

# Ancilla qubit wavefunctions for the pseudogap metal phase of the cuprates

Tensor Networks: From Simulations to Holography III

Perimeter Institute, Waterloo

November 16, 2020

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PHYSICS



HARVARD

Talk online: [sachdev.physics.harvard.edu](https://sachdev.physics.harvard.edu)



Yahui Zhang

# Luttinger theorem for Fermi liquids

Consider a general model of interacting electrons  $c_\uparrow, c_\downarrow$  and  $S = 1/2$  spins  $\vec{S} = (1/2)f_\alpha^\dagger \vec{\sigma}_{\alpha\beta} f_\beta$ ,  $\sum_\alpha f_\alpha^\dagger f_\alpha = 1$ .

$$c_\alpha c_\beta^\dagger + c_\beta^\dagger c_\alpha = \delta_{\alpha\beta}, \quad f_\alpha f_\beta^\dagger + f_\beta^\dagger f_\alpha = \delta_{\alpha\beta}, \quad c_\alpha f_\beta + f_\beta c_\alpha = 0$$

We can also think of the spins as qubits with  $\vec{S} = (1/2)(X, Y, Z)$  the Pauli qubit operators.

$$H = - \sum_{i \neq j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} - \mu \sum_i c_{i\alpha}^\dagger c_{i\alpha} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \\ + \sum_{i < j} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_i \frac{J_K}{2} \vec{S}_i \cdot c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta} \dots$$

# Luttinger theorem for Fermi liquids

Luttinger's theorem states that the momentum space volume enclosed by the Fermi surface (the location of a discontinuity in the electron distribution function) equals  $(1/2)(\text{density of all electrons}) \times (2\pi)^d$  modulo the density contained in filled bands (which can accommodate 2 electrons per unit cell).

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The traditional proofs rely upon a perturbative expansion about the free electron limit. In this proof we use the  $f_\alpha$  representation of  $\vec{S}_i$ , and replace the constraint  $\sum_\alpha f_\alpha^\dagger f_\alpha$  by an interaction  $U_f f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow$ , and expand about  $U_f = 0$ .

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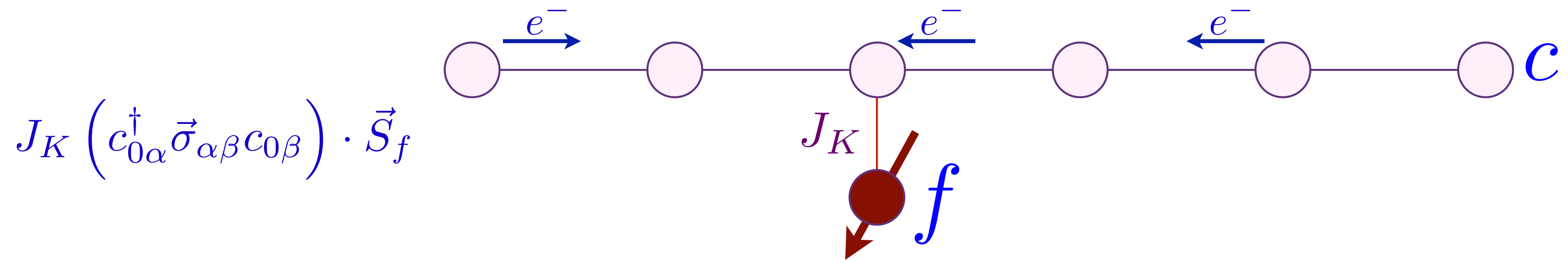
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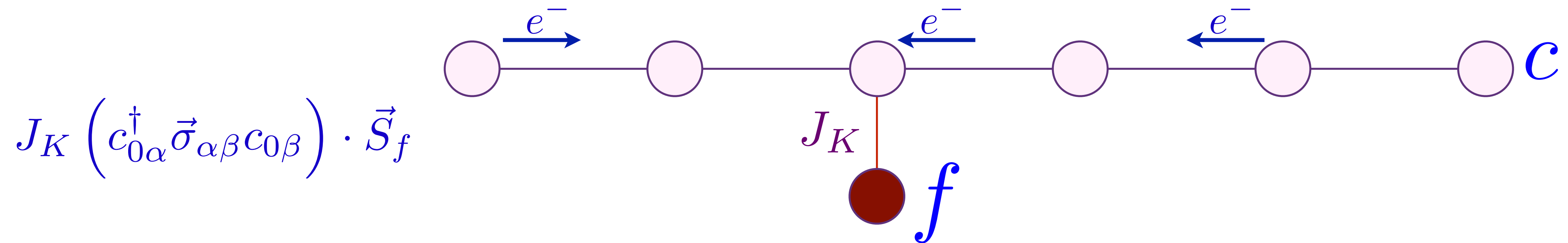
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More recent proofs (Oshikawa; Else, Thorngren, Senthil) use an 'anomaly' associated with the combination of translations and the U(1) symmetry of electron number conservation, and can work directly with spin qubits.

# Kondo model



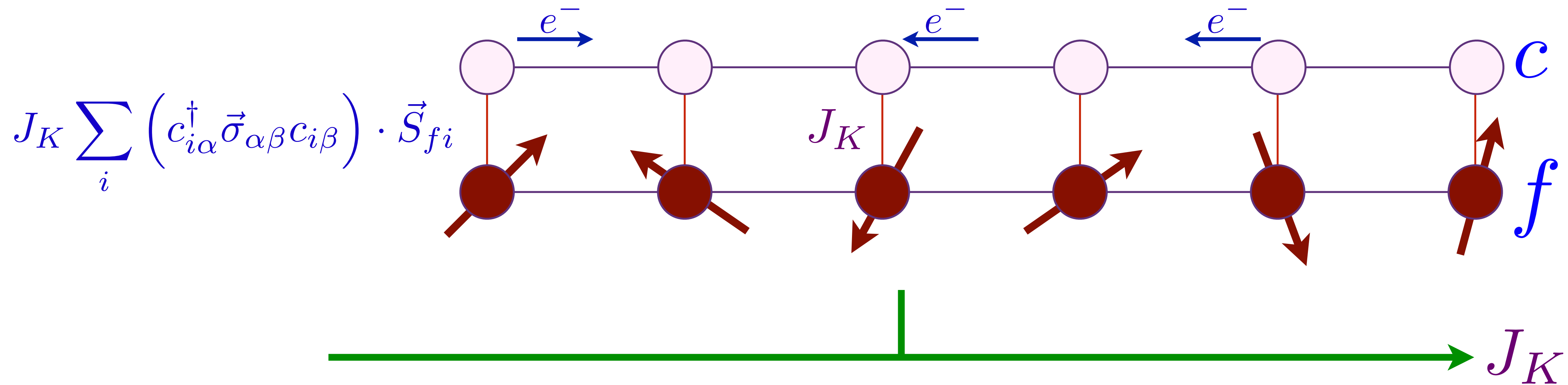
# Kondo model



The  $c$  electrons ‘Kondo screen’ the  $f$  spin at low energies:  
The  $f$  electron ‘dissolves’ into the Fermi sea.

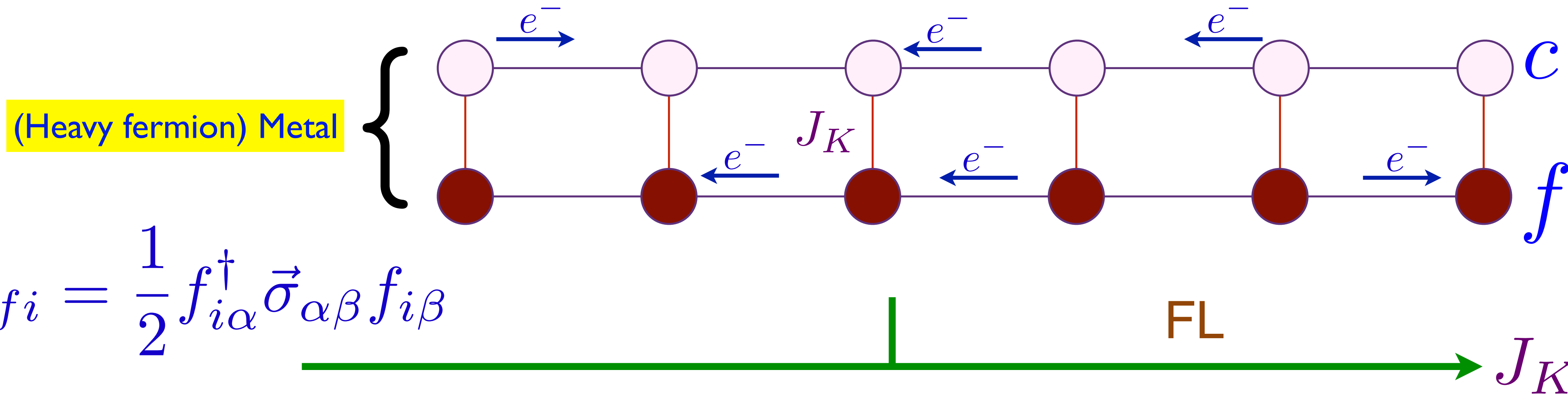
# Luttinger volume in **Kondo lattice** models

Kondo lattice of  $f$  electron spins coupled to a conduction band of  $c$  electrons of density  $p$ .



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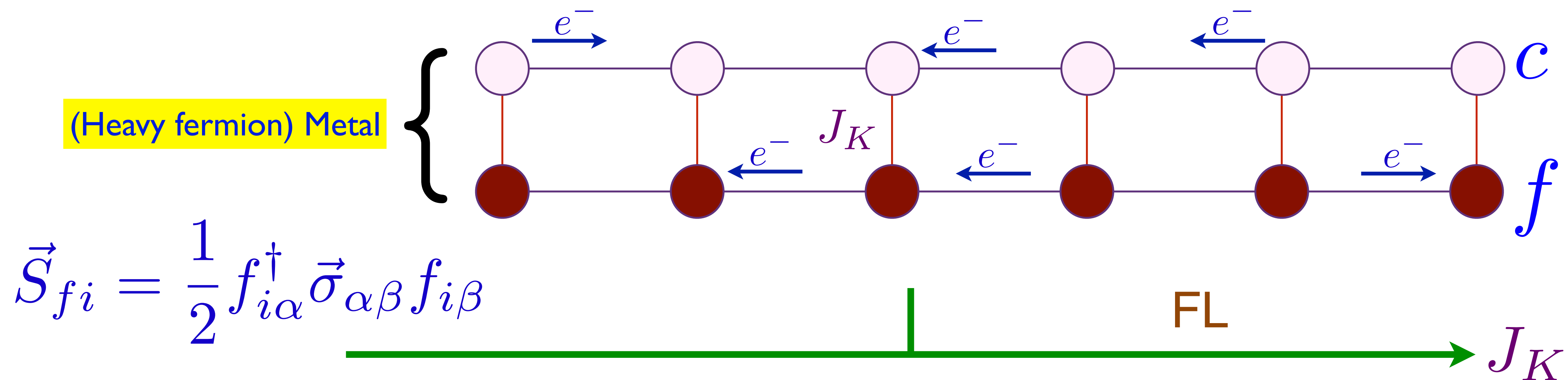
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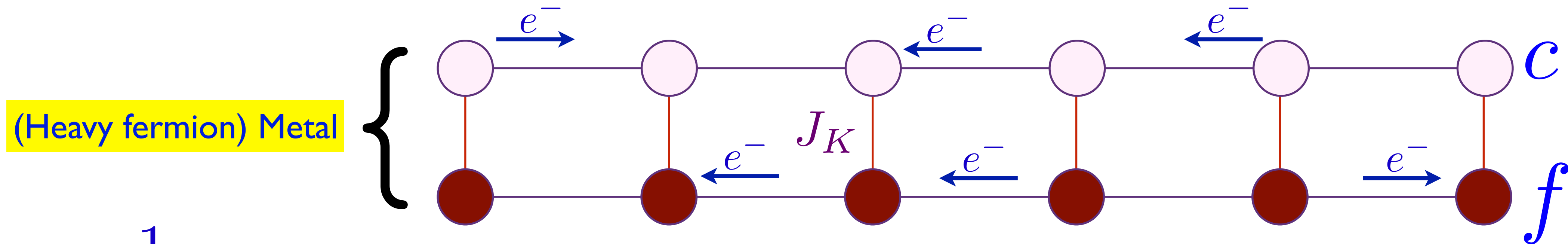
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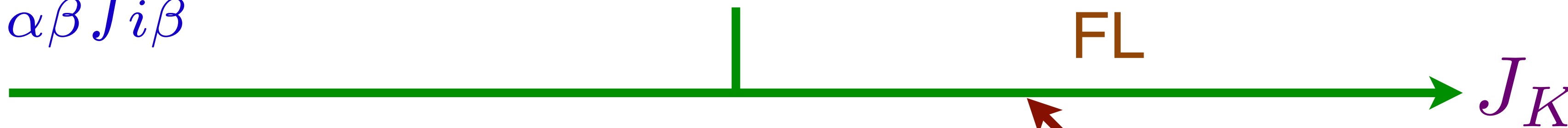
The  $c$  electrons ‘Kondo screen’ the  $f$  spins in the FL phase:  
 The  $f$  electrons ‘dissolve’ into the Fermi sea.  
 The Fermi surface is large: encloses volume of  $1 + p$  electrons.

# Luttinger volume in **Kondo lattice** models

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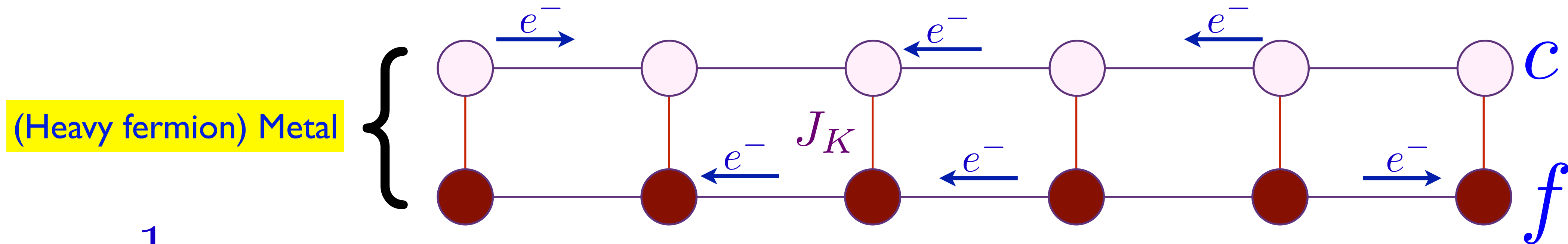


Large Fermi surface of size  $1 + p$

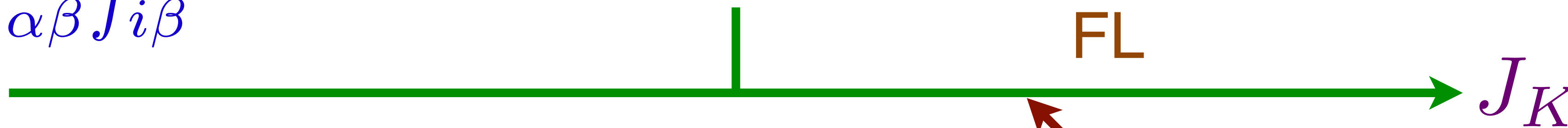
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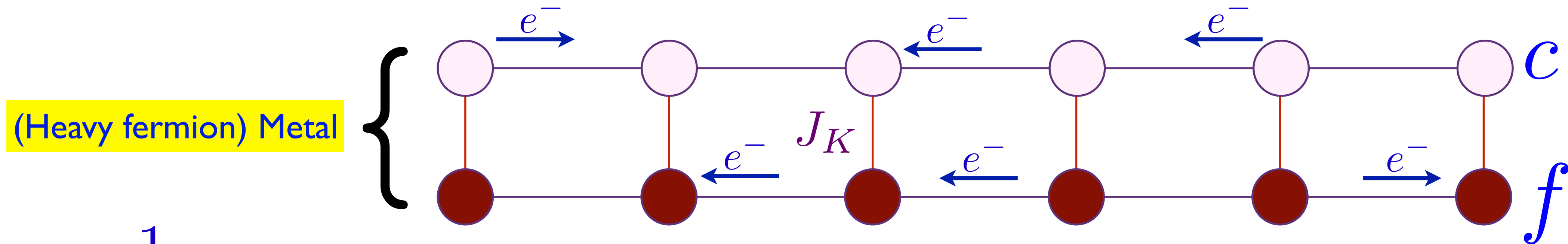
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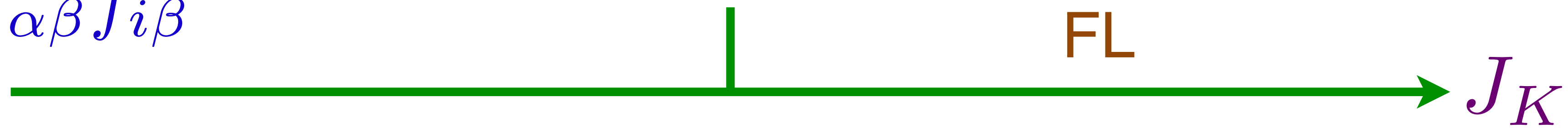
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$$\vec{S}_{fi} = \frac{1}{2} f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta}$$

$$\langle c_\alpha^\dagger f_\alpha \rangle \neq 0$$



The Kondo lattice model has a gauge symmetry:  $f_{i\alpha} \rightarrow e^{i\theta_i} f_{i\alpha}$

This gauge symmetry is fully broken by a Higgs condensate  $\langle c_\alpha^\dagger f_\alpha \rangle$  in the FL phase.

1. Luttinger volume violation in  
Kondo lattice models

*The FL\* phase*

2. Introduction to cuprates

*The pseudogap metal*

3. Luttinger volume violation a one-band model

*Ancilla qubits and ghost Fermi surfaces*

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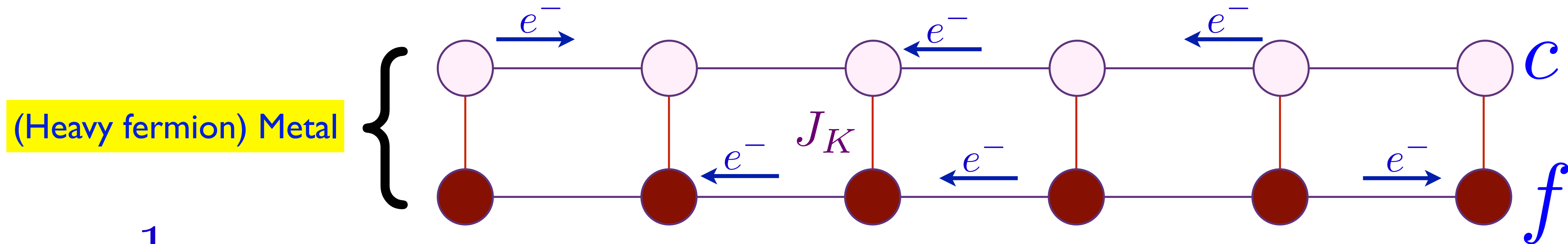
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In this manner we obtain the  $FL^*$  phase: a metallic phase with a Fermi surface of Fermi-liquid-like electronic quasiparticles, enclosing a non-Luttinger volume.

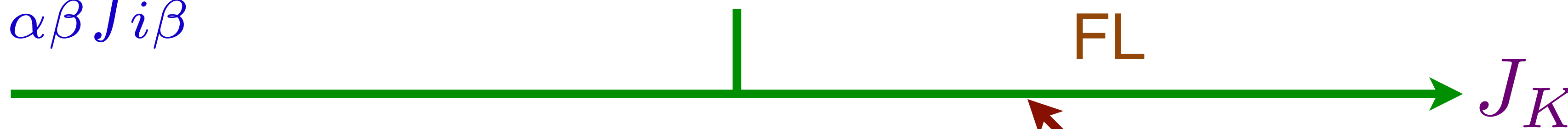
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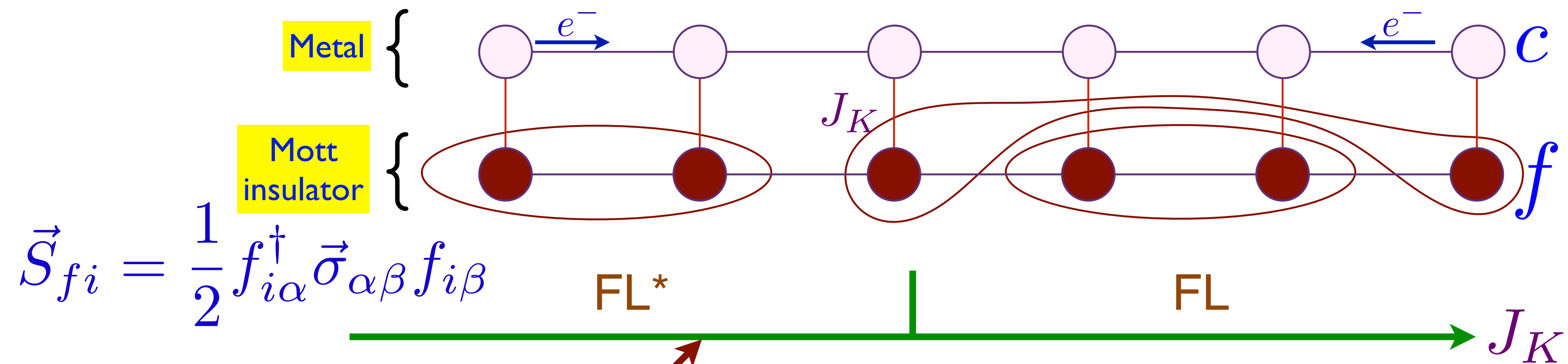
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Large Fermi surface of size  $1 + p$

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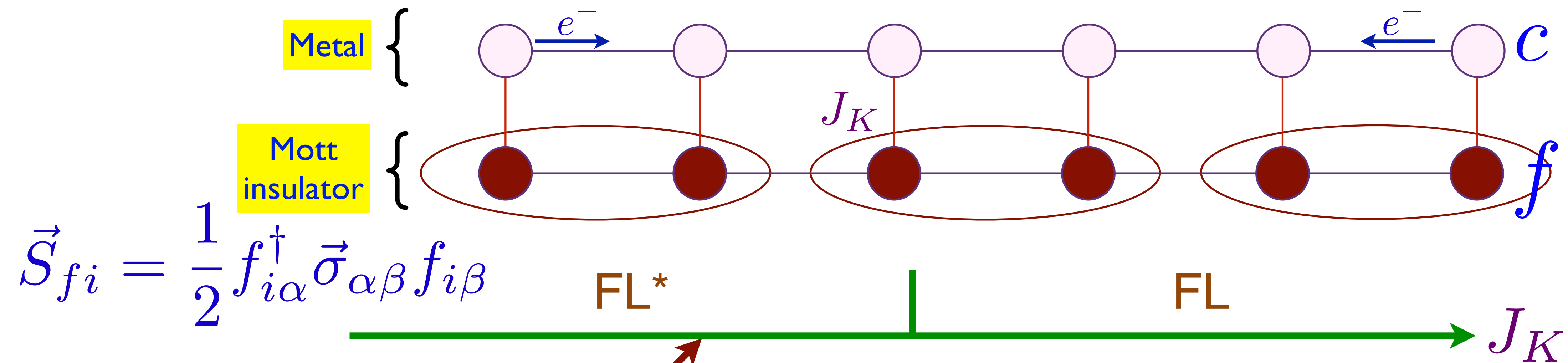
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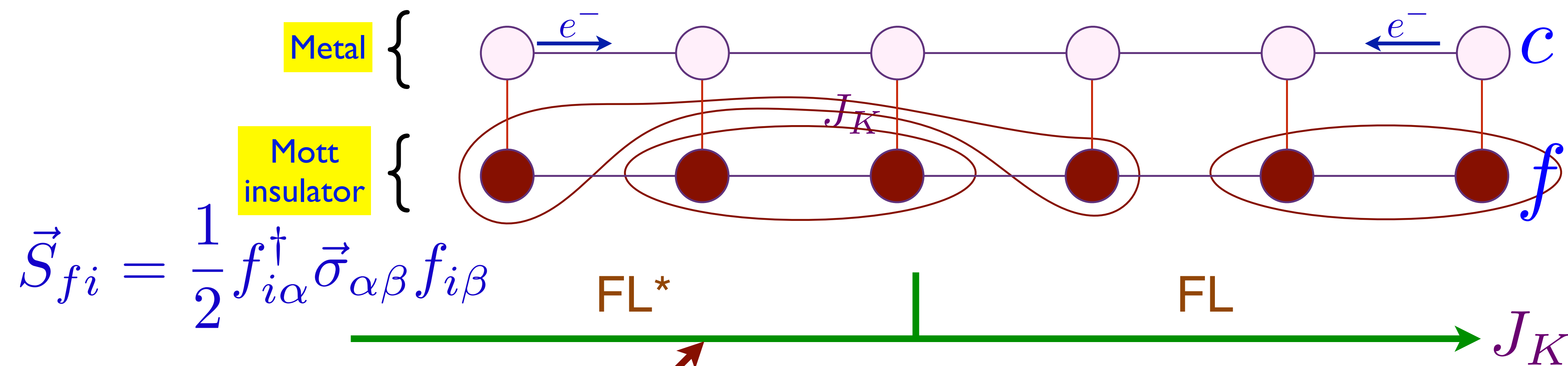
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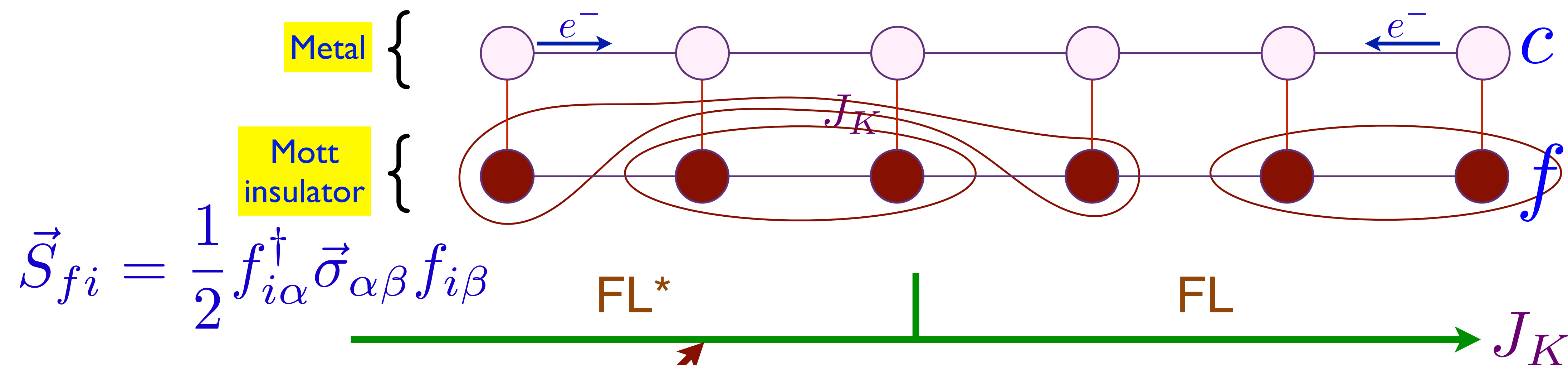
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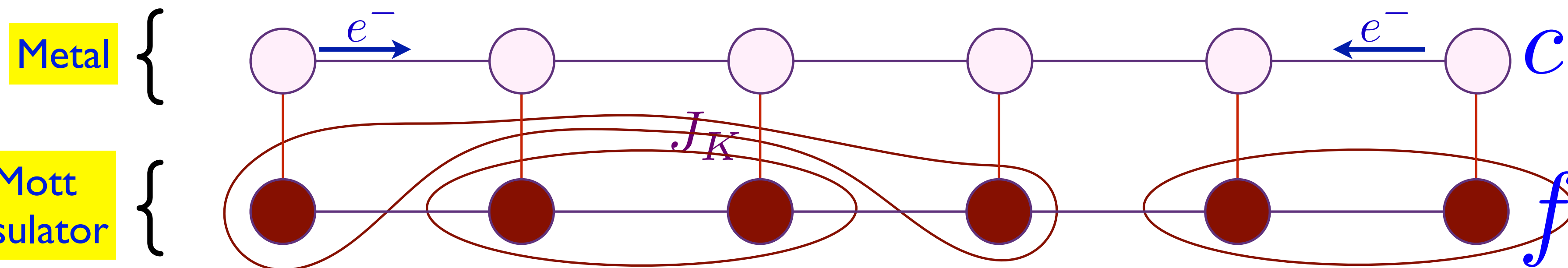
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V.I. Anisimov, I.A. Nekrasov,  
D.E. Kondakov, T.M. Rice & M. Sigrist,  
EPJB **25**, 191 (2002)  
L. de' Medici, A. Georges, S. Biermann,  
PRB **72**, 205124 (2005)

Kondo-breakdown or 'selective Mott' transition



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Kondo-breakdown or ‘selective Mott’ transition

U(1) gauge theory of a ‘hybridization-Higgs’ boson  $b \sim f_{\alpha}^{\dagger} c_{\alpha}$  which condenses on the ‘Large Fermi surface’ side.

$$\vec{S}_{fi} = \frac{1}{2} f_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} f_{i\beta}$$

FL\*

FL

$J_K$

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- No simple extension to one-band model.

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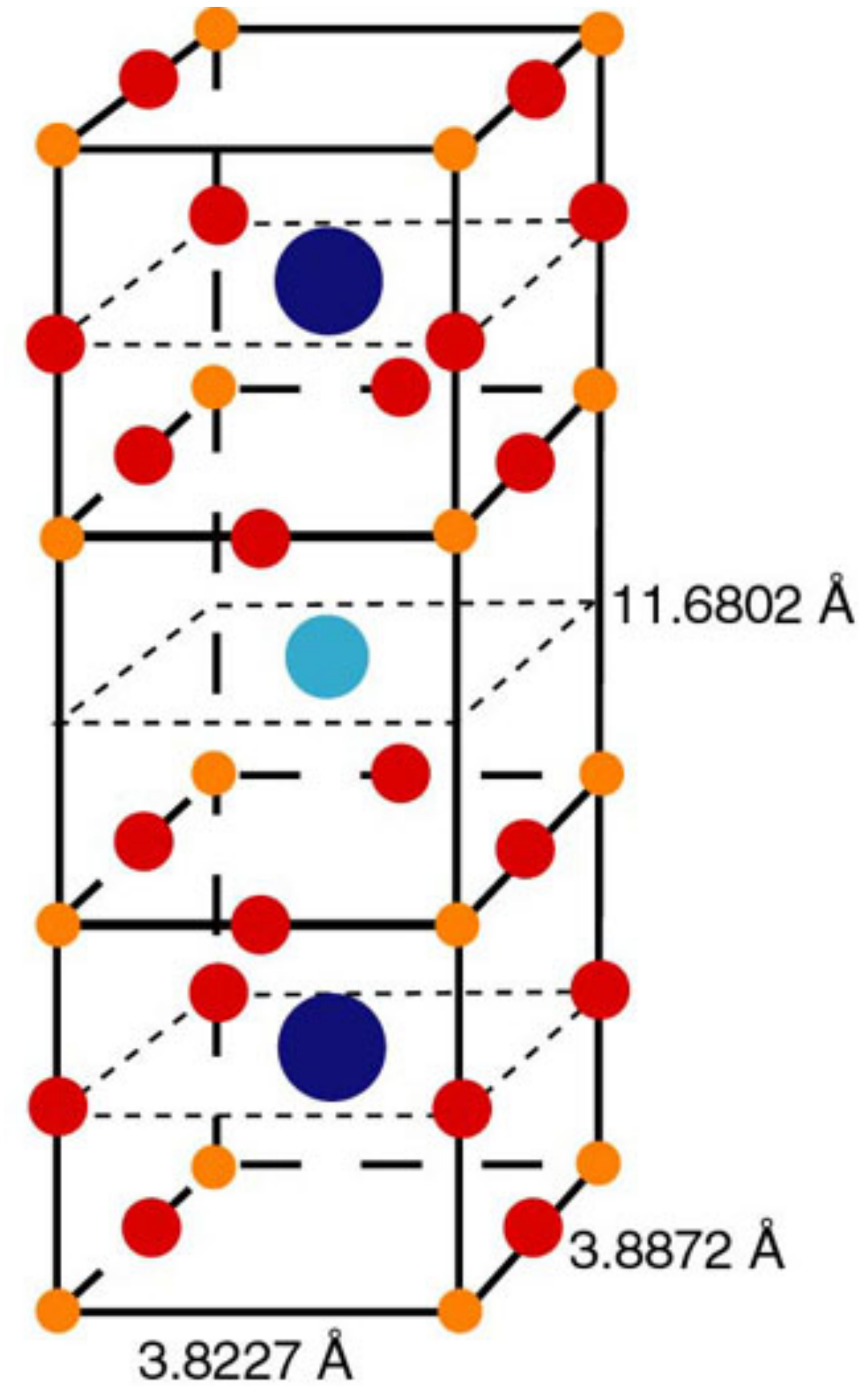
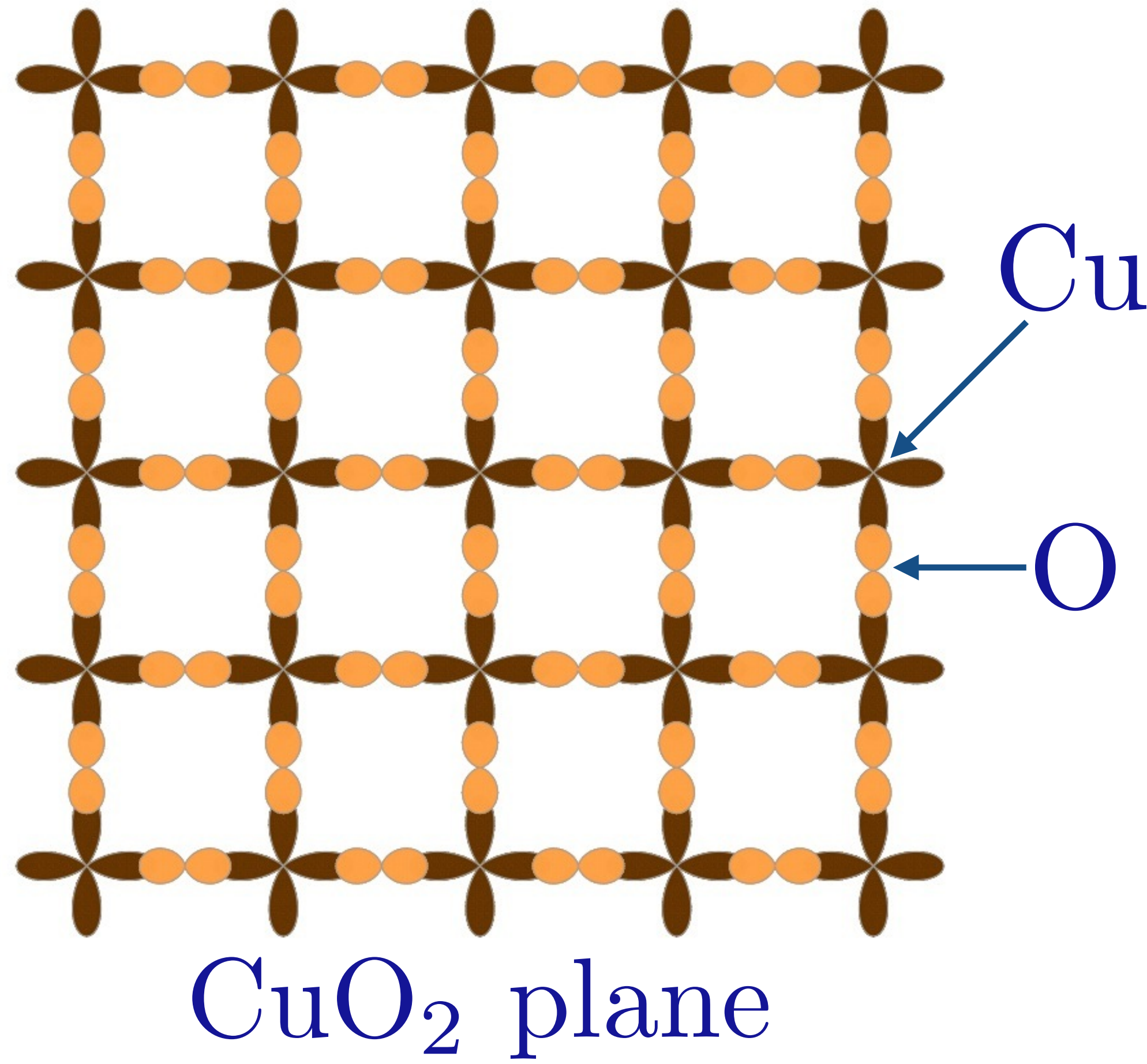
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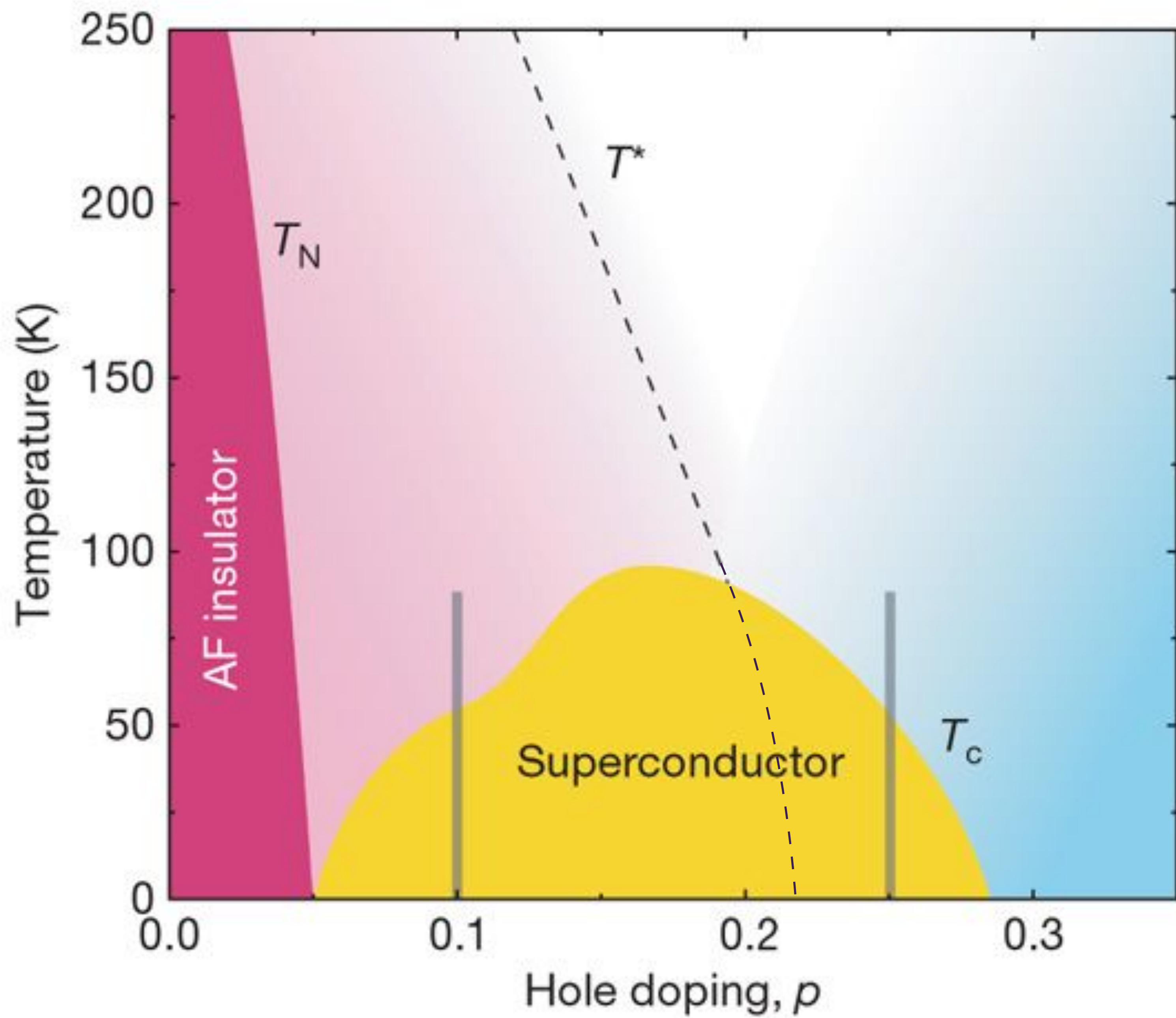
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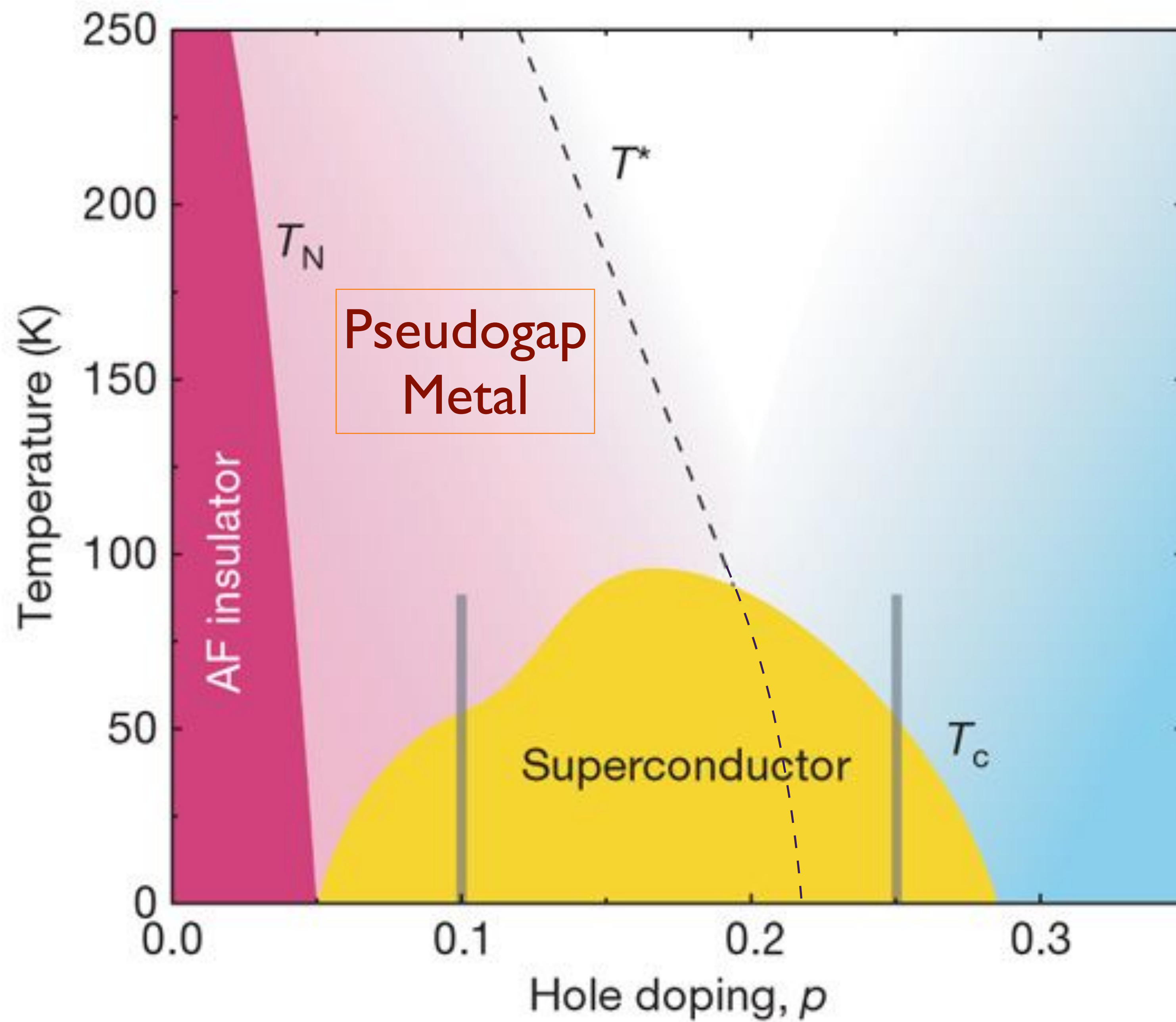
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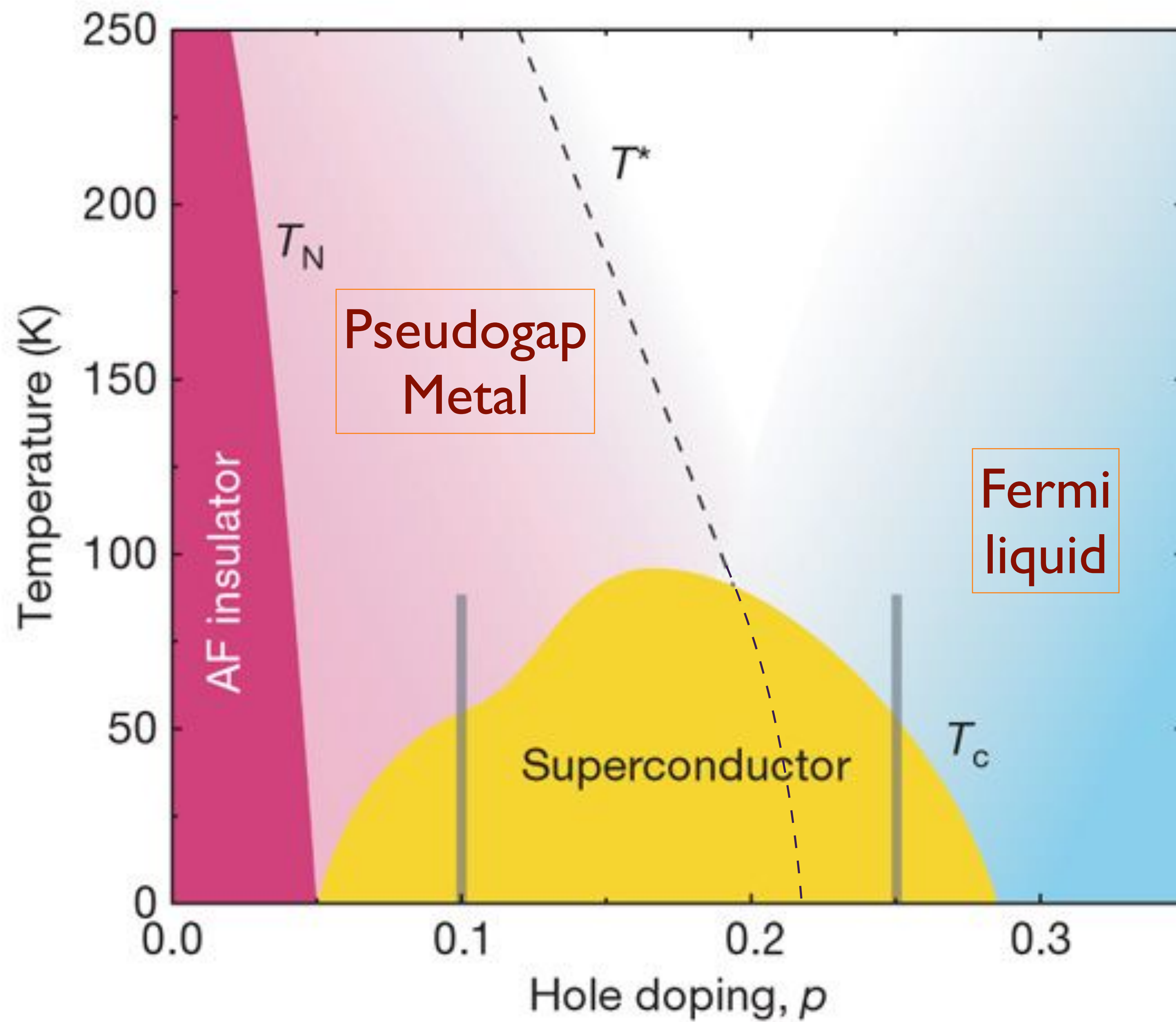
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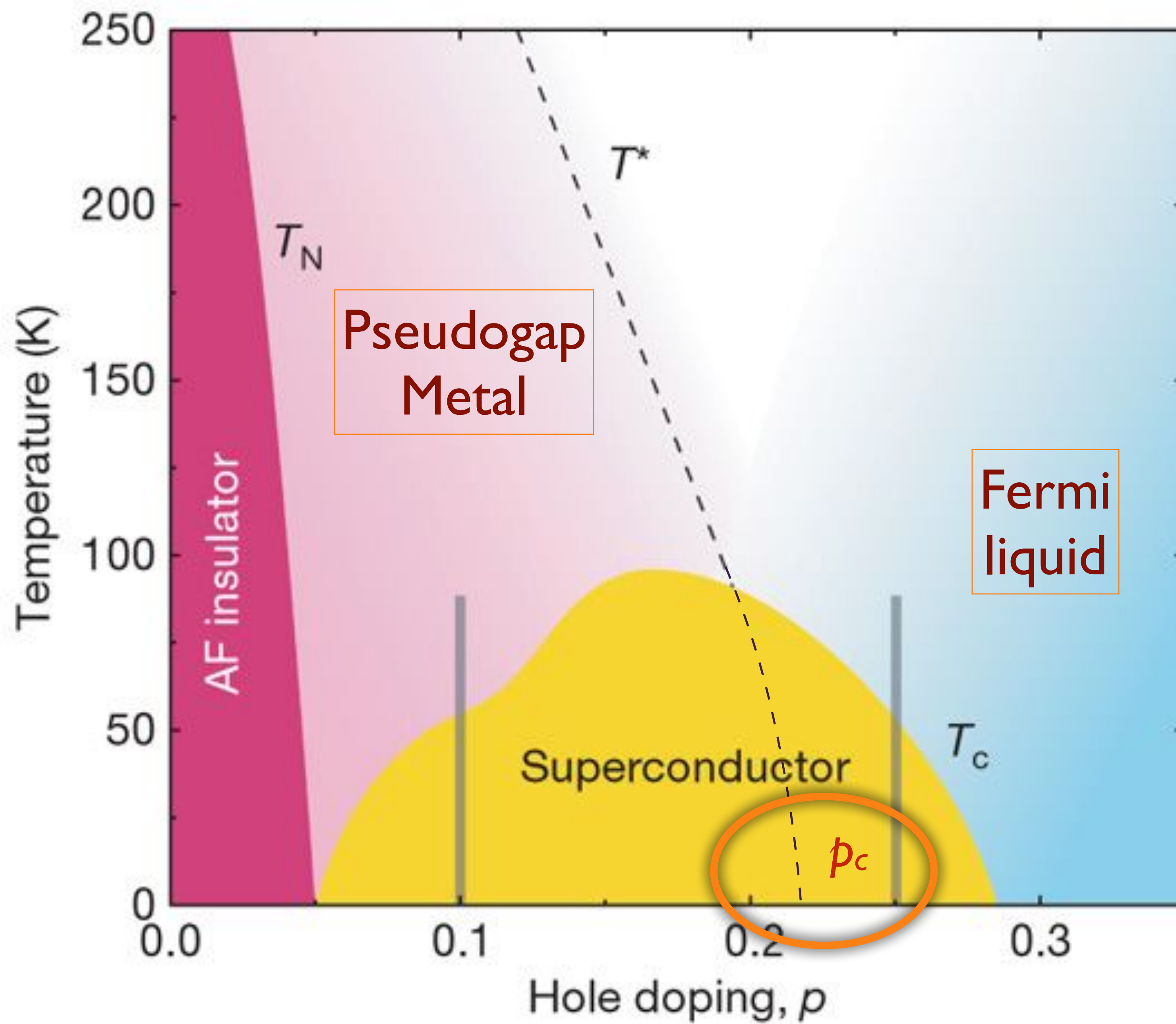
# High temperature superconductors

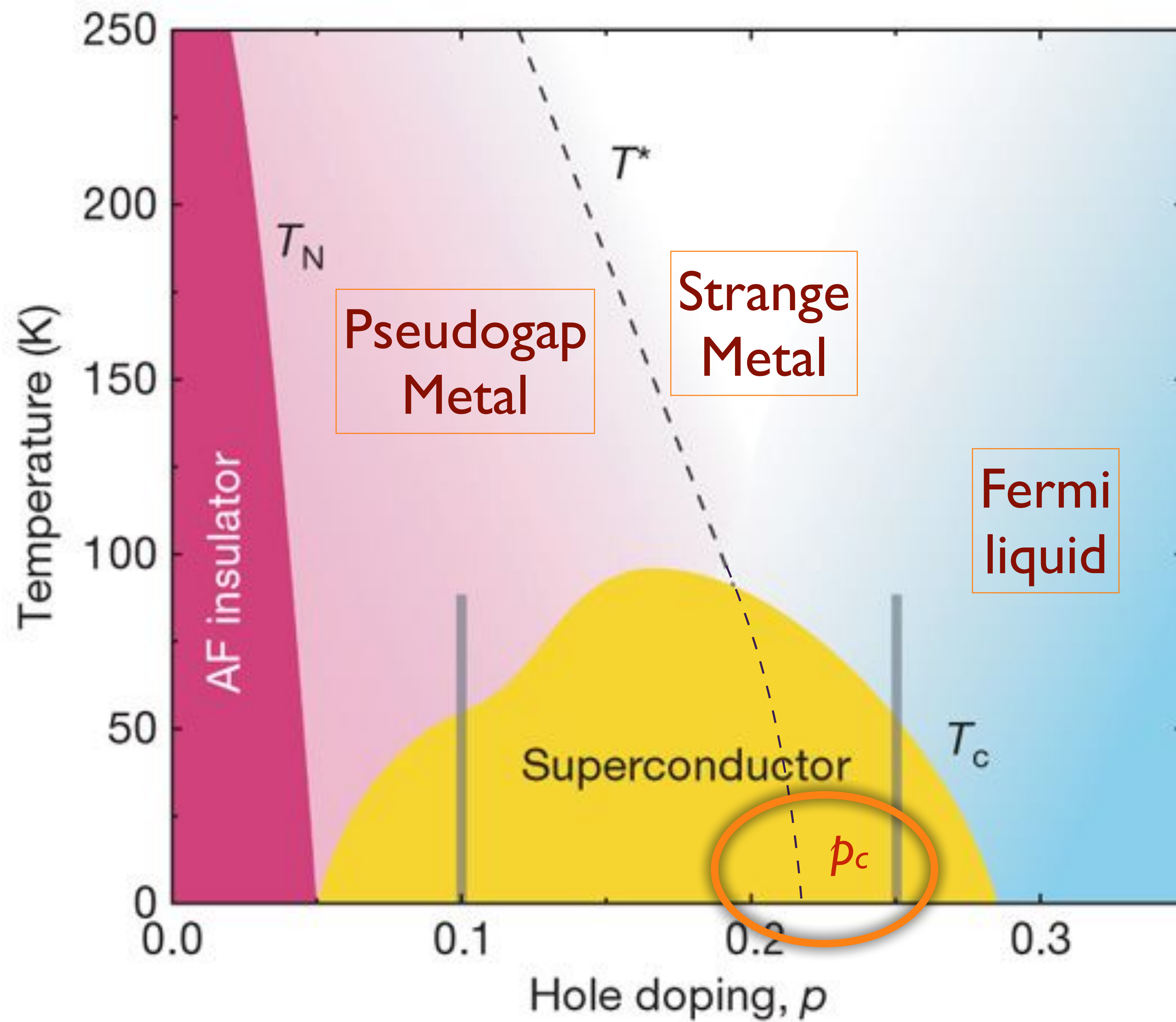




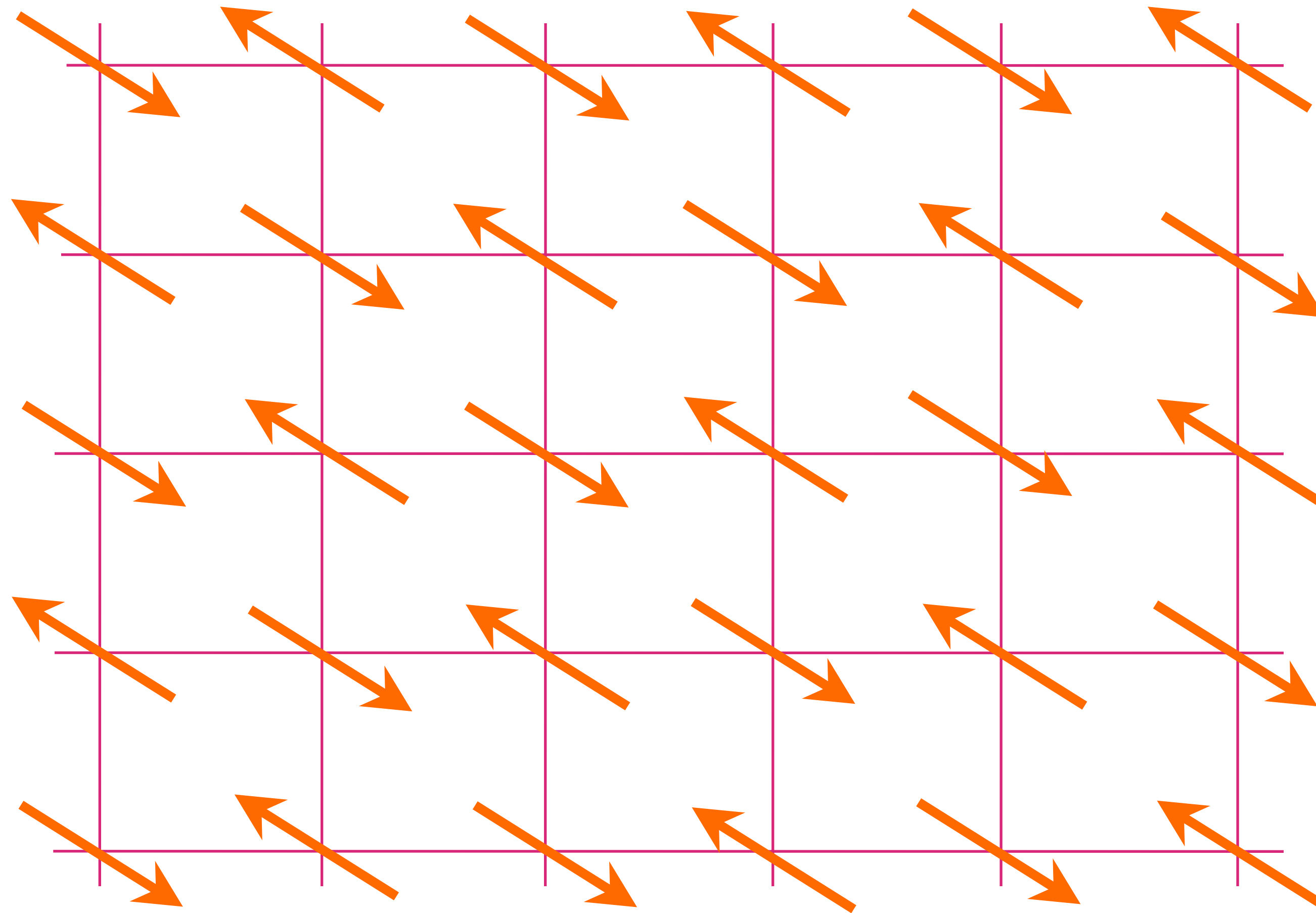




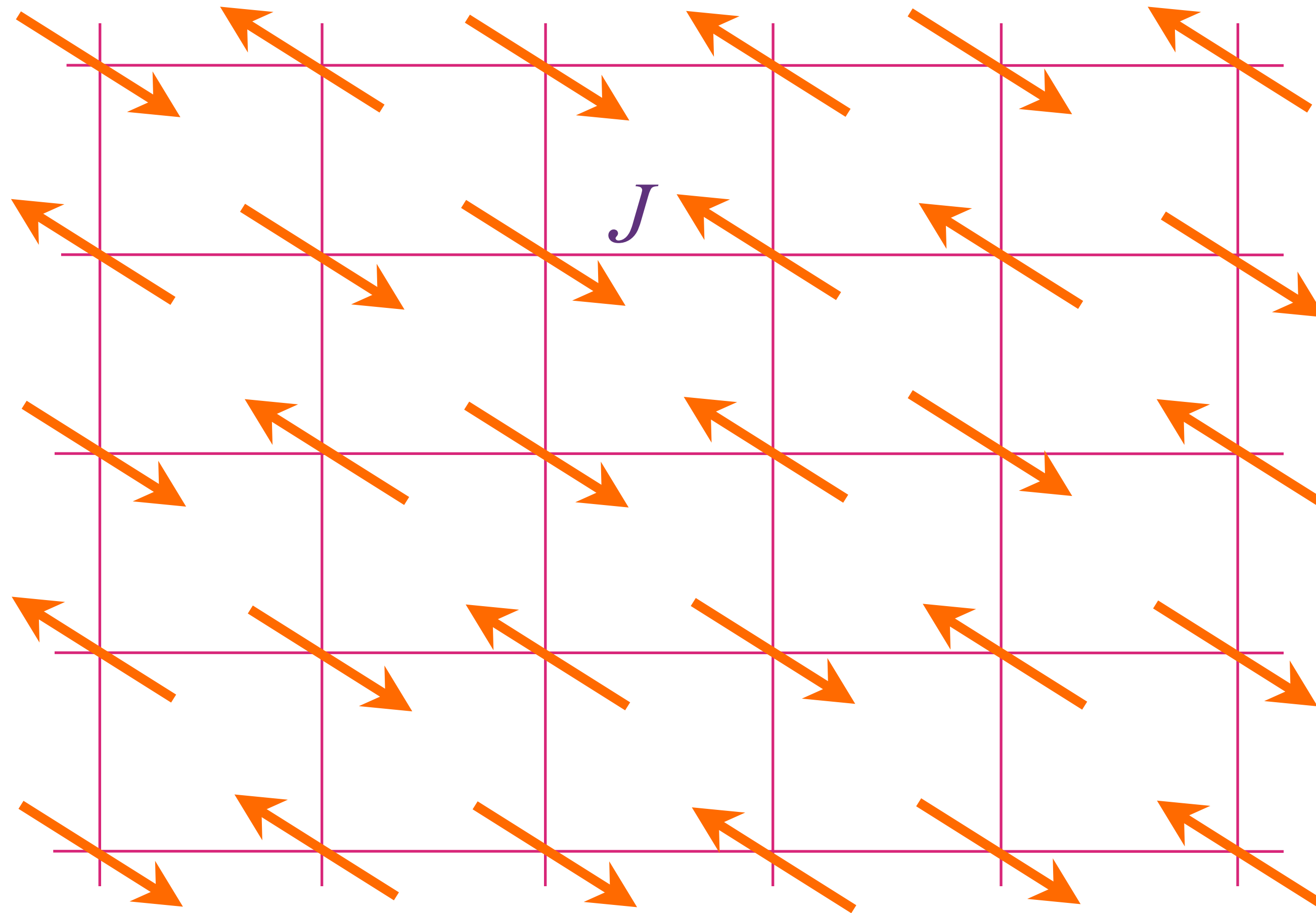




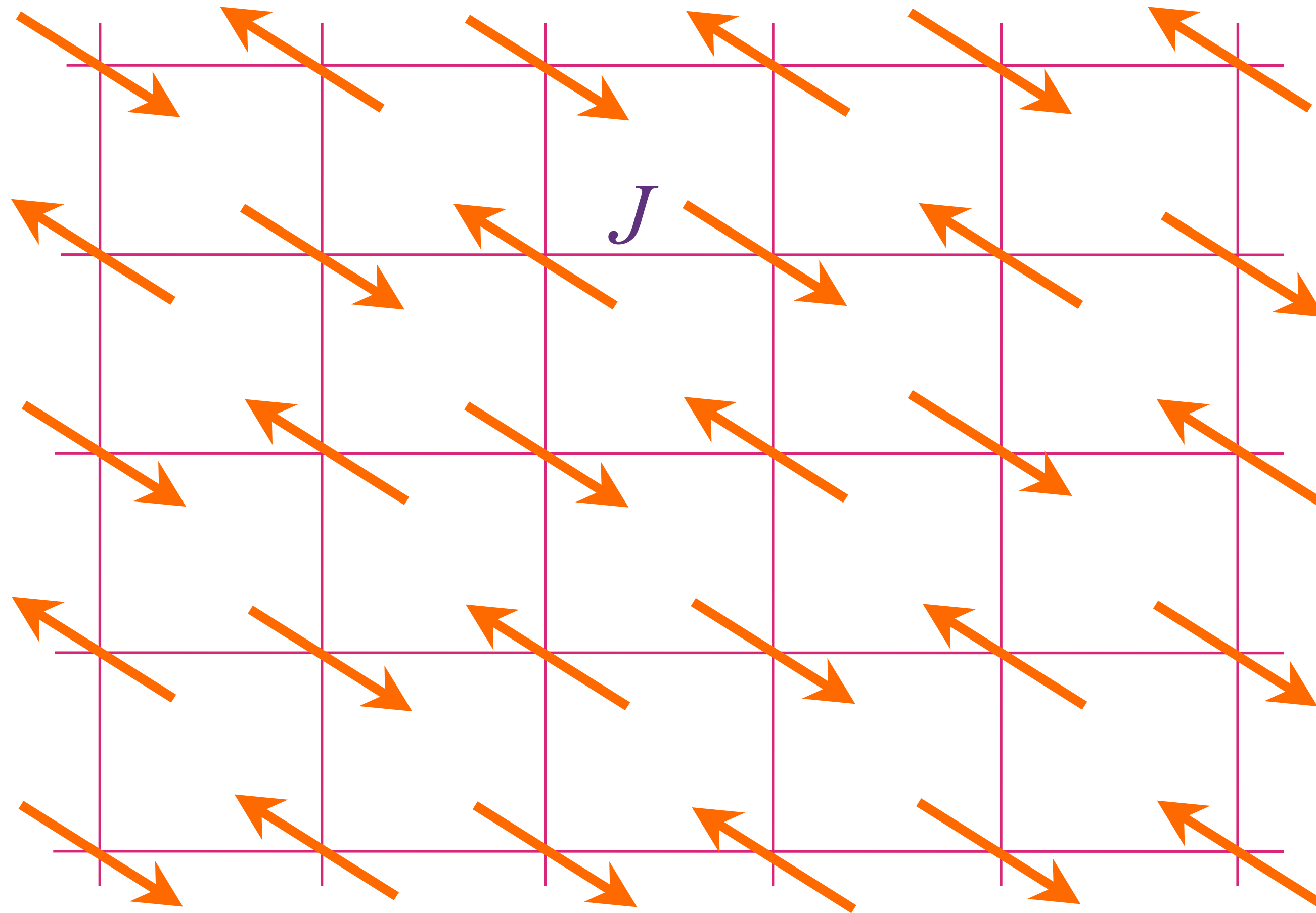
# Insulating antiferromagnet



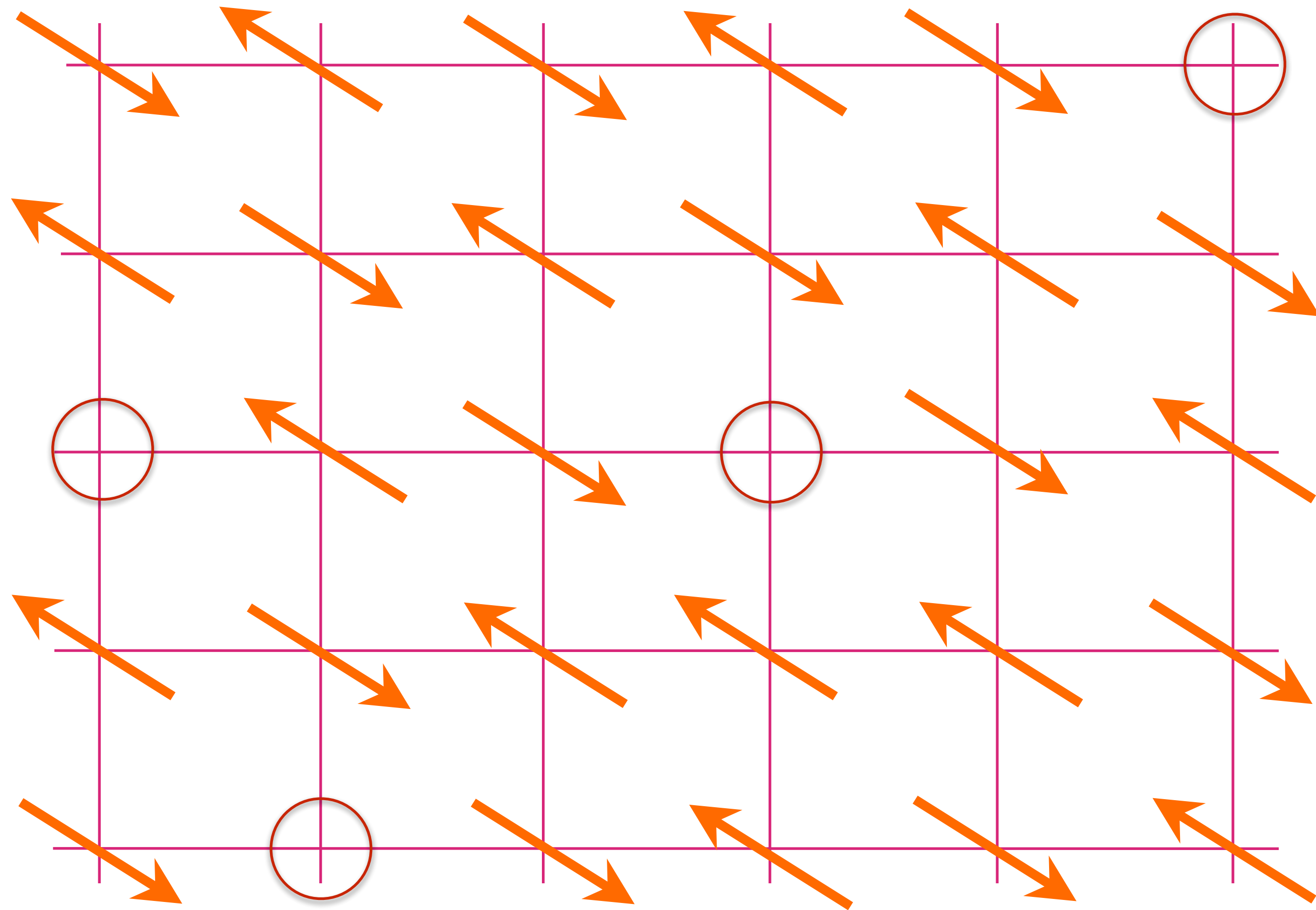
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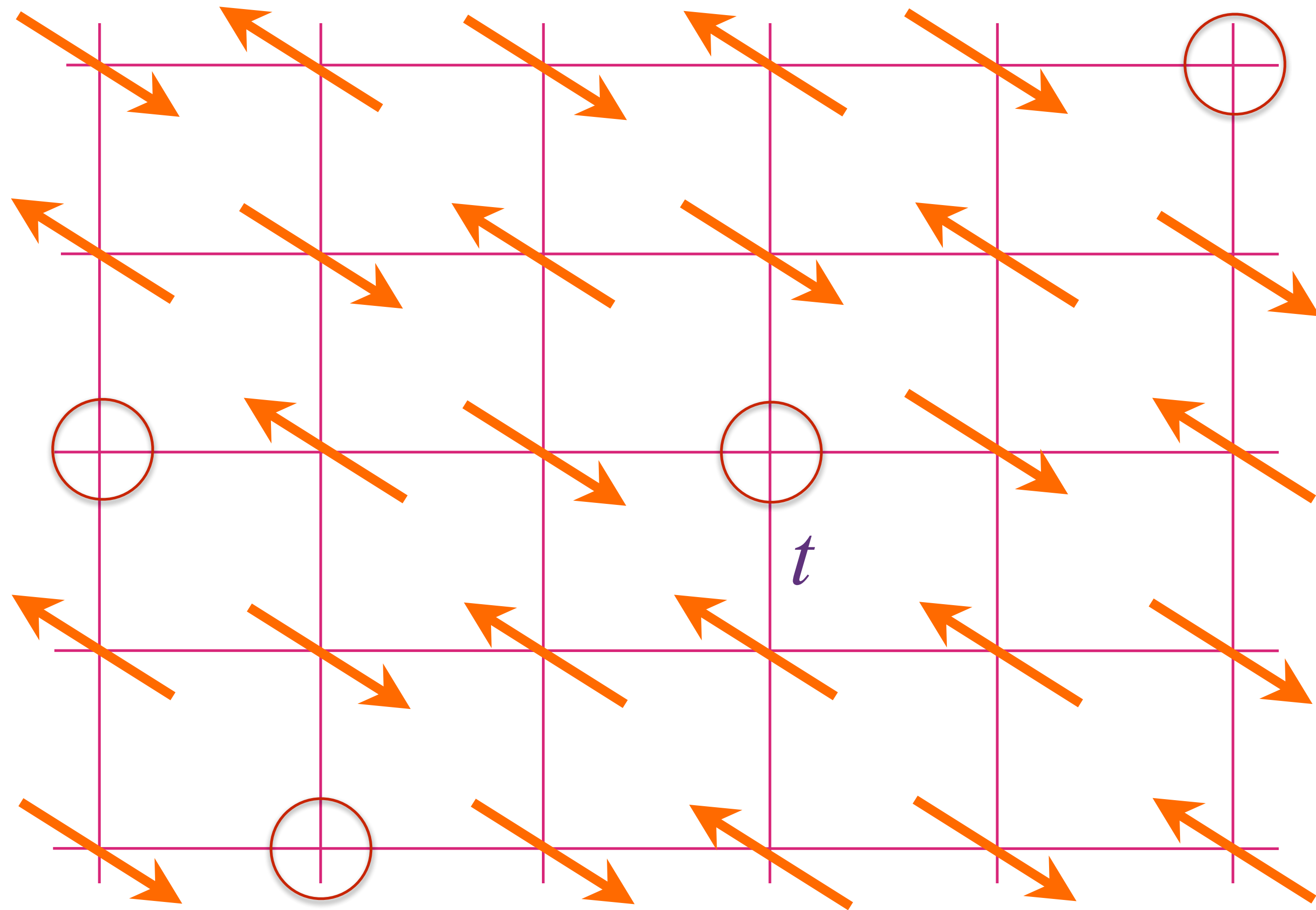
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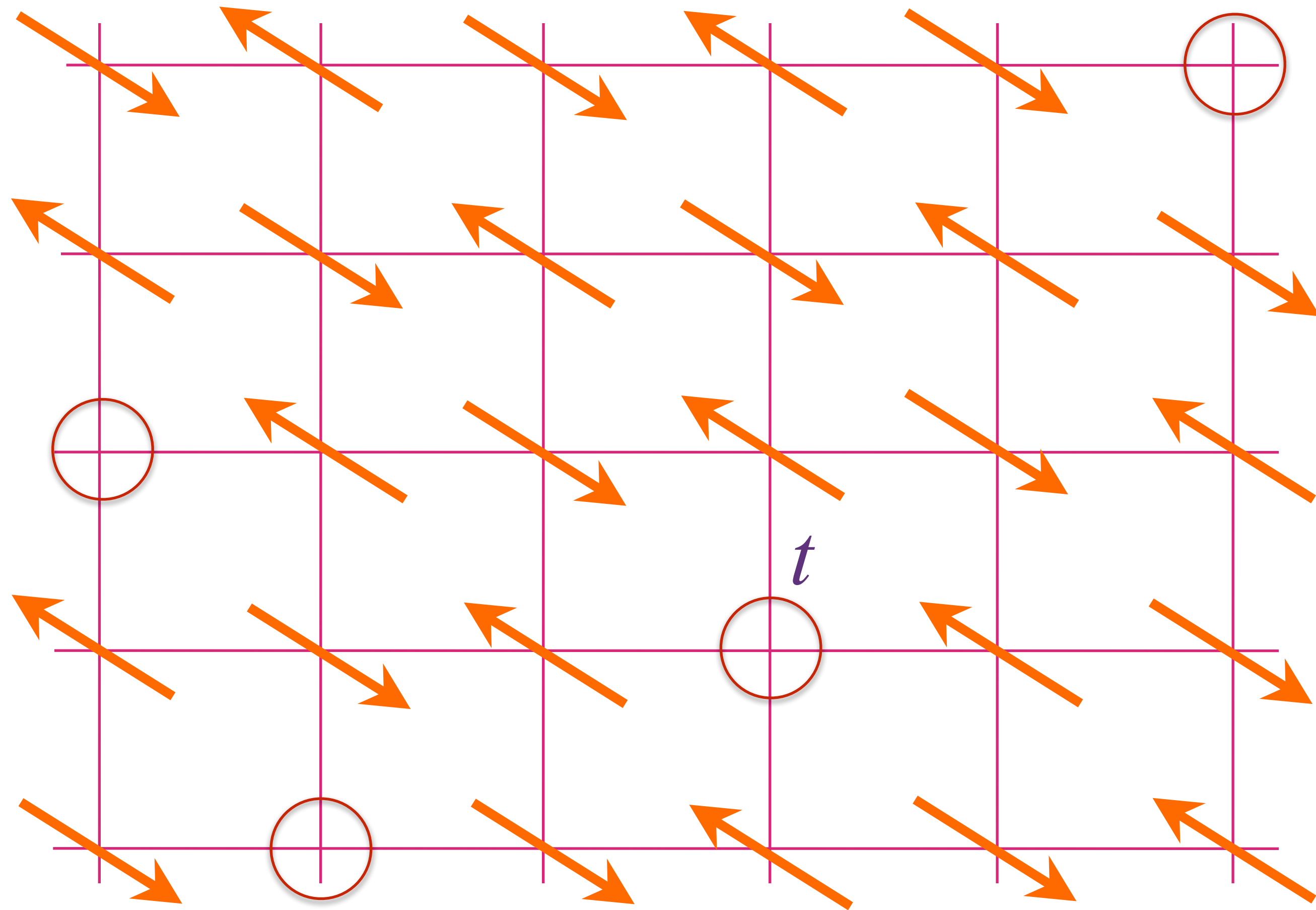
# Antiferromagnet doped with hole density $p$



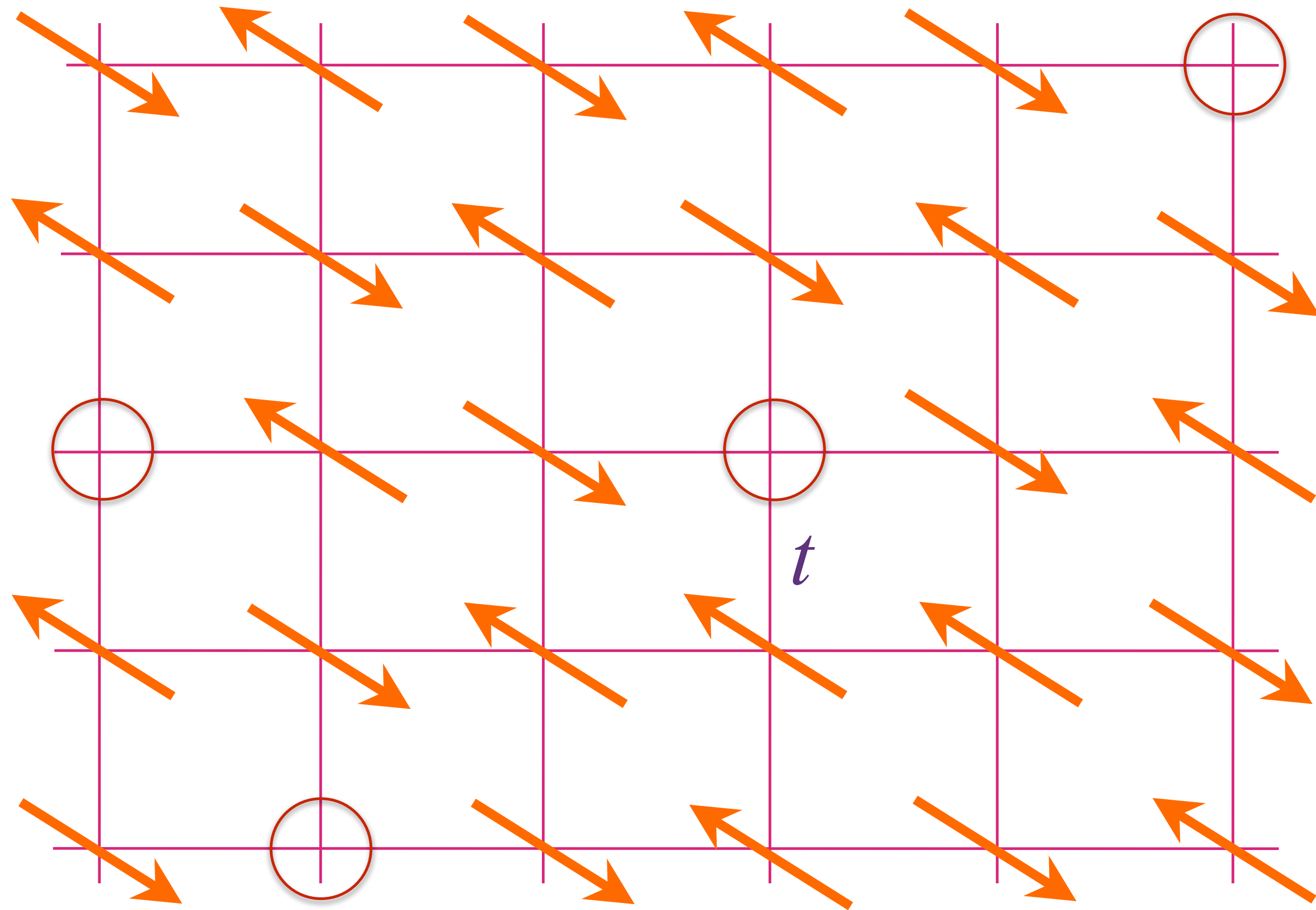
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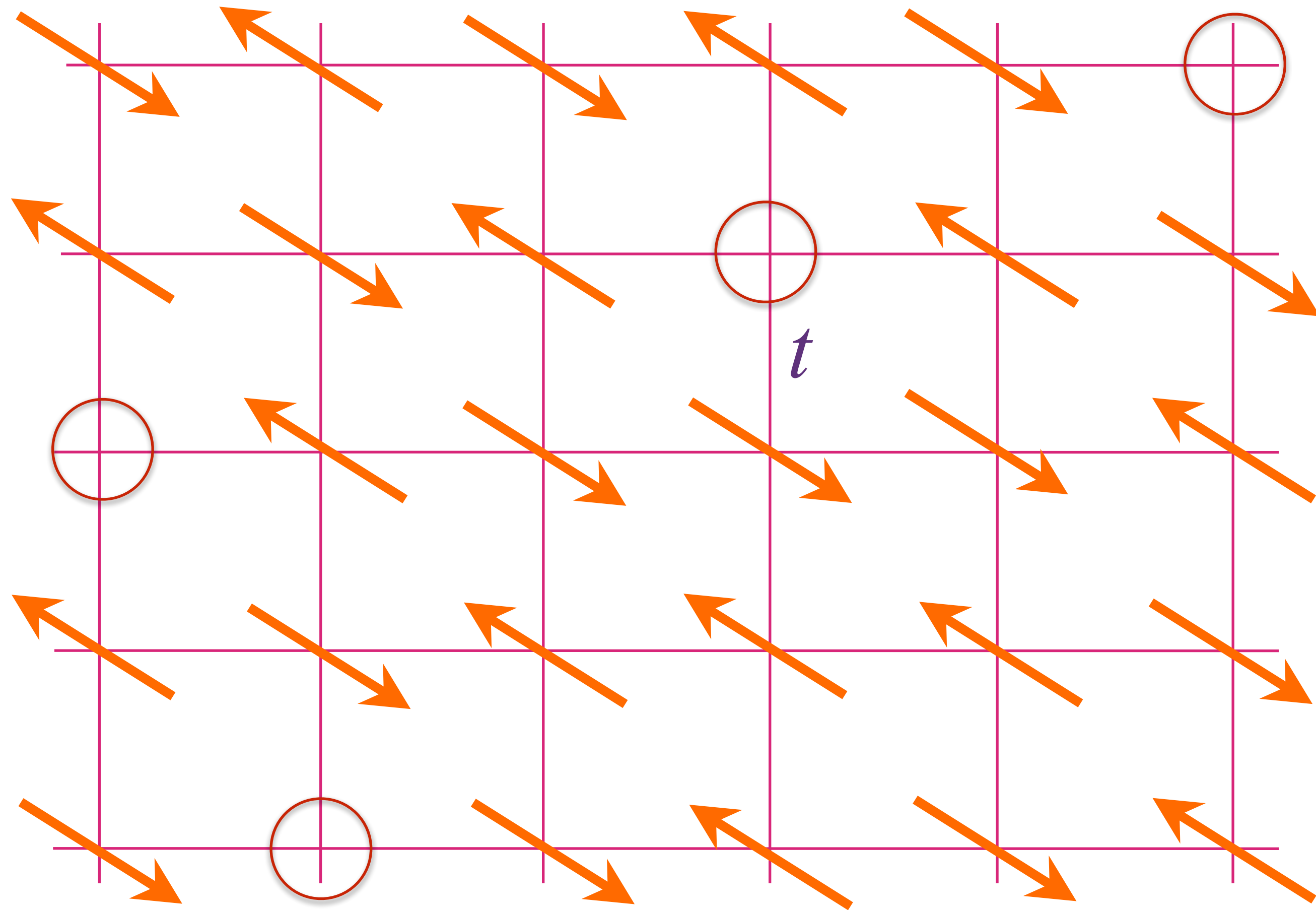


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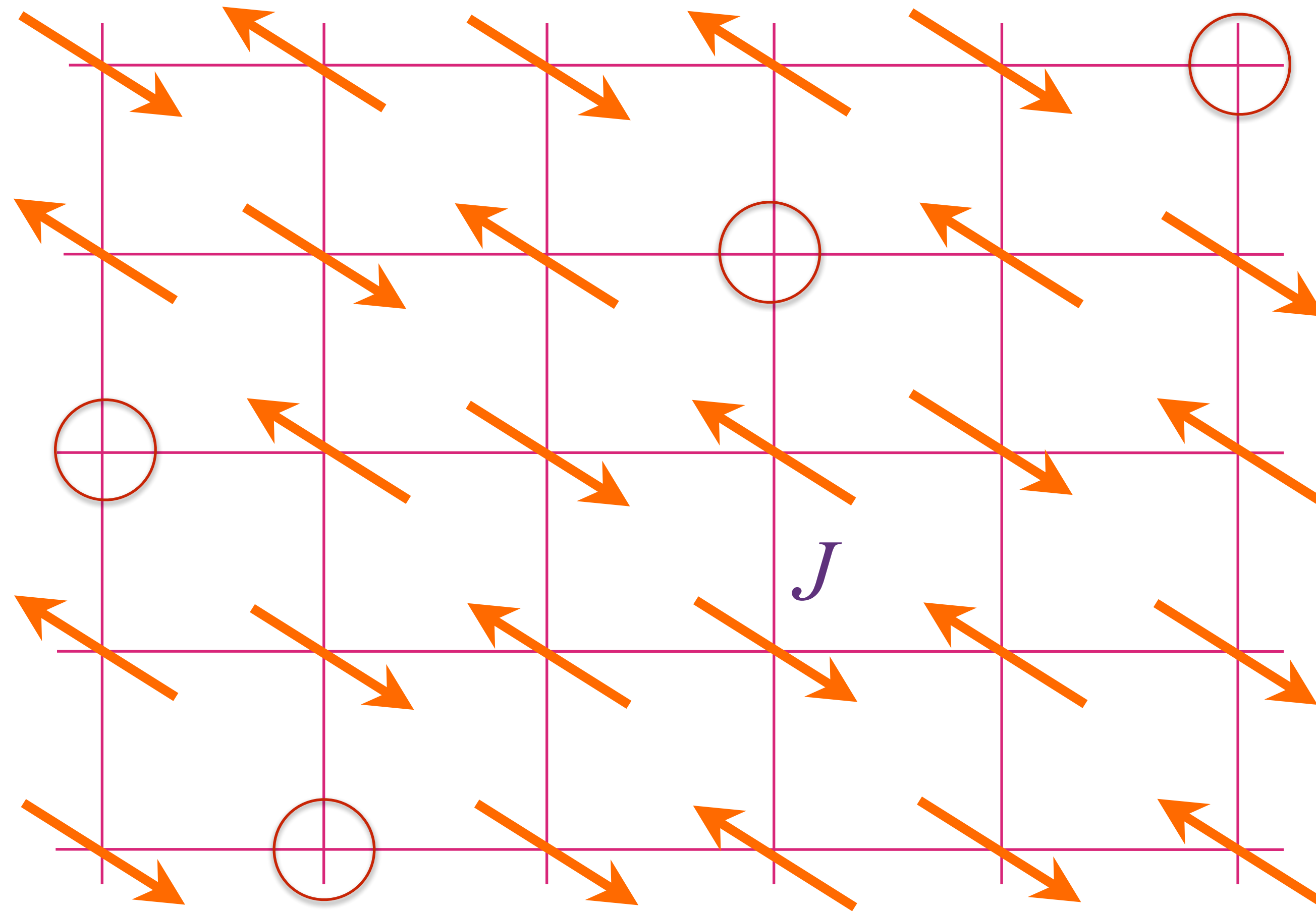
$p$  mobile holes in a background of  
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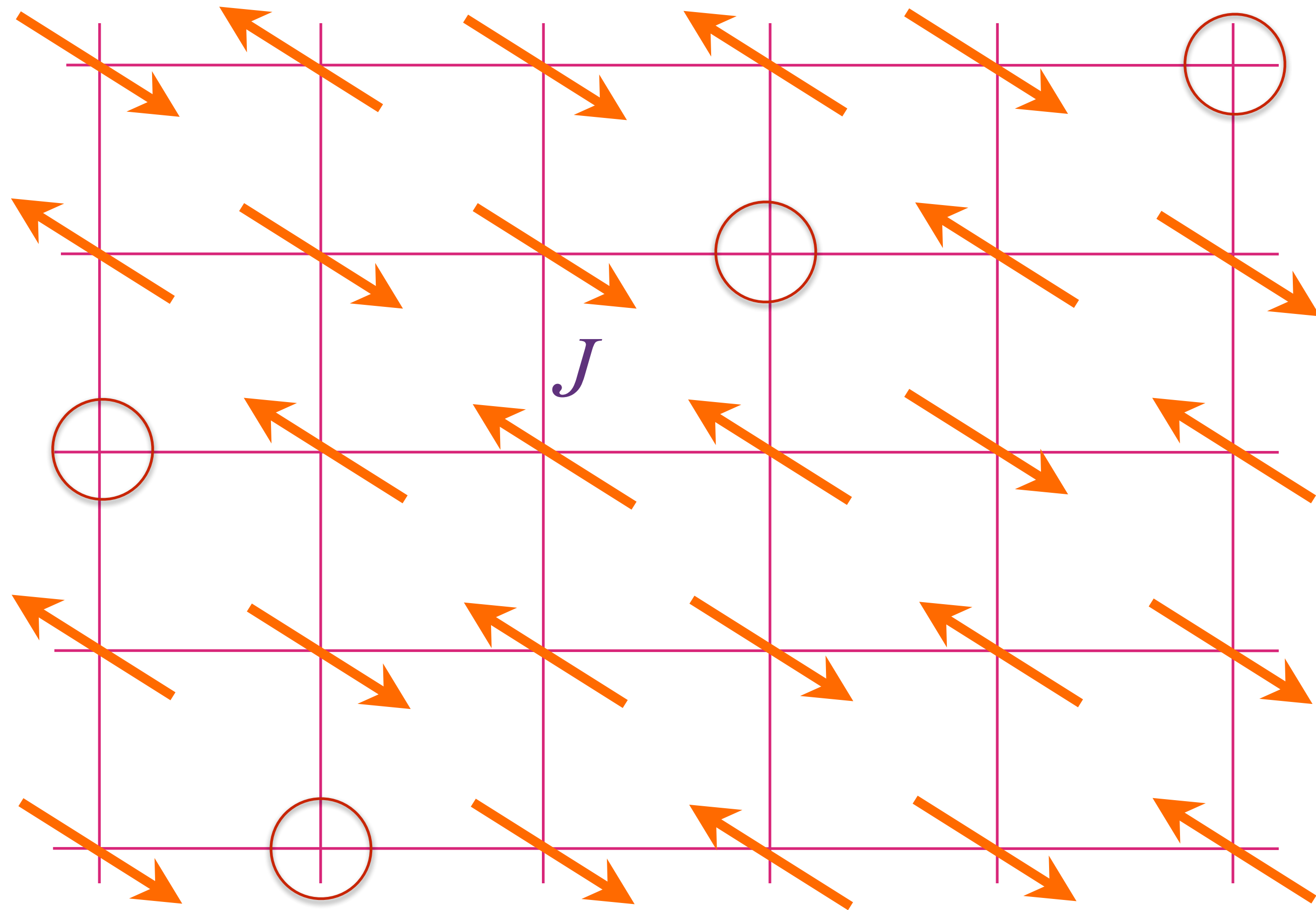
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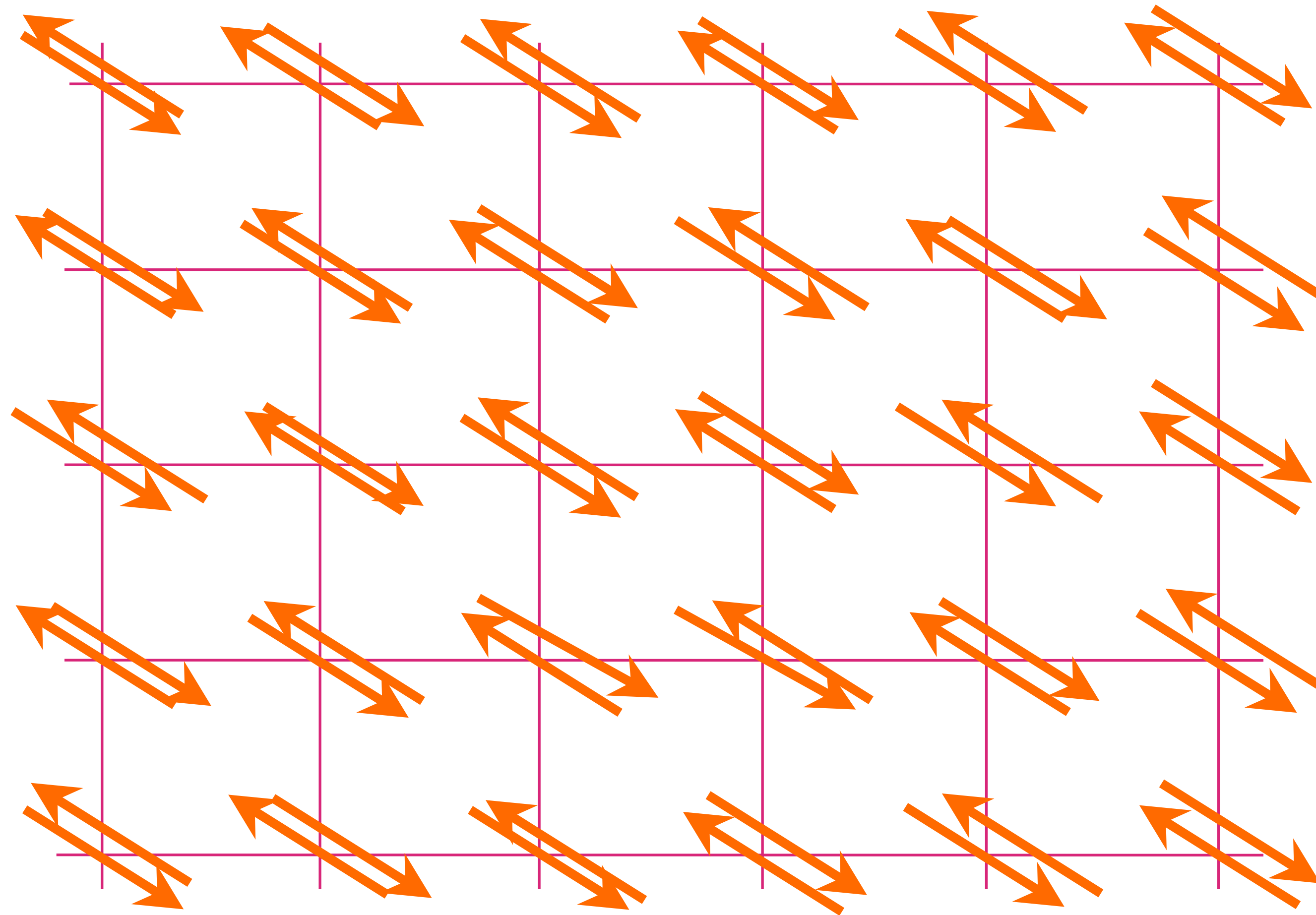
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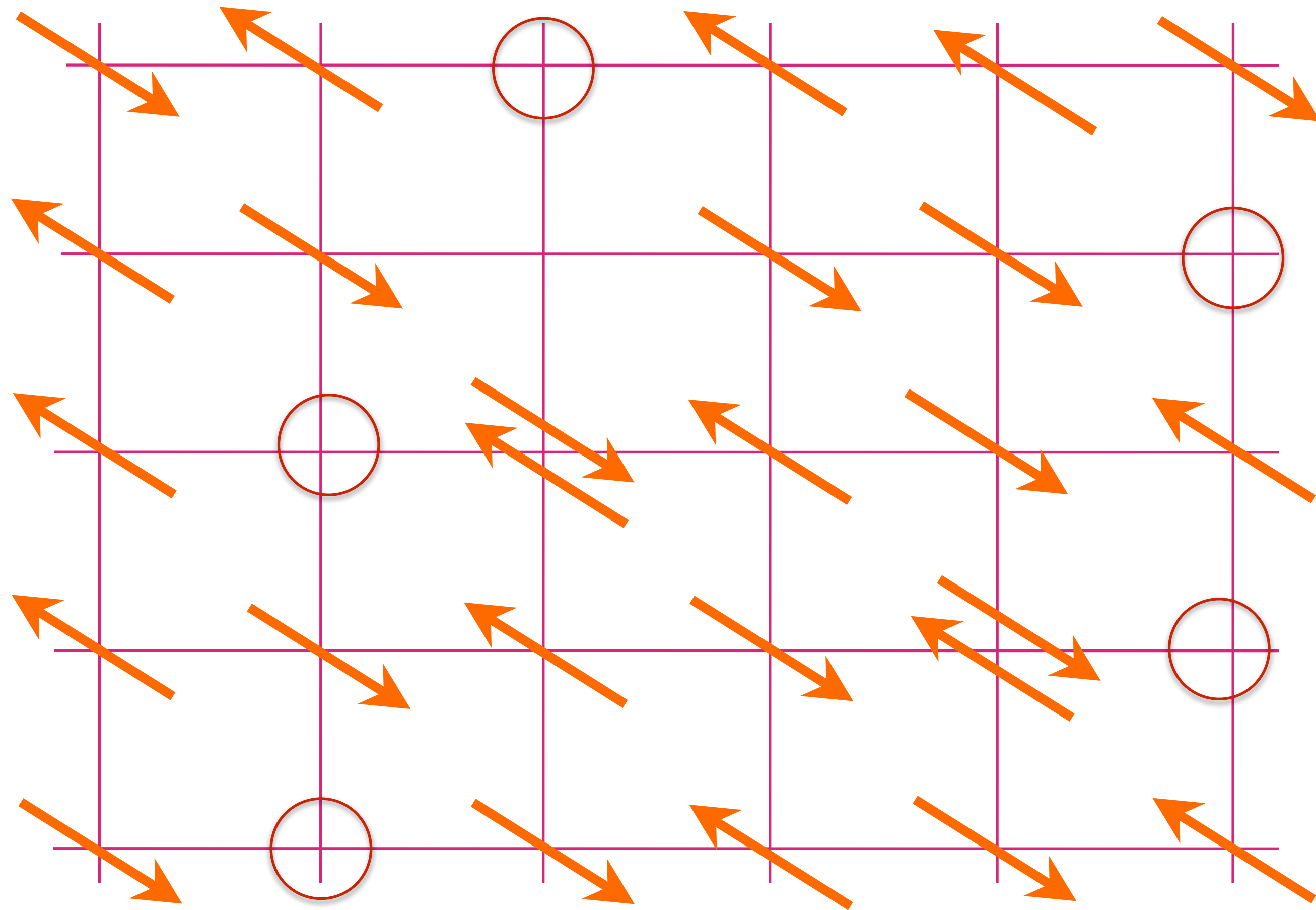
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# Momentum-space view at large $p$



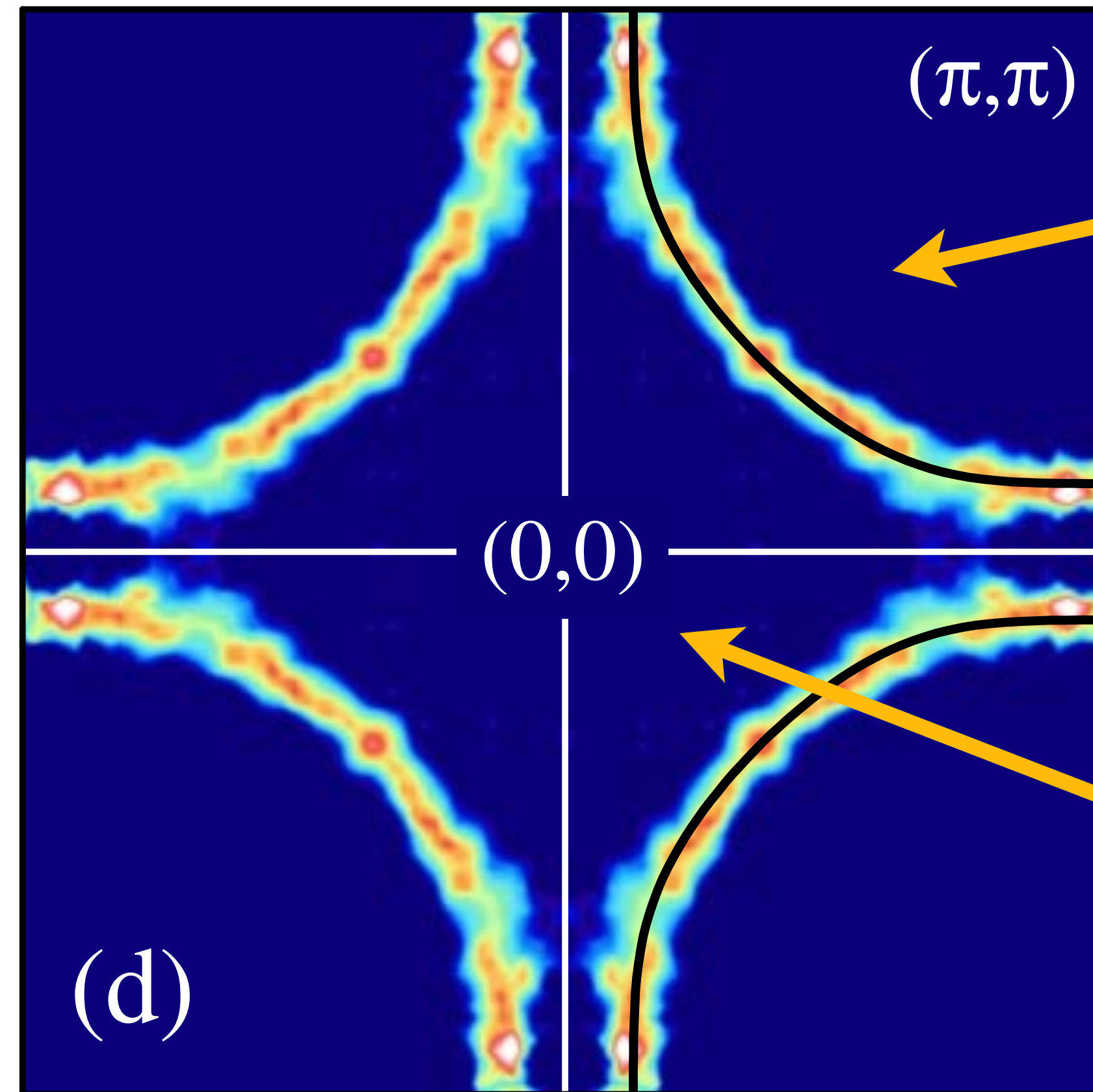
Filled  
Band

# Momentum-space view at large $p$



$1-p$  mobile electrons =  
 $1+p$  mobile holes in a filled band

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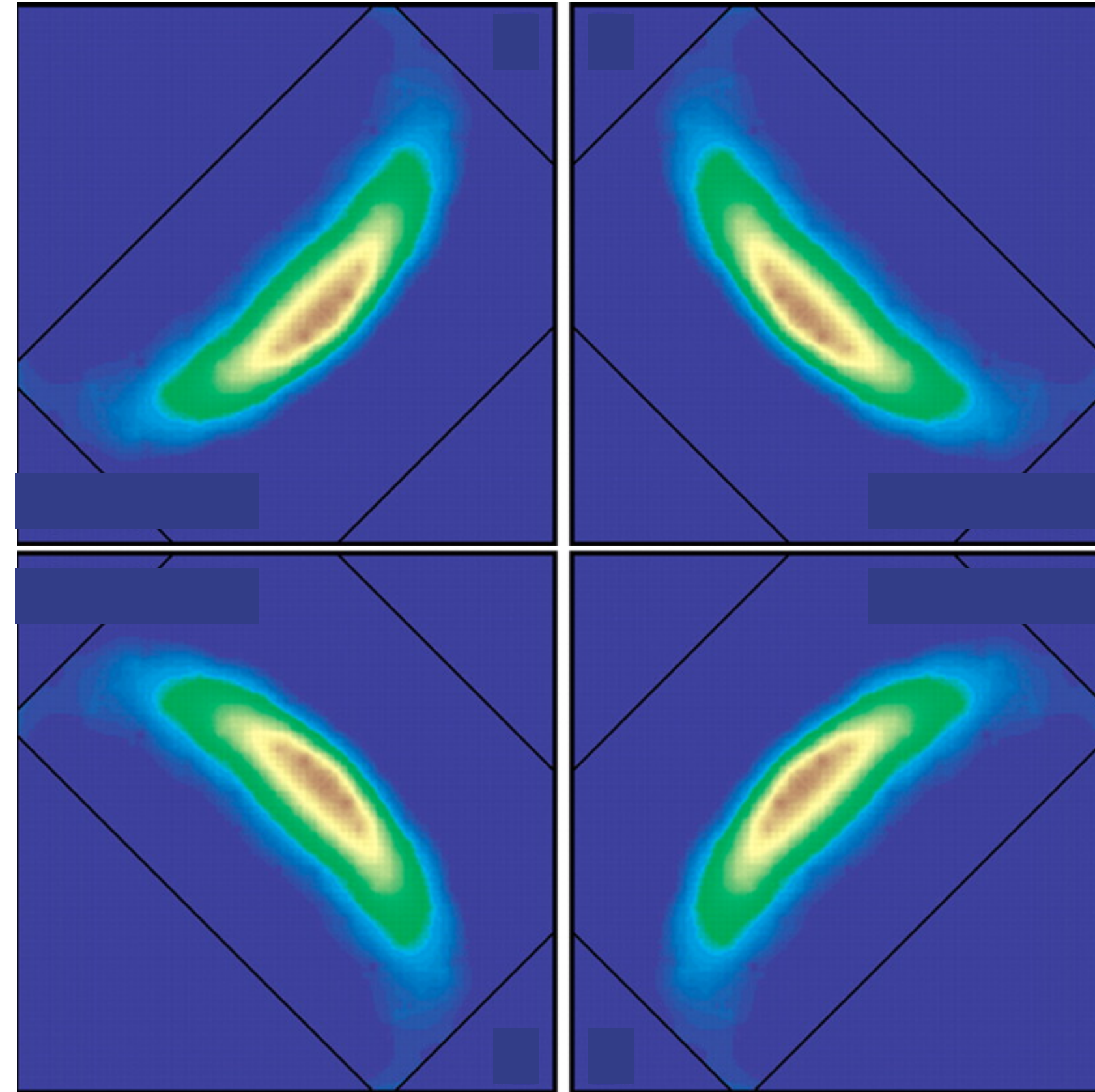
$l+p$  holes

Overdoped  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$   
 $T_c = 30\text{K}$

$l-p$  electrons

$l+p$  mobile holes in a filled band

# Momentum-space view at small $p$



$\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$   
at  $x = 0.10$

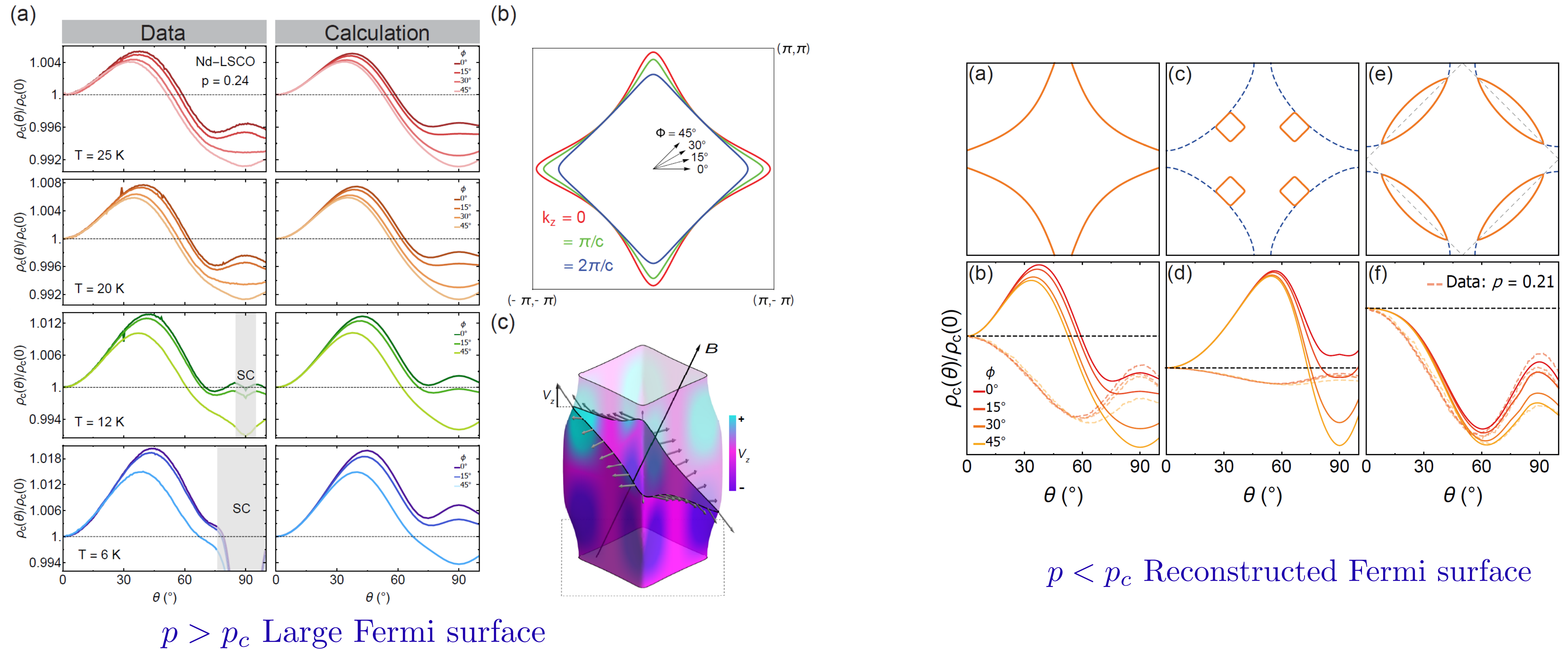
*“Fermi arcs”*

Kyle M. Shen, F. Ronning, D. H. Lu, F. Baumberger, N. J. C. Ingle, W. S. Lee, W. Meevasana, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, Z.-X. Shen, *Science* **307**, 901 (2005)

# 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, arXiv:2004.01725

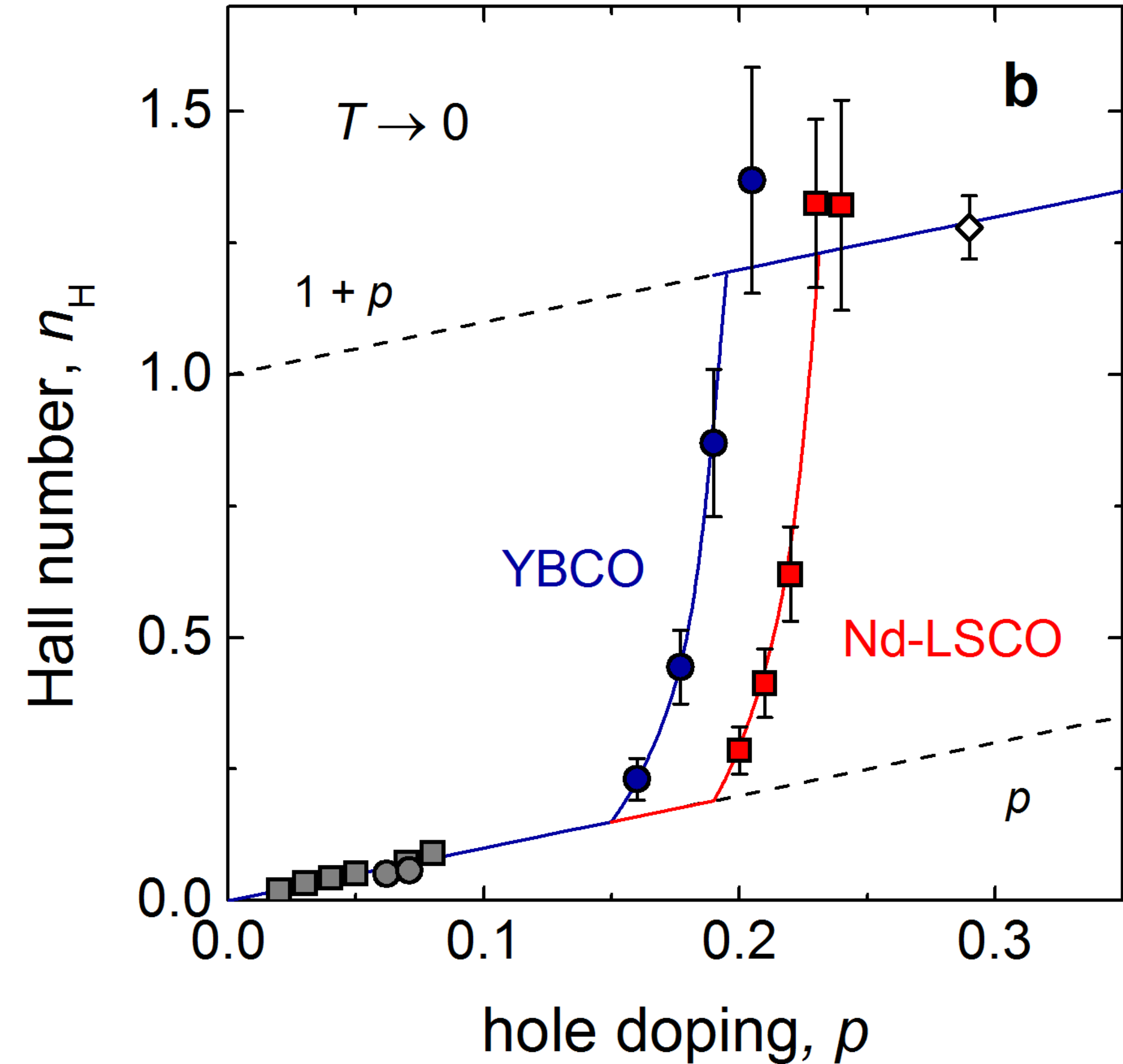
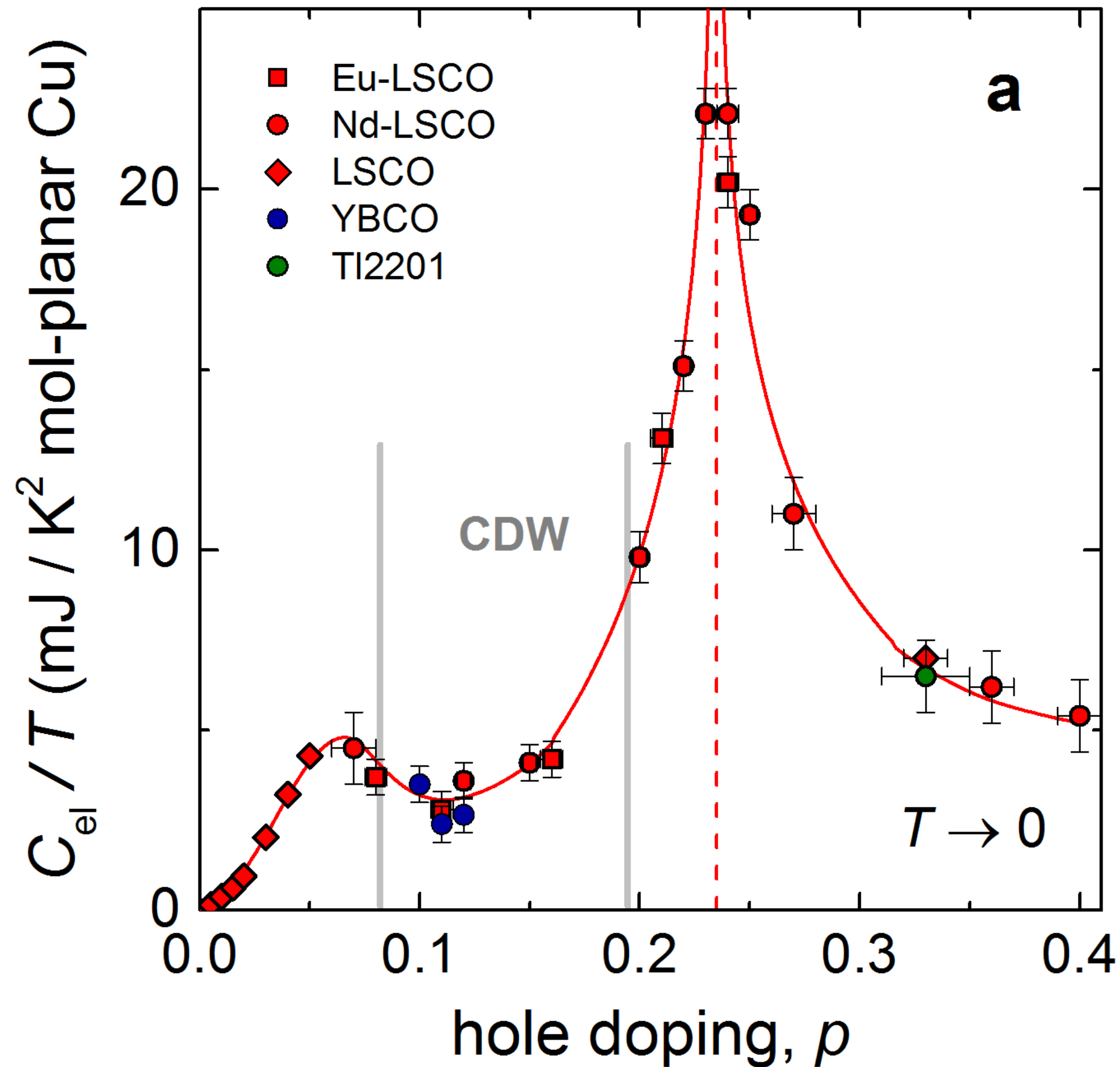
We use angle-dependent magnetoresistance (ADMR) to measure the Fermi surface of the cuprate  $\text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4$ . Above the critical doping  $p^*$  — outside of the pseudogap phase — we find a Fermi surface that is in quantitative agreement with angle-resolved photoemission. Below  $p^*$ , however, the ADMR is qualitatively different, revealing a clear change in Fermi surface topology. We find that our data is most consistent with a Fermi surface that has been reconstructed by a  $Q = (\pi, \pi)$  wavevector. While static  $Q = (\pi, \pi)$  antiferromagnetism is not found at these dopings, our results suggest that this wavevector is a fundamental organizing principle of the pseudogap phase.



# Hole doped cuprates

The remarkable underlying ground states of cuprate superconductors

Cyril Proust and Louis Taillefer, Annual Review Condensed Matter Physics **10**, 409 (2019)



1. Luttinger volume violation in  
Kondo lattice models

*The FL\* phase*

2. Introduction to cuprates

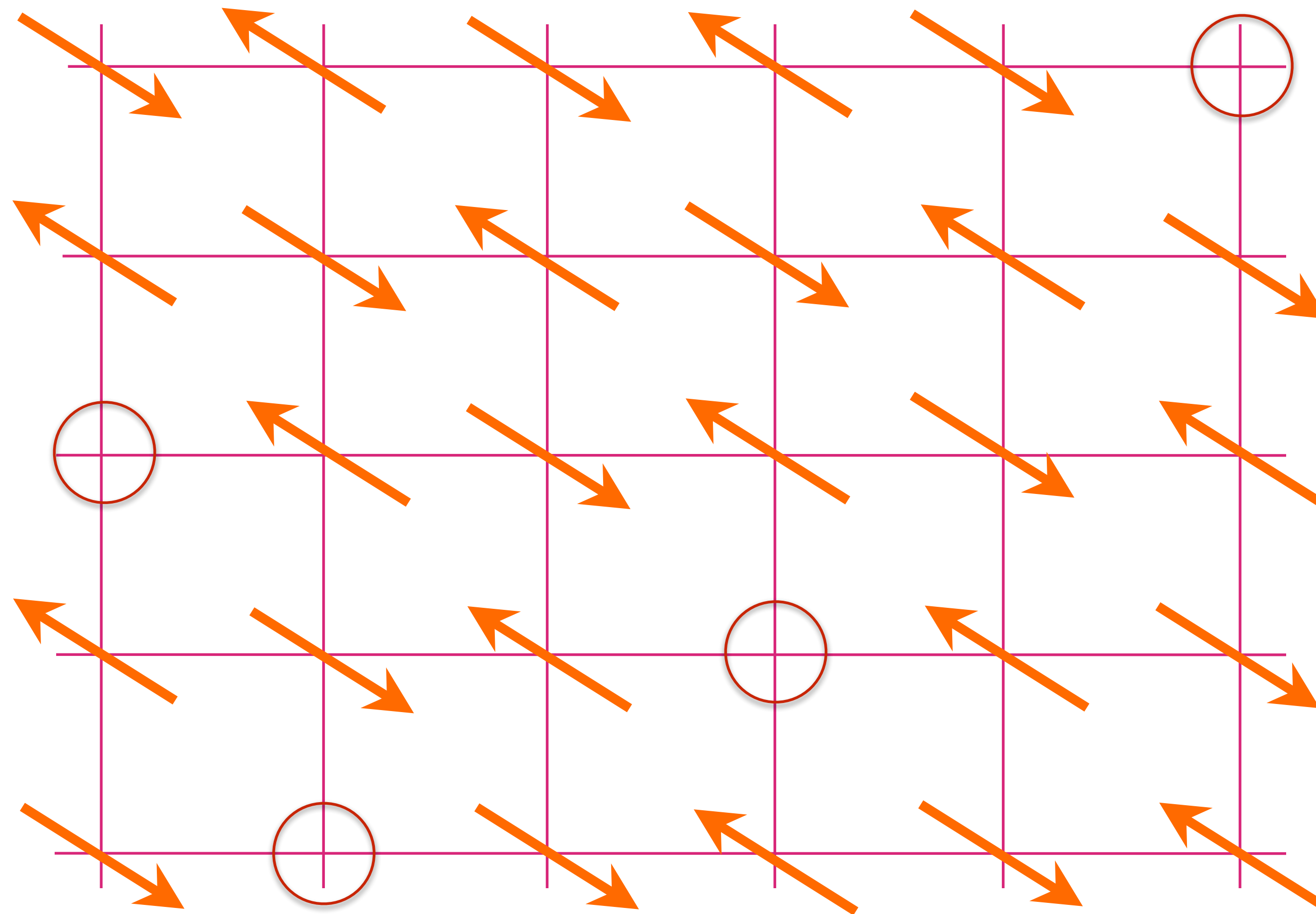
*The pseudogap metal*

3. Luttinger volume violation a one-band model

*Ancilla qubits and ghost Fermi surfaces*

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

- Can realize the FL\* state as a doped spin liquid in which spinons and holons bind to form ‘electrons’, which then form a small Fermi surface (X.-G. Wen and P. A. Lee, PRL **76**, 503 (1996)); but there is no complete description of this process, except in the very strong binding limit of dimer ‘electrons’ (M. Punk, A. Allais, and S. Sachdev, PNAS **112**, 9552 (2015)). This approach does not yield a theory of the transition to the FL state.

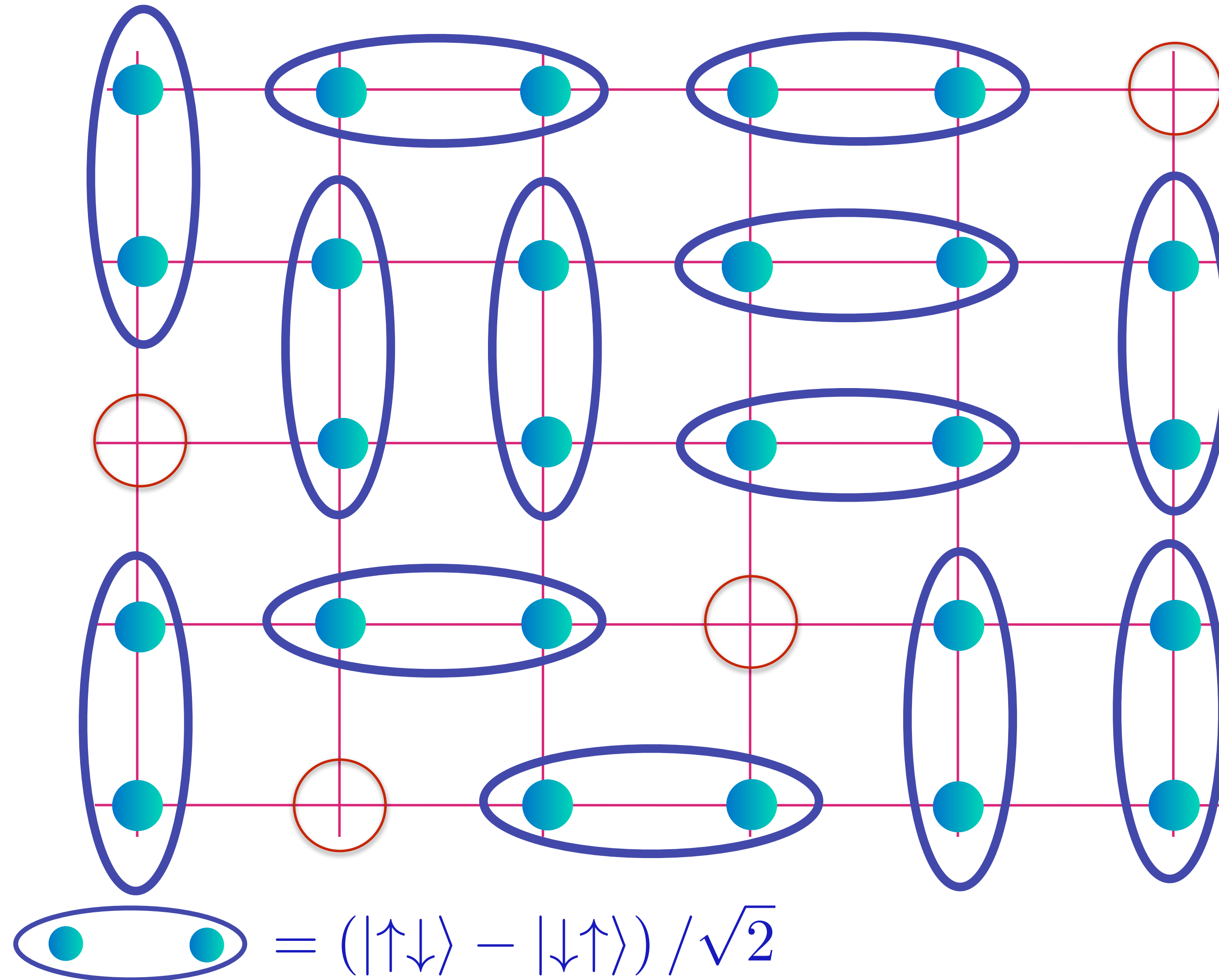


Anti-ferromagnet  
with  $p$  holes  
per square

# Holon metal

S.A. Kivelson, D.S. Rokhsar and J.P. Sethna, PRB **35**, 8865 (1987)

D. Rokhsar and S.A. Kivelson, PRL **61**, 2376 (1988)

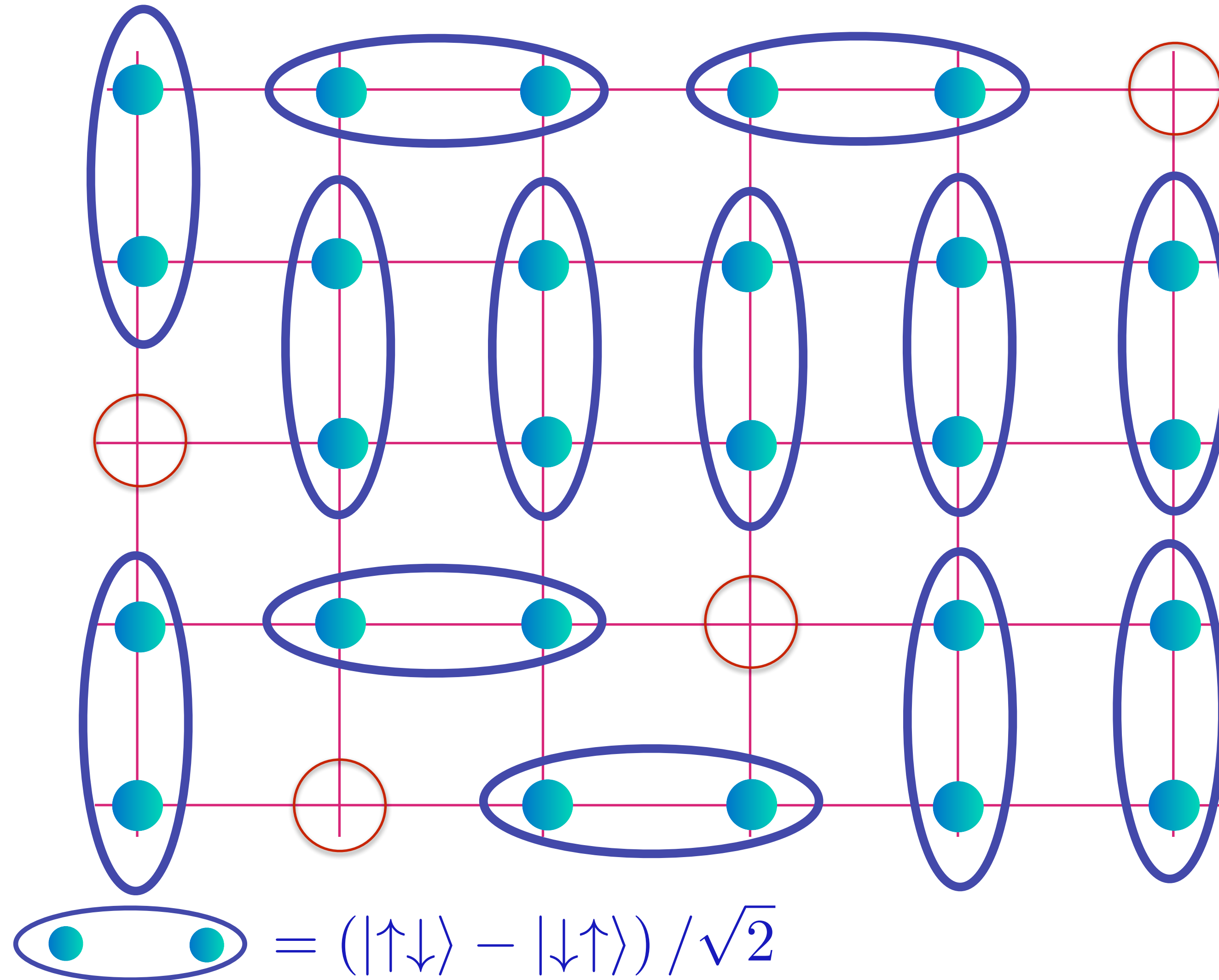


Spin liquid  
with density  
 $\rho$  of spinless,  
charge  $+e$   
“holons”.

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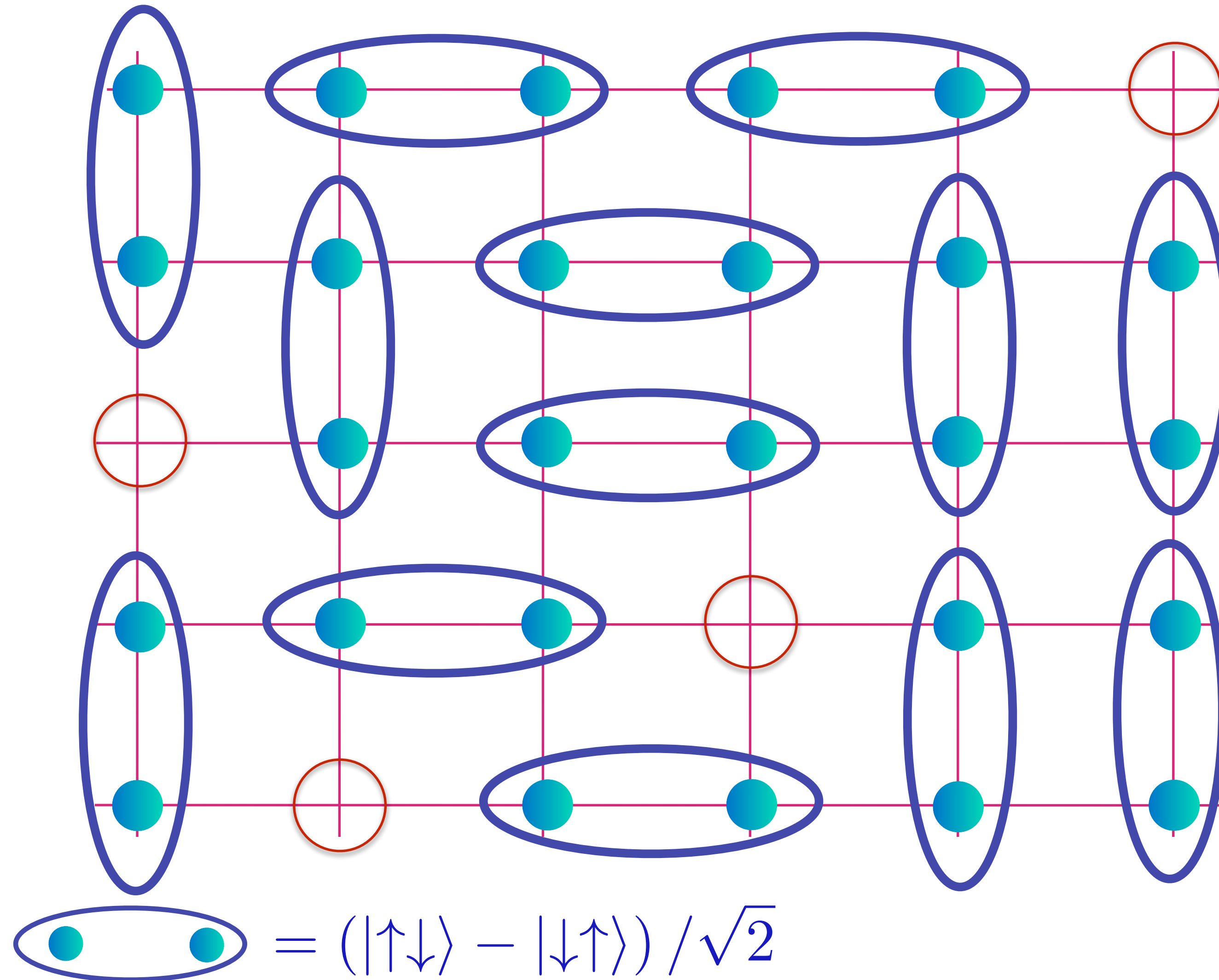


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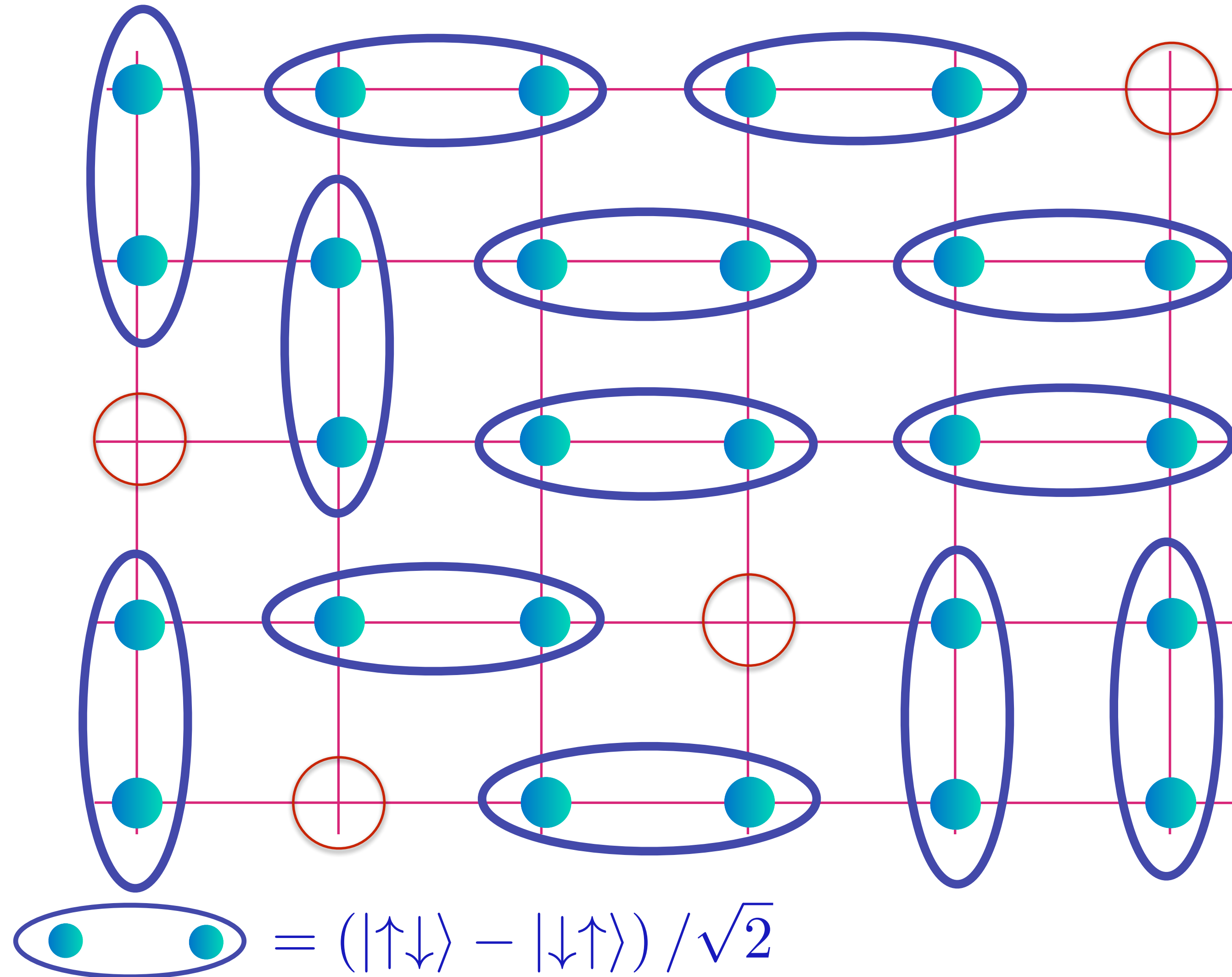


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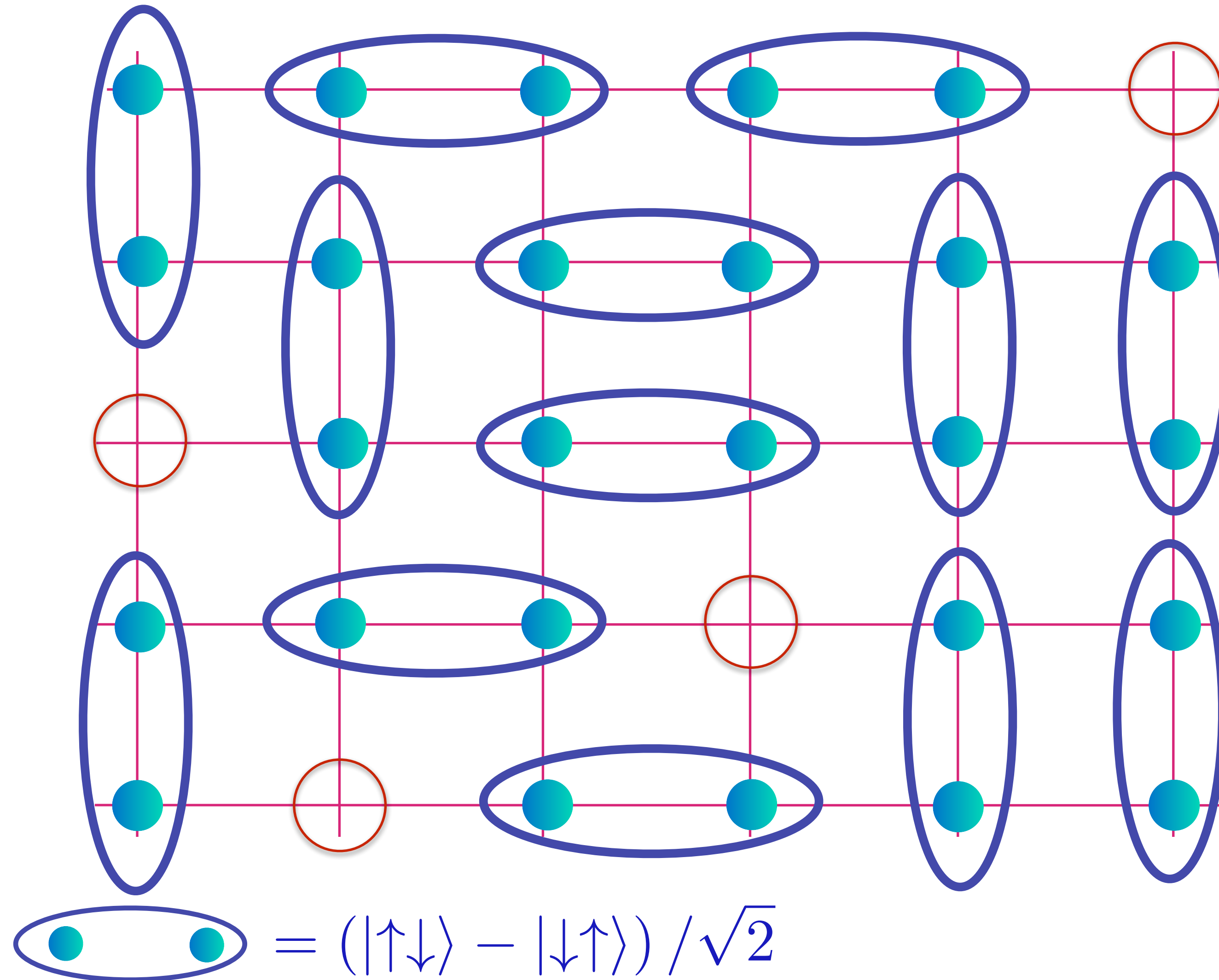


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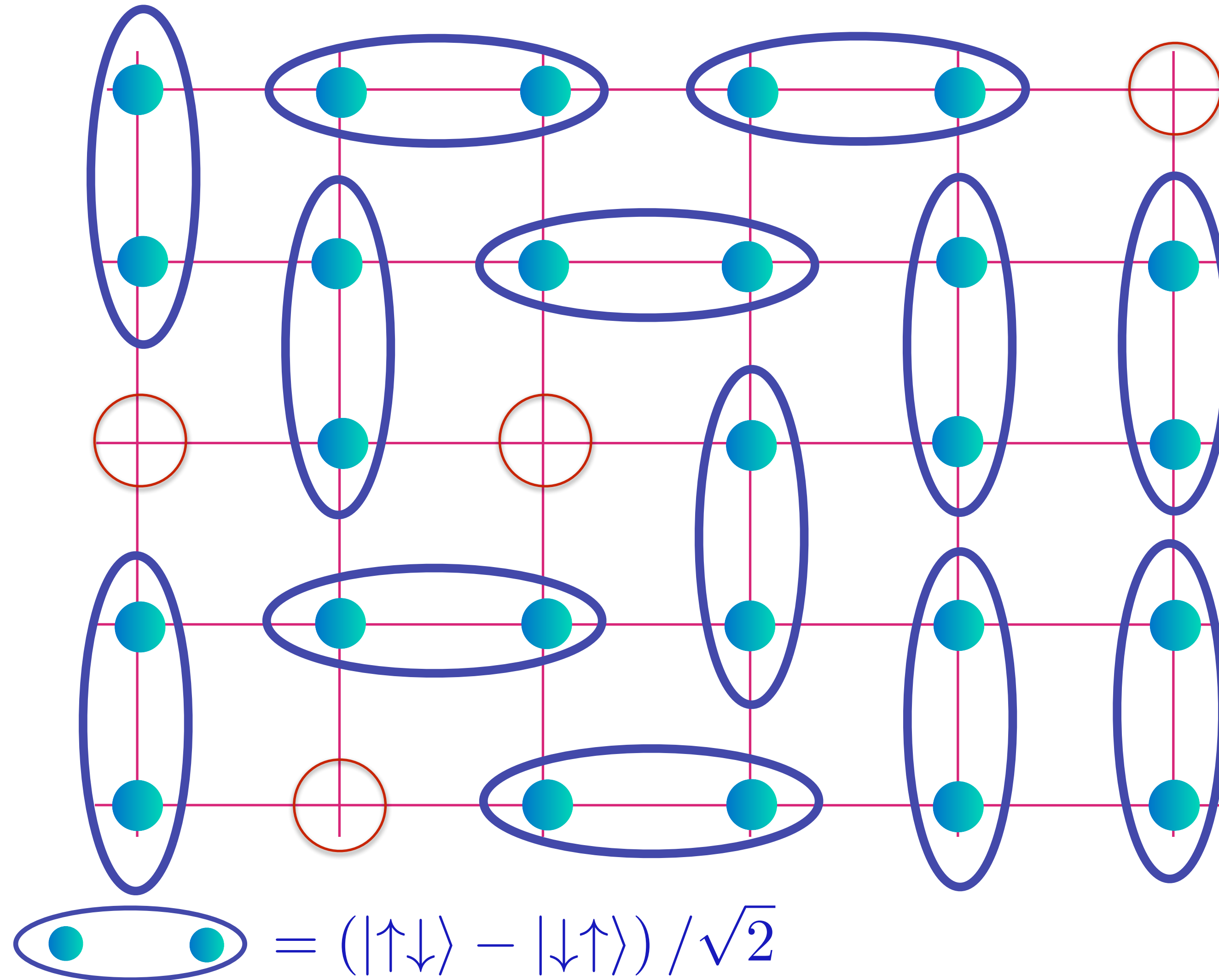


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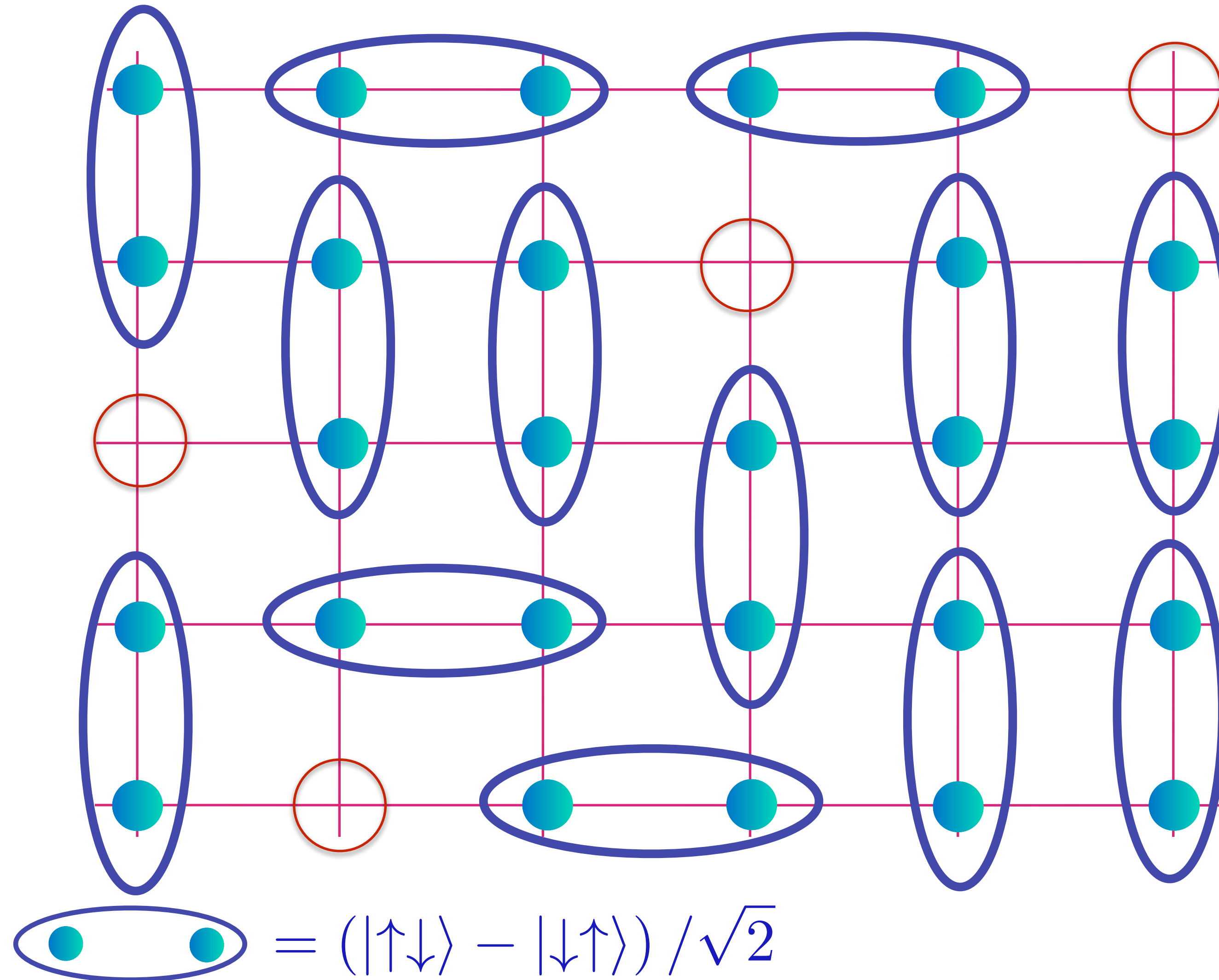


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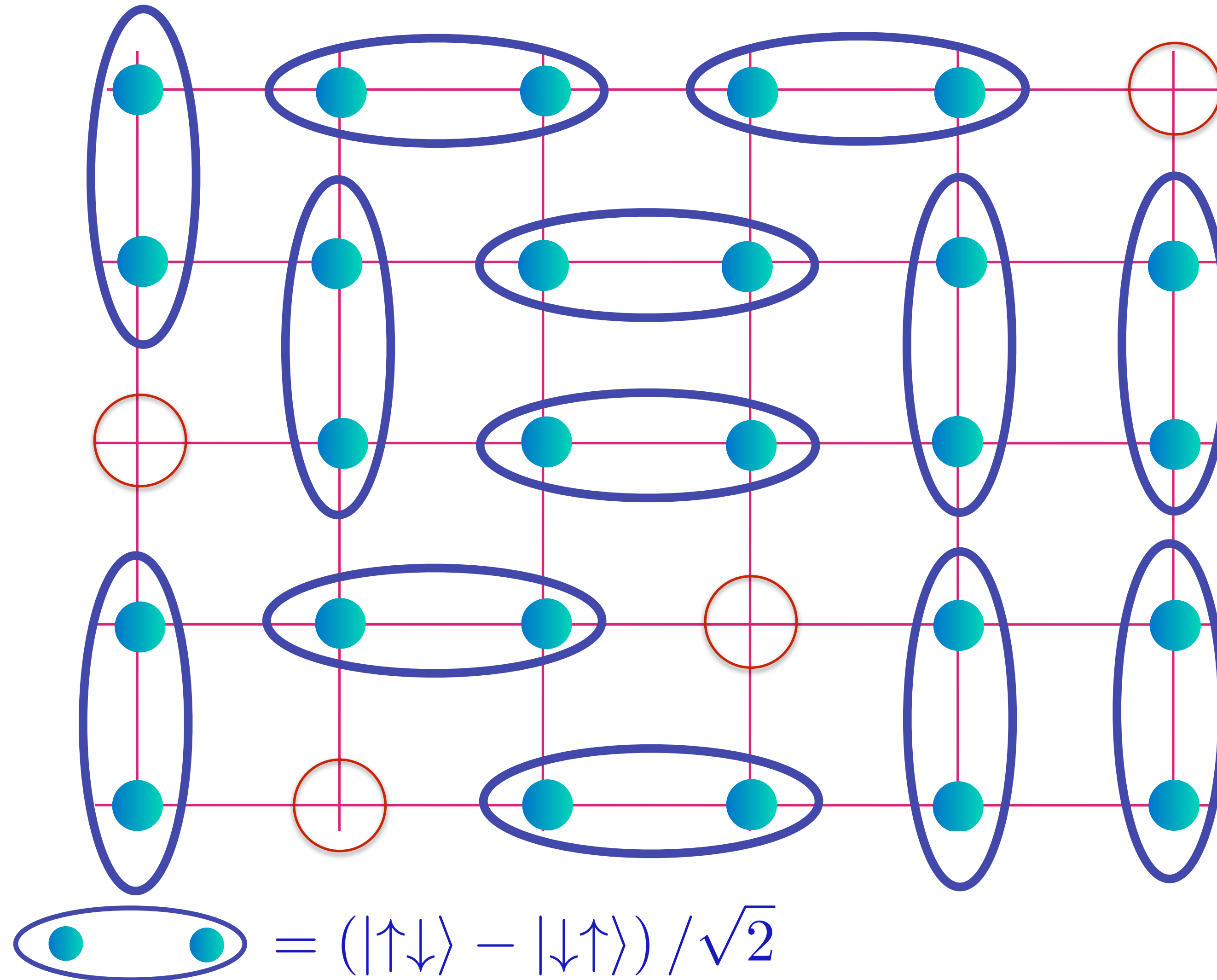


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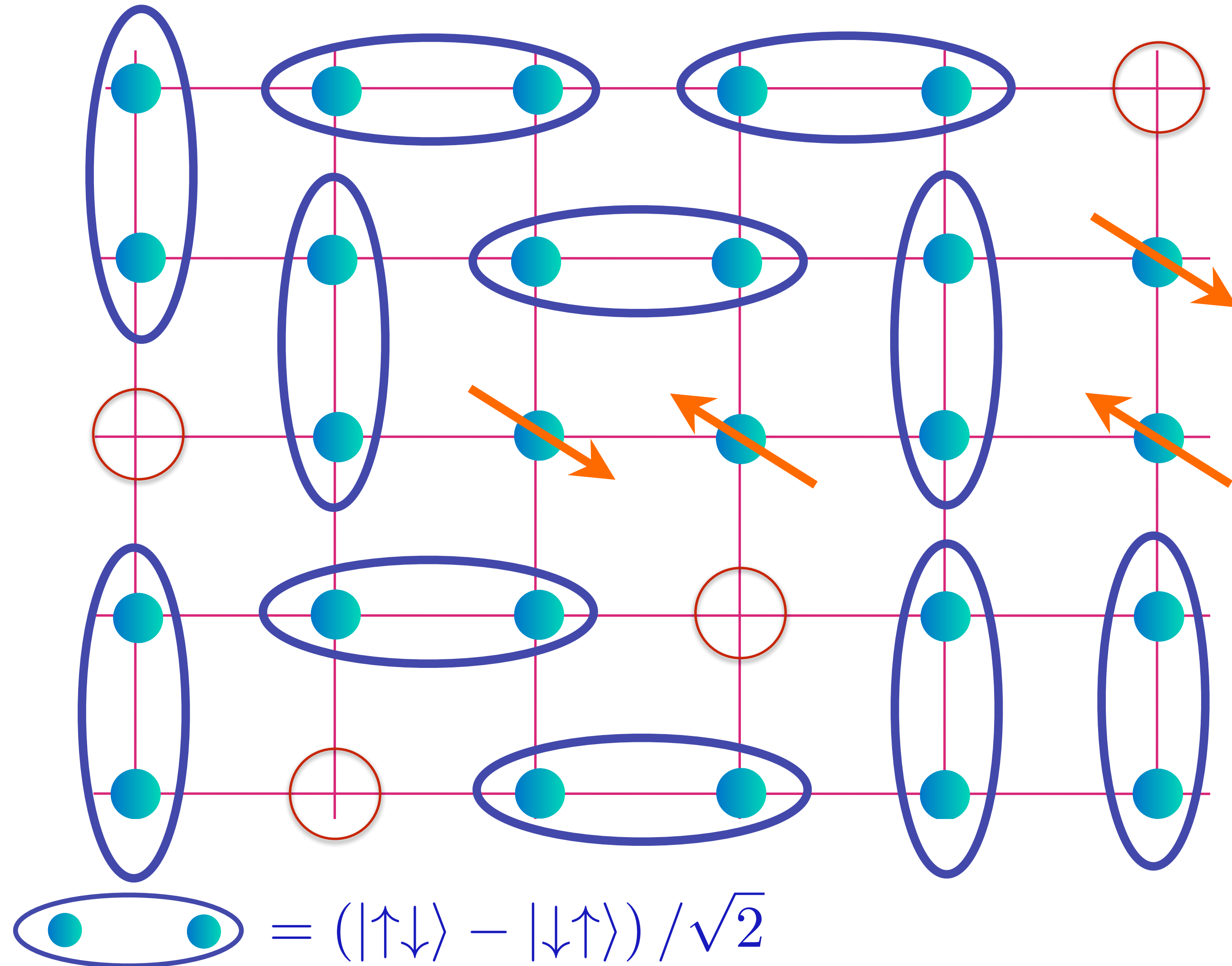


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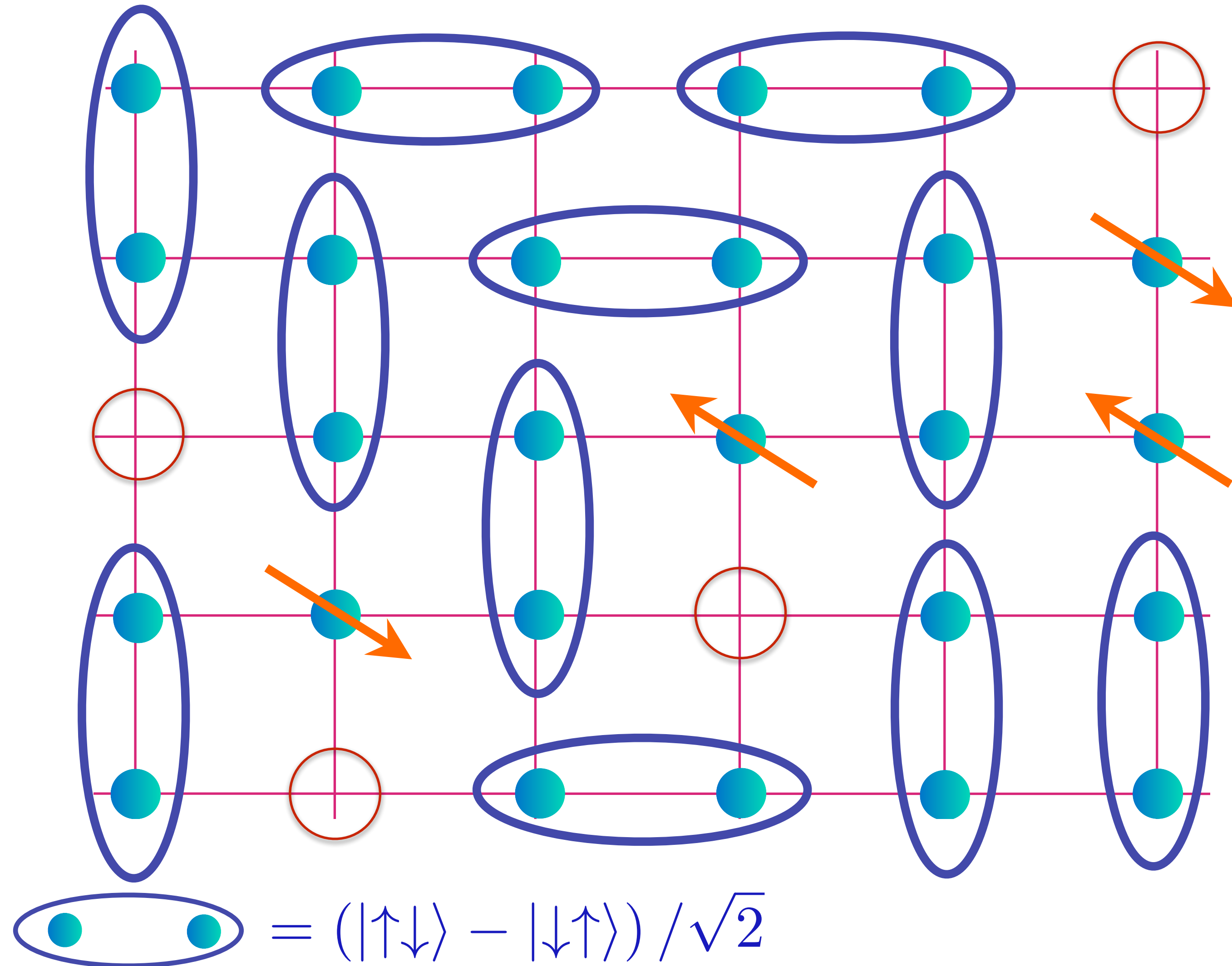


Spin liquid  
with density  
 $p$  of spinless,  
charge  $+e$   
“holons” and  
charge 0, spin-1/2  
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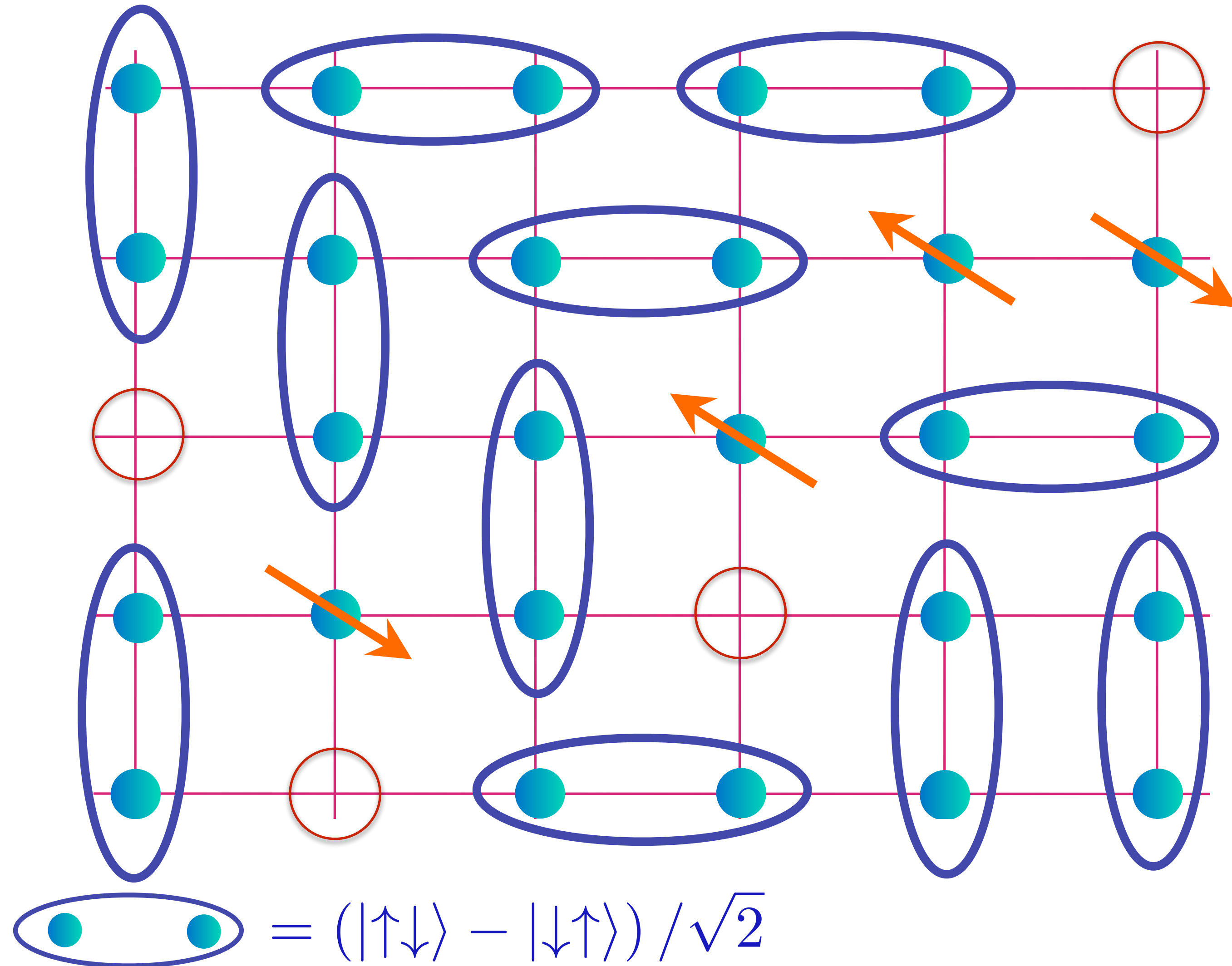


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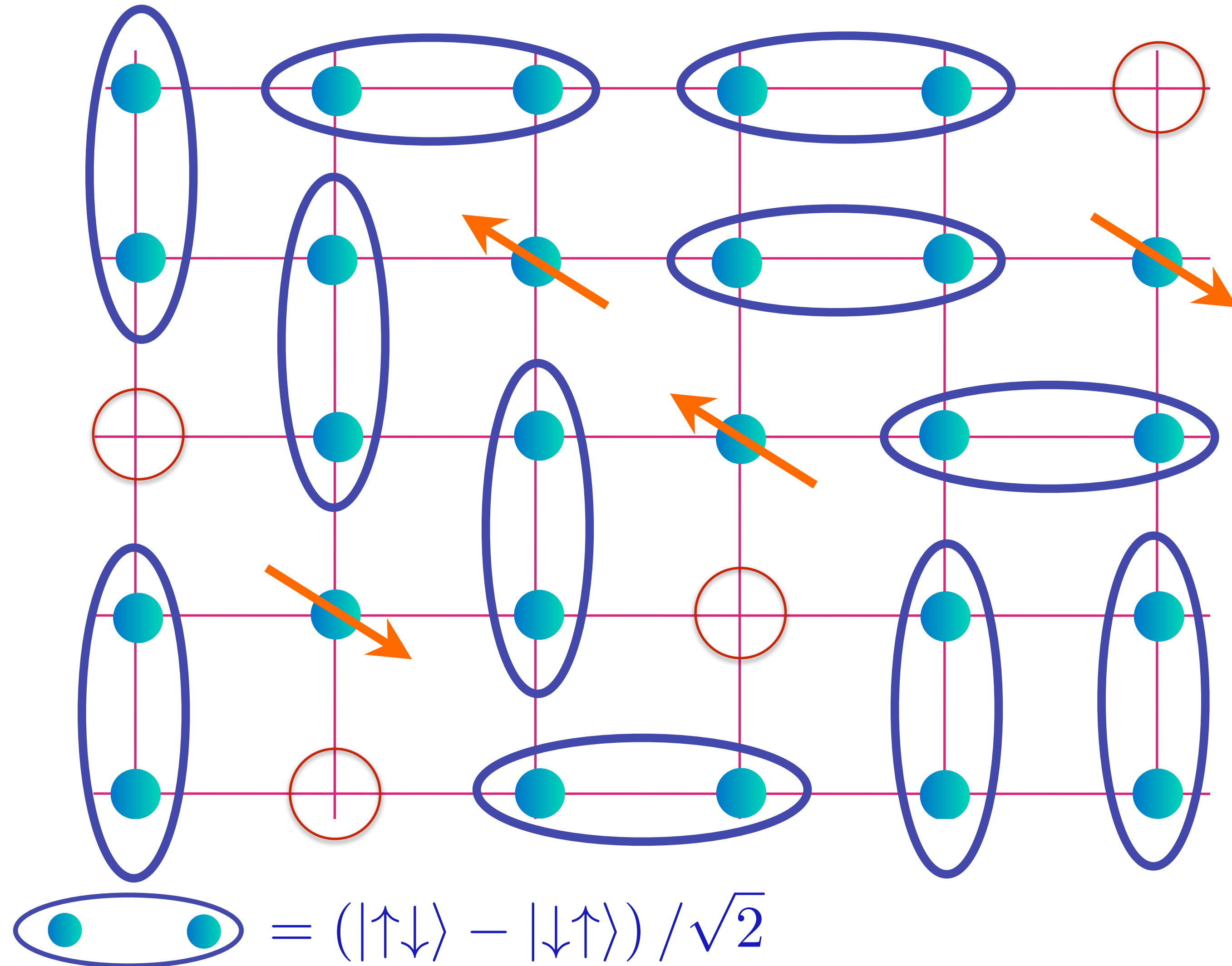


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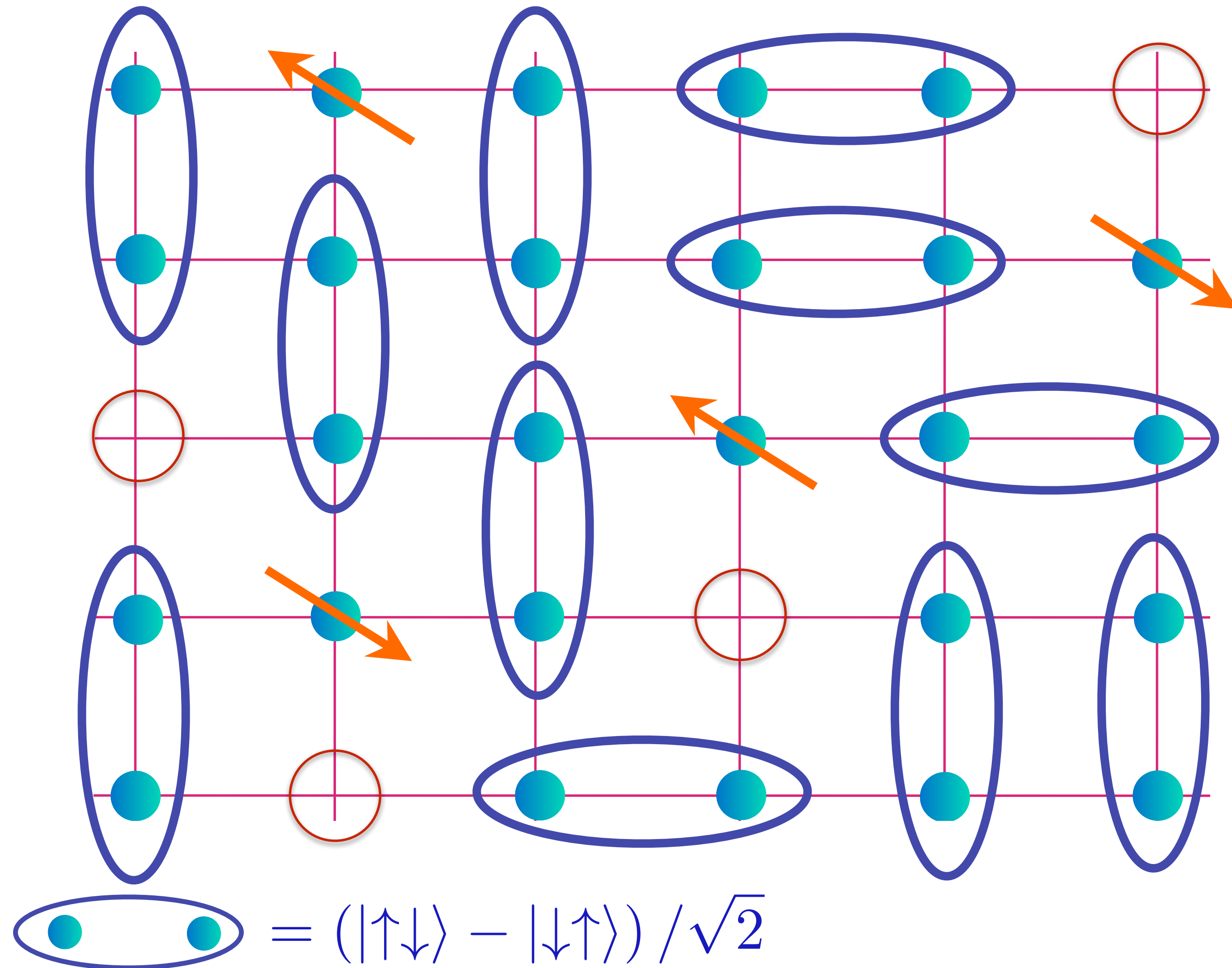


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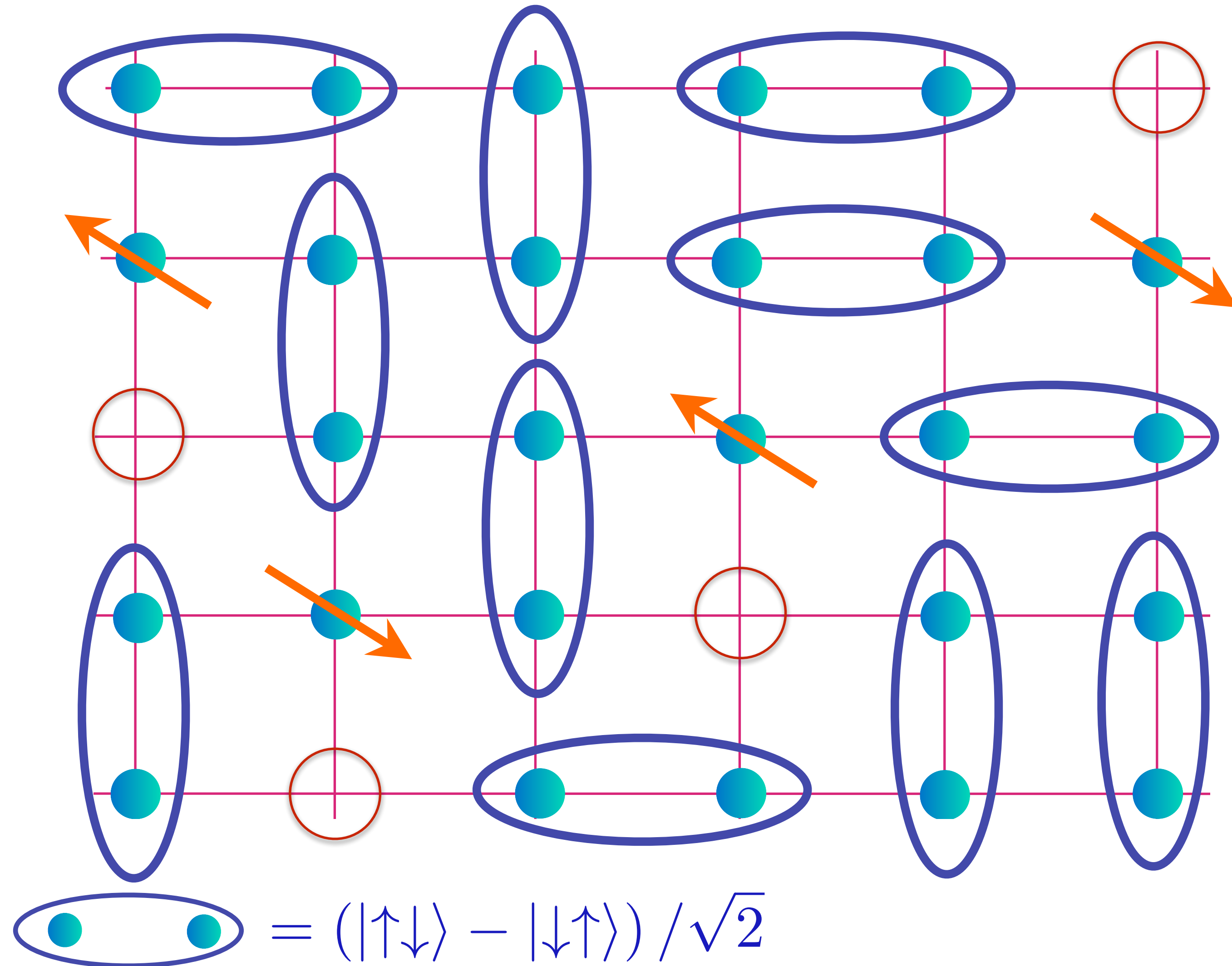


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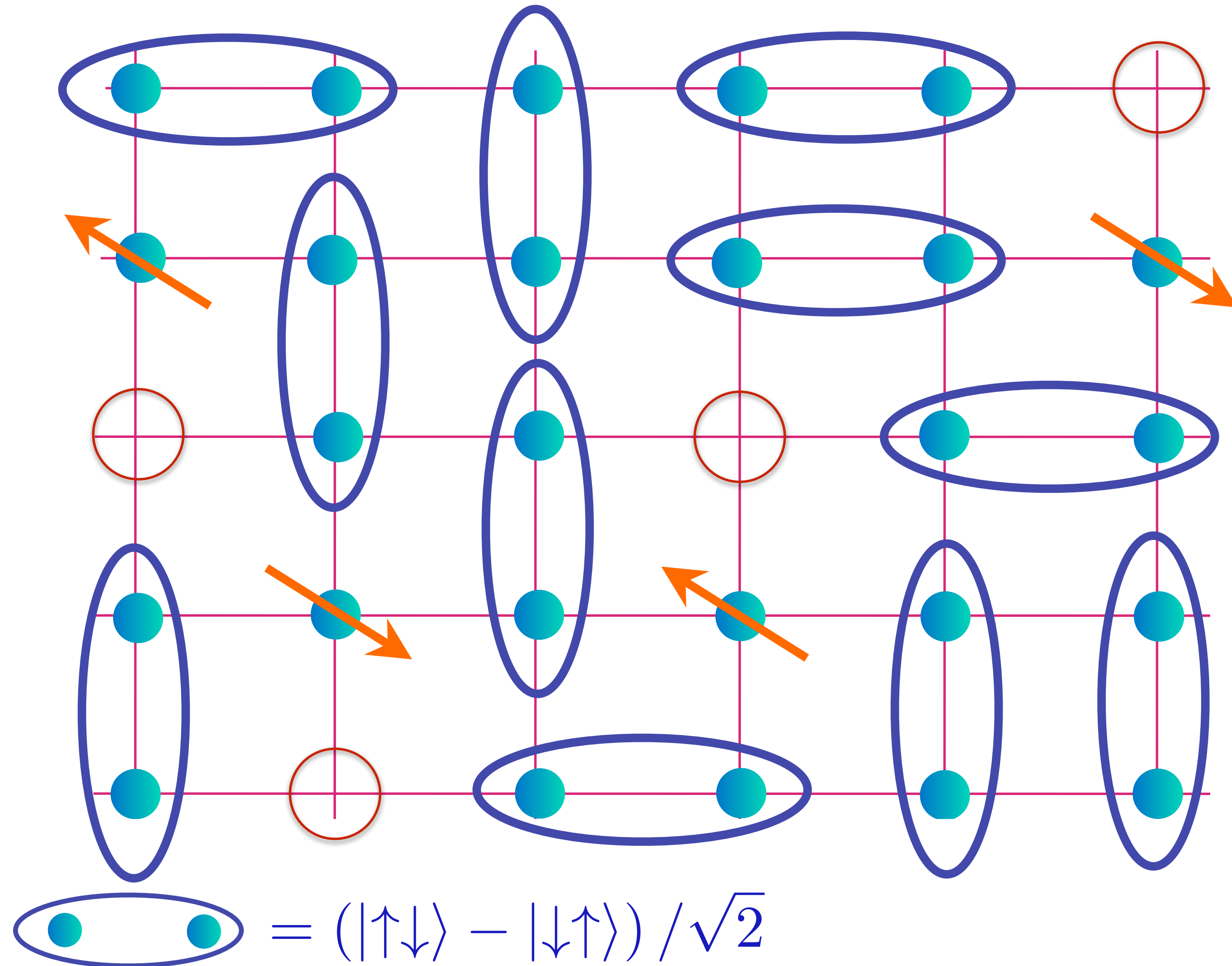


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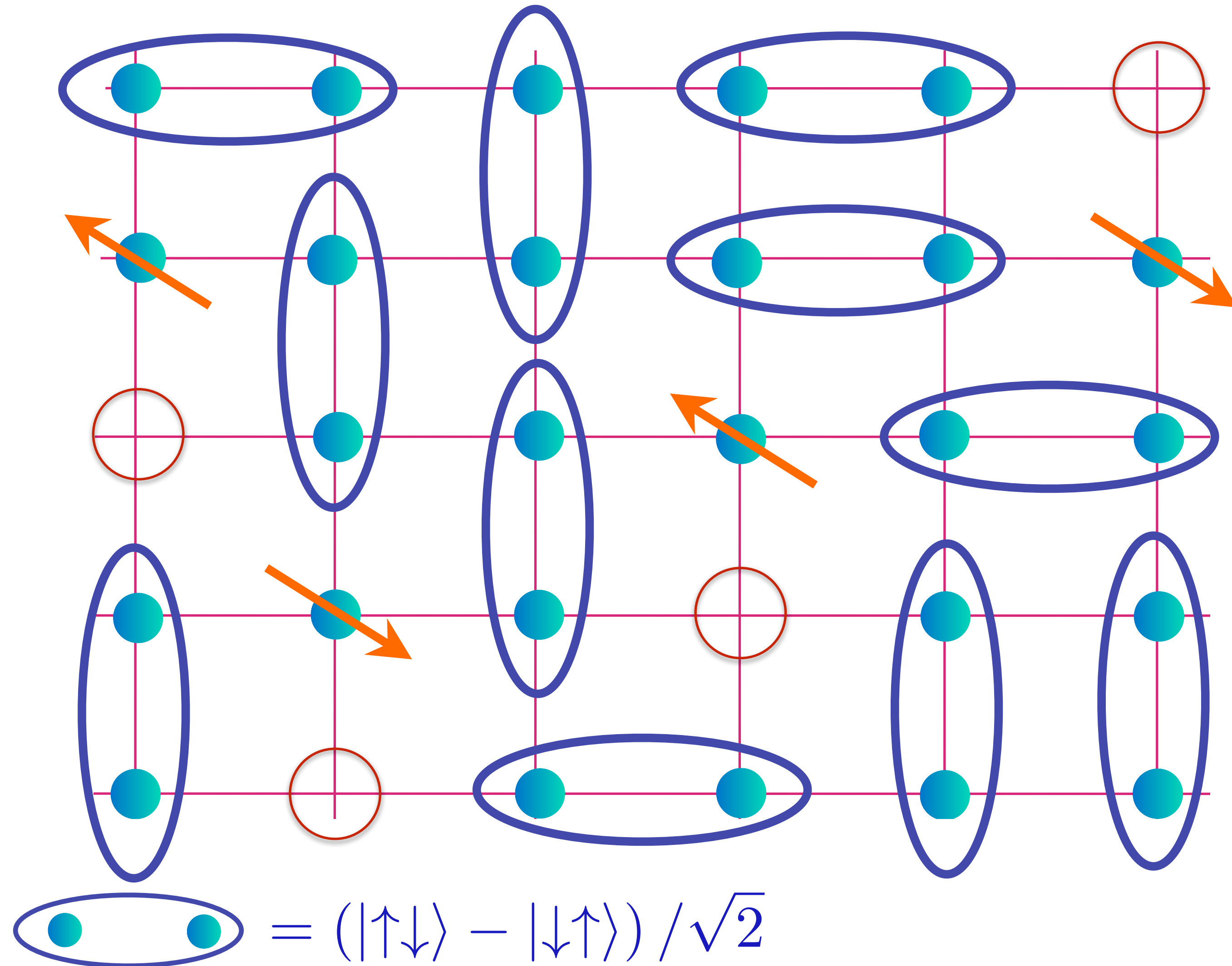


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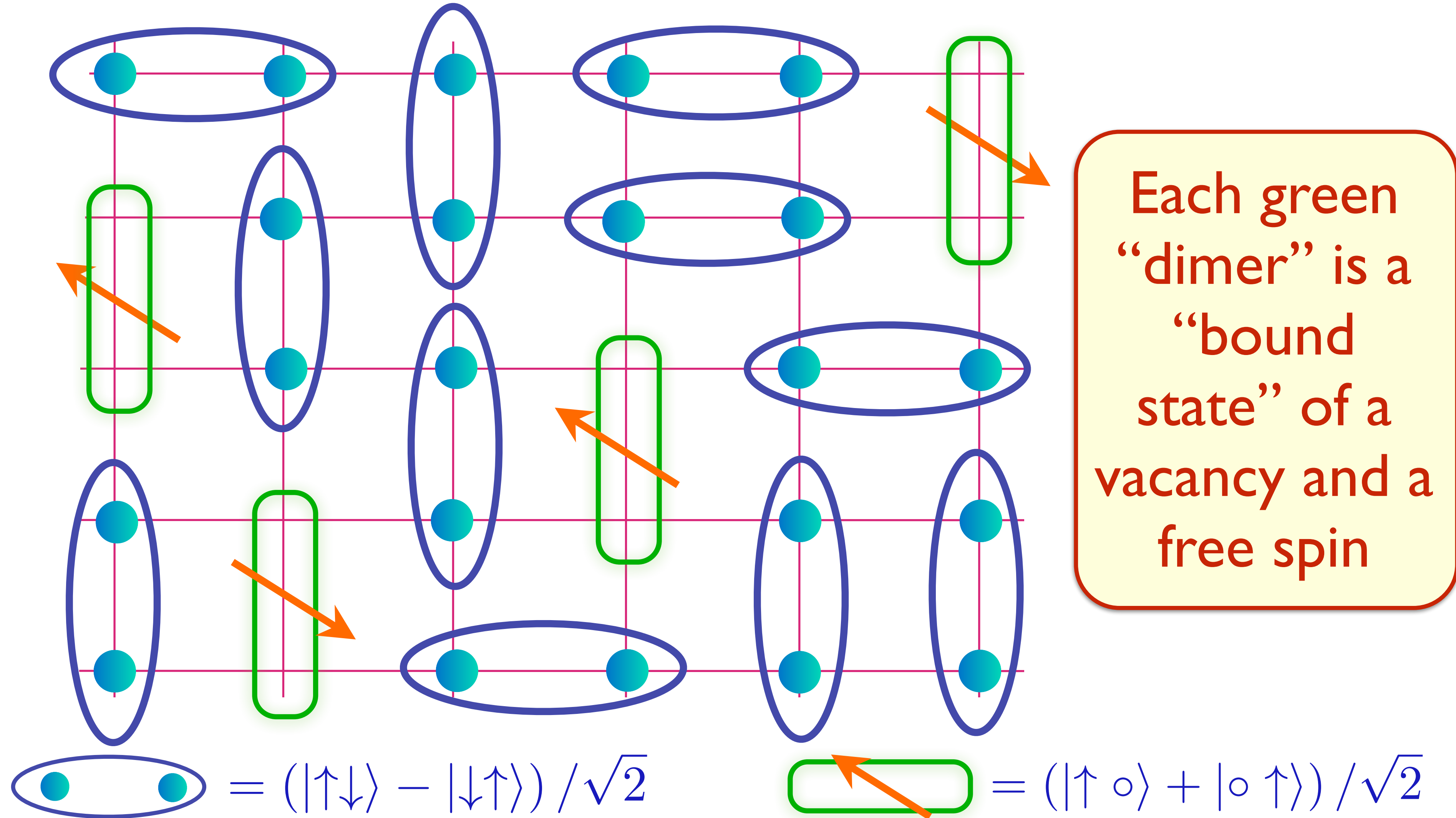


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# FL\*

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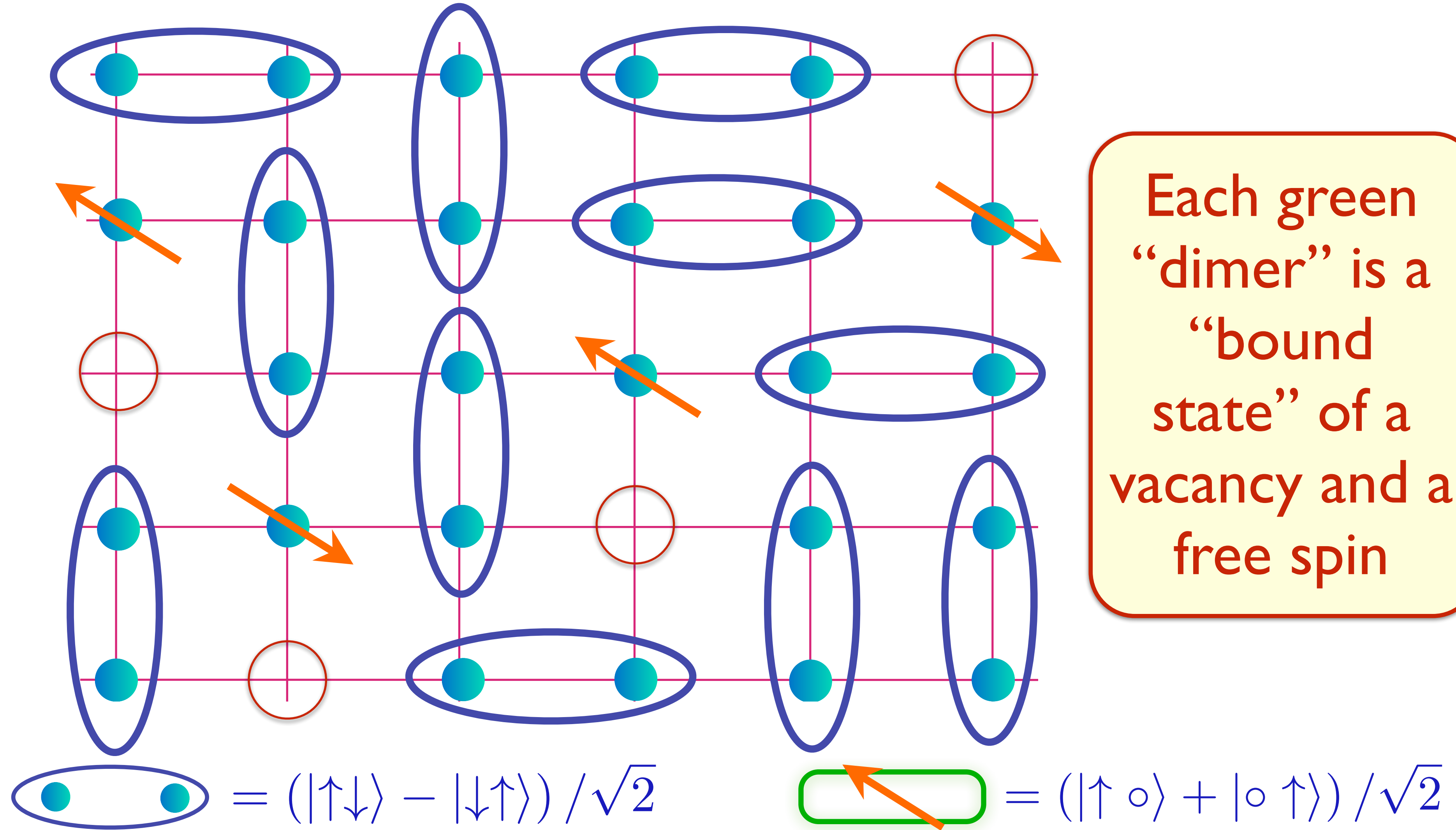
R. K. Kaul, A. Kolezhuk, M. Levin, S. Sachdev, and T. Senthil, PRB **75**, 235122 (2007)



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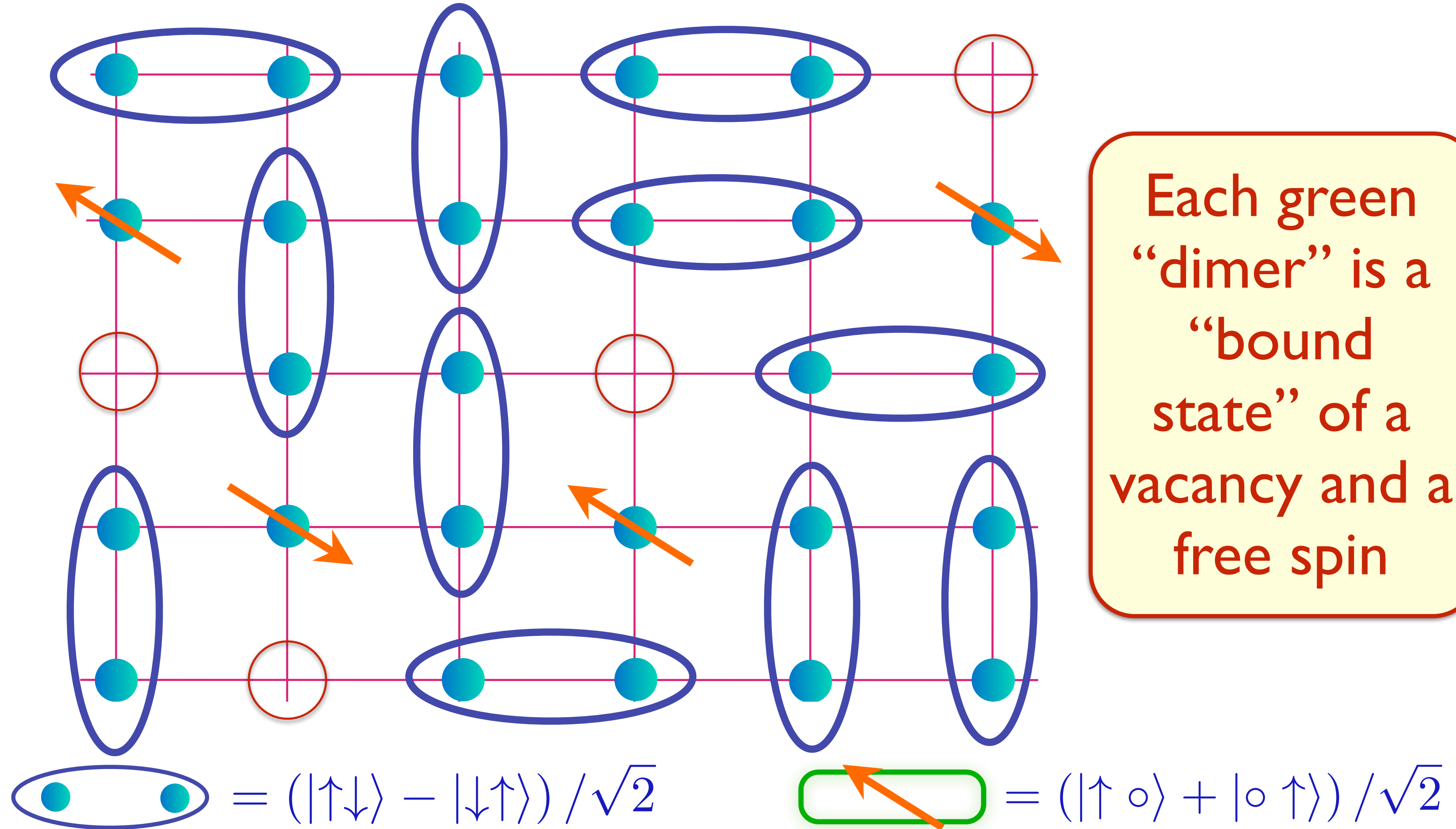
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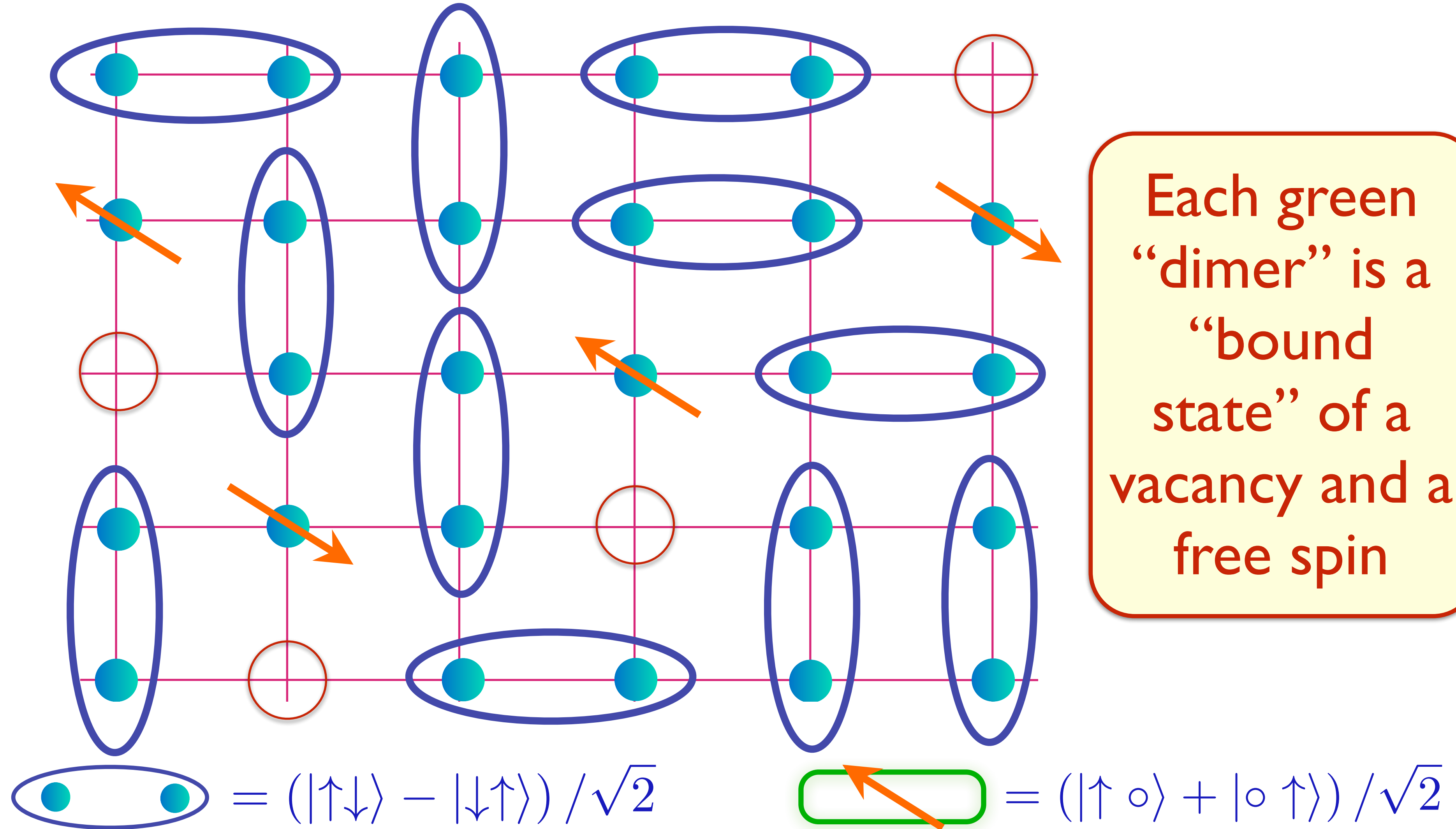
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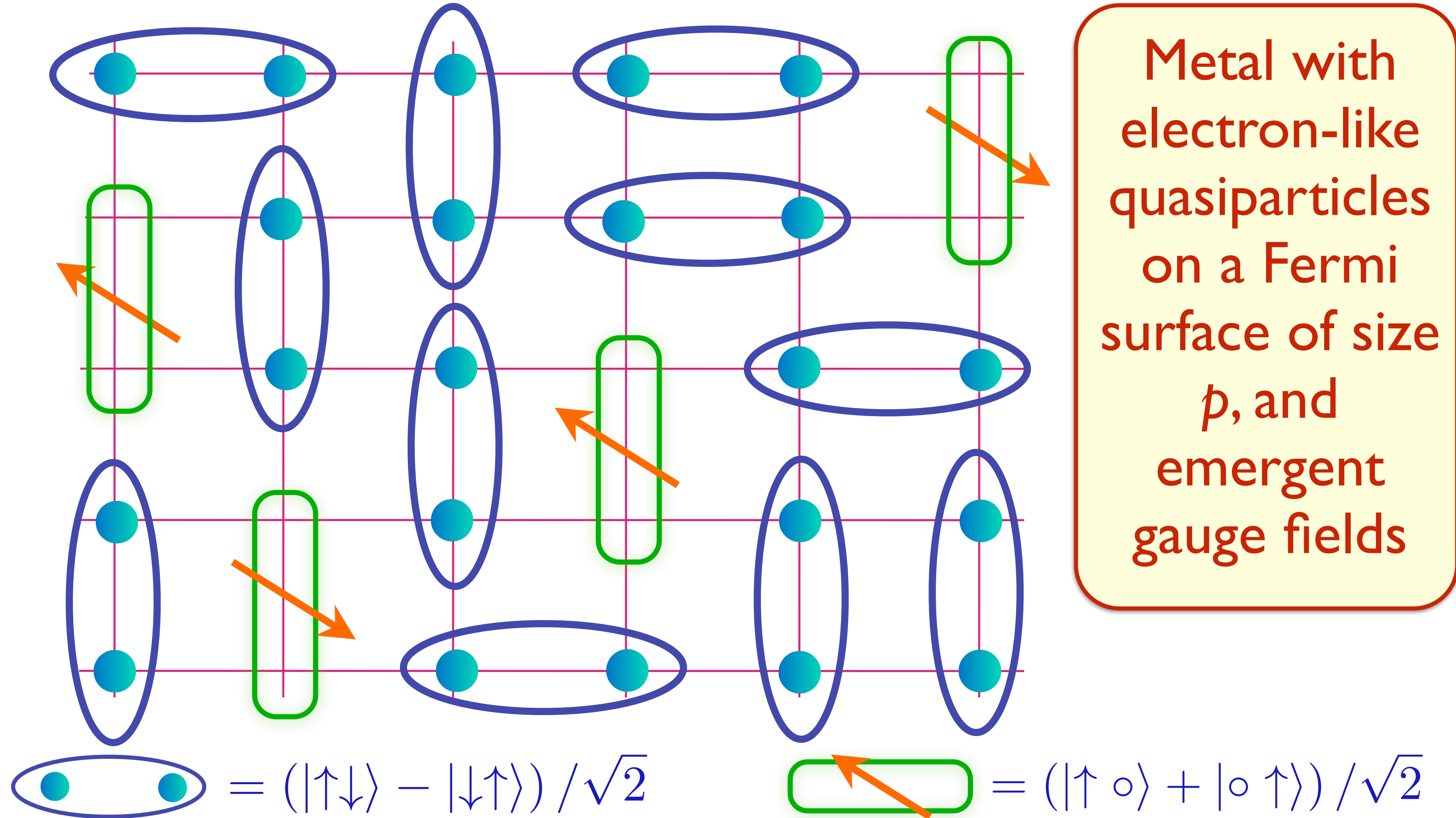
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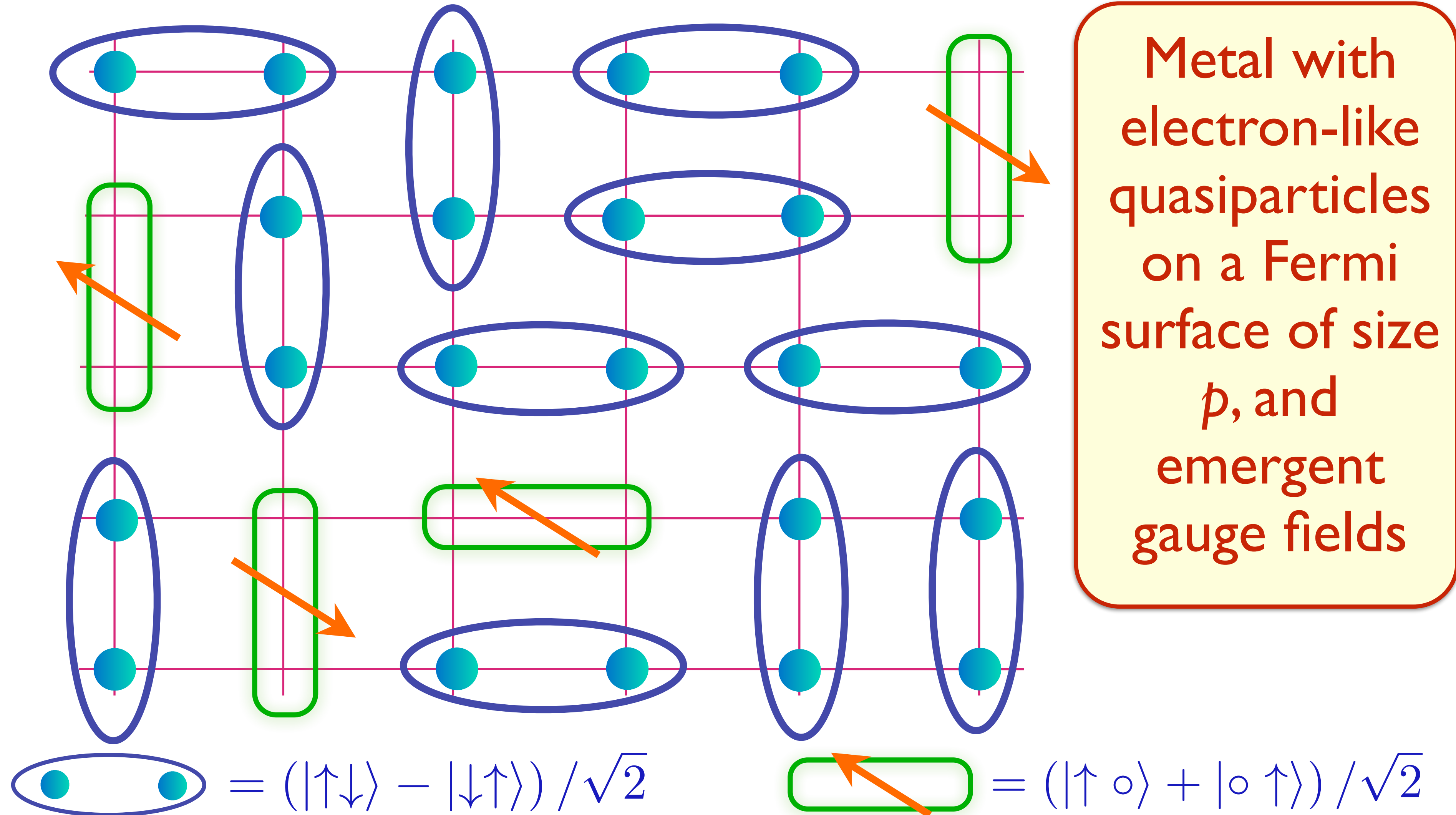
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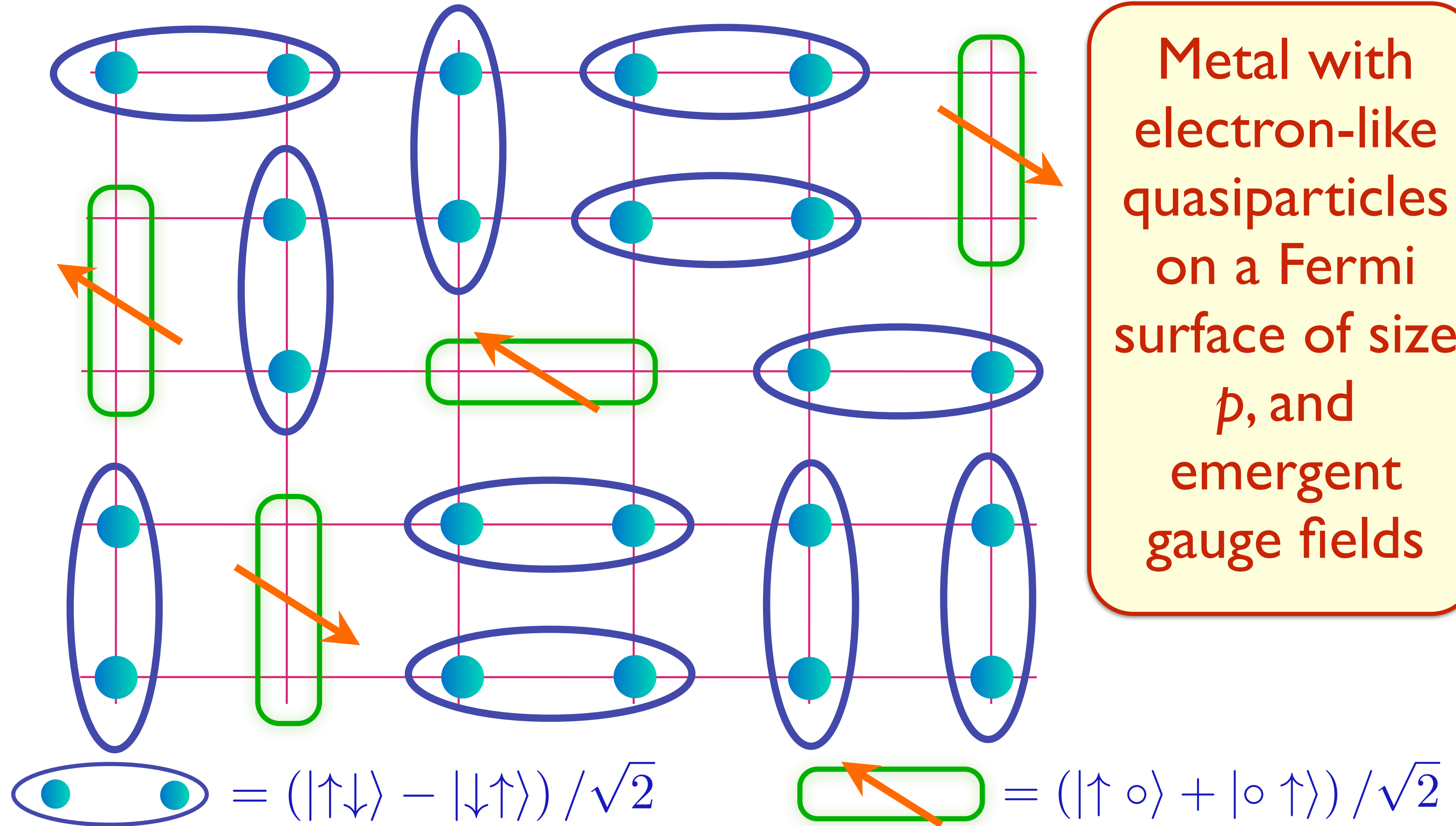
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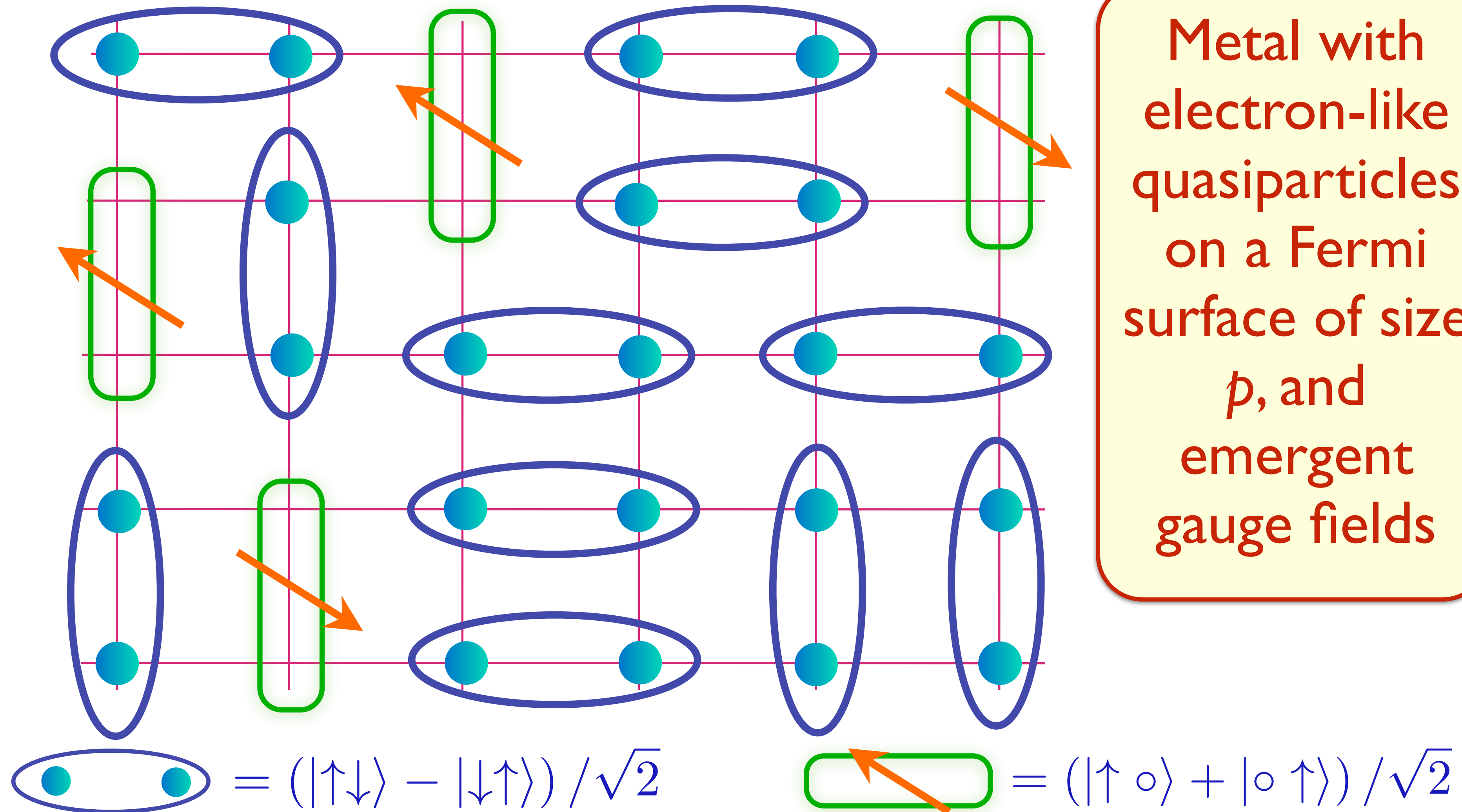
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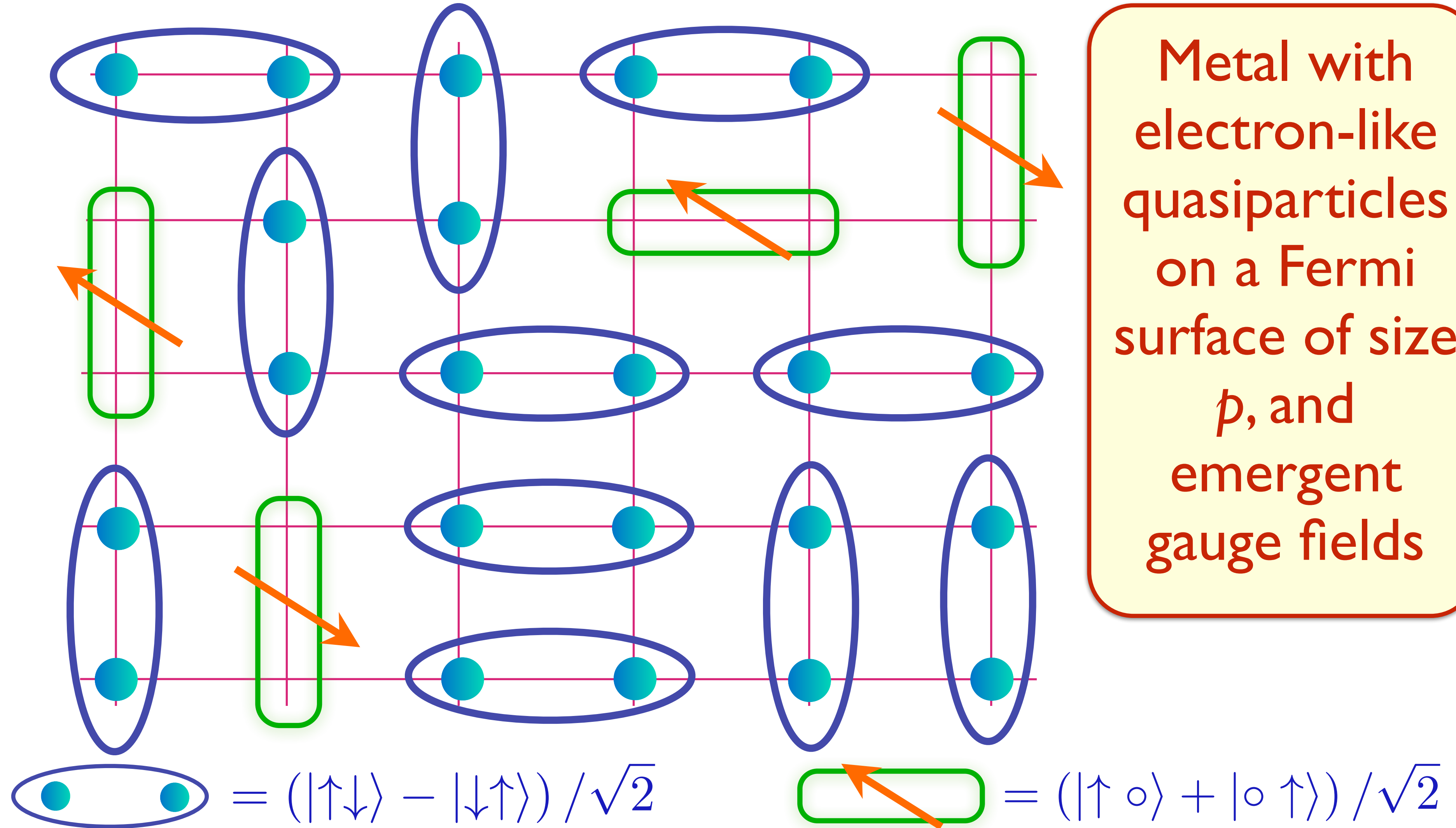
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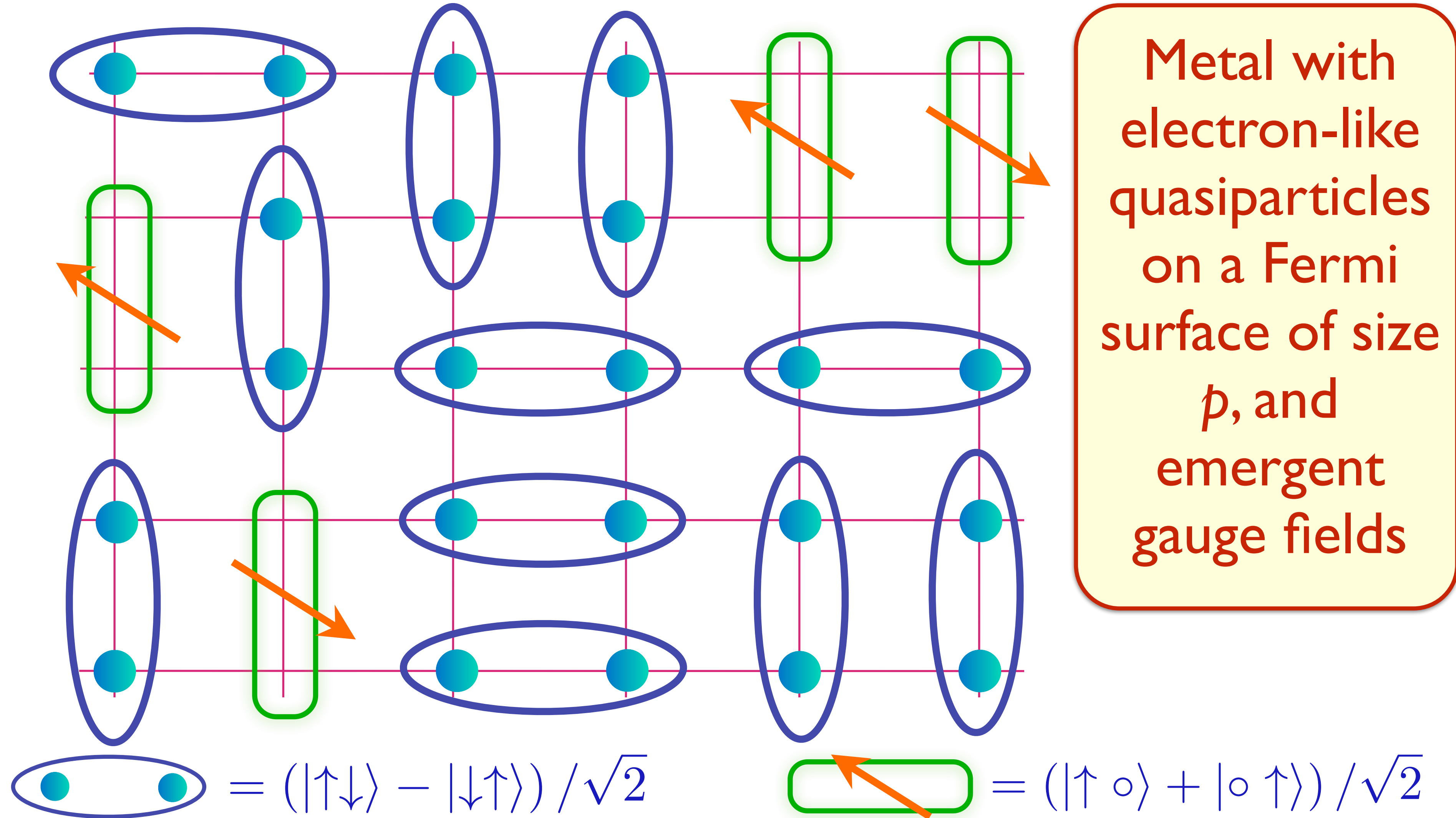
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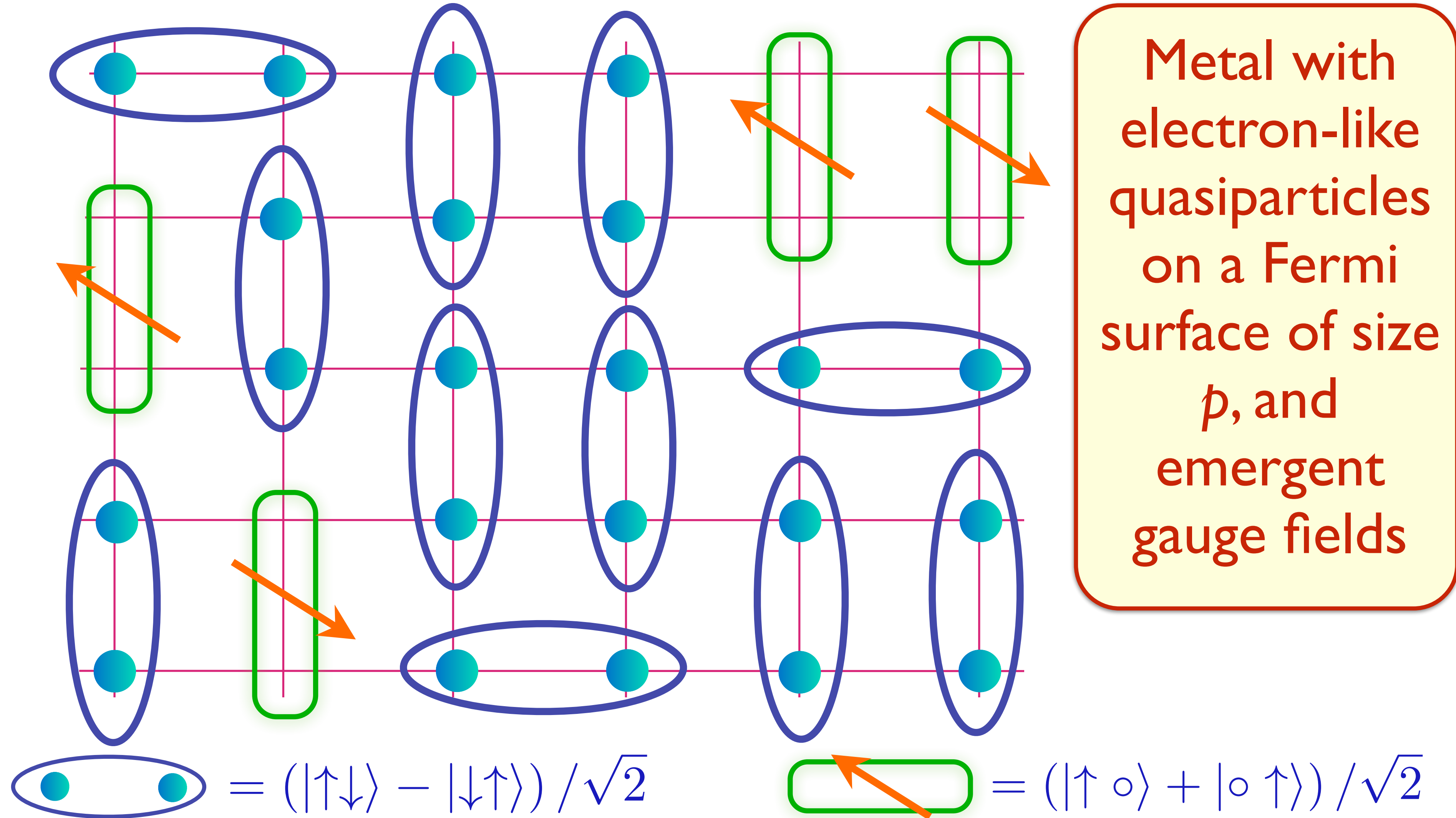
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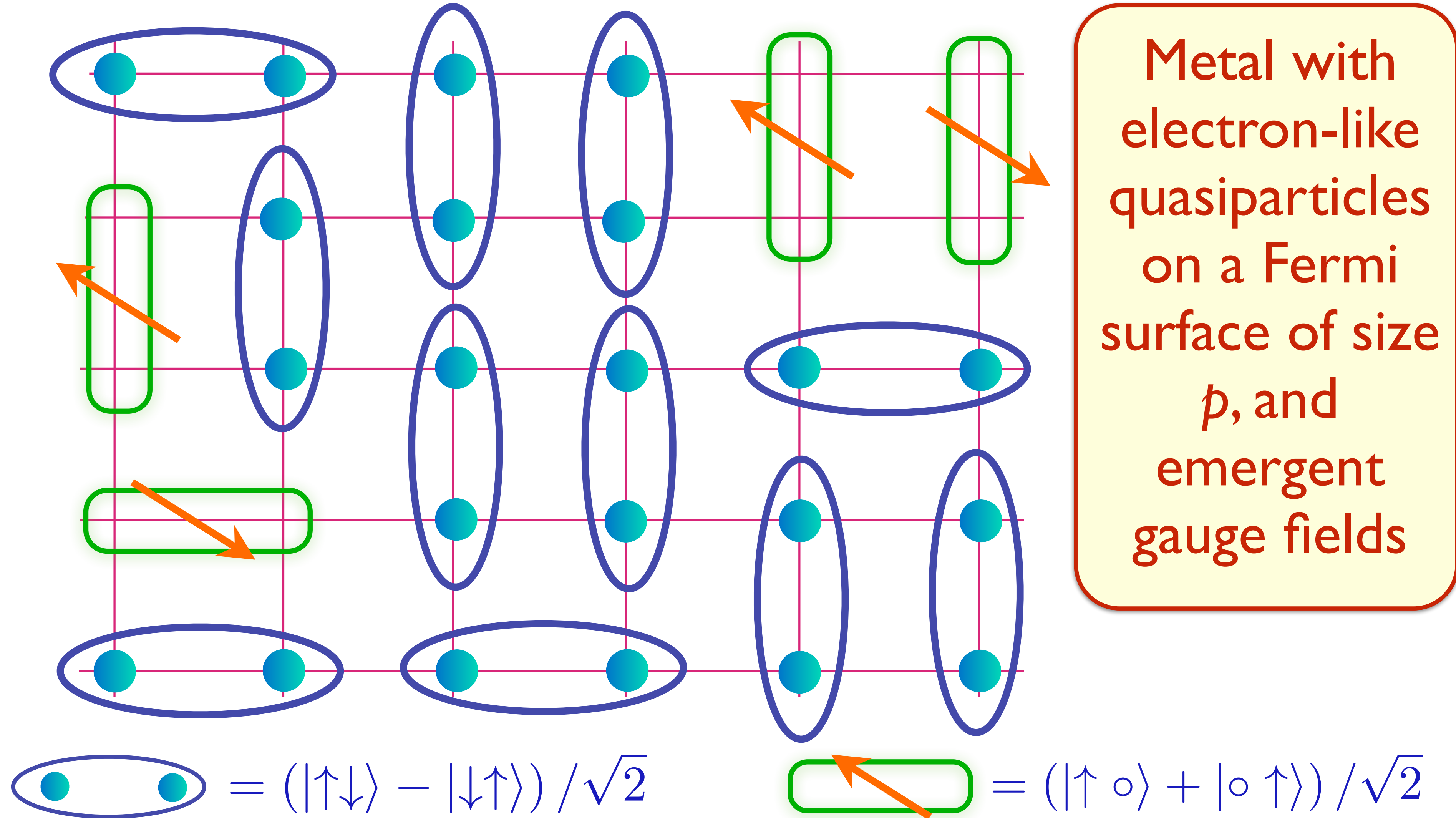


Metal with electron-like quasiparticles on a Fermi surface of size  $p$ , and emergent gauge fields

# FL\*

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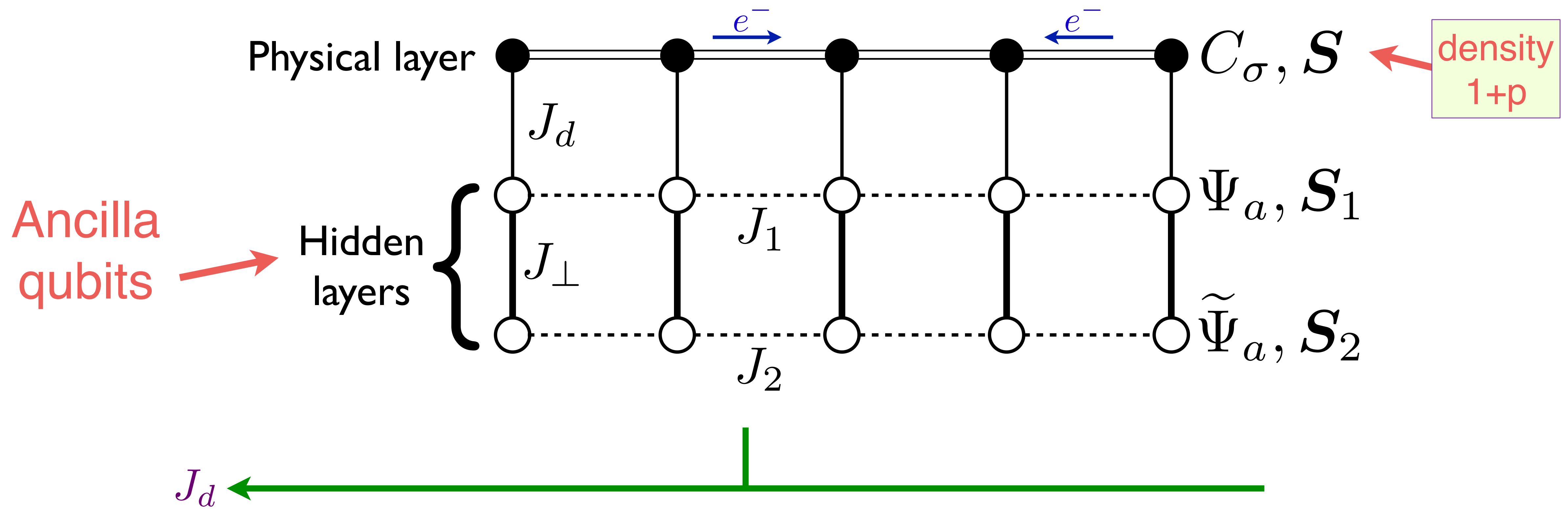
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## FL\* in a **one-band** model

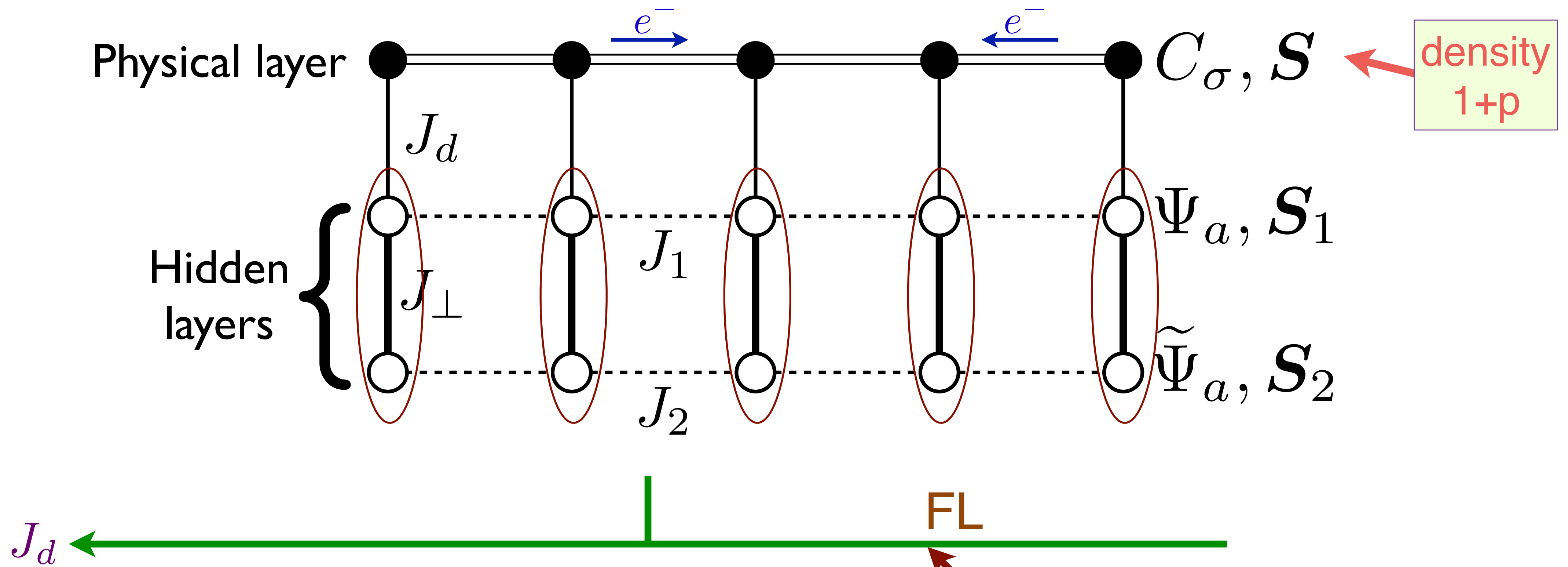
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# FL\* and FL in a **one-band** model



Ya-Hui Zhang

# FL\* and FL in a **one-band** model



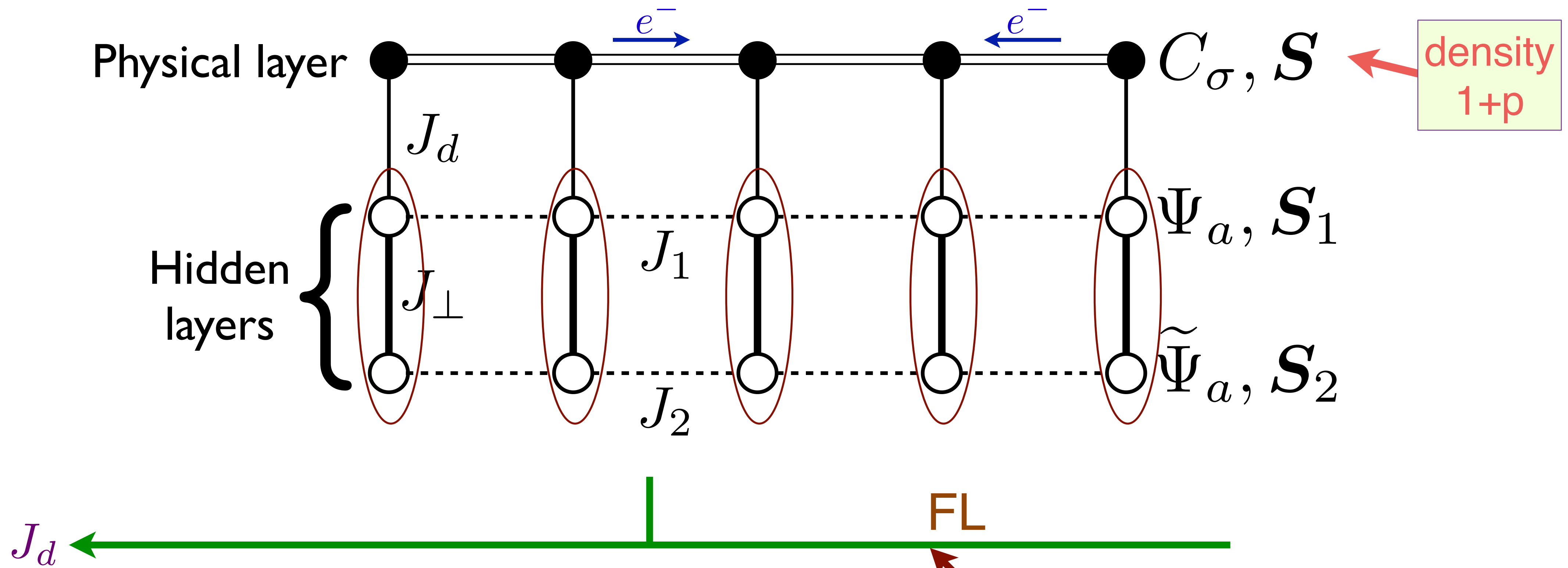
Large Fermi surface of size  $1 + p$

$$|\Phi\rangle = \left| \text{Rung singlets of } \Psi, \tilde{\Psi} \right\rangle \otimes \left| \text{Slater determinant of } C \right\rangle$$



Ya-Hui Zhang

# FL\* and FL in a **one-band** model



Ya-Hui Zhang

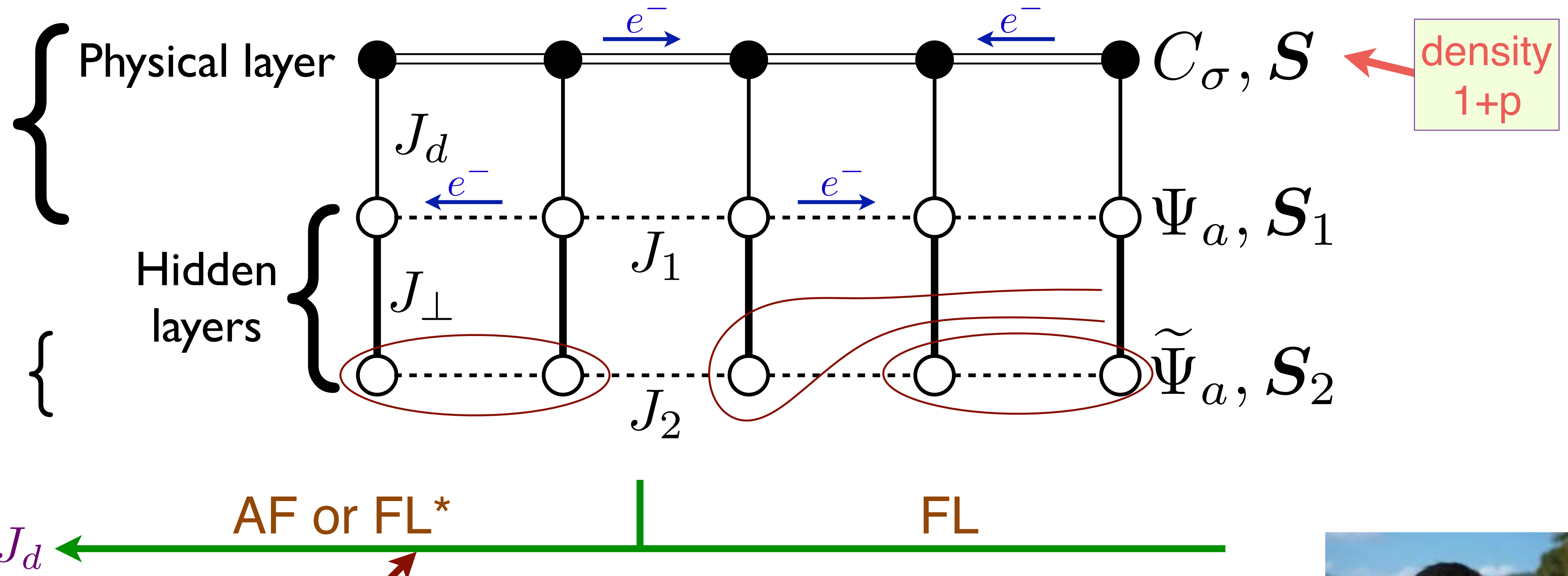
Luttinger  
Theorem  
obeyed

Large Fermi surface of size  $1 + p$

$$|\Phi\rangle = \left| \text{Rung singlets of } \Psi, \tilde{\Psi} \right\rangle \otimes \left| \text{Slater determinant of } C \right\rangle$$

# FL\* and FL in a **one-band** model

Metal.  
Density  
 $2 + p \cong p$



Small Fermi surface of size  $p$

$$|\Phi\rangle = \left[ \text{Projection onto rung singlets of } \Psi, \tilde{\Psi} \right] \otimes |\text{Slater determinant of } (C, \Psi)\rangle \otimes |\text{Slater determinant of } \tilde{\Psi}\rangle$$

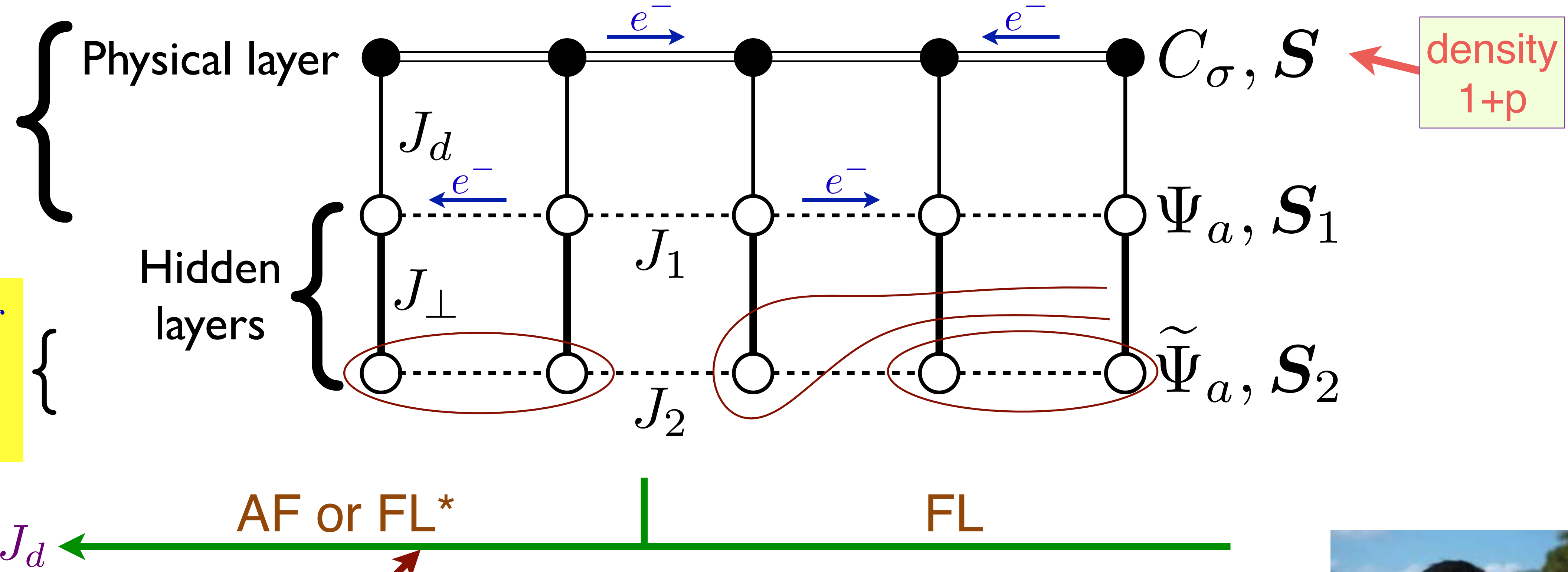


Ya-Hui Zhang

# FL\* and FL in a **one-band** model

Metal.  
Density  
 $2 + p \cong p$

Mott insulator  
Spin liquid  
or AF order



Small Fermi surface of size  $p$

$$|\Phi\rangle = \left[ \text{Projection onto rung singlets of } \Psi, \tilde{\Psi} \right] \otimes |\text{Slater determinant of } (C, \Psi)\rangle \otimes |\text{Slater determinant of } \tilde{\Psi}\rangle$$

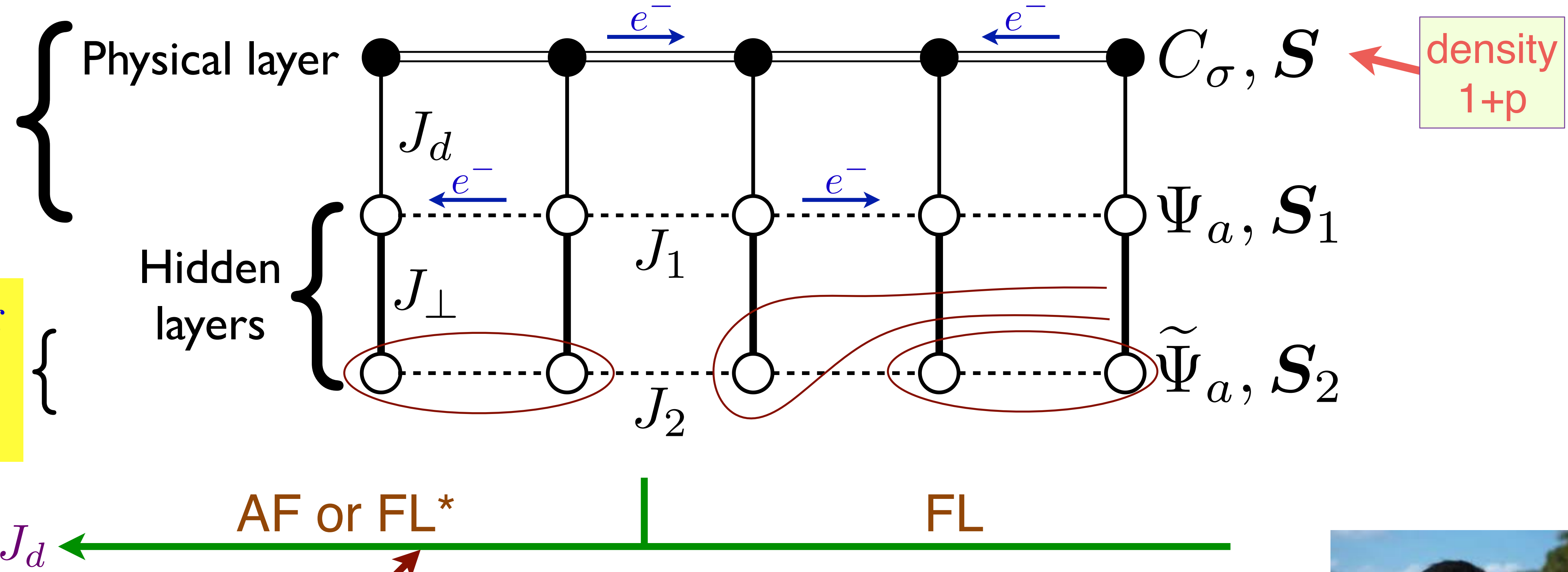


Ya-Hui Zhang

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Small Fermi surface of size  $p$

$|\Phi\rangle = \left[ \text{Projection onto rung singlets of } \Psi, \tilde{\Psi} \right]$   
 $\otimes |\text{Slater determinant of } (C, \Psi)\rangle$   
 $\otimes |\text{Slater determinant of } \tilde{\Psi}\rangle$

Luttinger Theorem violated;  
OK, because of topological order of  $\tilde{\Psi}$

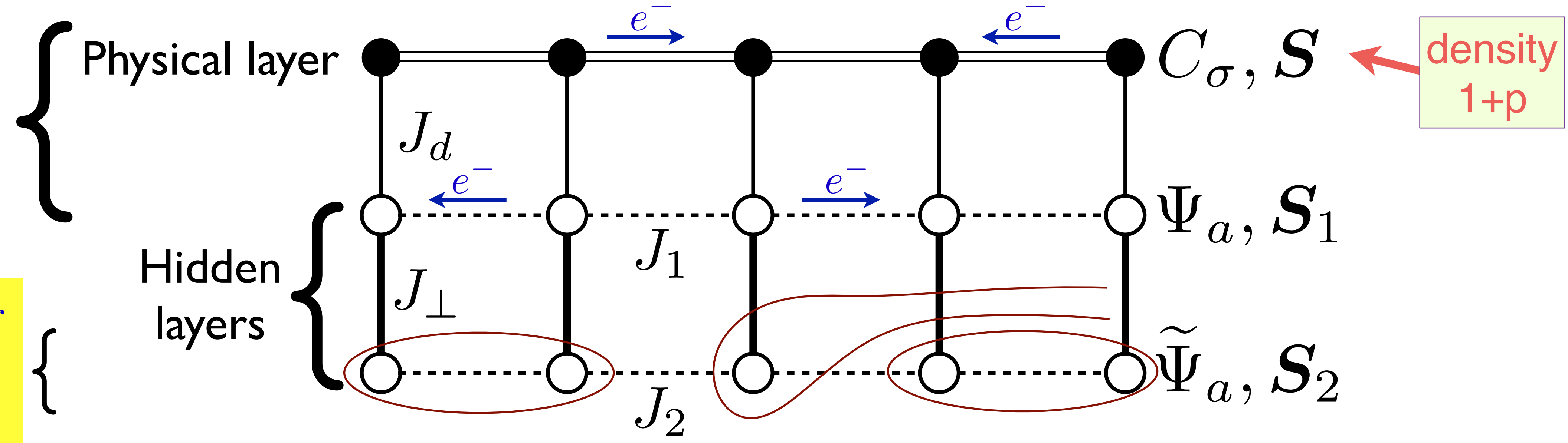


Ya-Hui Zhang

# FL\* and FL in a **one-band** model

Metal.  
Density  
 $2 + p \cong p$

Mott insulator  
Spin liquid  
or AF order



AF or FL\* | FL

$J_d$  ←

Small Fermi surface of size  $p$

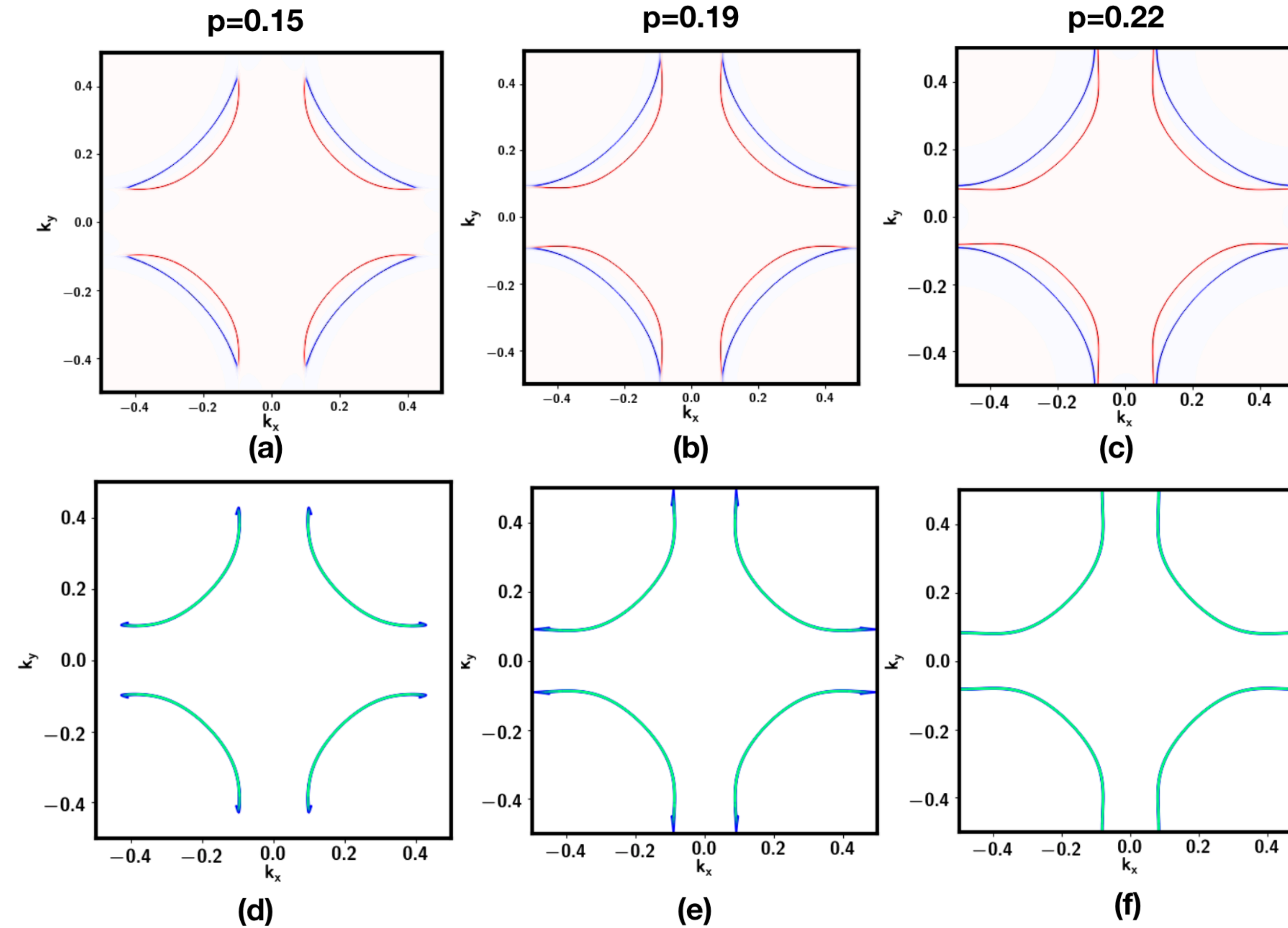
$$|\Phi\rangle = \left[ \text{Projection onto rung singlets of } \Psi, \tilde{\Psi} \right] \otimes |\text{Slater determinant of } (C, \Psi)\rangle \otimes |\text{Slater determinant of } \tilde{\Psi}\rangle$$

Similar to a selective Mott transition in hidden layer 1:  $\Psi$  fermions are insulating in FL phase, and metallic in FL\* phase.



Ya-Hui Zhang

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



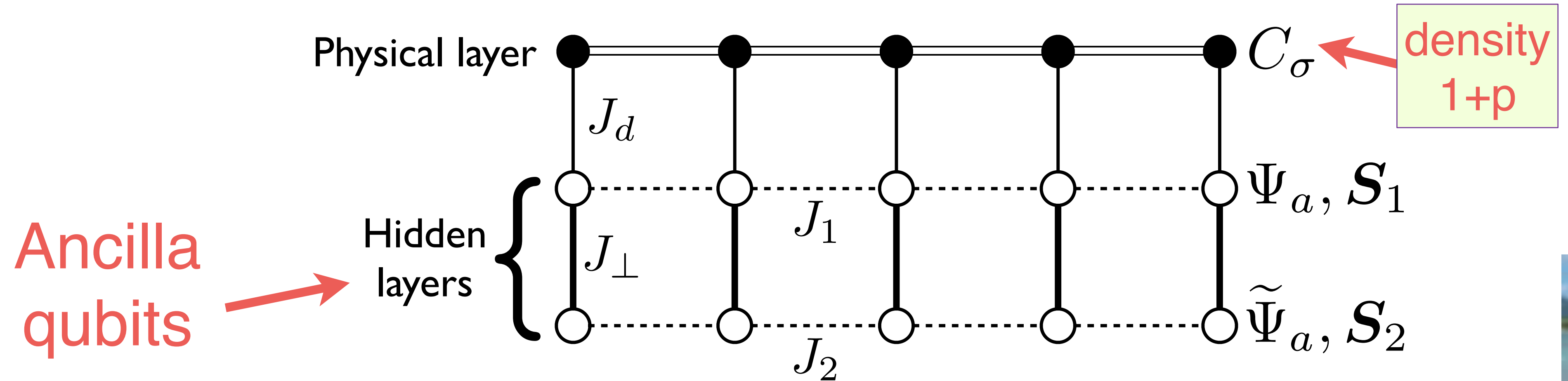
“Fermi arc”  
spectral functions  
in the FL\* phase



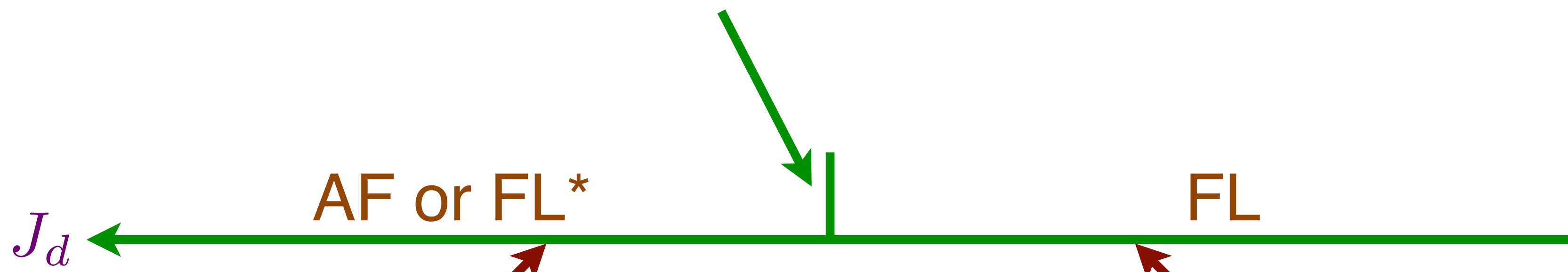
Ya-Hui Zhang

Zero frequency spectral density of electrons (red) and ghosts (blue)

# FL\* and FL in a **one-band** model



Yahui Zhang



Small Fermi surface of size  $p$

$$|\Phi\rangle = \left[ \text{Projection onto rung singlets of } \Psi, \tilde{\Psi} \right] \otimes |\text{Slater determinant of } (C, \Psi)\rangle \otimes |\text{Slater determinant of } \tilde{\Psi}\rangle$$

Large Fermi surface of size  $1 + p$

$$|\Phi\rangle = |\text{Rung singlets of } \Psi, \tilde{\Psi}\rangle \otimes |\text{Slater determinant of } C\rangle$$

# FL\* and FL in a **one-band** model

Write fermion operators as  $2 \times 2$  matrices

$$\Psi = \begin{pmatrix} \Psi_{\uparrow} & -\Psi_{\downarrow}^{\dagger} \\ \Psi_{\downarrow} & \Psi_{\uparrow}^{\dagger} \end{pmatrix}, \quad \tilde{\Psi} = \begin{pmatrix} \tilde{\Psi}_{\uparrow} & -\tilde{\Psi}_{\downarrow}^{\dagger} \\ \tilde{\Psi}_{\downarrow} & \tilde{\Psi}_{\uparrow}^{\dagger} \end{pmatrix}$$

Single occupancy constraints of  $\Psi$ ,  $\tilde{\Psi}$  leads to  $SU(2)_1 \times SU(2)_2$  gauge symmetry:

$$\begin{aligned} SU(2)_1 : \quad & \Psi \rightarrow \Psi U_1, & \tilde{\Psi} & \rightarrow \tilde{\Psi} \\ SU(2)_2 : \quad & \Psi & \rightarrow \Psi, & \tilde{\Psi} \rightarrow \tilde{\Psi} U_2 \end{aligned}$$

P.A. Lee, N. Nagaosa, and X.-G. Wen, RMP **78**, 17 (2006)

Local singlet formation ('antiferromagnetism')  $\mathcal{S}_1 + \mathcal{S}_2 \approx 0$  leads to  $SU(2)_S$  gauge symmetry:

$$SU(2)_S : \quad \Psi \rightarrow U_S \Psi, \quad \tilde{\Psi} \rightarrow U_S \tilde{\Psi}$$

S. Sachdev, M.A. Metlitski, Yang Qi, and Cenke Xu, PRB **80**, 155129 (2009)

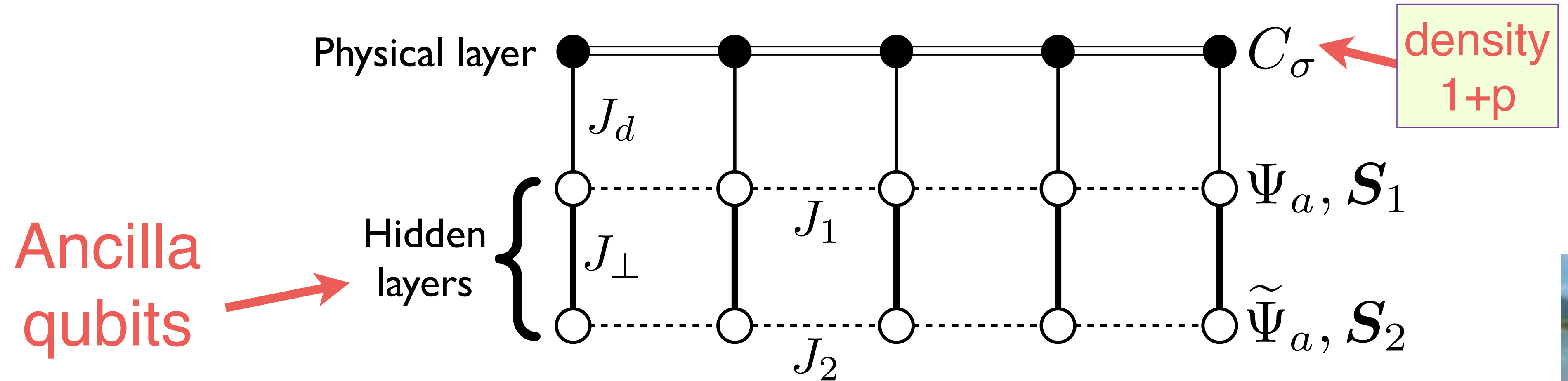
S. Sachdev, H. D. Scammell, M. S. Scheurer, and G. Tarnopolsky, PRB **99**, 054516 (2019)



Yahui Zhang

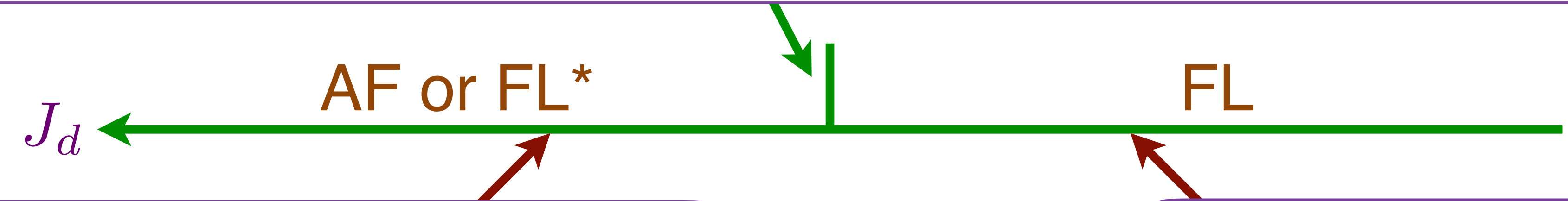
Ya-Hui Zhang, S. Sachdev, PRR **2**, 023172; PRB **102**, 155124 (2020)

# Metal-metal transitions in a **one-band** model



Yahui Zhang

$(U(1)_S \times U(1)_1)/Z_2$  or  $(SU(2)_S \times U(1)_1)/Z_2$  gauge theory of a  $\Psi$  ghost Fermi surface and a ‘hybridization-Higgs’ boson  $\sim C_\sigma^\dagger \Psi_a$  which condenses on the ‘Small Fermi surface’ side.



Small Fermi surface of size  $p$

$|\Phi\rangle = \left[ \text{Projection onto rung singlets of } \Psi, \tilde{\Psi} \right]$   
 $\otimes |\text{Slater determinant of } (C, \Psi)\rangle$   
 $\otimes |\text{Slater determinant of } \tilde{\Psi}\rangle$

Large Fermi surface of size  $1+p$

$|\Phi\rangle = |\text{Rung singlets of } \Psi, \tilde{\Psi}\rangle$   
 $\otimes |\text{Slater determinant of } C\rangle$

# Ancilla qubit theory of FL\* and FL phases in a one-band model

- FL\* as the pseudogap metal with carrier density  $p$ . Variants of the theory can have broken symmetries (*e.g.* antiferromagnetism) without fractionalization in the pseudogap metal.

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- Ghost fermions, carrying neither spin nor charge, emerge as additional low energy excitations near the critical point to the FL phase. While the ancilla qubits are gauged away as ‘fake’ in the UV theory, the ghost fermions are physical excitations in the IR theory, which can be detected by thermal probes.
- The ghost fermions are coupled to 2 gauge fields: the first arising from the no double occupancy constraint, and the second from transforming to a rotating reference frame in spin space. These gauge fields lead respectively to repulsive and attractive interactions between the ghost fermions.

## Ancilla qubits for the cuprates

- By introducing a double layer of ancilla qubits, we are able to describe a FL\* phase in a single band model: some of the electrons localize into an insulator of spins, while the others form a Luttinger-volume-violating Fermi surface.

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- It would be interesting to use PEPS/tensor-network technology to compute properties of the ancilla wavefunctions for FL\*!