Order and quantum phase transitions in the cuprate superconductors

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Talk online at
http://pantheon.yale.edu/~subir

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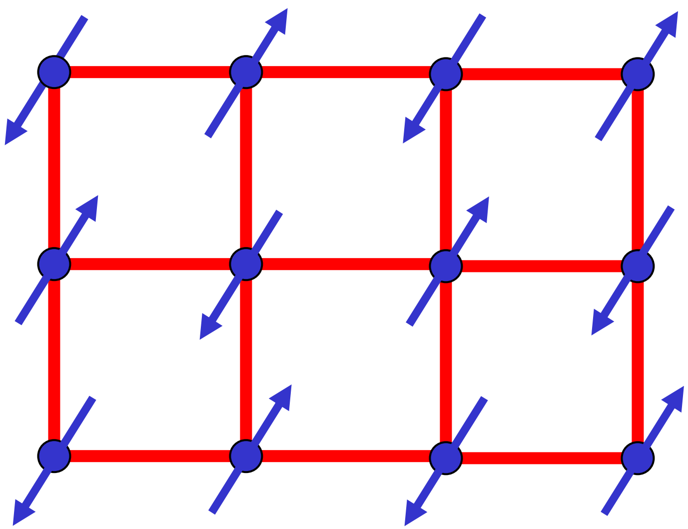
Parent compound of the high temperature superconductors: La_2CuO_4

Mott insulator: square lattice antiferromagnet



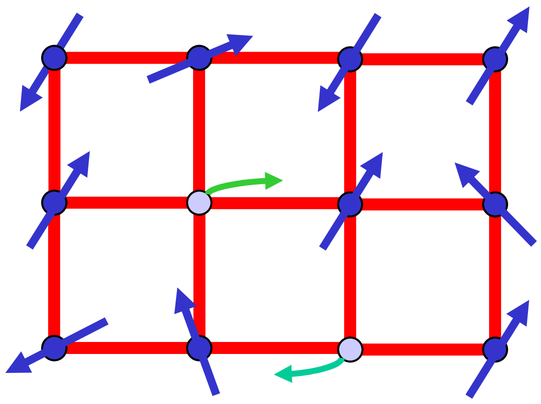
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Ground state has long-range magnetic Néel order, or a "spin density wave (SDW)"

Néel order parameter: $\vec{\phi} = (-1)^{i_x + i_y} \vec{S}_i$

$$\langle \vec{\phi} \rangle \neq 0 \quad ; \quad \langle \vec{S}_i \rangle \neq 0$$

Introduce mobile carriers of density δ by substitutional doping of out-of-plane ions *e.g.* $La_{2-\delta}Sr_{\delta}CuO_4$

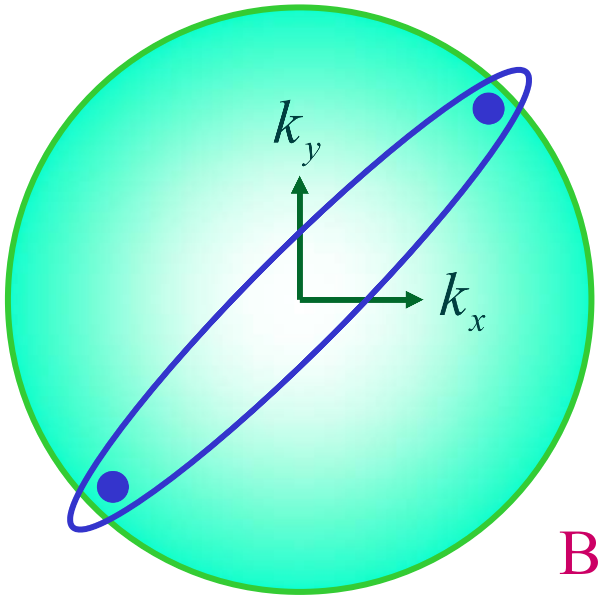


$$\left\langle \vec{S} \right\rangle = 0$$

Exhibits superconductivity below a high critical temperature T_c

Superconductivity in a doped Mott insulator

BCS superconductor obtained by the Cooper instability of a *metallic Fermi liquid*



Pair wavefunction

$$\Psi = \left(k_x^2 - k_y^2\right)\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$$

$$\left\langle \vec{S} \right\rangle = 0$$

Bose-Einstein condensation of Cooper pairs

Several *low* temperature properties of the cuprate superconductors appear to be qualitatively similar to those predicted by BCS theory.

Superconductivity in a doped Mott insulator

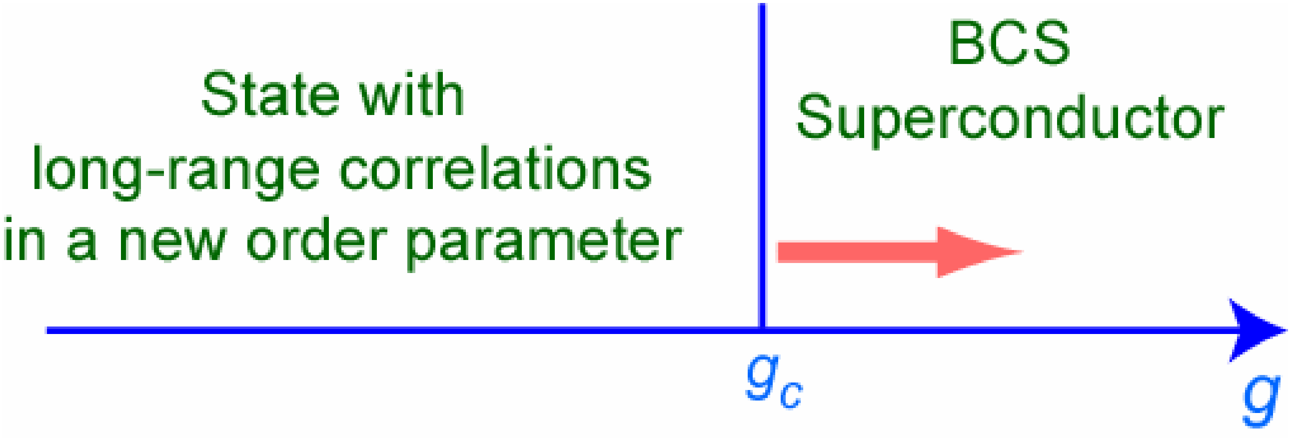
Review: S. Sachdev, *Science* **286**, 2479 (1999).

Hypothesis: cuprate superconductors are characterized by additional order parameters, associated with the proximate Mott insulator, along with the familiar order associated with the Bose condensation of Cooper pairs in BCS theory. These orders lead to new low energy excitations.

Predictions of BCS associated with underlying Fermi surface do not apply

Superconductivity in a doped Mott insulator

Review: S. Sachdev, *Science* **286**, 2479 (1999).



Study physics in a generalized phase diagram which includes new phases (which need not be experimentally accessible) with long-range correlations in the additional order parameters. Expansion away from quantum critical points provides a systematic and controlled theory of the low energy excitations (including their behavior near imperfections such as impurities and vortices and their response to applied fields) and of crossovers into "incoherent" regimes at finite temperature.

Outline

I. **What is a quantum phase transition ?**

II. The simplest quantum phase transition
    Quantum Ising Chain

III. Coupled Ladder Antiferromagnet

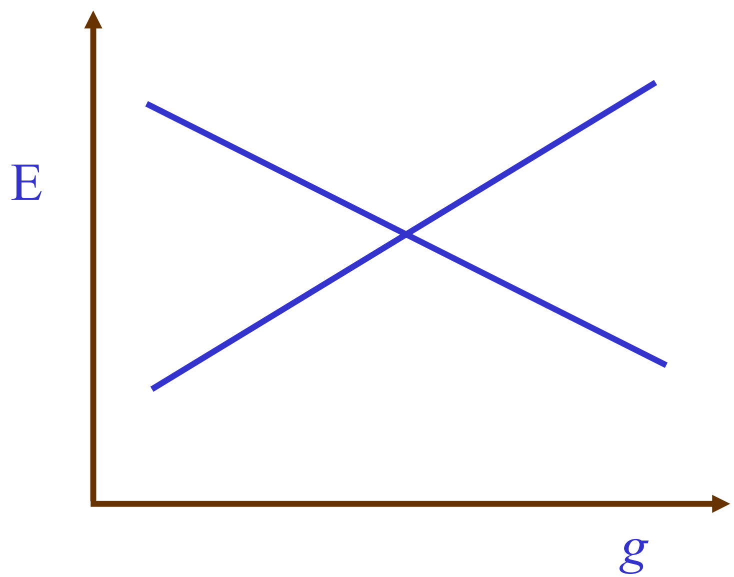
IV. A global phase diagram

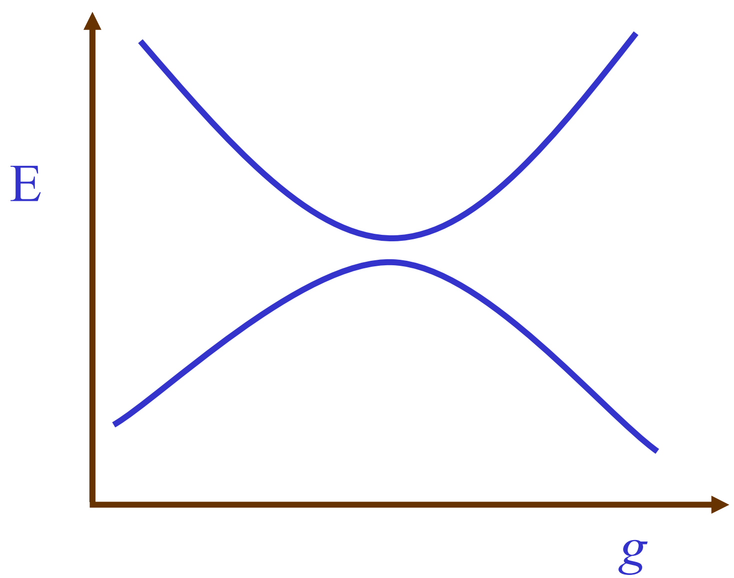
V. Recent neutron scattering and STM experiments on the cuprates.

VI. Conclusions

What is a quantum phase transition ?

Non-analyticity in ground state properties as a function of some control parameter *g*





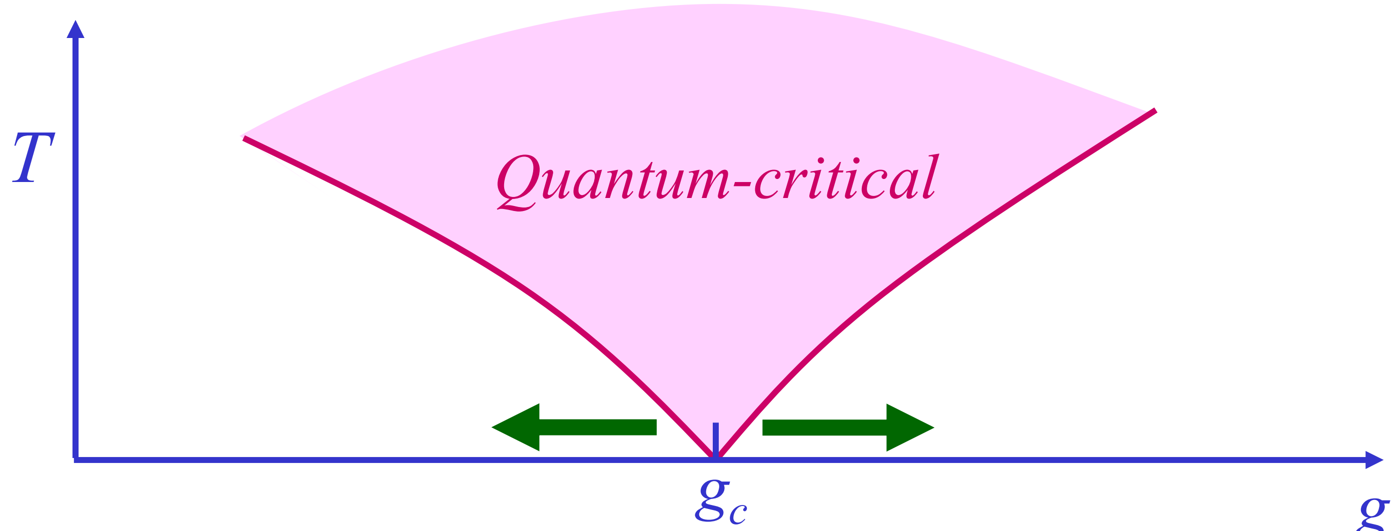
True level crossing:

Usually a *first*-order transition

Avoided level crossing which becomes sharp in the infinite volume limit:

second-order transition

Why study quantum phase transitions ?



• Theory for a quantum system with strong correlations: describe phases on either side of g_c by expanding in deviation from the quantum critical point.

• Critical point is a novel state of matter without quasiparticle excitations

• Critical excitations control dynamics in the wide *quantum-critical* region at non-zero temperatures.
No collective classical variables for large scale dynamics.

Important property of ground state at $g=g_c$: temporal and spatial scale invariance; characteristic energy scale at other values of g: $\Delta \sim |g - g_c|^{z\nu}$

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I. Quantum Ising Chain

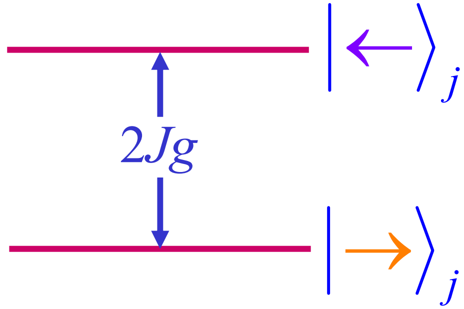
Degrees of freedom: $j = 1 \ldots N$ qubits, N "large"

$$|\uparrow\rangle_j \, , \; |\downarrow\rangle_j$$

or $$|\rightarrow\rangle_j = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_j + |\downarrow\rangle_j\right) \, , \; |\leftarrow\rangle_j = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_j - |\downarrow\rangle_j\right)$$

Hamiltonian of decoupled qubits:

$$H_0 = -Jg \sum_j \sigma_j^x$$



Coupling between qubits:

$$H_1 = -J \sum_j \sigma_j^z \sigma_{j+1}^z$$

$$\Big(\left| \rightarrow \right\rangle_j \left\langle \leftarrow \right| + \left| \leftarrow \right\rangle_j \left\langle \rightarrow \right| \Big) \Big(\left| \rightarrow \right\rangle_{j+1} \left\langle \leftarrow \right| + \left| \leftarrow \right\rangle_{j+1} \left\langle \rightarrow \right| \Big)$$

Prefers neighboring qubits

are *either* $\left| \uparrow \right\rangle_j \left| \uparrow \right\rangle_{j+1}$ *or* $\left| \downarrow \right\rangle_j \left| \downarrow \right\rangle_{j+1}$

(not entangled)

Full Hamiltonian

$$H = H_0 + H_1 = -J \sum_j \left(g \sigma_j^x + \sigma_j^z \sigma_{j+1}^z \right)$$

leads to entangled states at g of order unity

Weakly-coupled qubits $\left(g \gg 1\right)$

Ground state:

$$\left|G\right\rangle = \left|\cdots\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\cdots\right\rangle$$

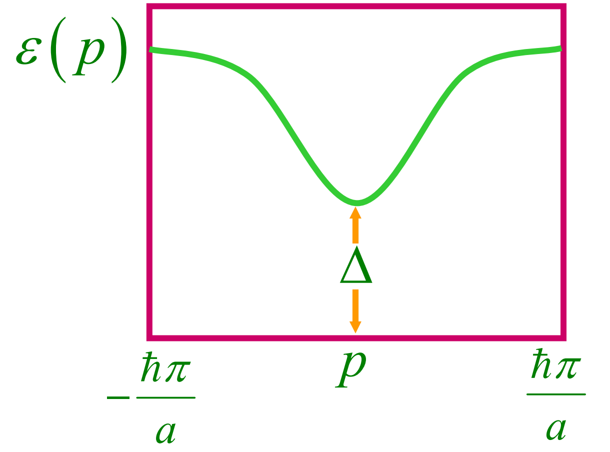
$$-\frac{1}{2g}\left|\cdots\rightarrow\rightarrow\rightarrow\rightarrow\leftarrow\leftarrow\rightarrow\rightarrow\rightarrow\rightarrow\cdots\right\rangle - \cdots$$

Lowest excited states:

$$\left|\ell_j\right\rangle = \left|\cdots\rightarrow\rightarrow\rightarrow\rightarrow\underset{j}{\leftarrow}\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\cdots\right\rangle + \cdots$$

Coupling between qubits creates "flipped-spin" *quasiparticle* states at momentum p

$$\left|p\right\rangle = \sum_j e^{ipx_j/\hbar}\left|\ell_j\right\rangle$$



Excitation energy $\varepsilon(p) = \Delta + 4J\sin^2\left(\frac{pa}{2\hbar}\right) + O\left(g^{-1}\right)$

Excitation gap $\Delta = 2gJ - 2J + O\left(g^{-1}\right)$

Entire spectrum can be constructed out of multi-quasiparticle states

Strongly-coupled qubits $(g \ll 1)$

Ground states:

$$|G\uparrow\rangle = |\cdots\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\rangle$$

$$-\frac{g}{2}|\cdots\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\rangle-\cdots$$

Ferromagnetic moment

$N_0 = \langle G|\sigma^z|G\rangle \neq 0$

Second state $|G\downarrow\rangle$ obtained by $\uparrow \Leftrightarrow \downarrow$

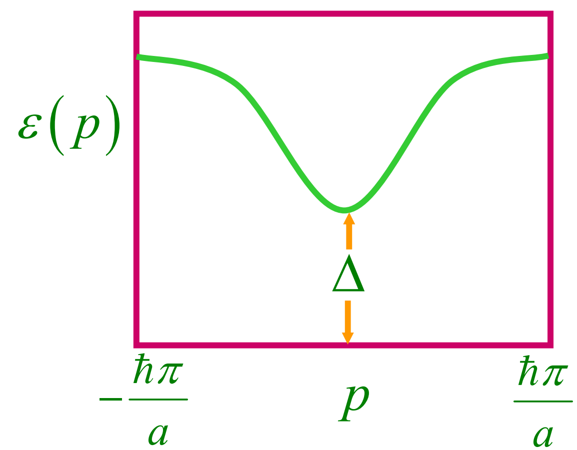
$|G\downarrow\rangle$ and $|G\uparrow\rangle$ mix only at order g^N

Lowest excited states: domain walls

$$|d_j\rangle = |\cdots\uparrow\uparrow\uparrow\uparrow\uparrow_j\downarrow\downarrow\downarrow\downarrow\downarrow\cdots\rangle+\cdots$$

Coupling between qubits creates new "domain-wall" *quasiparticle* states at momentum p

$$|p\rangle = \sum_j e^{ipx_j/\hbar}|d_j\rangle$$

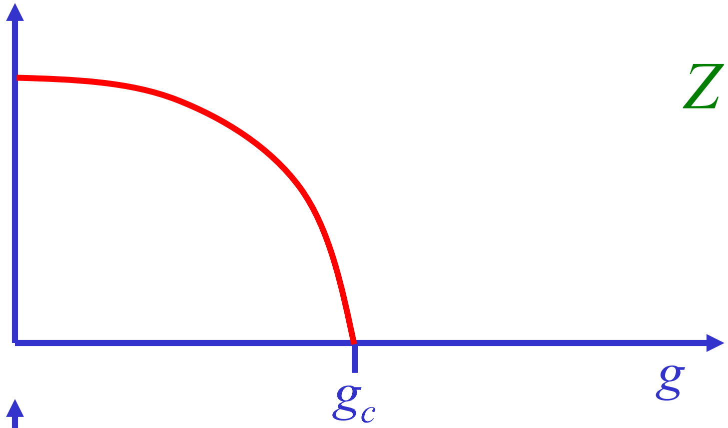


Excitation energy $\varepsilon(p) = \Delta + 4Jg\sin^2\left(\frac{pa}{2\hbar}\right) + O(g^2)$

Excitation gap $\Delta = 2J - 2gJ + O(g^2)$

Entangled states at g of order unity

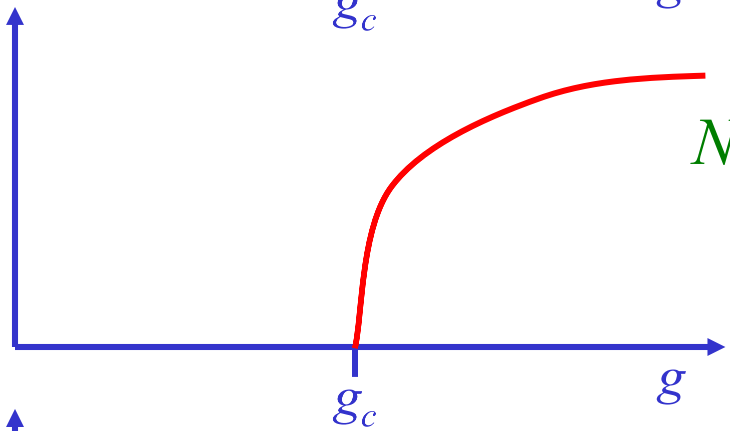
"Flipped-spin" Quasiparticle weight Z



$$Z \sim (g_c - g)^{1/4}$$

A.V. Chubukov, S. Sachdev, and J.Ye, *Phys. Rev.* B **49**, 11919 (1994)

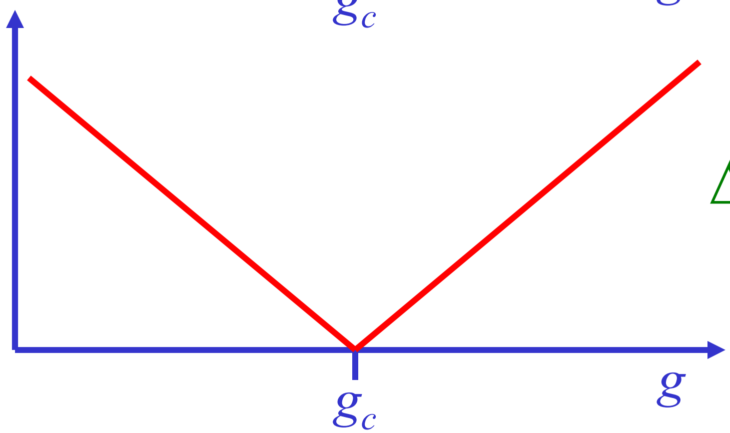
Ferromagnetic moment N_0



$$N_0 \sim (g - g_c)^{1/8}$$

P. Pfeuty *Annals of Physics*, **57**, 79 (1970)

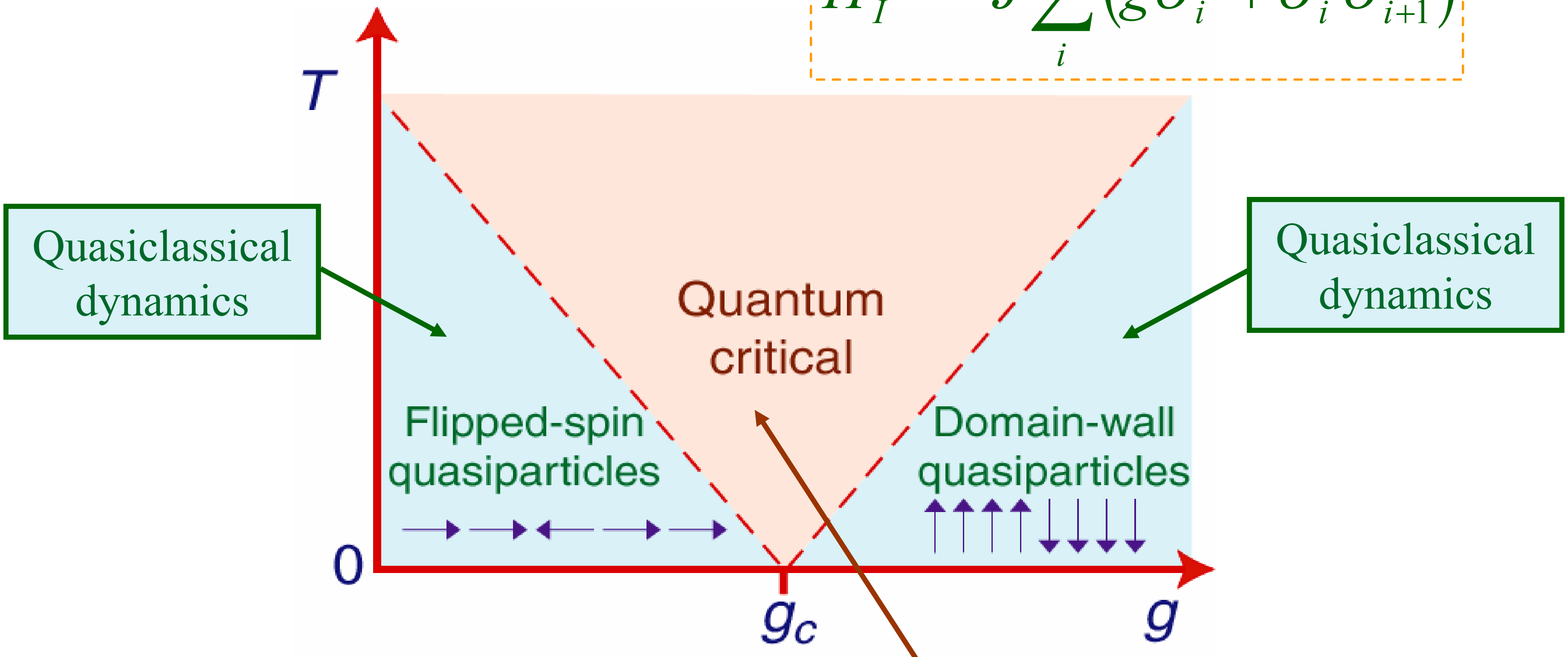
Excitation energy gap Δ



$$\Delta \sim |g - g_c|$$

Crossovers at nonzero temperature

$$H_I = -J\sum_i \left(g\sigma_i^x + \sigma_i^z \sigma_{i+1}^z \right)$$



$$\chi(\omega) = \frac{i}{\hbar}\sum_k \int_0^\infty dt \left\langle \left[\sigma_j^z(t), \sigma_k^z(0) \right] \right\rangle e^{i\omega t}$$

$$= \frac{A}{T^{7/4}\left(1 - i\omega\tau_\varphi + \ldots\right)}$$

Phase coherence time τ_φ given by $\frac{1}{\tau_\varphi} = \left(2\tan\frac{\pi}{16} \right)\frac{k_B T}{\hbar}$

S. Sachdev and J. Ye, *Phys. Rev. Lett*. **69**, 2411 (1992).
S. Sachdev and A.P. Young, *Phys. Rev. Lett*. **78**, 2220 (1997).

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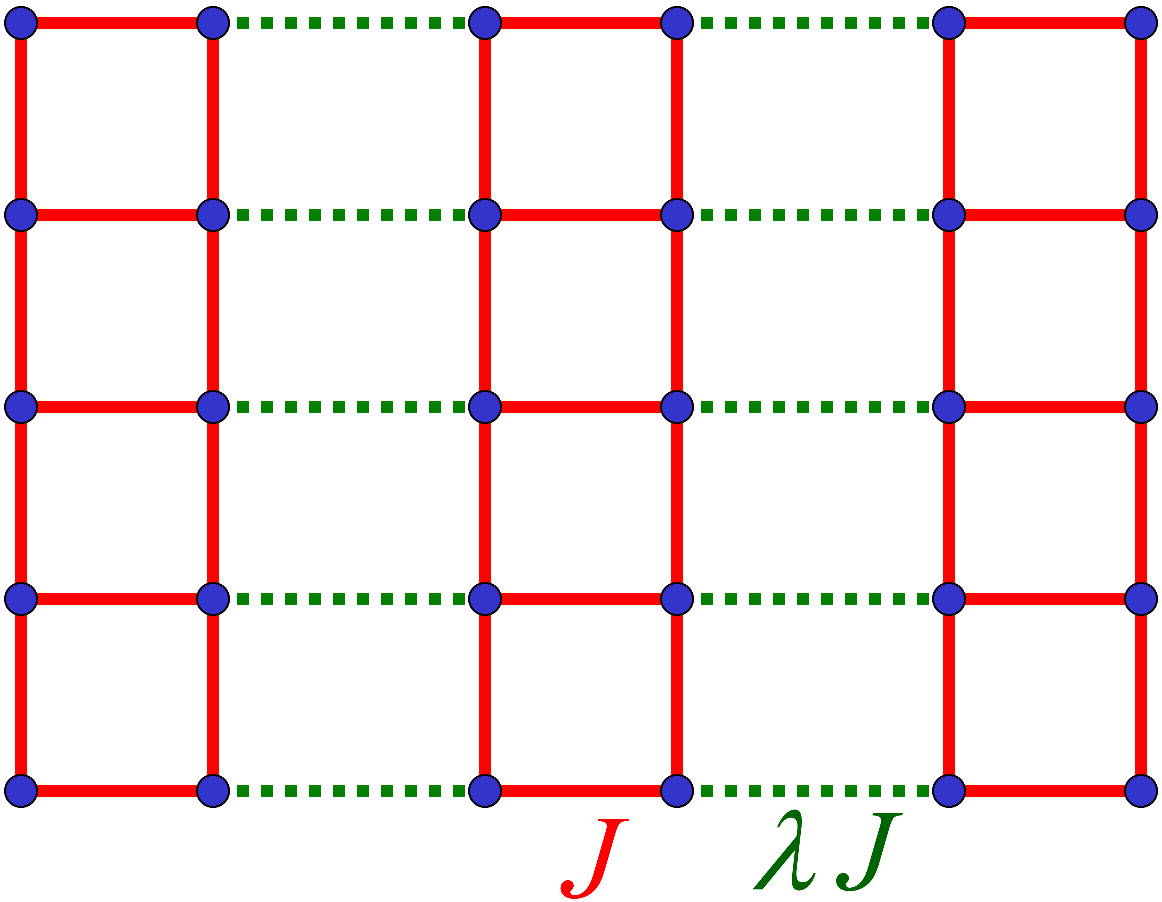
II. Coupled Ladder Antiferromagnet

N. Katoh and M. Imada, *J. Phys. Soc. Jpn.* **63**, 4529 (1994).
J. Tworzydlo, O. Y. Osman, C. N. A. van Duin, J. Zaanen, *Phys. Rev*. B **59**, 115 (1999).
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev.* B **65**, 014407 (2002).

S=1/2 spins on coupled 2-leg ladders



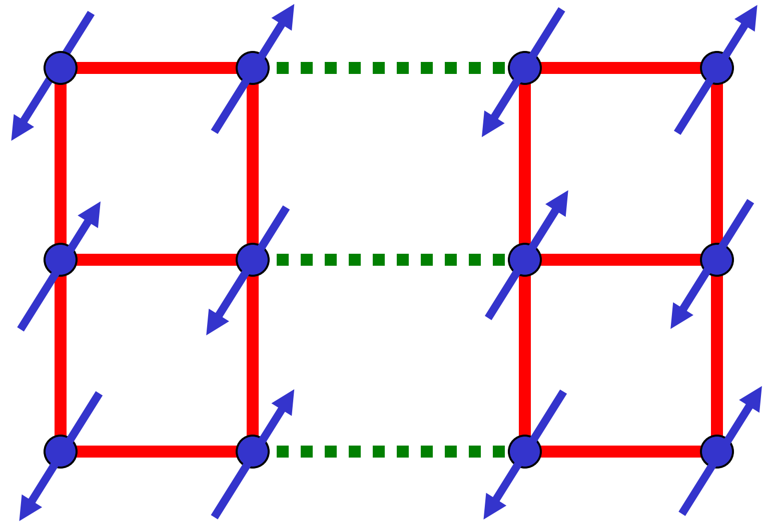
$$H = \sum_{<ij>} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

$$0 \le \lambda \le 1$$

λ close to 1

Square lattice antiferromagnet

Experimental realization: La_2CuO_4



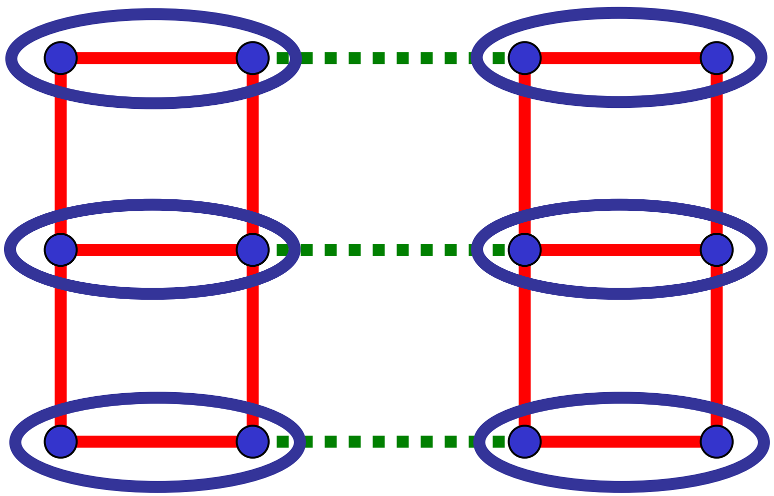
Ground state has long-range magnetic (Neel) order

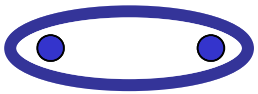
$$\left\langle \vec{S}_i \right\rangle = (-1)^{i_x + i_y} N_0 \neq 0$$

Excitations: 2 spin waves $\varepsilon_p = \sqrt{c_x^2 p_x^2 + c_y^2 p_y^2}$

λ close to 0

Weakly coupled ladders





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

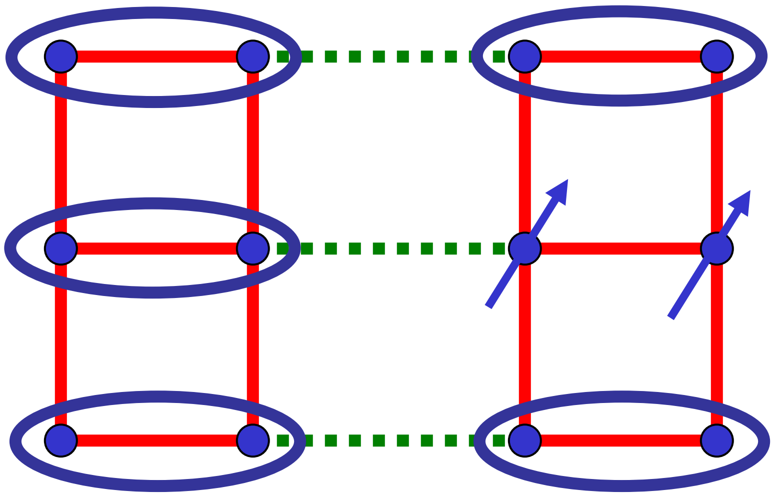
Real space Cooper pairs with their charge localized. Upon doping, motion and Bose-Einstein condensation of Cooper pairs leads to superconductivity

Paramagnetic ground state

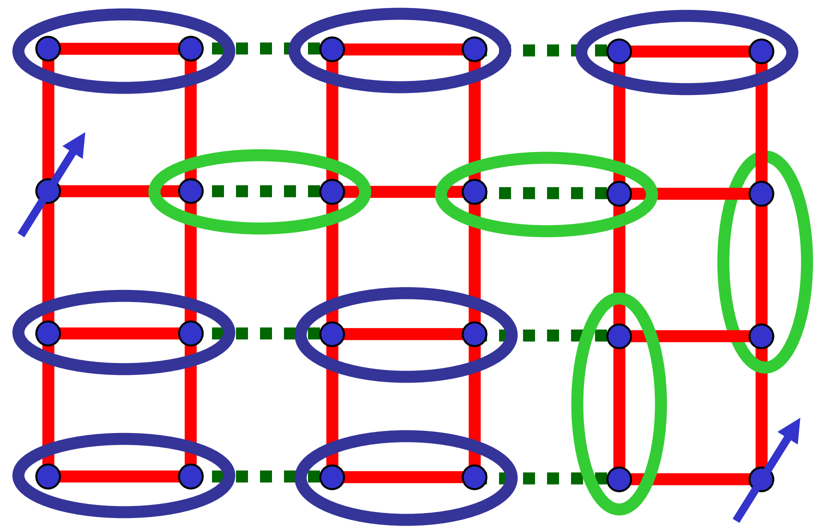
$$\left\langle \vec{S}_i \right\rangle = 0$$

λ close to 0

Excitations

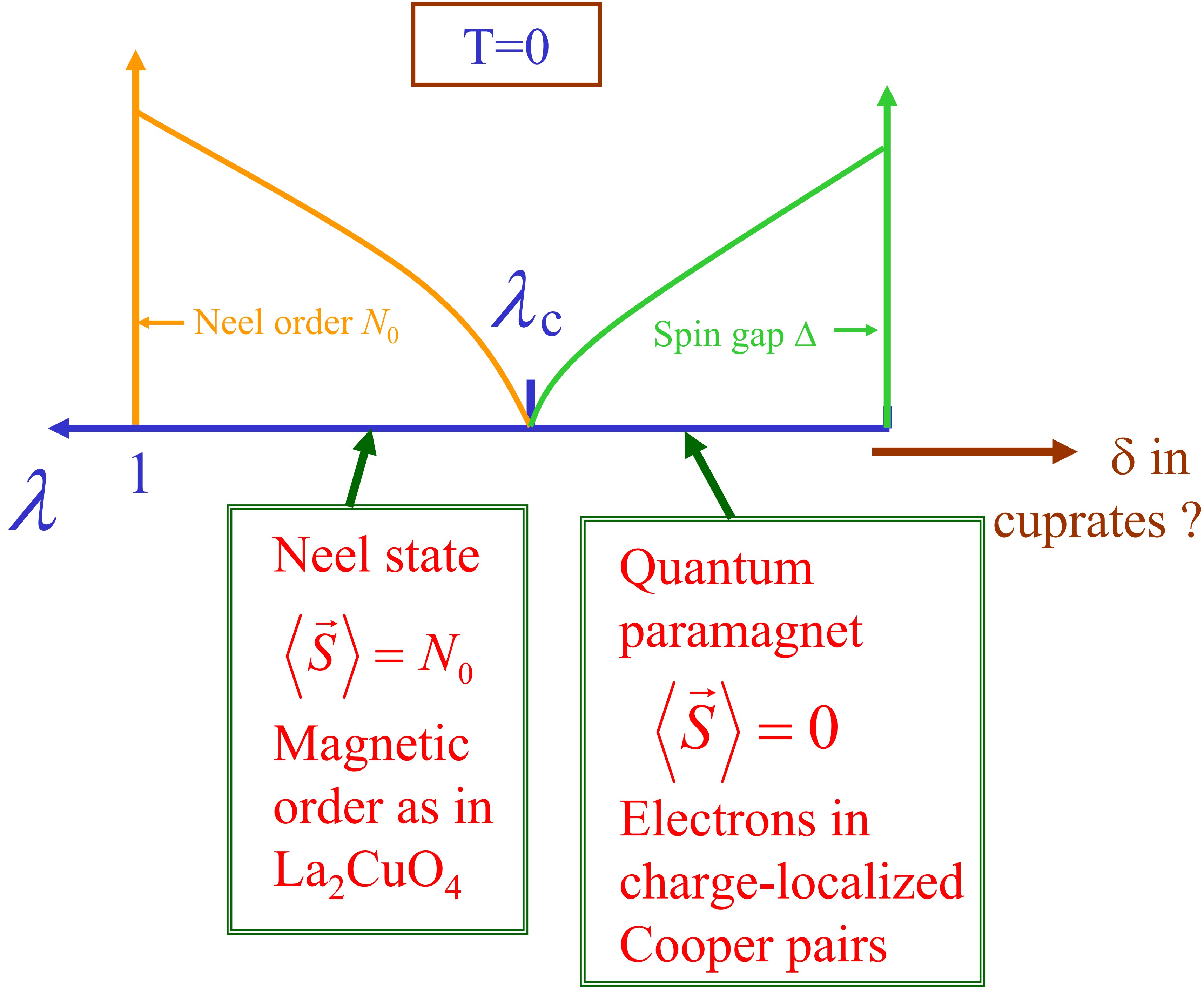


Excitation: S=1 ***exciton***
(spin collective mode)

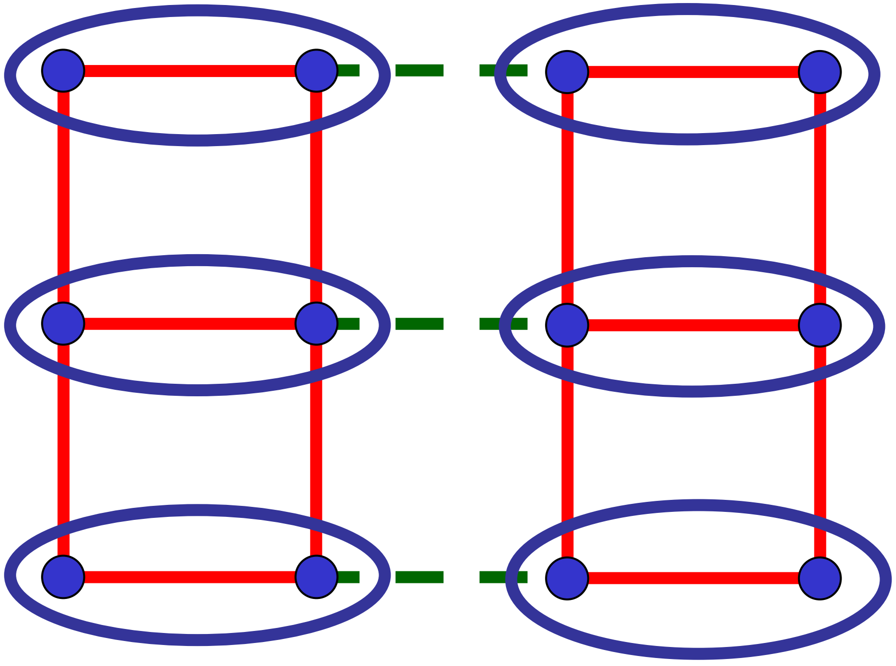


S=1/2 spinons are ***confined*** by a linear potential.

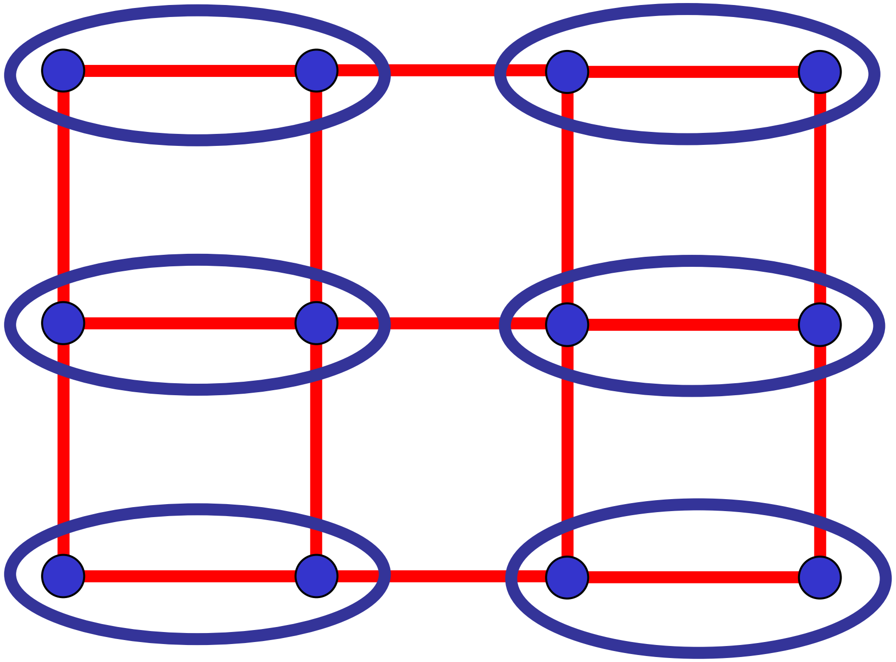
Energy dispersion away from antiferromagnetic wavevector $\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$


T=0
Neel order N_0
λ_c
Spin gap Δ
λ
1
δ in
cuprates ?
Neel state
$\langle \vec{S} \rangle = N_0$
Magnetic
order as in
La_2CuO_4
Quantum
paramagnet
$\langle \vec{S} \rangle = 0$
Electrons in
charge-localized
Cooper pairs

Paramagnetic ground state of coupled ladder model



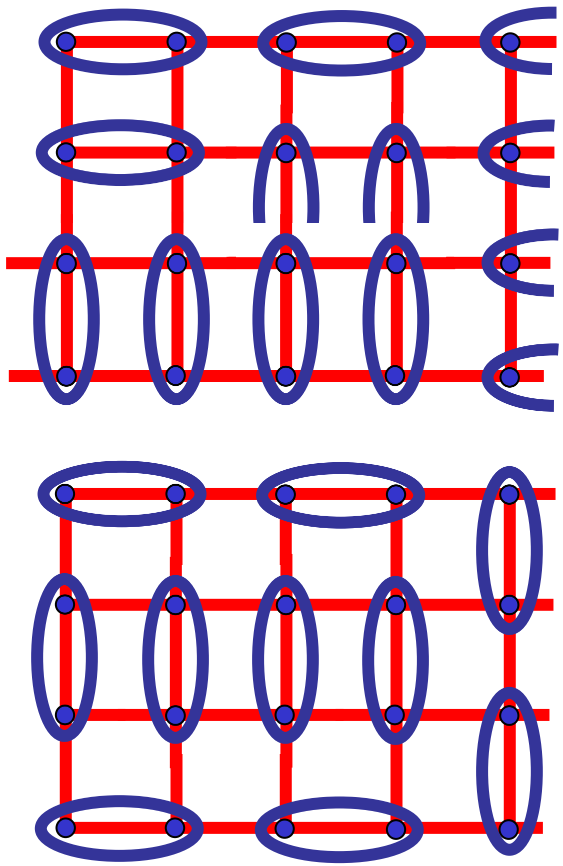
Can this be a paramagnetic ground state of a system with full square lattice symmetry ?



Such a state breaks lattice symmetry by the appearance of ***bond order***

Such ***bond order*** is generic in paramagnetic states proximate to a magnetic state with collinear spins

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



Origin of bond order

Quantum "entropic" effects prefer bond-ordered configurations in which the largest number of singlet pairs can resonate. The state on the upper left has more flippable pairs of singlets than the one on the lower left.
These effects lead to a broken square lattice symmetry near the transition to the magnetically ordered states with collinear spins.

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Order parameters in the cuprate superconductors

1. Pairing order of BCS theory

Bose-Einstein condensation of Cooper pairs

Orders associated with proximate Mott insulator

2. Collinear magnetic order

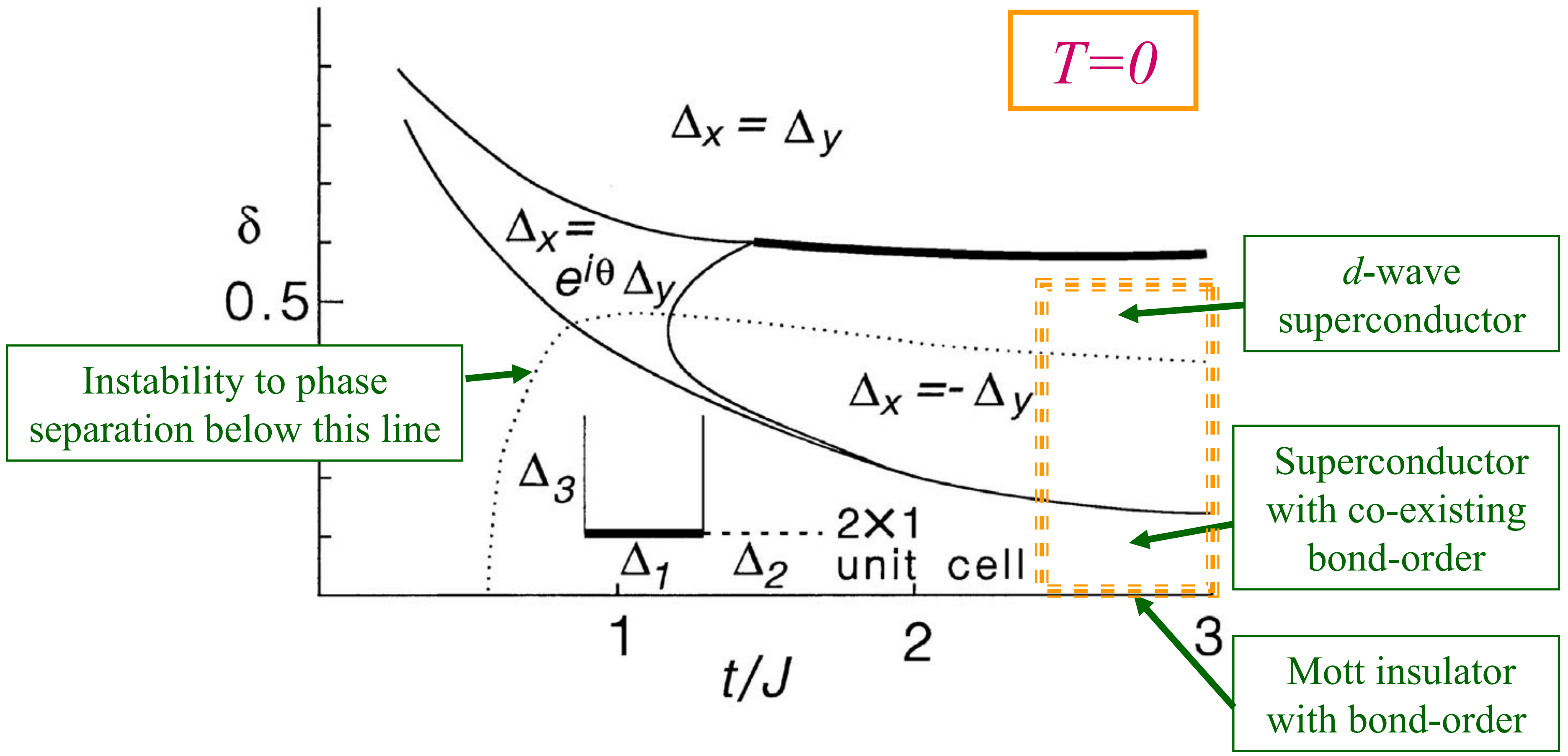
3. Bond order

For most wavevectors, these orders also imply a modulation in the site charge density ("charge order"). However, the amplitude of the charge order should be strongly suppressed by Coulomb interactions.

S. Sachdev and N. Read, *Int. J. Mod. Phys.* B **5**, 219 (1991).

Doping a paramagnetic bond-ordered Mott insulator

Systematic Sp(*N*) theory of translational symmetry breaking, while preserving spin rotation invariance.

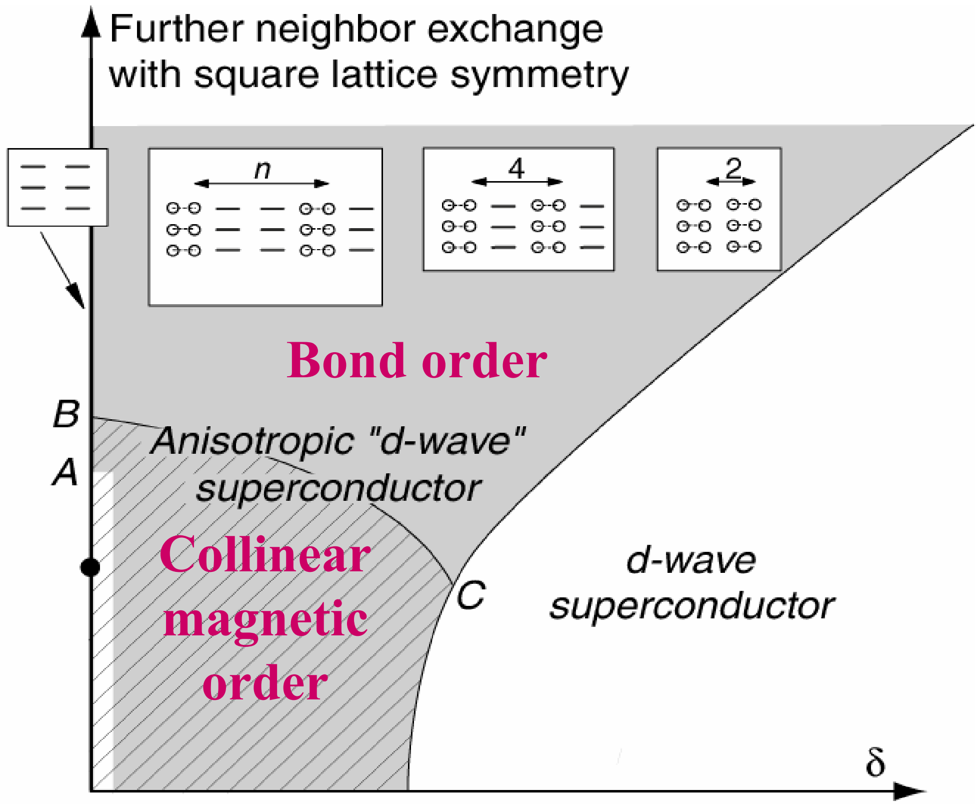


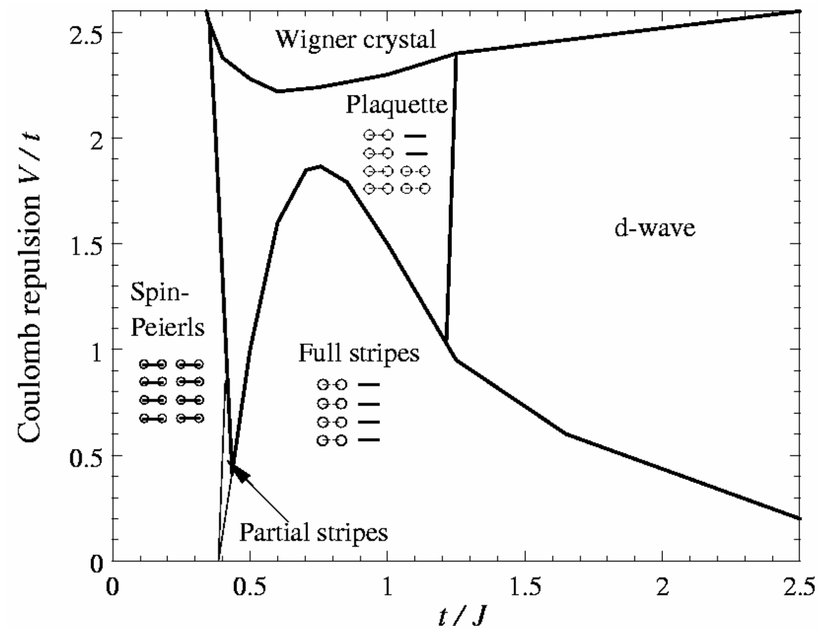
S. Sachdev and N. Read, *Int. J. Mod. Phys.* B **5**, 219 (1991).

IV. A global phase diagram

Include long-range Coulomb interactions: frustrated phase separation

V.J. Emery, S.A. Kivelson, and H.Q. Lin, *Phys. Rev. Lett*. 64, 475 (1990).





M. Vojta and S. Sachdev, *Phys. Rev. Lett*. **83**, 3916 (1999)
M. Vojta, Y. Zhang, and S. Sachdev, *Phys. Rev.* B **62**, 6721 (2000).
M. Vojta, Phys. Rev. B **66**, 104505 (2002).

See also J. Zaanen, *Physica* C **217**, 317 (1999),
S. White and D. J. Scalapino, *Phys. Rev. Lett*. **80**, 1272 (1998).
C. Castellani, C. Di Castro, and M. Grilli, *Phys.Rev. Lett*. **75**, 4650 (1995).
S. Mazumdar, R.T. Clay, and D.K. Campbell, Phys. Rev. B **62**, 13400 (2000).

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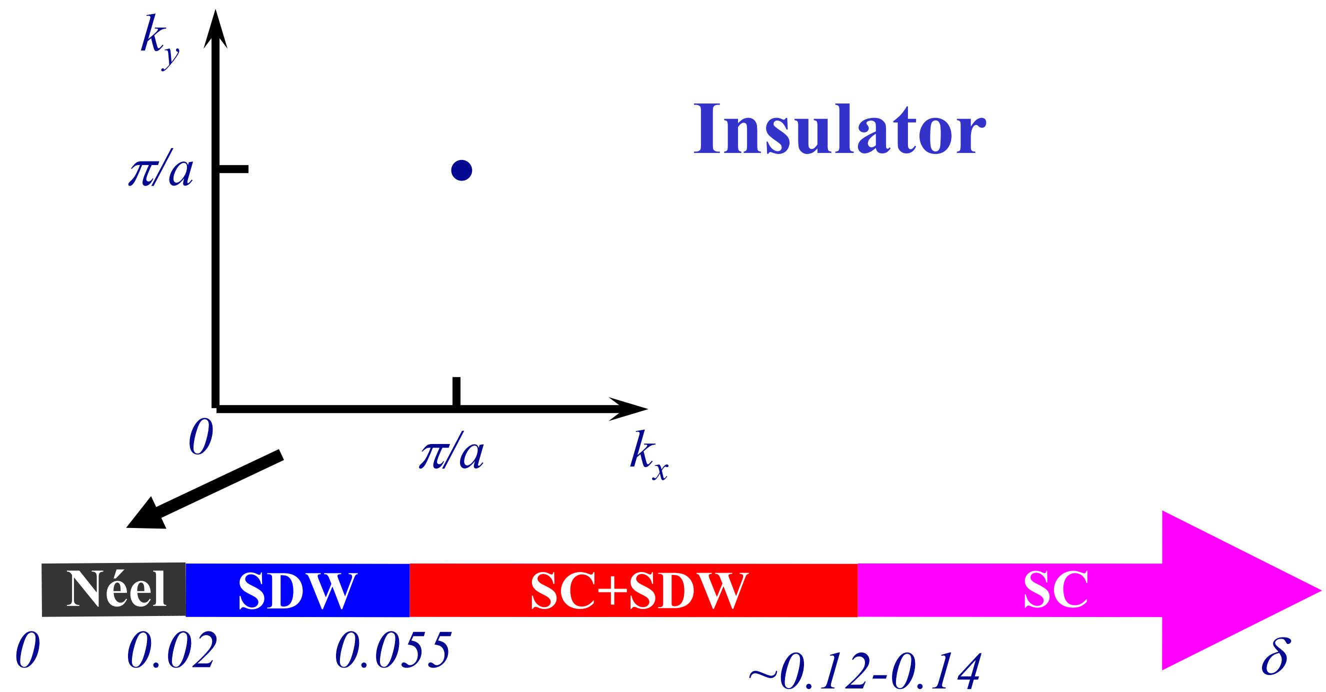
V. Tuning magnetic order in LSCO by a magnetic field

T=0 phases of LSCO



(additional commensurability effects near δ=0.125)

J. M. Tranquada *et al*., *Phys. Rev*. B **54**, 7489 (1996).

G. Aeppli, T.E. Mason, S.M. Hayden, H.A. Mook, J. Kulda, *Science* **278**, 1432 (1997).

S. Wakimoto, G. Shirane *et al*., *Phys. Rev*. B **60**, R769 (1999).

Y.S. Lee, R. J. Birgeneau, M. A. Kastner *et al., Phys. Rev*. B **60**, 3643 (1999)

S. Wakimoto, R.J. Birgeneau, Y.S. Lee, and G. Shirane, *Phys. Rev*. B **63**, 172501 (2001).

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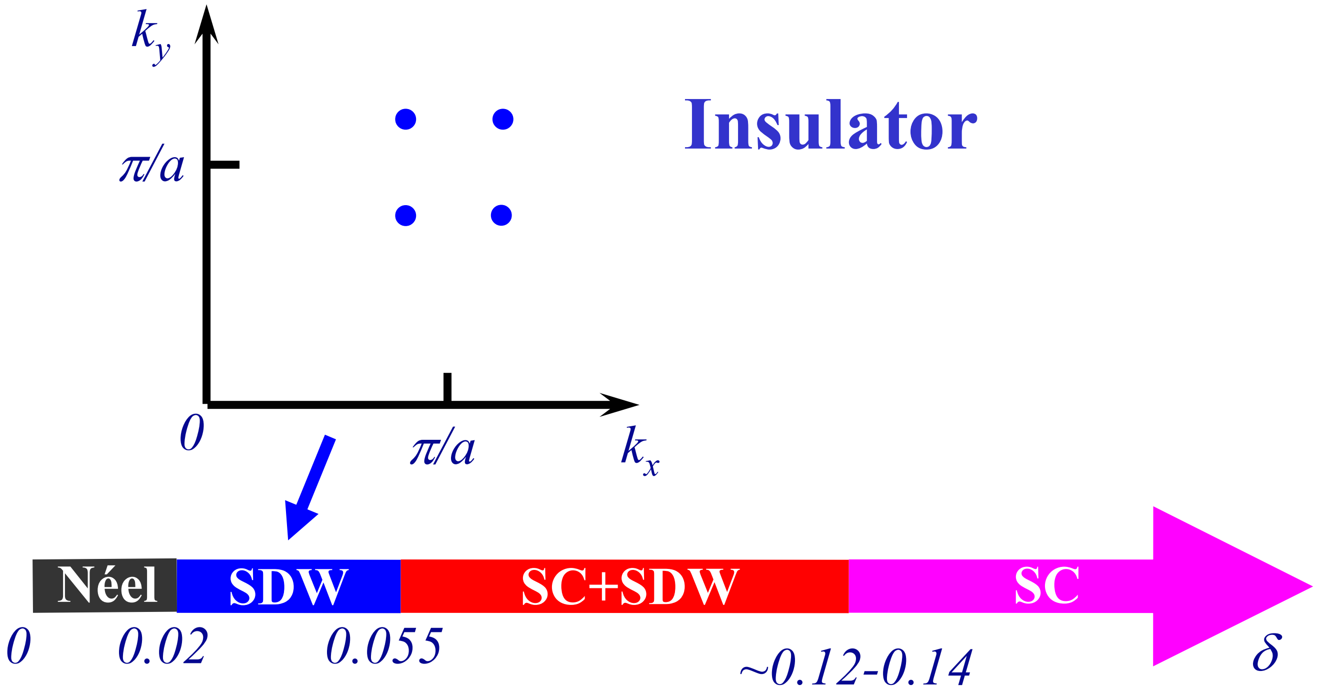

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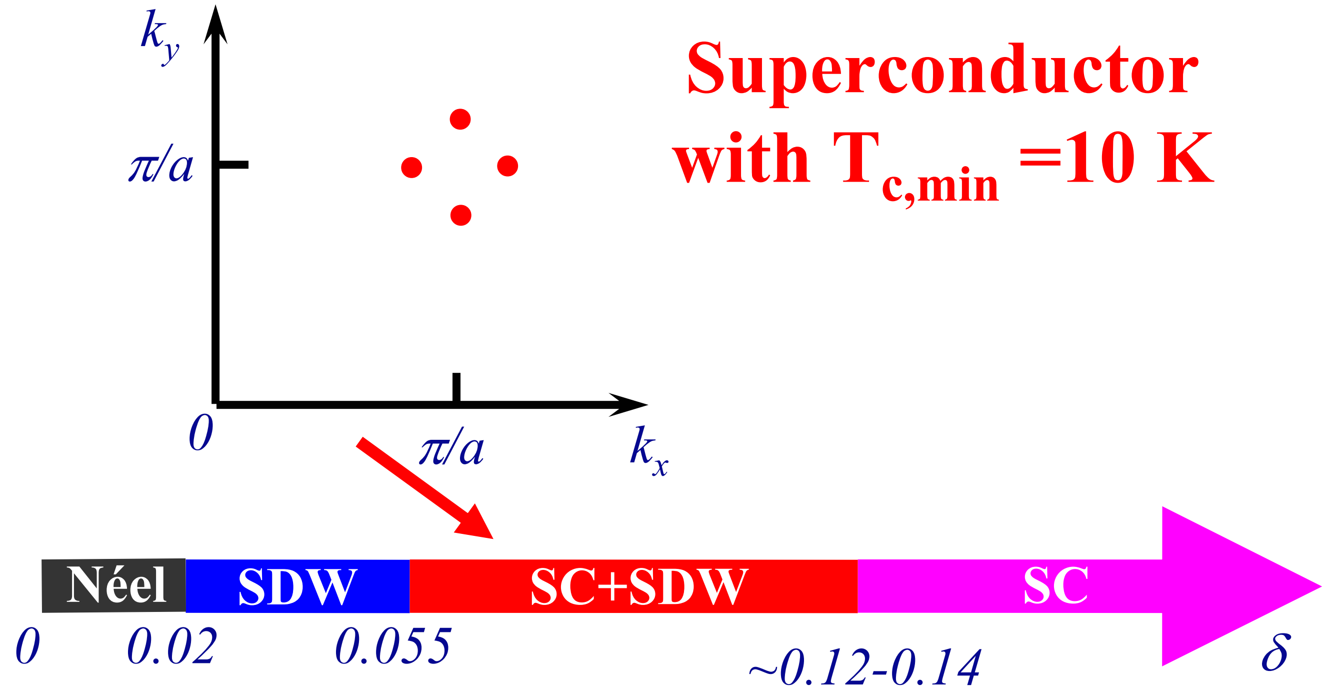

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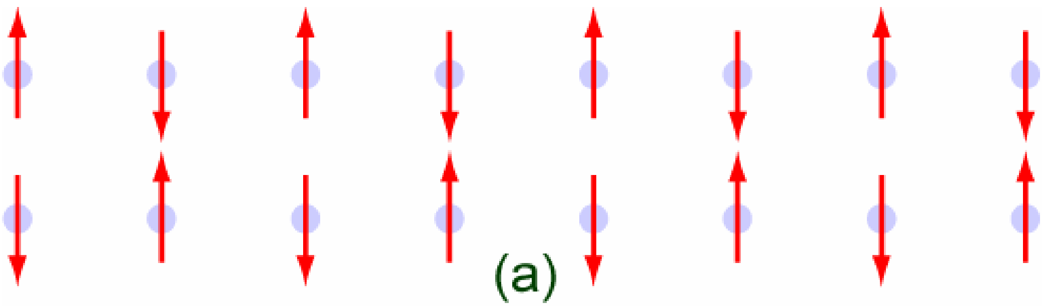
S. Wakimoto, G. Shirane *et al*., *Phys. Rev*. B **60**, R769 (1999).
Y.S. Lee, R. J. Birgeneau, M. A. Kastner *et al., Phys. Rev*. B **60**, 3643 (1999)
S. Wakimoto, R.J. Birgeneau, Y.S. Lee, and G. Shirane, *Phys. Rev*. B **63**, 172501 (2001).

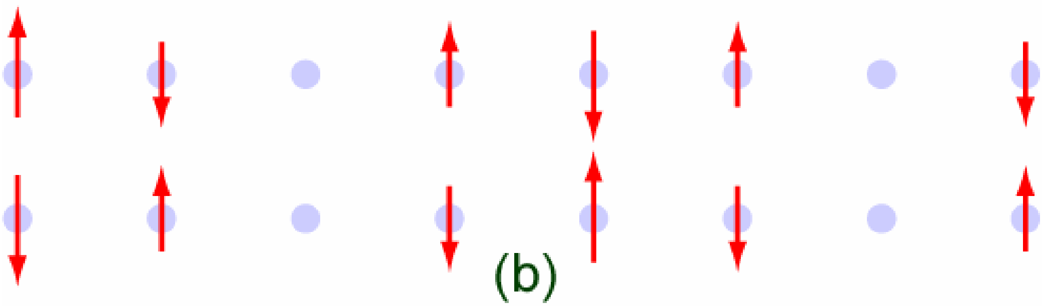
Spin density wave order

$$\langle \boldsymbol{S}_j \rangle = \boldsymbol{N}_1 \cos\left(\vec{K}\cdot\vec{r}_j\right) + \boldsymbol{N}_2 \sin\left(\vec{K}\cdot\vec{r}_j\right)$$

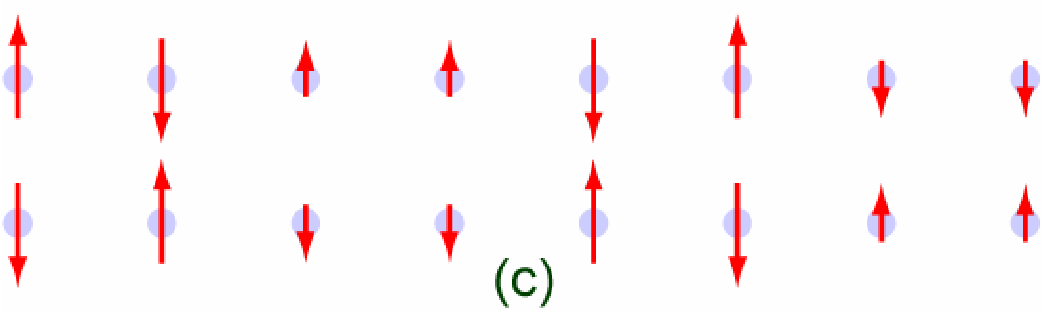
Collinear spins



$$\vec{K} = (\pi, \pi) \;\; ; \;\; \boldsymbol{N}_2 = 0$$



$$\vec{K} = (3\pi/4, \pi) \;\; ; \;\; \boldsymbol{N}_2 = 0$$

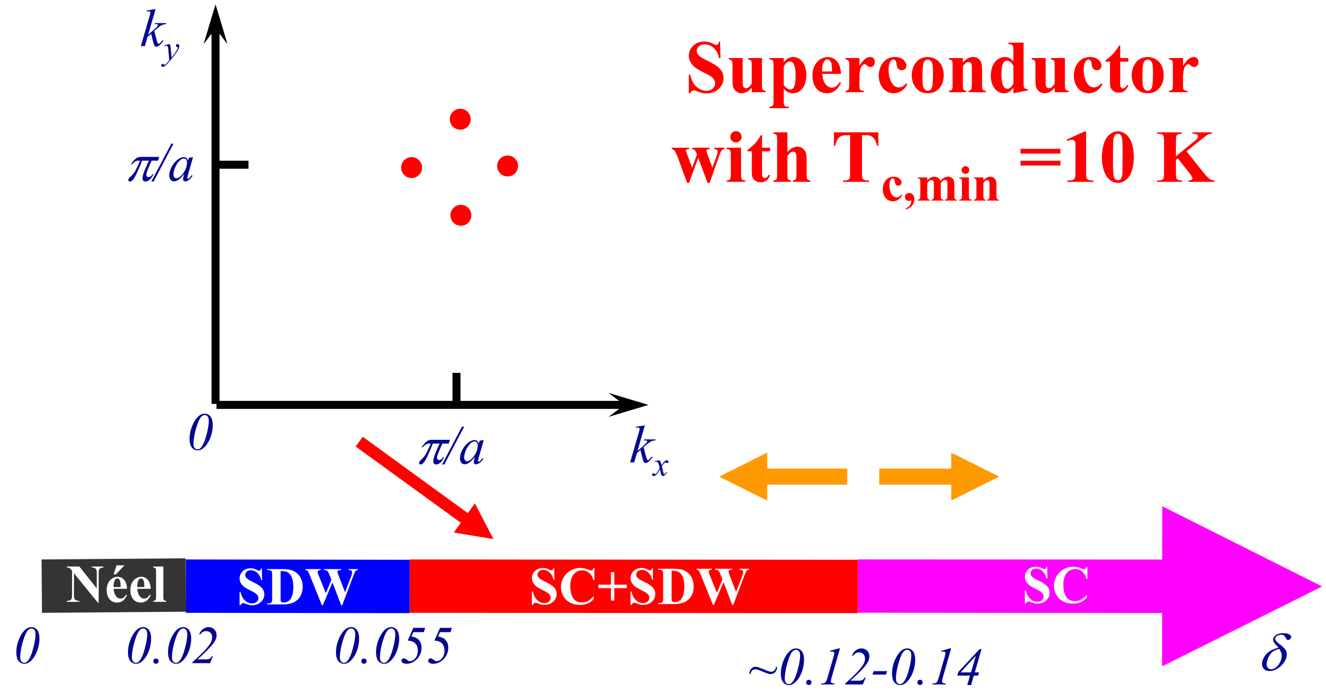


$$\vec{K} = (3\pi/4, \pi) \;\; ;$$

$$\boldsymbol{N}_2 = \left(\sqrt{2} - 1\right) \boldsymbol{N}_1$$

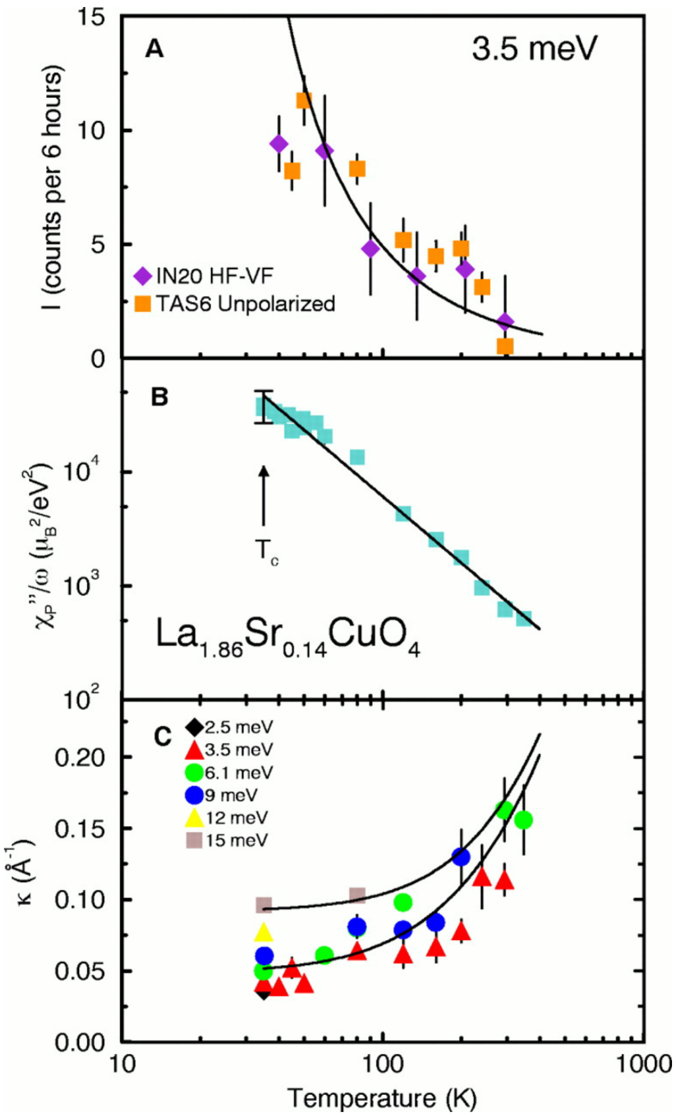
V. Tuning magnetic order in LSCO by a magnetic field

T=0 phases of LSCO

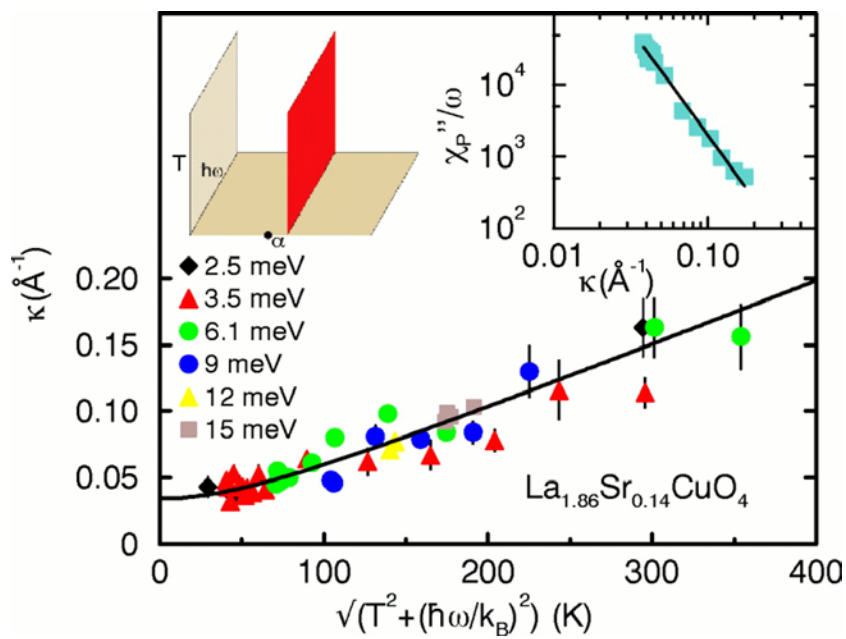


Use simplest assumption of a direct second-order quantum phase transition between SC and SC+SDW phases

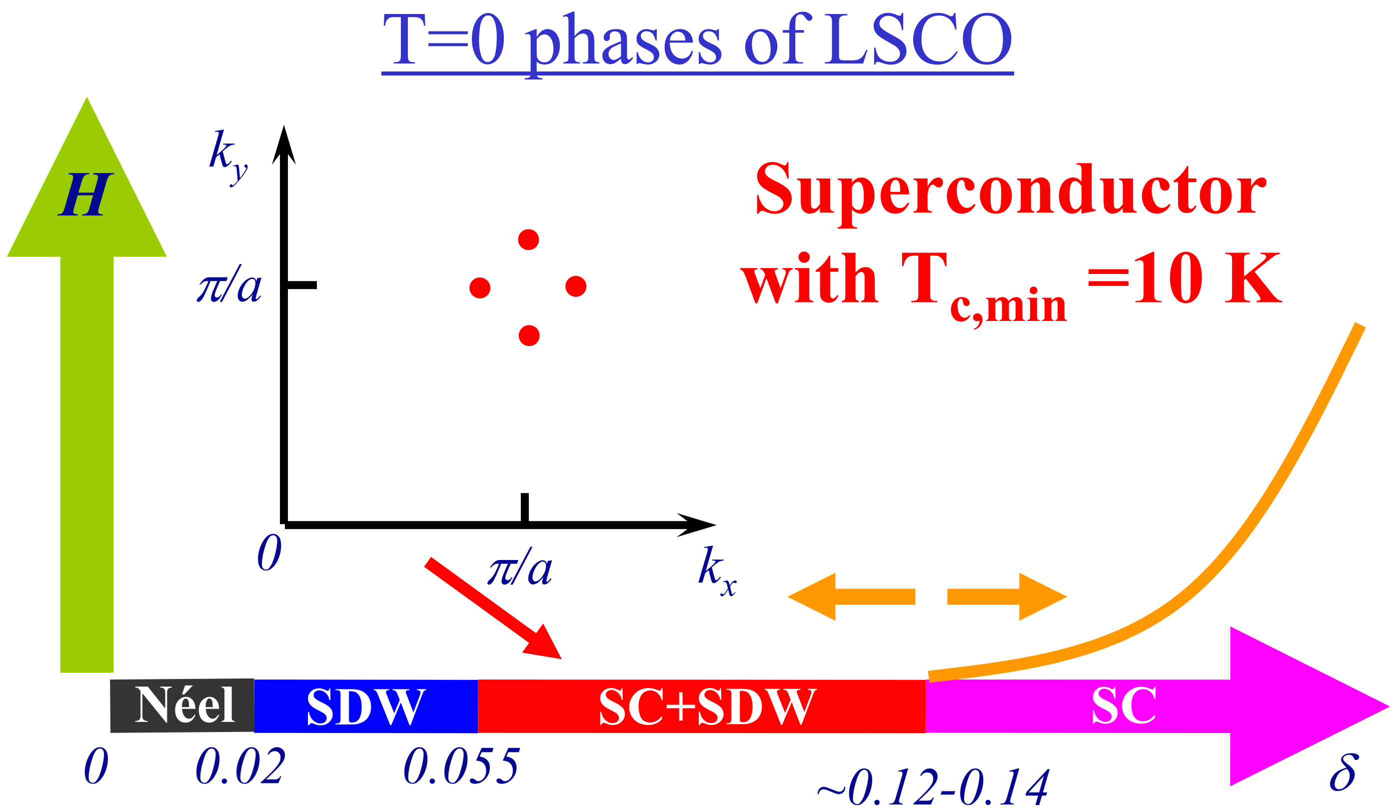
Neutron scattering measurements of dynamic spin susceptibility at an incommensurate wavevector: T and ω dependent divergence scaling as a function of $\hbar\omega/k_BT$ as in the quantum-critical region of Ising chain



G. Aeppli, T.E. Mason, S,M. Hayden, H.A. Mook, and J. Kulda, *Science* **278**, 1432 (1998).



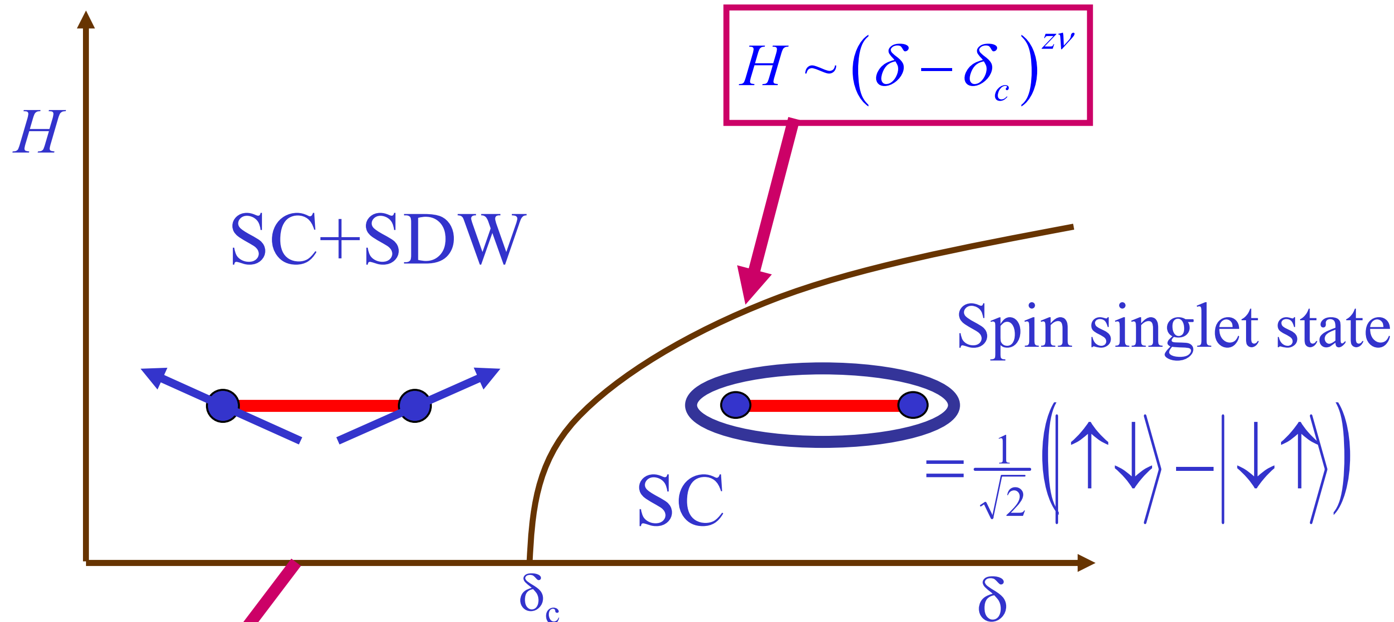
V. Tuning magnetic order in LSCO by a magnetic field



Use simplest assumption of a direct second-order quantum phase transition between SC and SC+SDW phases

Follow intensity of elastic Bragg spots in a magnetic field

Zeeman term: only effect in coupled ladder system



Elastic scattering intensity

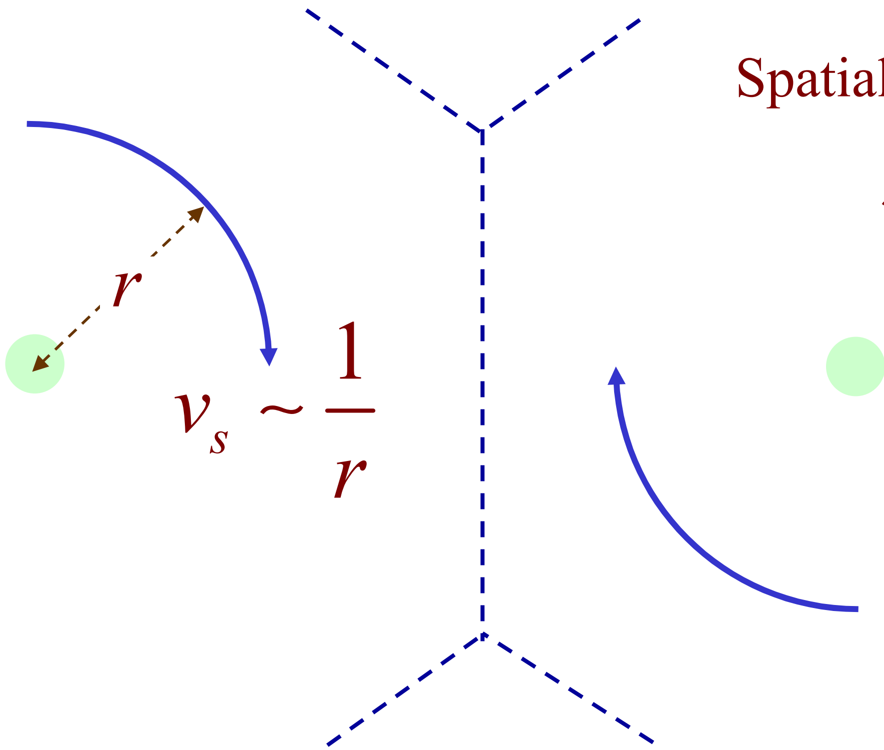
$$I(H) = I(0) + a\left(\frac{H}{J}\right)^2$$

Characteristic field $g\mu_B H = \Delta$, the spin gap

1 Tesla = 0.116 meV

Effect is negligible over experimental field scales

Dominant effect with coexisting superconductivity: **uniform** softening of spin excitations by superflow kinetic energy



Spatially averaged superflow kinetic energy

$$\sim \left\langle v_s^2 \right\rangle \sim \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H}$$

The suppression of SC order appears to the SDW order as an effective δ :

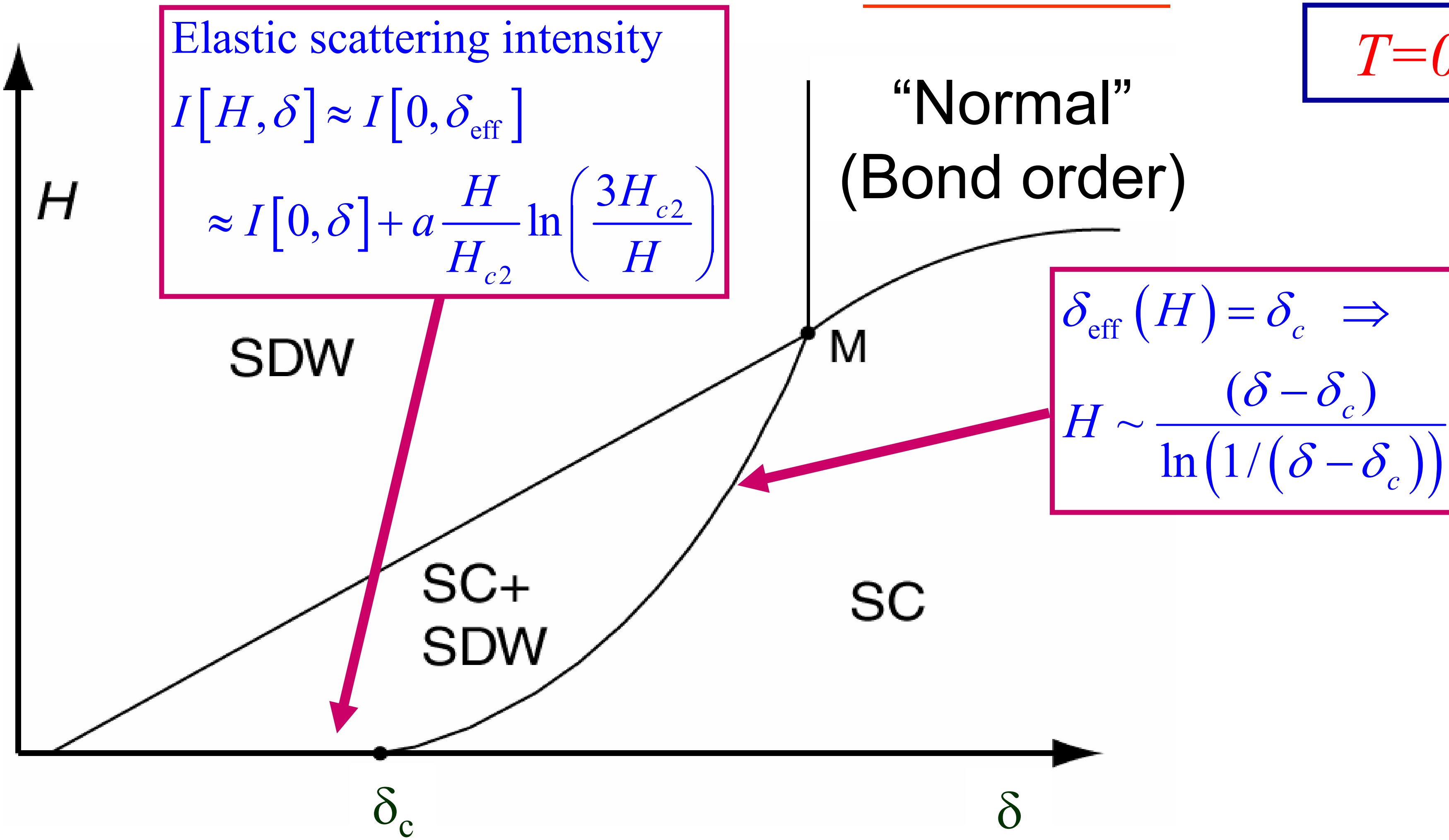
$$\delta_{\text{eff}}\left(H\right) = \delta - C \frac{H}{H_{c2}} \ln\left(\frac{3H_{c2}}{H}\right)$$

Competing order is enhanced in a "halo" around each vortex

E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

Main results

$T=0$



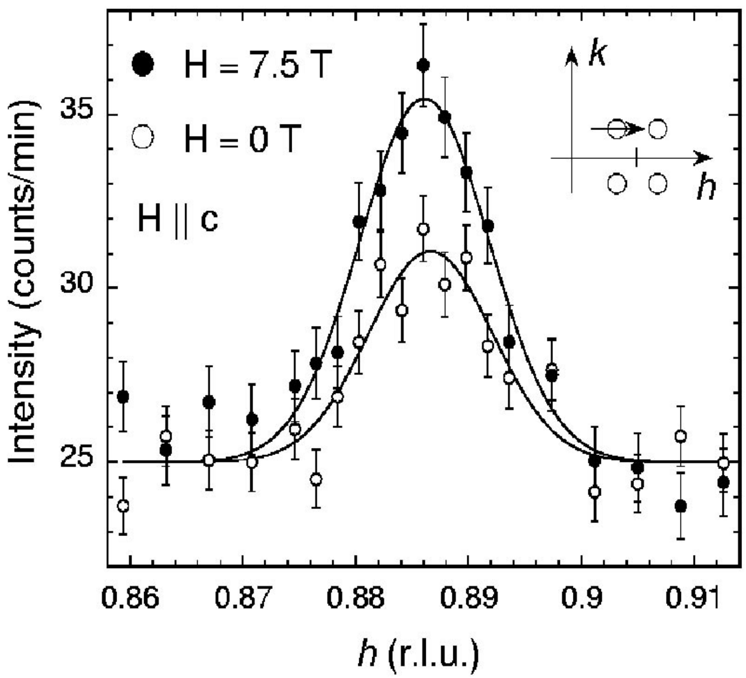
E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

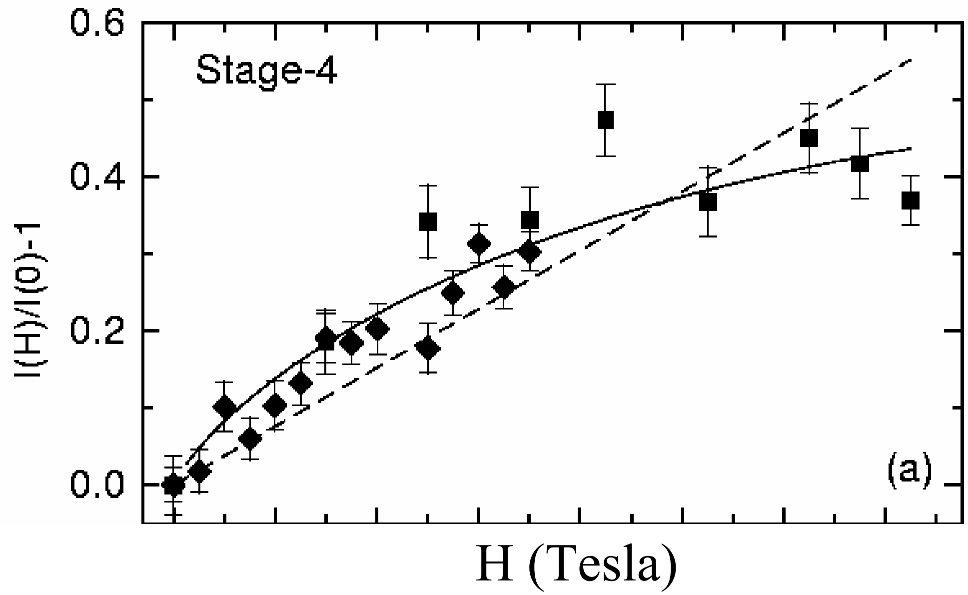
D. P. Arovas, A. J. Berlinsky, C. Kallin, and S.-C. Zhang, *Phys. Rev. Lett.* **79**, 2871 (1997) proposed static local spins within vortex cores in SC phase

Neutron scattering measurements of static spin correlations of the superconductor+spin-density-wave (SC+SDW) in a magnetic field

Elastic neutron scattering off La_2CuO_{4+y}

B. Khaykovich, Y. S. Lee, S. Wakimoto, K. J. Thomas, M. A. Kastner, and R.J. Birgeneau, *Phys. Rev.* B **66**, 01452



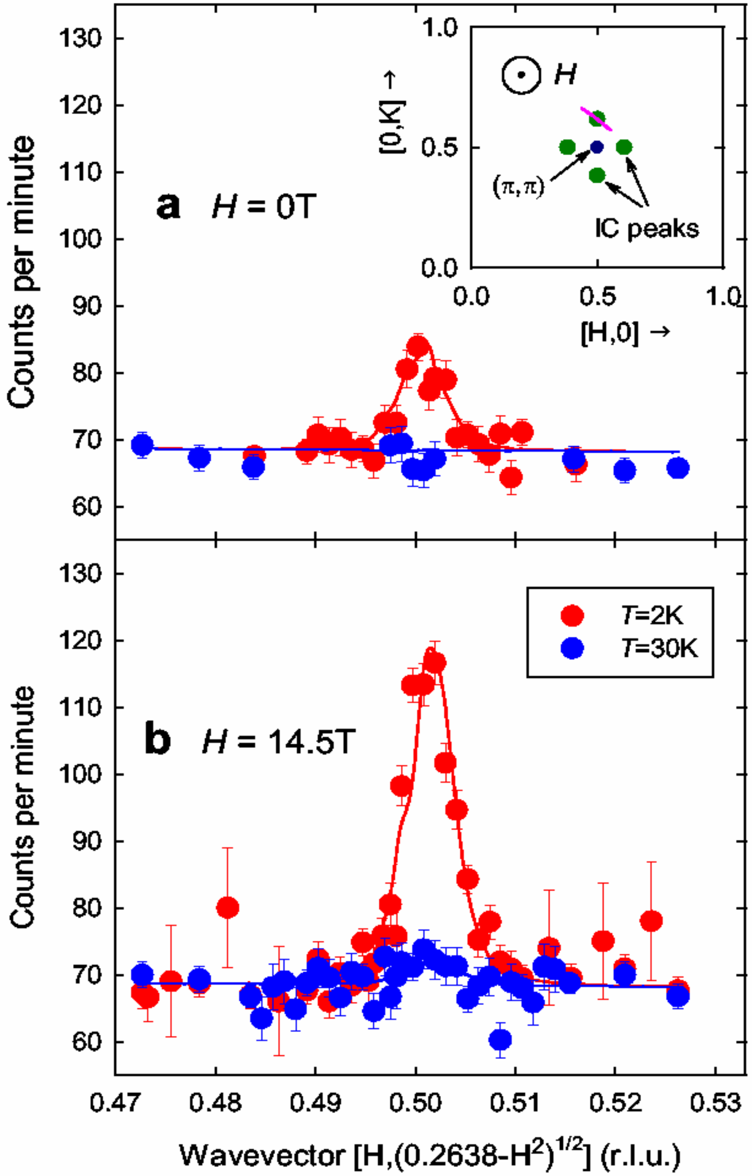


Solid line --- fit to : $\dfrac{I(H)}{I(0)} = 1 + a\dfrac{H}{H_{c2}}\ln\left(\dfrac{3.0H_{c2}}{H}\right)$

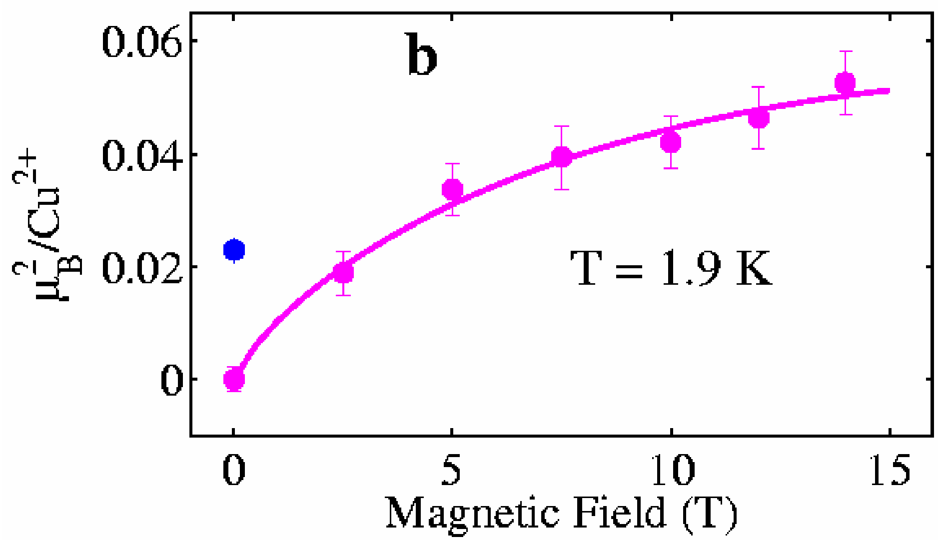
a is the only fitting parameter

Best fit value - a = 2.4 with H_{c2} = 60 T

Neutron scattering of $La_{2-x}Sr_xCuO_4$ at x=0.1

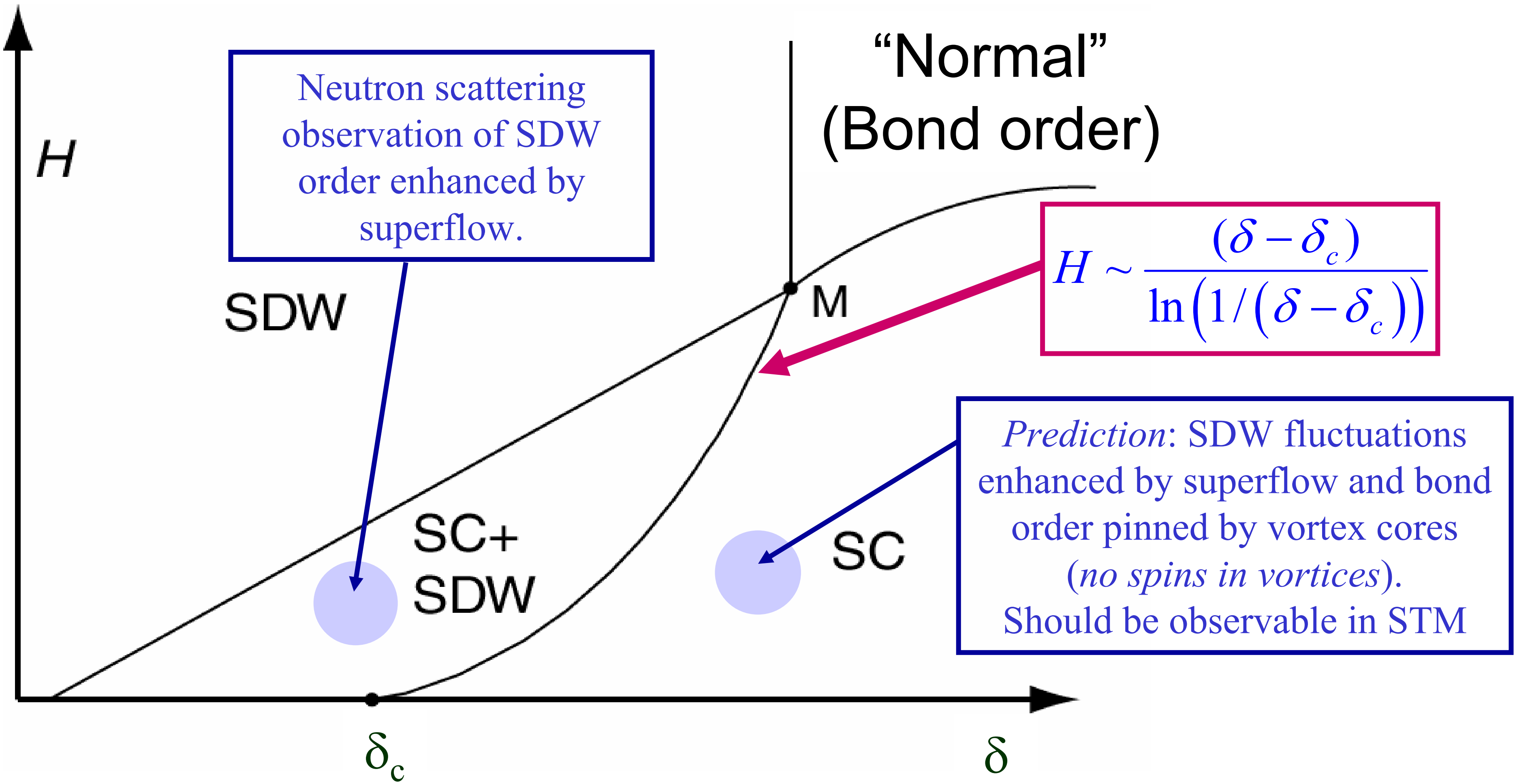


B. Lake, H. M. Rønnow, N. B. Christensen, G. Aeppli, K. Lefmann, D. F. McMorrow, P. Vorderwisch, P. Smeibidl, N. Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, T. E. Mason, *Nature*, **415**, 299 (2002).



Solid line - fit to : $I(H) = a\frac{H}{H_{c2}}\ln\left(\frac{H_{c2}}{H}\right)$

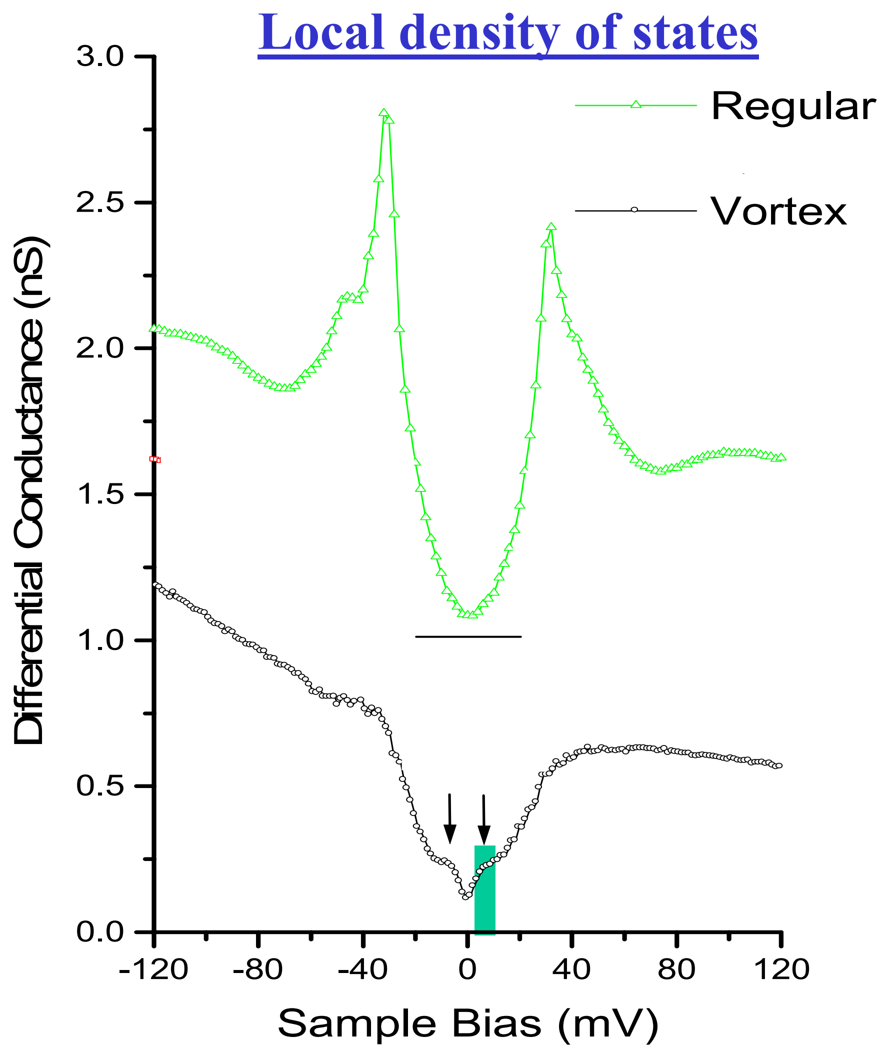
See also S. Katano, M. Sato, K. Yamada, T. Suzuki, and T. Fukase, *Phys. Rev.* B **62**, R14677 (2000).



K. Park and S. Sachdev *Phys. Rev*. B **64**, 184510 (2001).
Y. Zhang, E. Demler and S. Sachdev, *Phys. Rev*. B **66,** 094501 (2002).

STM around vortices induced by a magnetic field in the superconducting state

J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan,
H. Eisaki, S. Uchida, and J. C. Davis, *Science* **295**, 466 (2002).

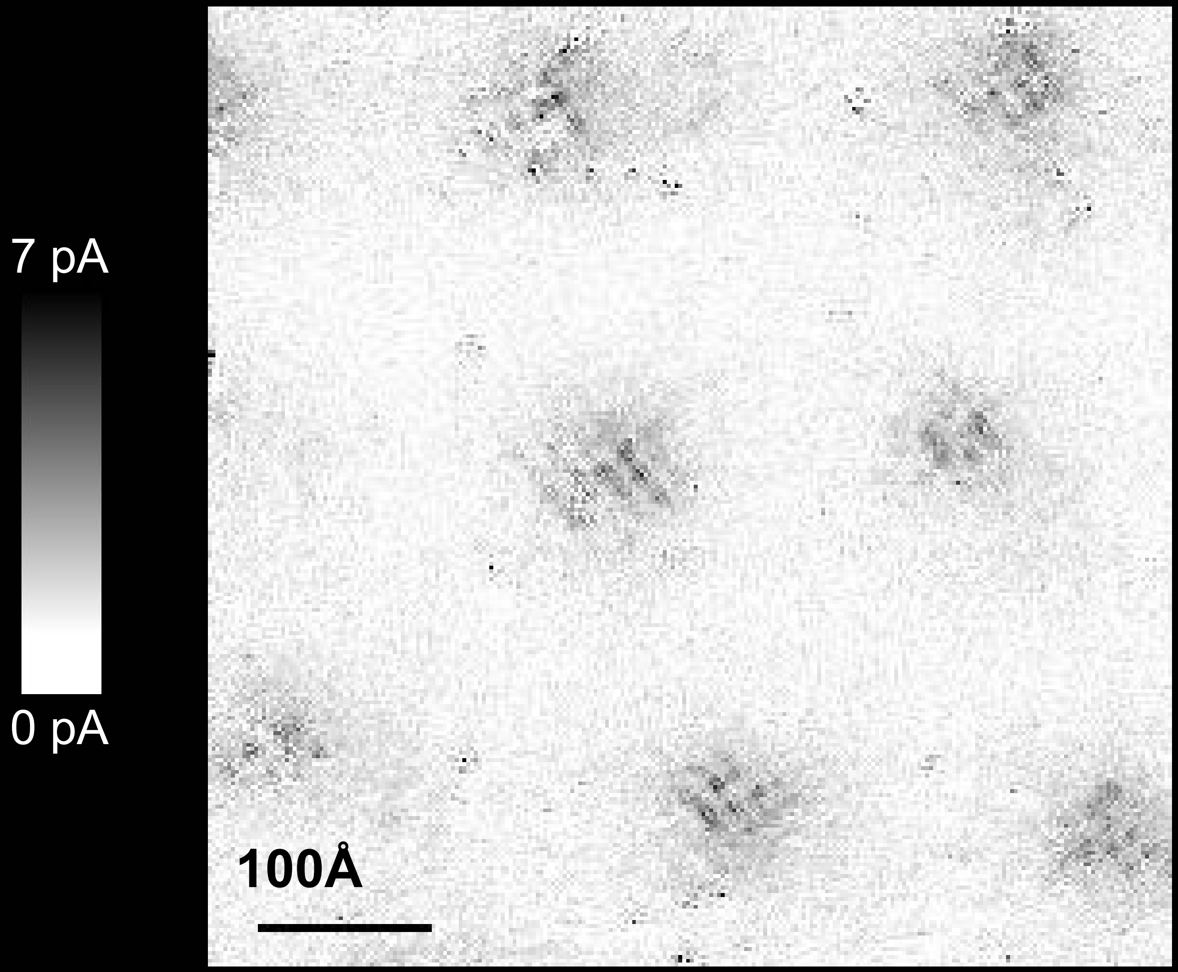


S.H. Pan *et al*. *Phys. Rev. Lett*. **85**, 1536 (2000).

1Å spatial resolution image of integrated LDOS of $Bi_2Sr_2CaCu_2O_{8+\delta}$

(1meV to 12 meV) at B=5 Tesla.

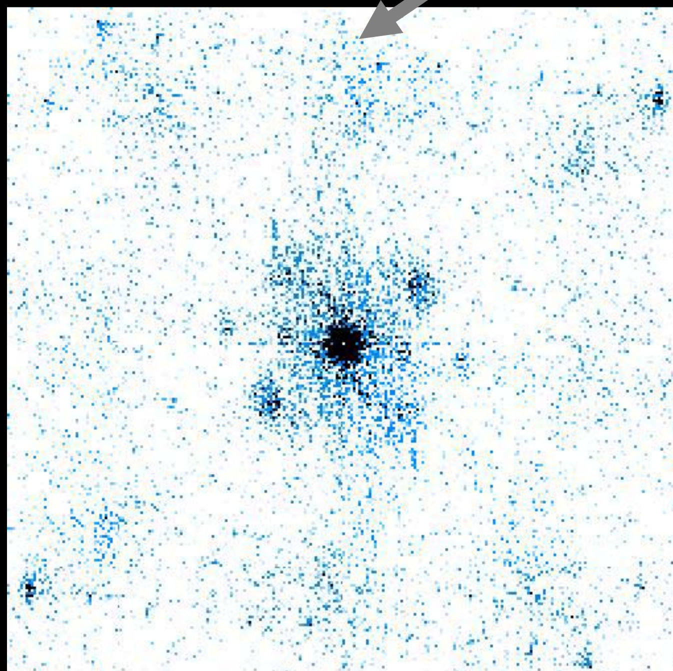
Vortex-induced LDOS of $Bi_2Sr_2CaCu_2O_{8+\delta}$ integrated from 1meV to 12meV

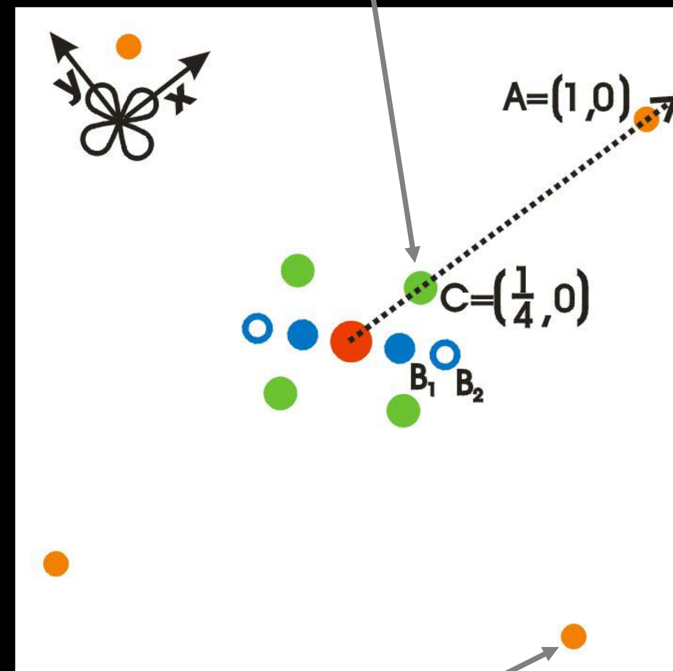


J. Hoffman E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan, H. Eisaki, S. Uchida, and J. C. Davis, *Science* 295, 466 (2002).

Fourier Transform of Vortex-Induced LDOS map

K-space locations of vortex induced LDOS





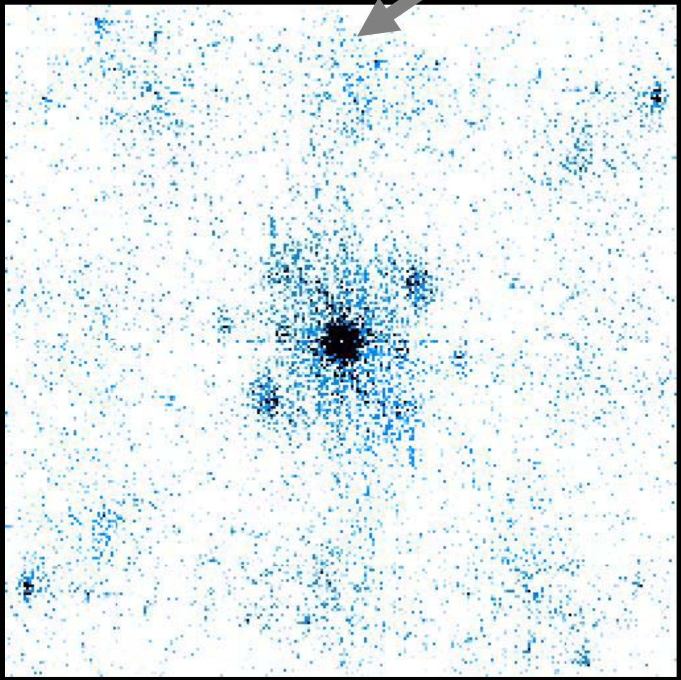
K-space locations of Bi and Cu atoms

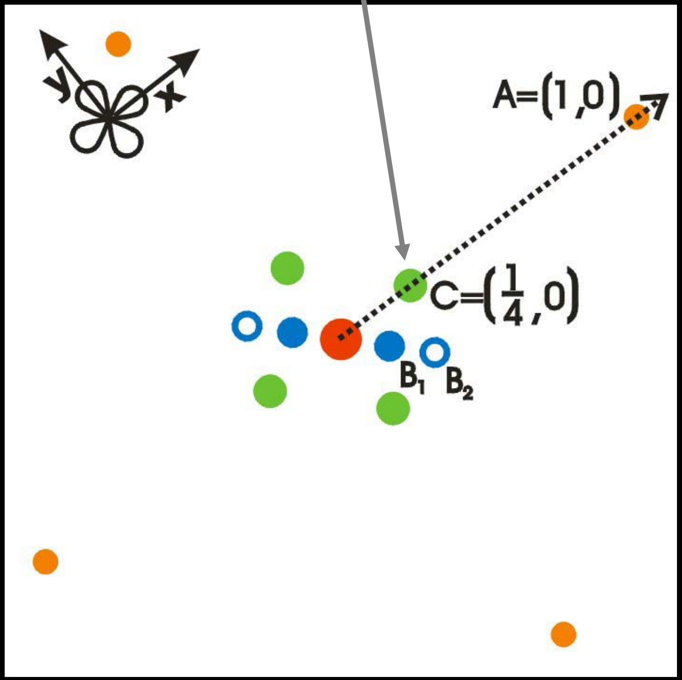
Distances in k –space have units of $2\pi/a_0$
a_0=3.83 Å is Cu-Cu distance

J. Hoffman *et al. Science*, **295**, 466 (2002).

Fourier Transform of Vortex-Induced LDOS map

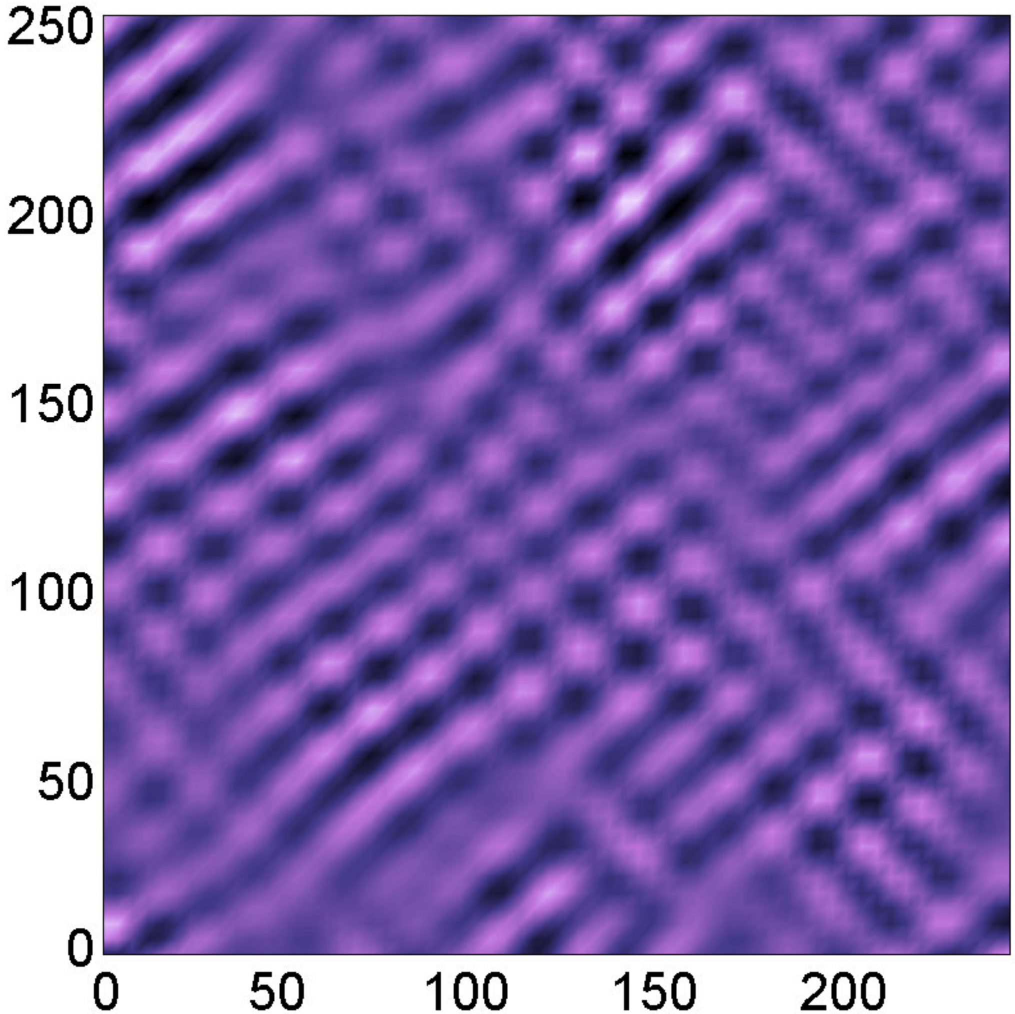
K-space locations of vortex induced LDOS

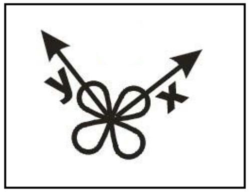




Our interpretation: LDOS modulations are signals of bond order of period 4 revealed in vortex halo

V. STM image of LDOS modulations in $Bi_2Sr_2CaCu_2O_{8+\delta}$ in zero magnetic field

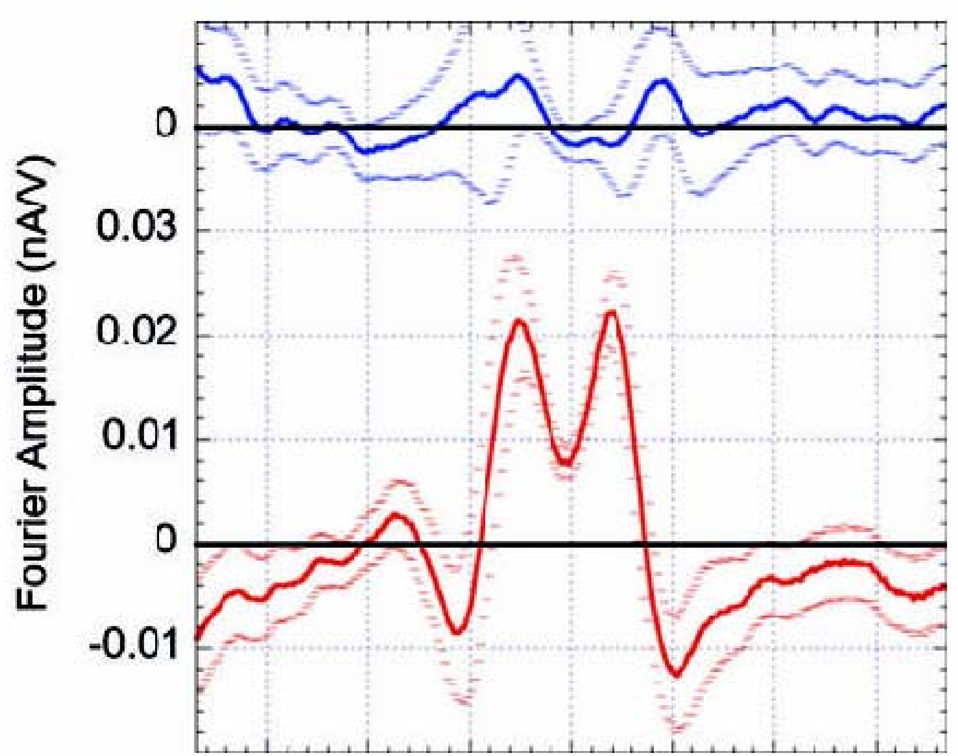




Period = 4 lattice spacings

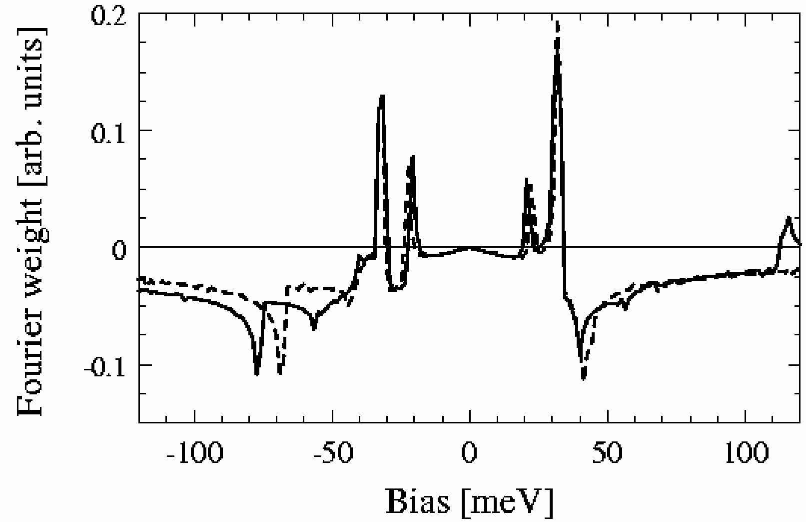
C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, cond-mat/0201546

Spectral properties of the STM signal are sensitive to the microstructure of the charge order



Measured energy dependence of the Fourier component of the density of states which modulates with a period of 4 lattice spacings

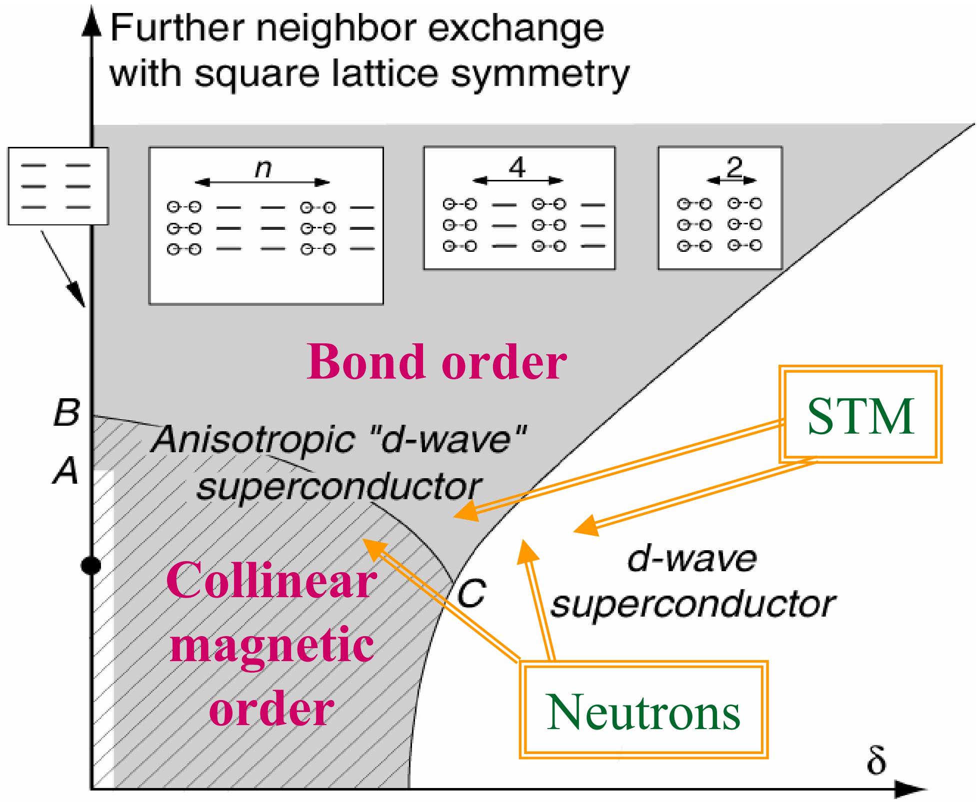
C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, cond-mat/0201546

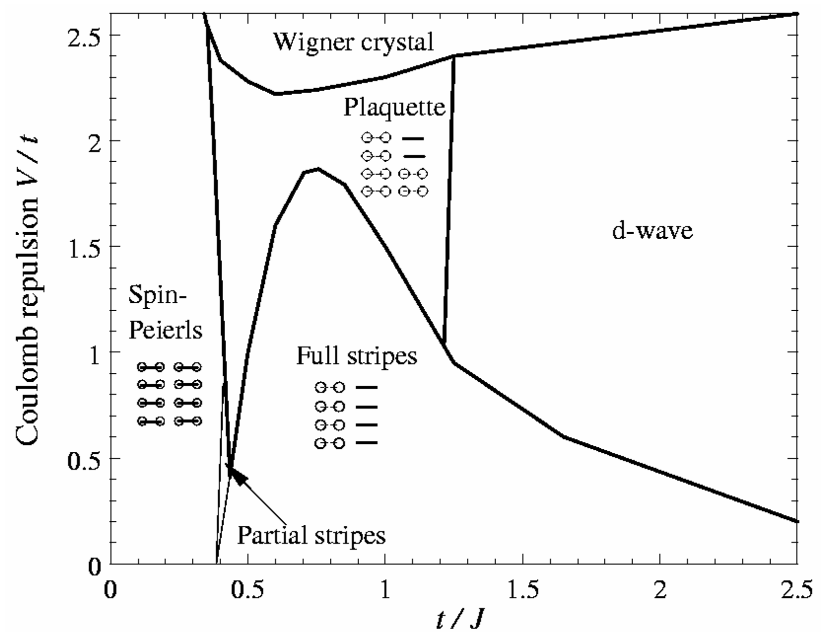


Theoretical modeling shows that this spectrum is best obtained by a modulation of bond variables, such as the exchange, kinetic or pairing energies.

M. Vojta, Phys. Rev. B **66**, 104505 (2002); D. Podolsky, E. Demler, K. Damle, and B.I. Halperin, cond-mat/0204011

Global phase diagram





M. Vojta and S. Sachdev, *Phys. Rev. Lett*. **83**, 3916 (1999)
M. Vojta, Y. Zhang, and S. Sachdev, *Phys. Rev*. B **62**, 6721 (2000).
M. Vojta, Phys. Rev. B **66**, 104505 (2002); .

See also J. Zaanen, *Physica* C **217**, 317 (1999),
V.J. Emery, S.A. Kivelson, and H.Q. Lin, *Phys. Rev. Lett*. **64**, 475 (1990).
S. White and D. Scalapino, *Phys. Rev. Lett*. **80**, 1272 (1998).
C. Castellani, C. Di Castro, and M. Grilli, *Phys.Rev. Lett*. **75**, 4650 (1995).
S. Mazumdar, R.T. Clay, and D.K. Campbell, Phys. Rev. B **62**, 13400 (2000).

Conclusions

I. Cuprate superconductivity is associated with doping Mott insulators with charge carriers.

II. Order parameters characterizing the Mott insulator compete with the order associated with the Bose-Einstein condensation of Cooper pairs.

III. Classification of Mott insulators shows that the appropriate order parameters are collinear magnetism and bond order.

IV. Theory of quantum phase transitions provides semi-quantitative predictions for neutron scattering measurements of spin-density-wave order in superconductors; theory also proposes a connection to STM experiments.

V. Future experiments should search for SC+SDW to SC quantum transition driven by a magnetic field.