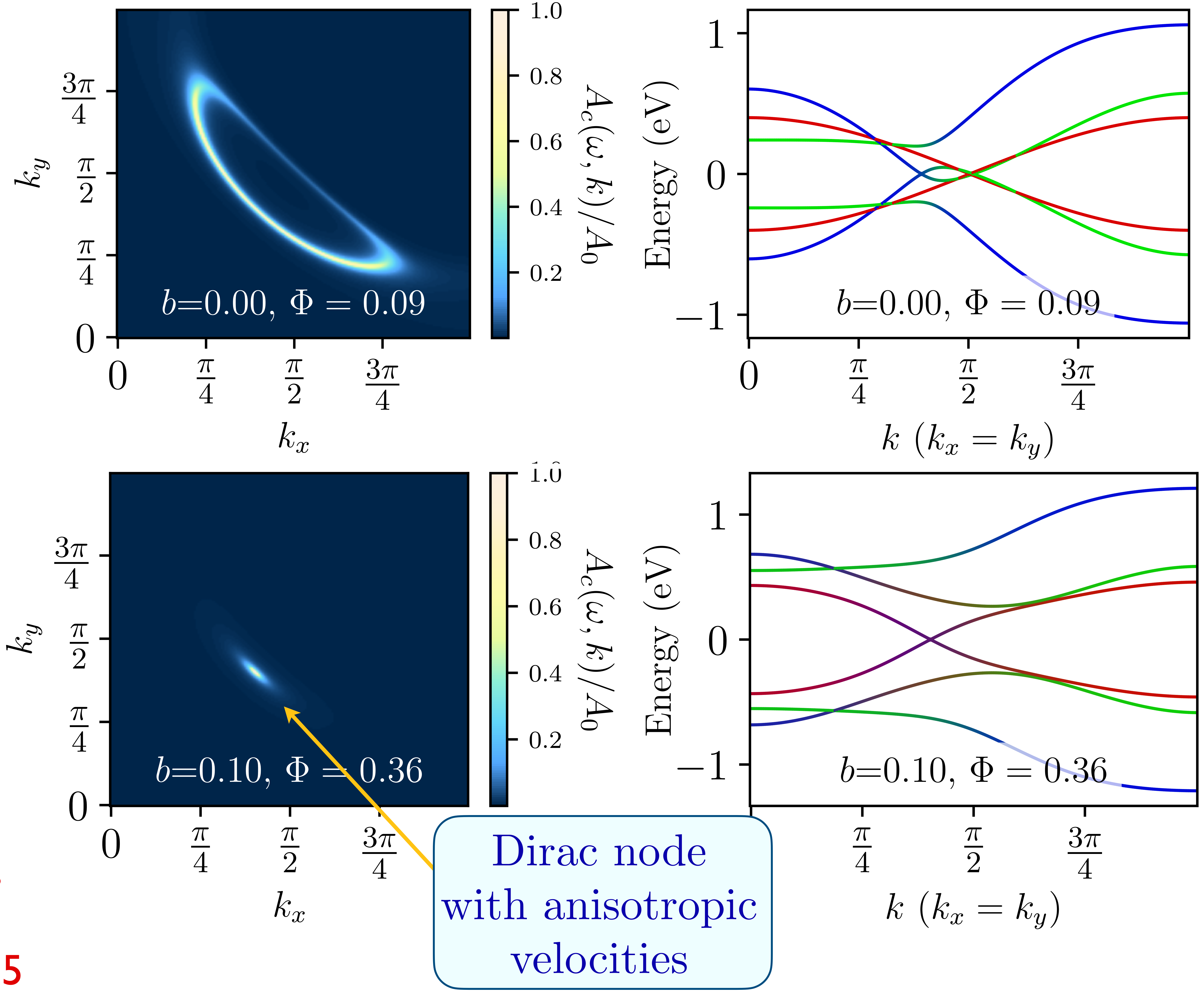
Predictions

Electron spectral density in hole-doped cuprates



FL*

dSC

Maine Christos and S.Sachdev, arXiv:2308.03835

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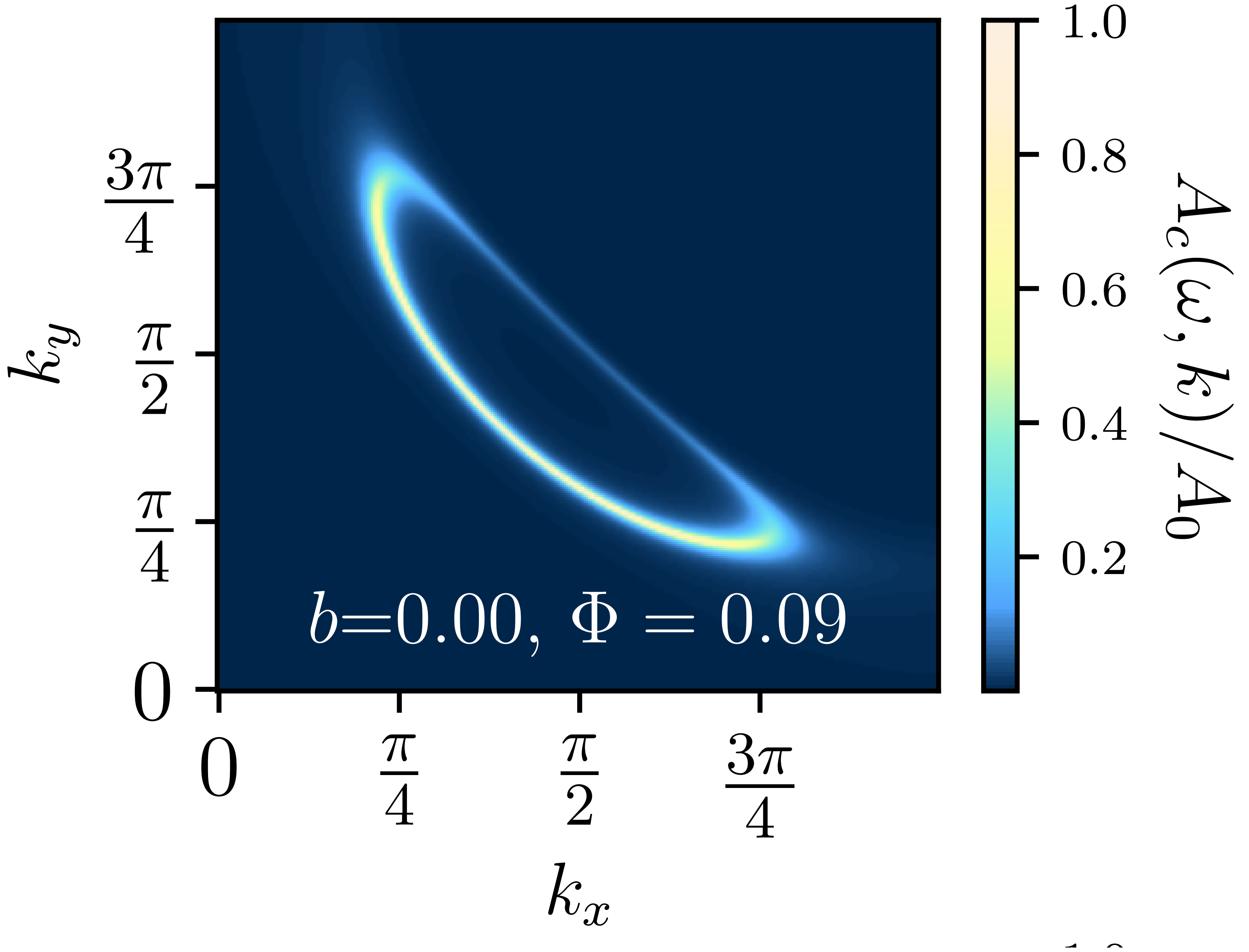
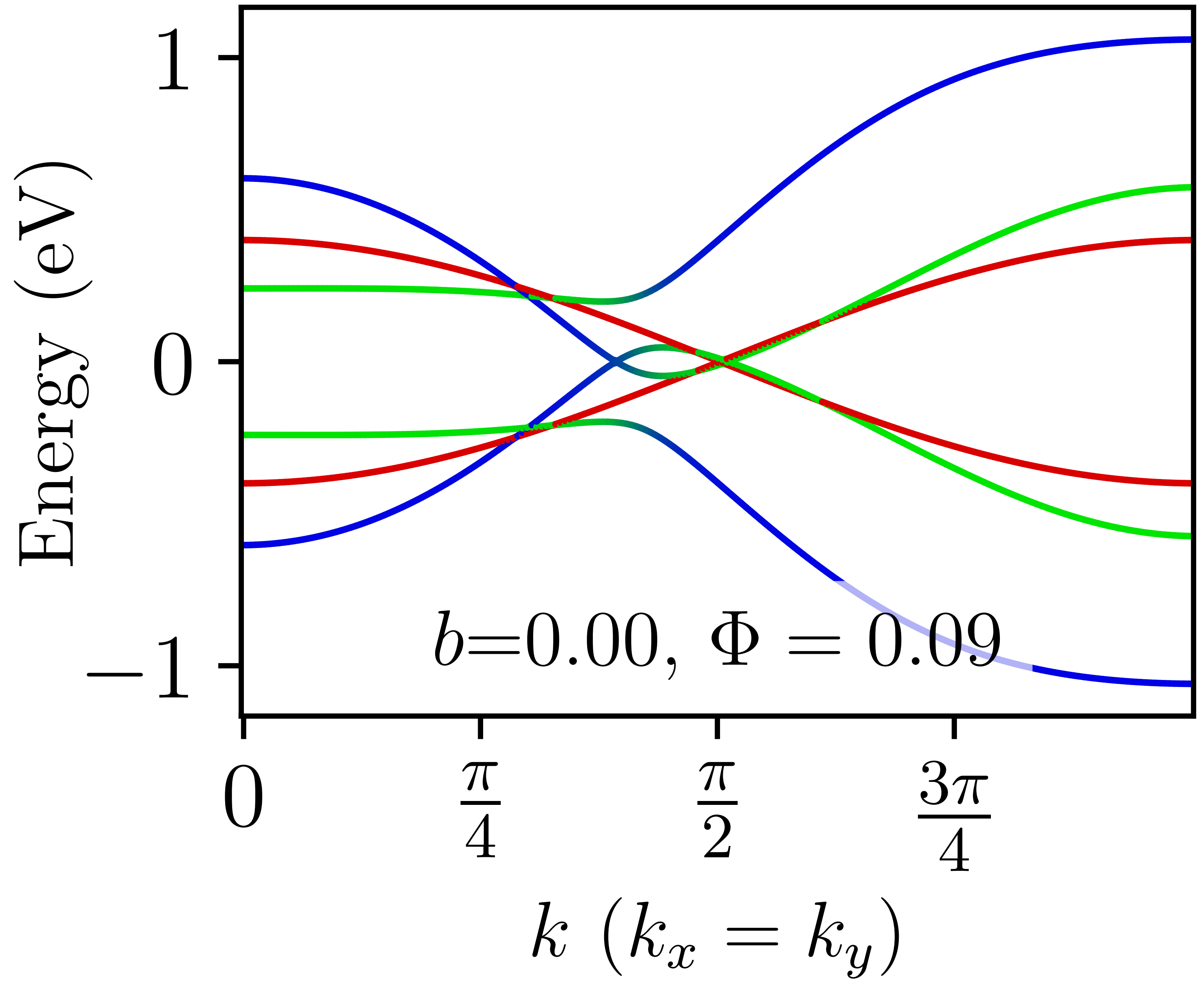
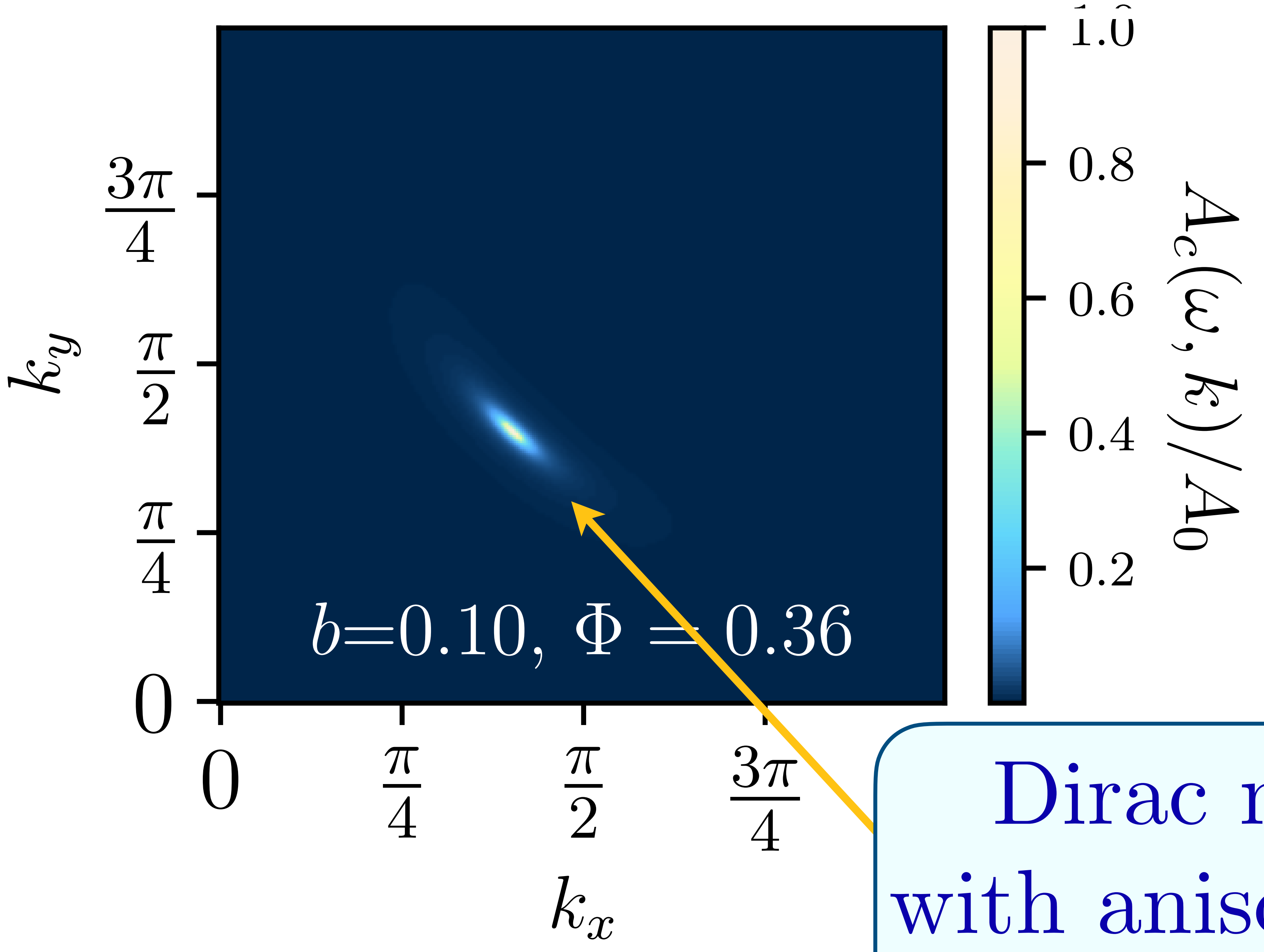
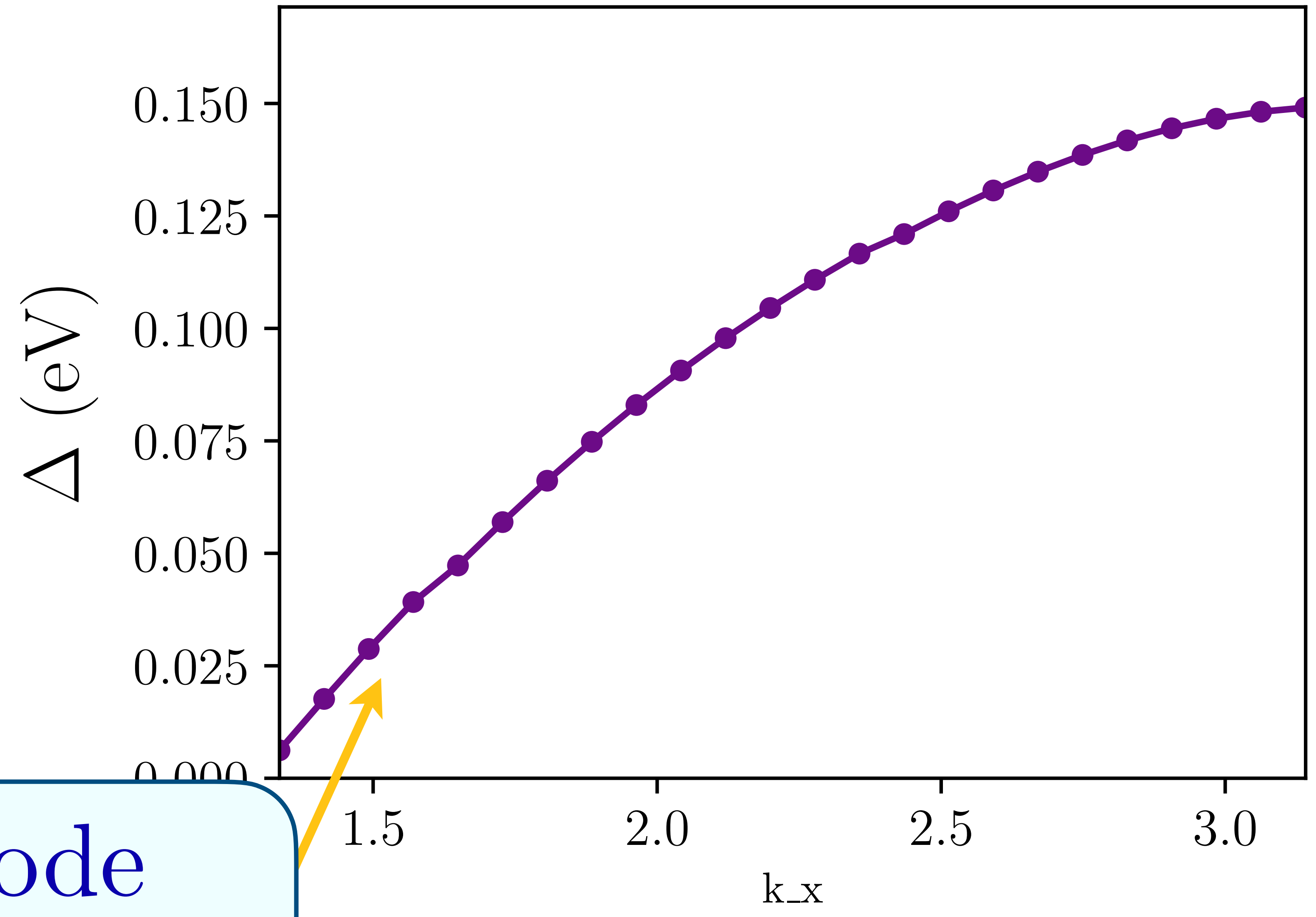




FL*



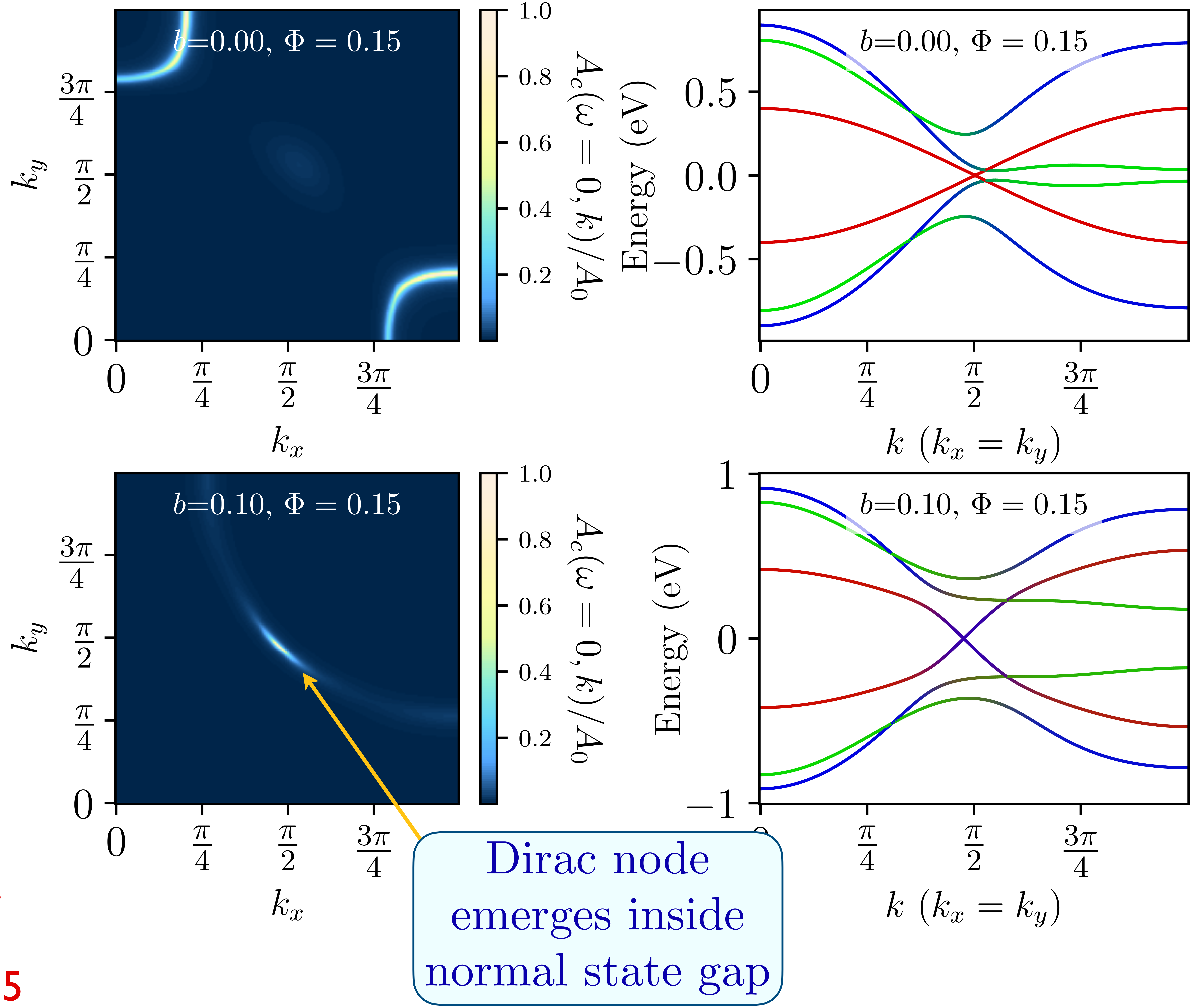


Dirac node with anisotropic velocities

dSC

Maine Christos and S.Sachdev, arXiv:2308.03835

Electron spectral density in electron-doped cuprates



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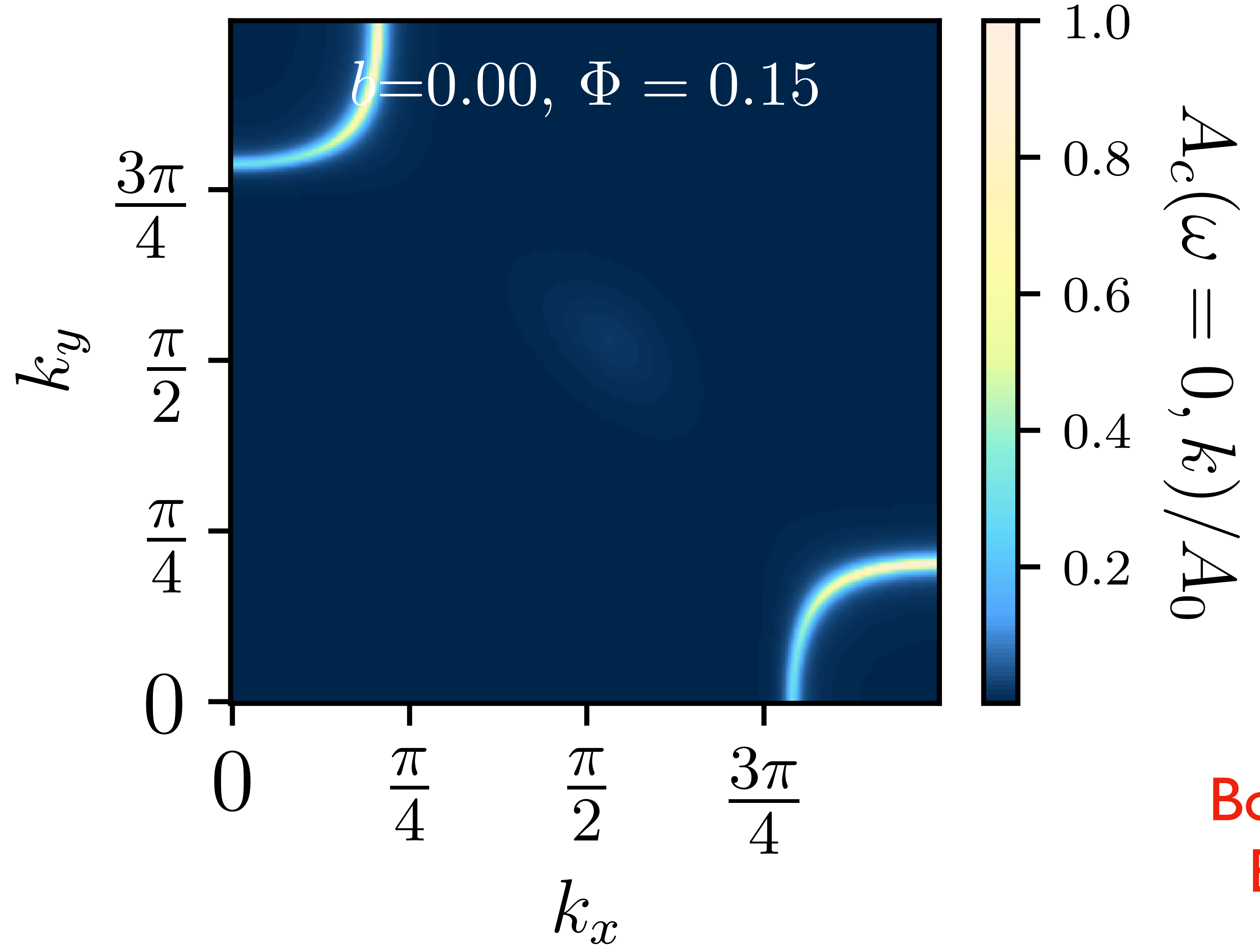
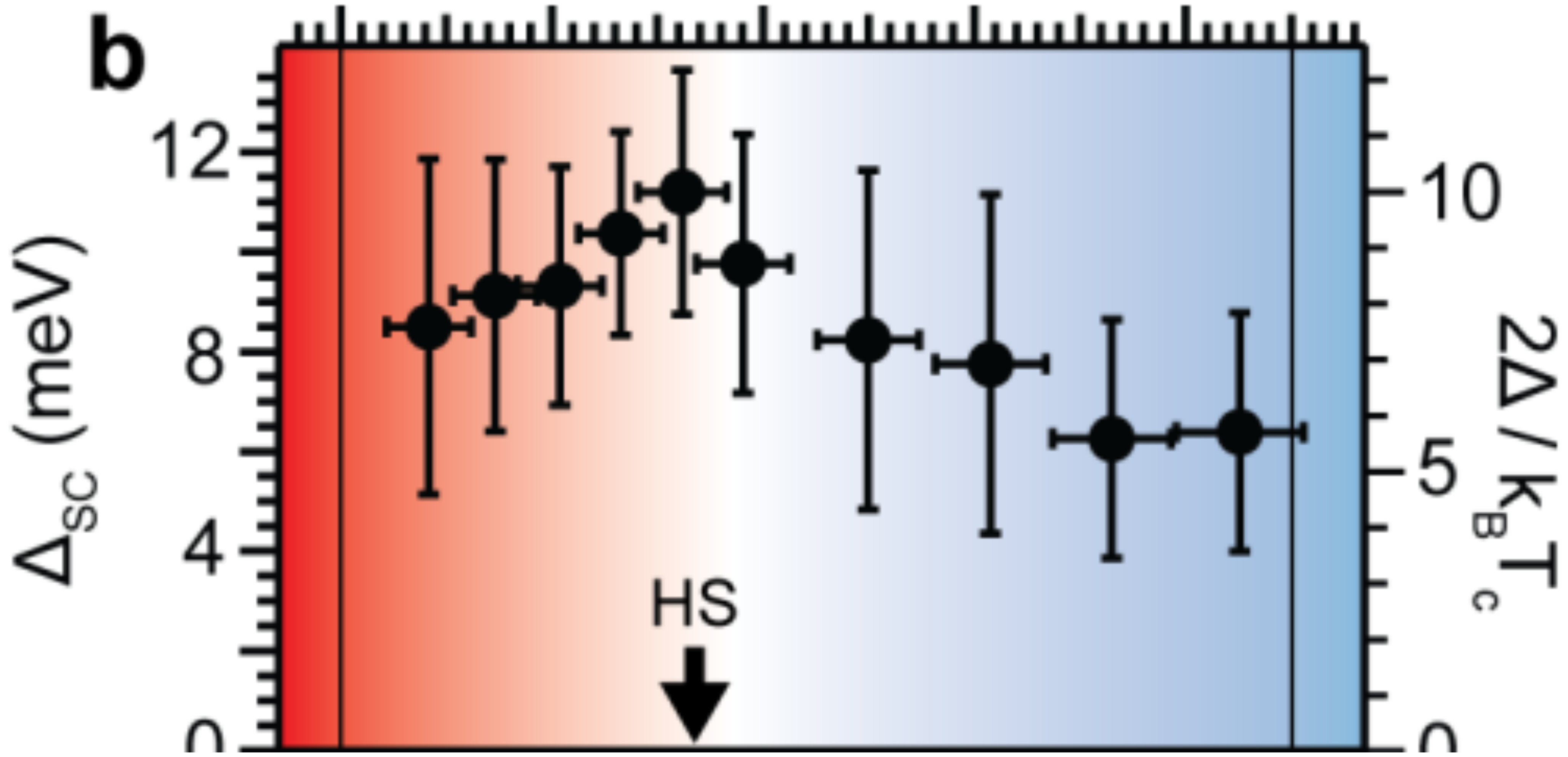
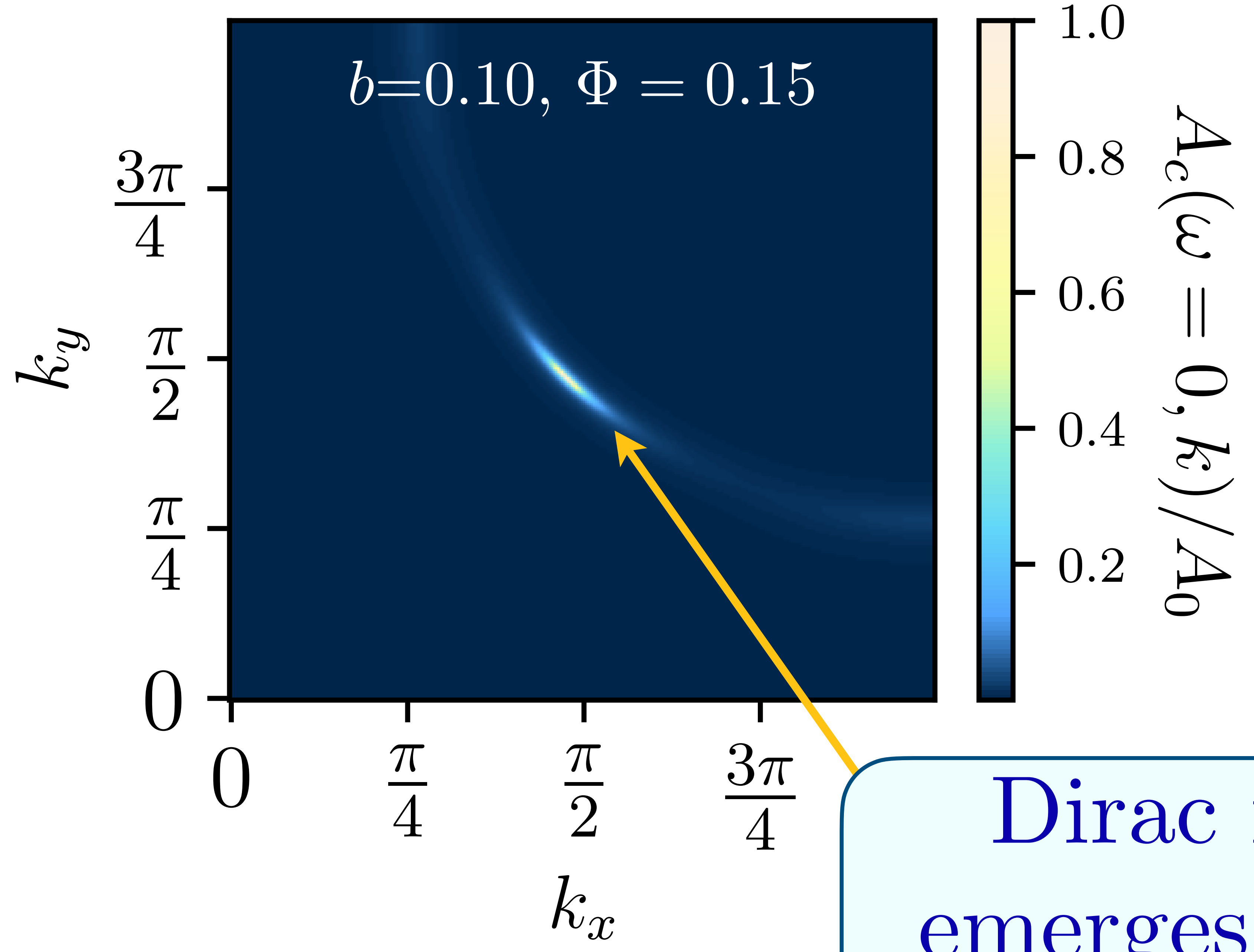
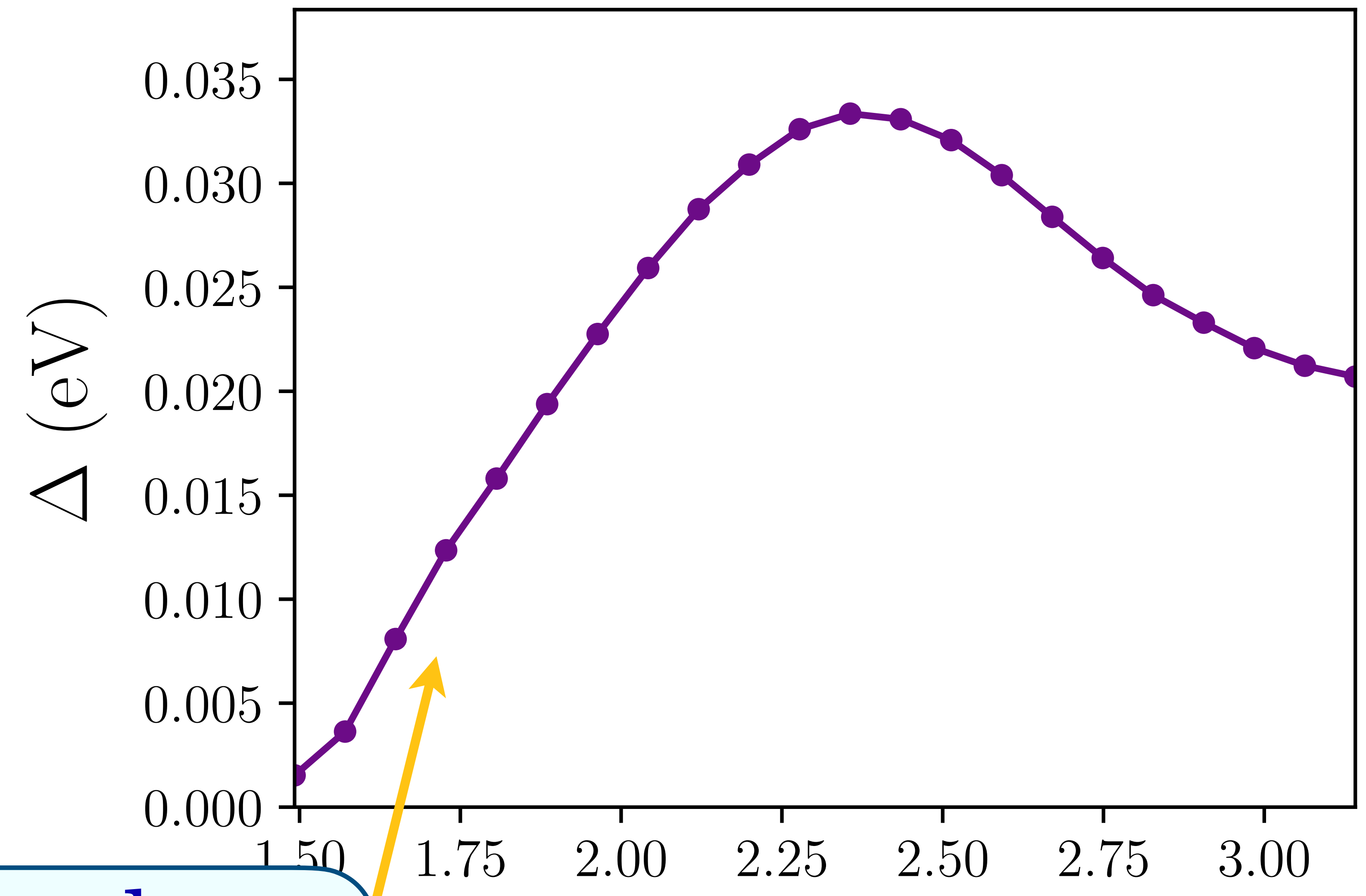




Bogoliubov Quasiparticle on the Gossamer Fermi Surface in Electron-Doped Cuprates, Ke-Jun Xu……Z.-X. Shen, Nature Physics (2023)



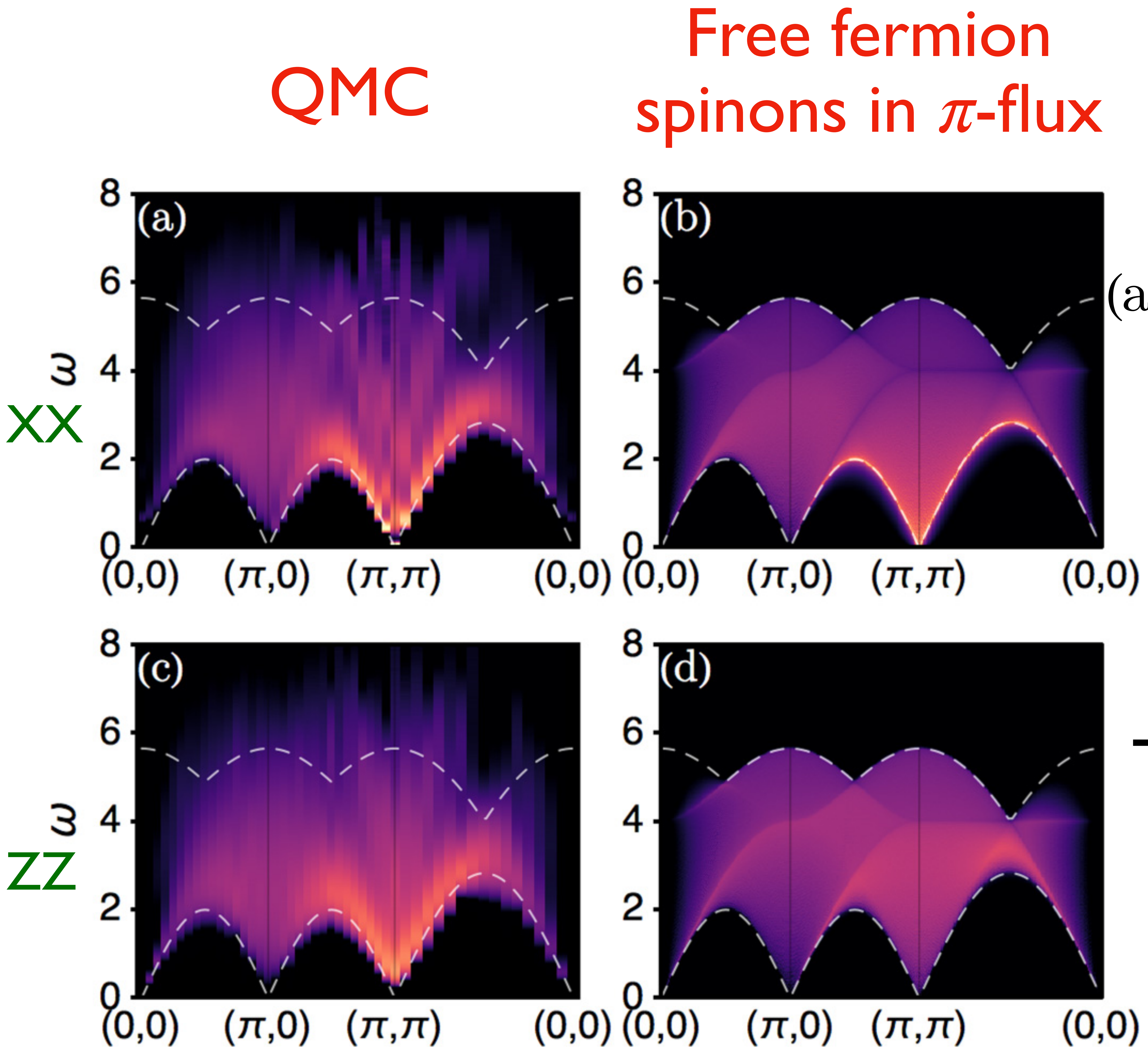


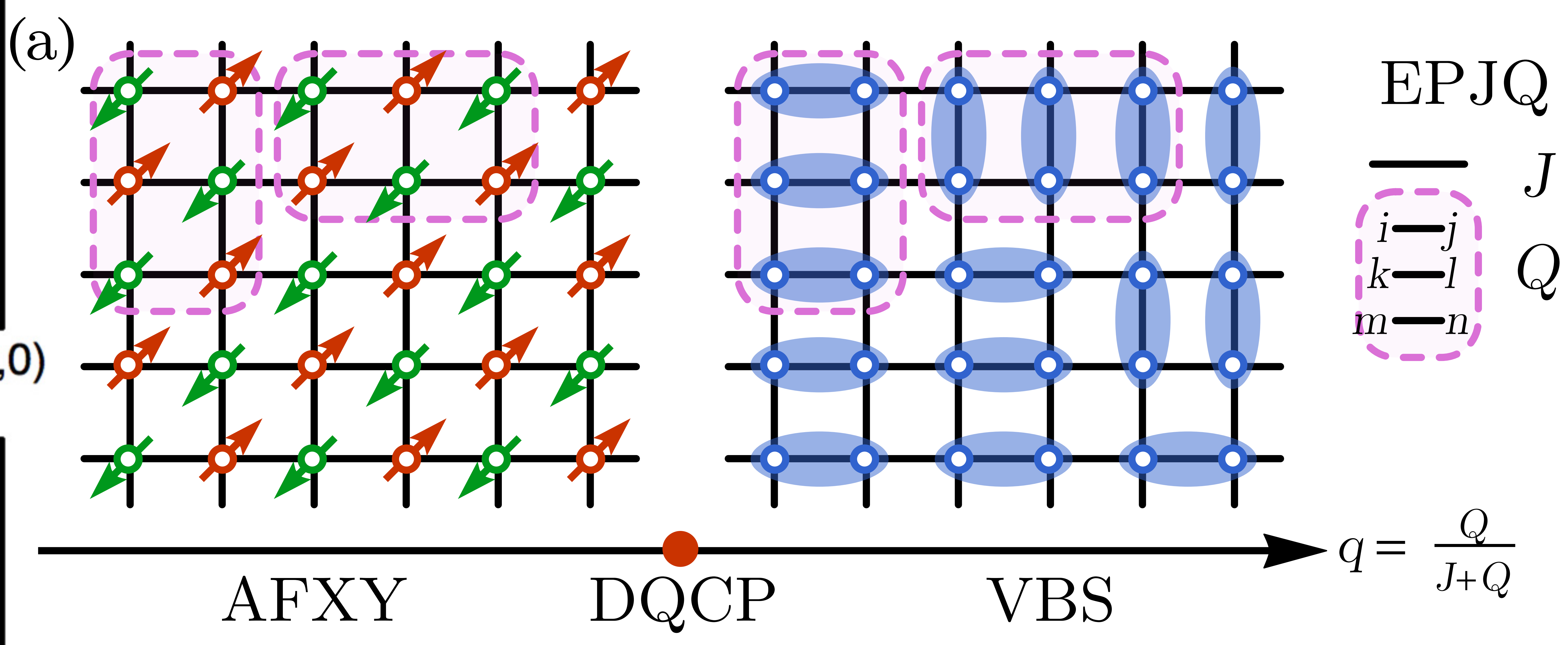
dSC

Dirac node emerges inside normal state gap

Maine Christos and S.Sachdev, arXiv:2308.03835

Observable by neutron scattering in pseudogap ?





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)

Summary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