

Spin correlations in Mott insulators and
d-wave superconductors:
implications of recent experiments

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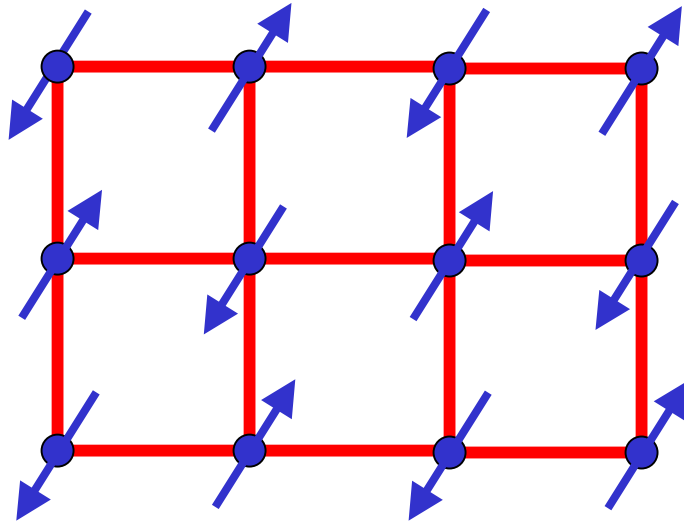
Science **286**, 2479 (1999).

Transparencies on-line at
<http://pantheon.yale.edu/~subir>



Parent compound of the high temperature superconductors: La_2CuO_4

Square lattice antiferromagnet

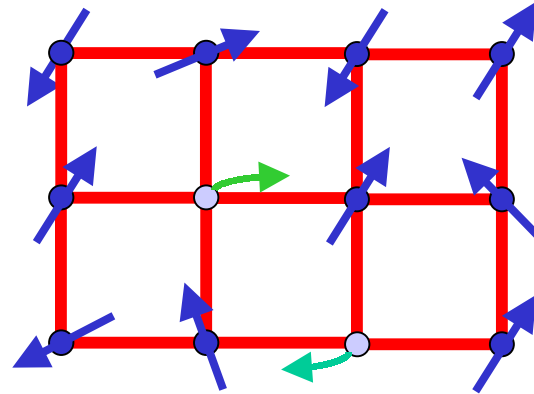


$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Ground state has long-range magnetic (Neel) order

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

Introduce mobile carriers of density δ
by substitutional doping of out-of-plane
ions e.g. $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$



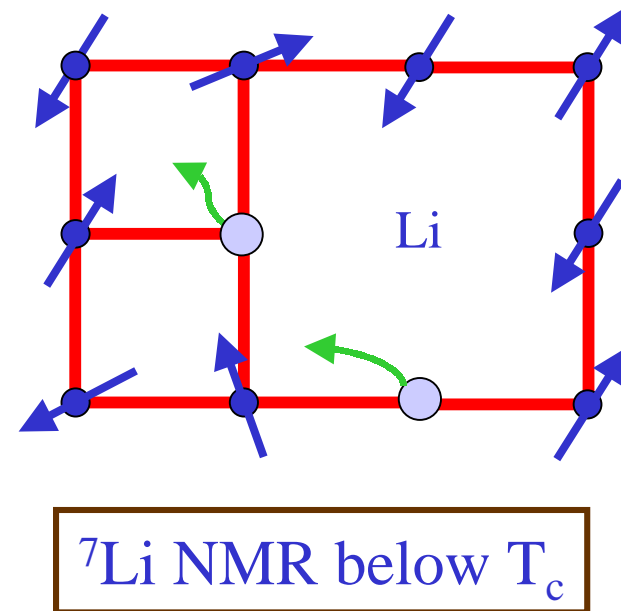
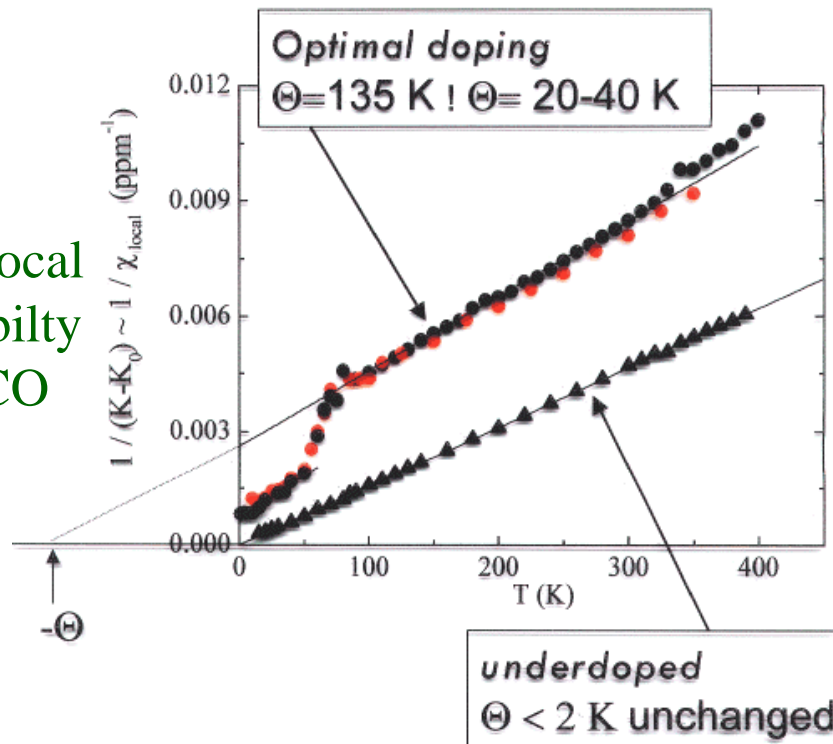
Exhibits superconductivity below a high critical temperature T_c

Almost all $T \rightarrow 0$ properties can be understood in the framework of a standard BCS theory in which the electrons form spin-singlet, d -wave Cooper pairs. However, many $T > T_c$ properties are anomalous.

$$\text{As } T \rightarrow 0, \quad \langle S_i \rangle = 0 \quad \text{and} \quad \chi_{\text{spin}} = 0$$

Measurement of spin susceptibility near non-magnetic (Zn/Li) impurities

Inverse local susceptibility in YBCO



J. Bobroff, H. Alloul, W.A. MacFarlane, P. Mendels, N. Blanchard, G. Collin, and J.-F. Marucco, cond-mat/0010234.

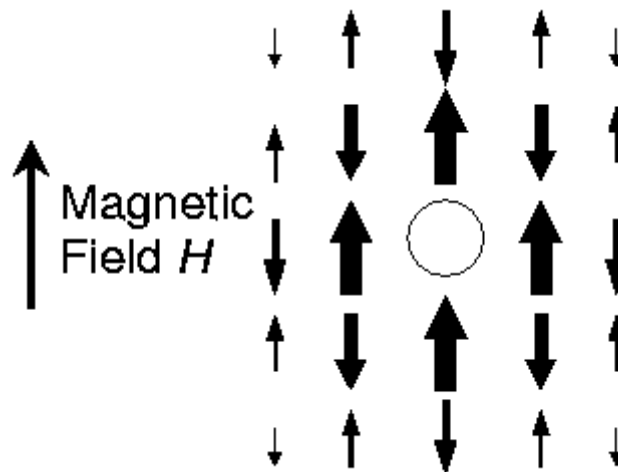
Measured $\chi_{\text{impurity}}(T \rightarrow 0) = \frac{S(S+1)}{3k_B T}$ with $S = 1/2$ in underdoped sample.

Not expected from BCS theory, which predicts $\chi_{\text{impurity}}(T \rightarrow 0) \neq \infty$ for a non-magnetic impurity with strong potential scattering.

Zn impurity in $\text{YBa}_2\text{Cu}_3\text{O}_{6.7}$

Moments measured by
analysis of Knight shifts

M.-H. Julien, T. Feher,
M. Horvatic, C. Berthier,
O. N. Bakharev, P. Segransan,
G. Collin, and J.-F. Marucco,
Phys. Rev. Lett. **84**, 3422
(2000); also earlier work of
the group of H. Alloul and the
original experiment of
A.M Finkelstein, V.E. Kataev,
E.F. Kukovitskii, and
G.B. Teitel'baum, *Physica C*
168, 370 (1990).



Berry phases of precessing spins do not cancel
between the sublattices in the vicinity of the
impurity: net uncanceled phase of $S=1/2$

S=1 resonance mode in YBCO

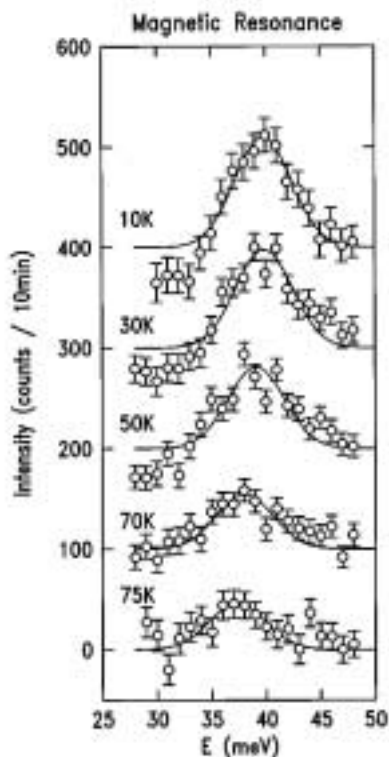
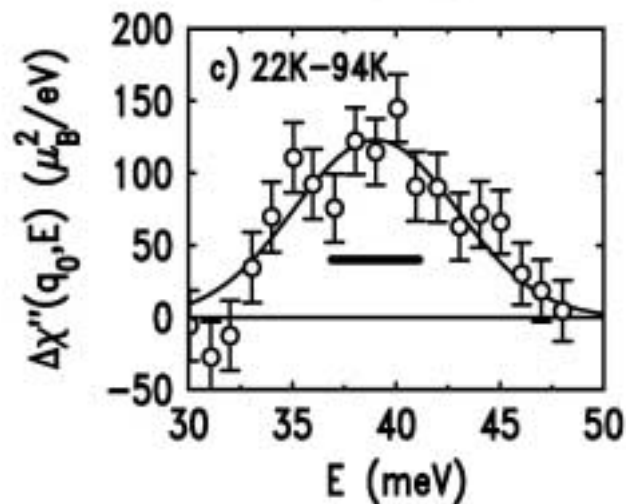


FIG. 8. Unpolarized beam, constant-Q data [$Q=(3/2, 1/2, -1.7)$] of the 40 meV magnetic resonance obtained by subtracting the signal below T_c from the $T=100$ K background. The lines are fits to Gaussians, as described in the text. For clarity successive scans are offset by 100.

Resolution limited width

H.F. Fong, B. Keimer, D. Reznik, D.L. Milius, and I.A. Aksay, Phys. Rev. B **54**, 6708 (1996)



Zn induced half-width = 4.25 meV

H. F. Fong, P. Bourges, Y. Sidis, L. P. Regnault, J. Bossy, A. Ivanov, D.L. Milius, I. A. Aksay, and B. Keimer, Phys. Rev. Lett. **82**, 1939 (1999)

Questions

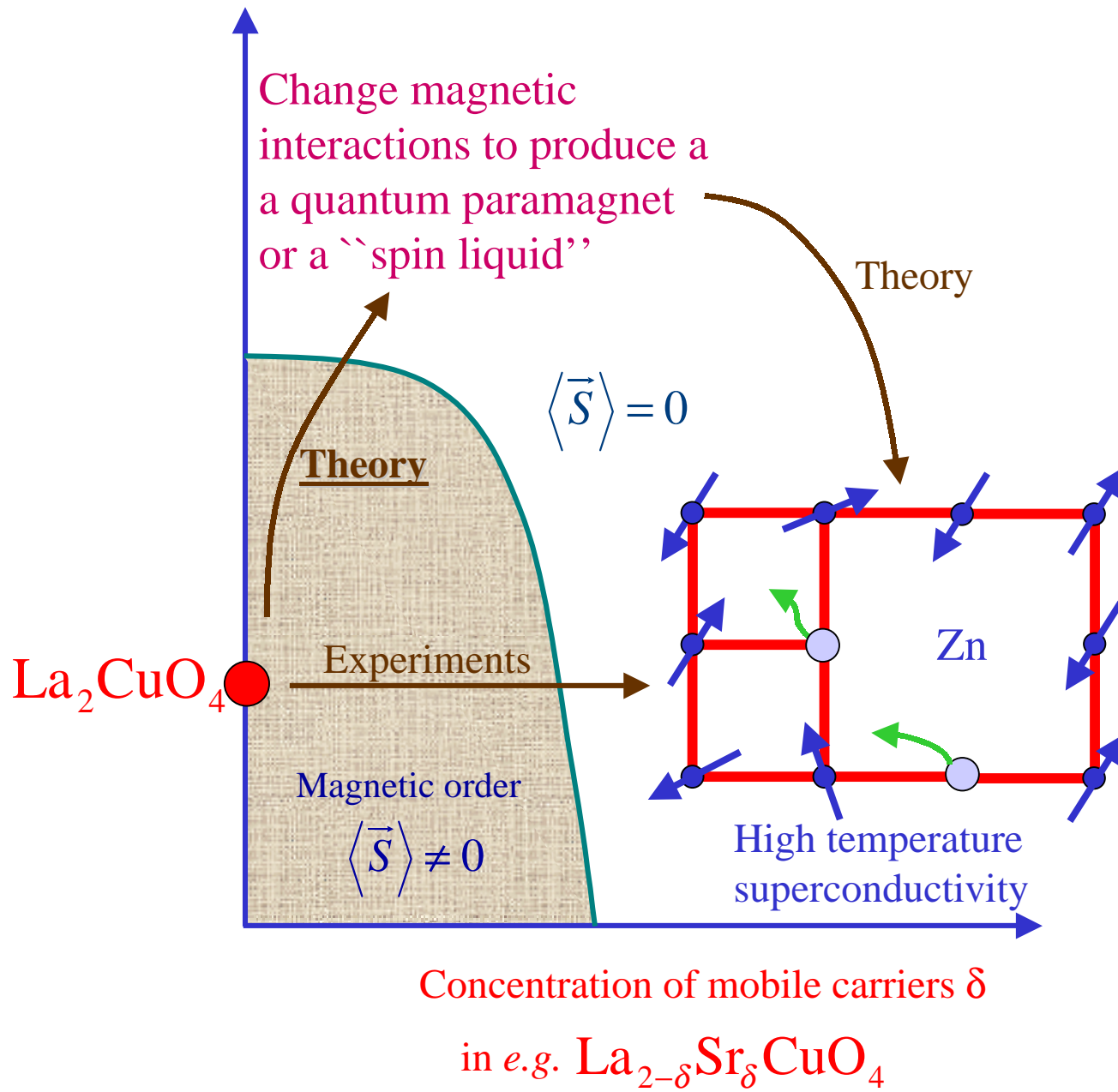
- I. Why do non-magnetic impurities acquire a $S=1/2$ moment ?
- II. What is the energy scale at which the collective spin resonance is broadened by Zn impurities ?

"Swiss cheese" model

$$\text{Inverse } Q \text{ of resonance} = C n_{\text{imp}} \xi^2$$

$C \rightarrow$ universal number

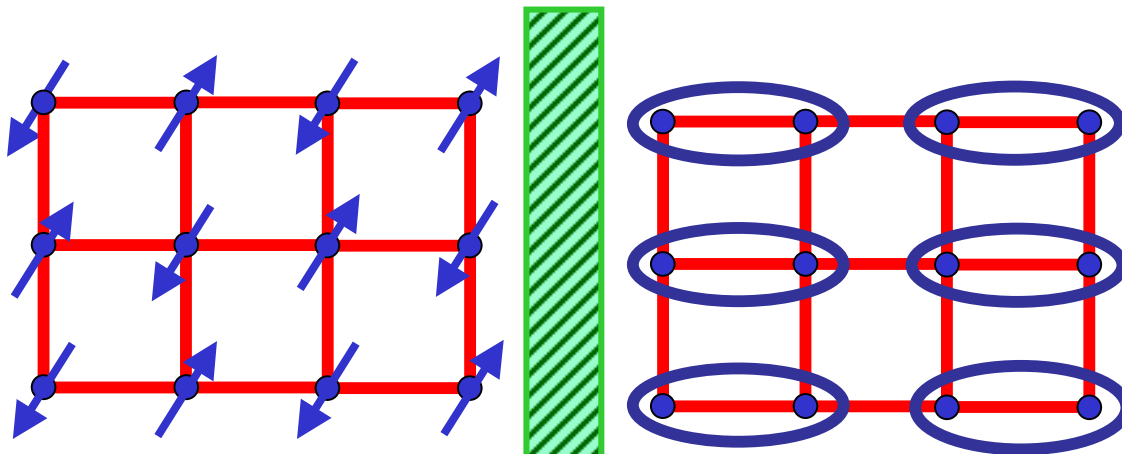
- III. Does the $S=1/2$ moment near a non-magnetic impurity have any implications for STM measurements of a single Zn impurity ?
- IV. Does our theoretical framework have any implications for order parameters which compete with the d-wave superconductivity ? Neutron scattering measurements of phonon spectra.



I. Why do non-magnetic impurities acquire a $S=1/2$ moment ?

I.A Insulating quantum paramagnets

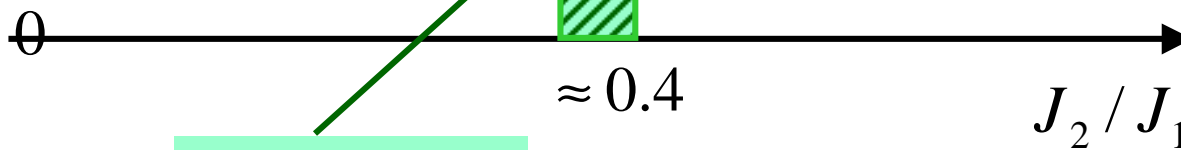
Square lattice with first (J_1) and second (J_2) neighbor exchange interactions



Neel state

Spin-Peierls state

“Bond-centered charge stripe”



Co-existence ?

$$\text{Singlet pair} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

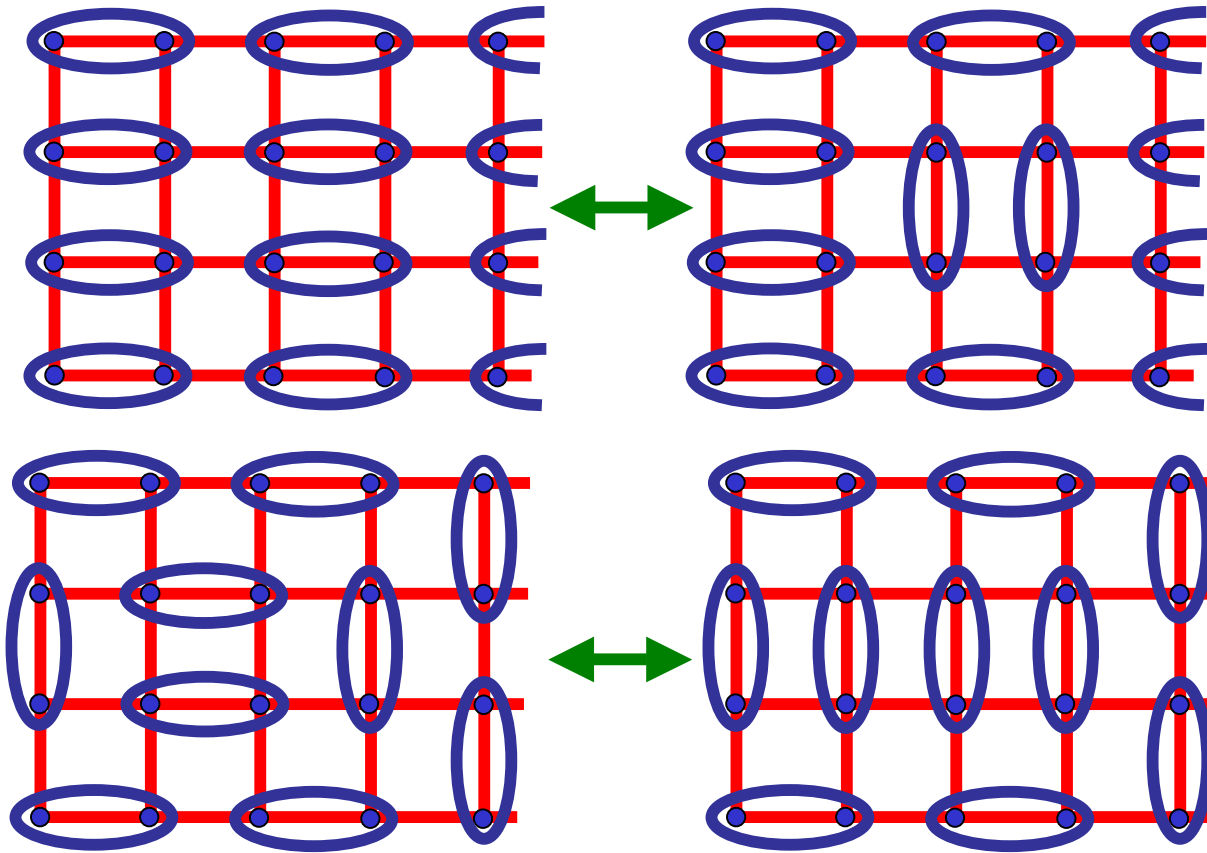
N. Read and S. Sachdev,
Phys. Rev. Lett. **62**, 1694
(1989).

O. P. Sushkov, J. Oitmaa,
and Z. Weihong,
condmat/0007329.

M.S.L. du Croo de Jongh,
J.M.J. van Leeuwen, W.
van Saarloos, cond-
mat/0002116.

Quantum dimer model –

D. Rokhsar and S. Kivelson Phys. Rev. Lett. **61**, 2376 (1988)



Quantum “entropic” effects prefer one-dimensional striped structures 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 always lead to a broken square lattice symmetry near the transition to the Neel state.

N. Read and S. Sachdev Phys. Rev. B **42**, 4568 (1990).

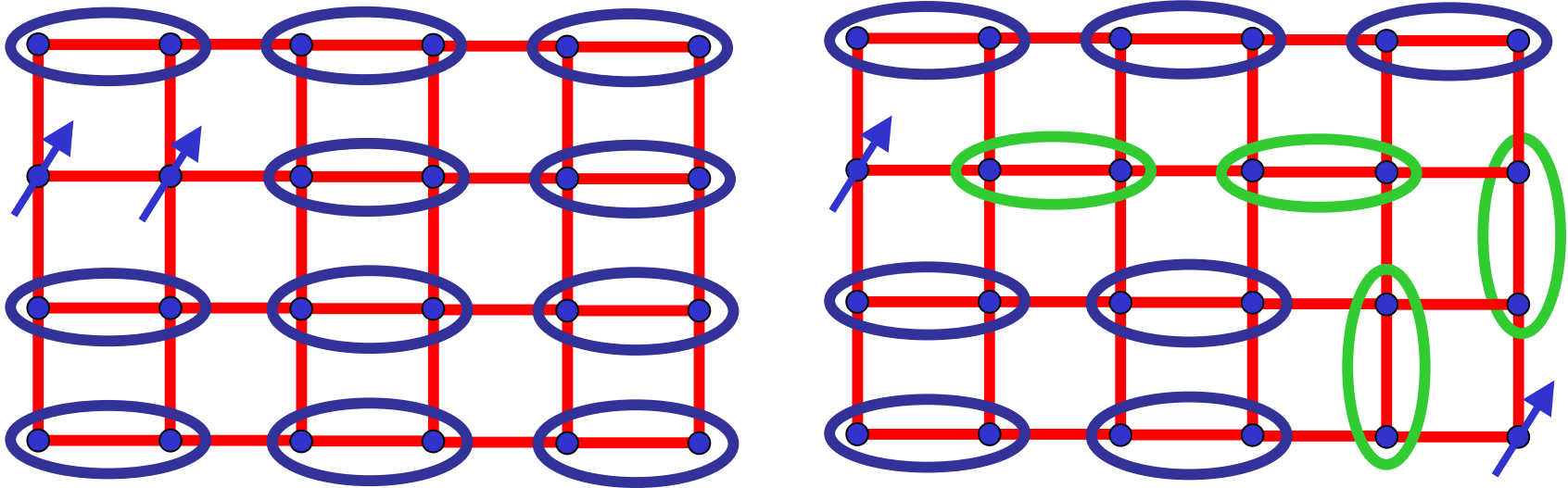
Excitations

Stable $S=1$ particle

Energy dispersion

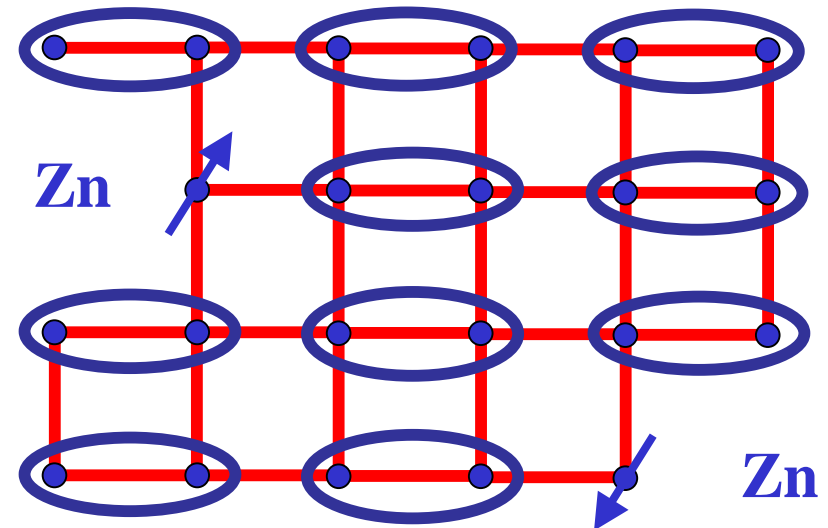
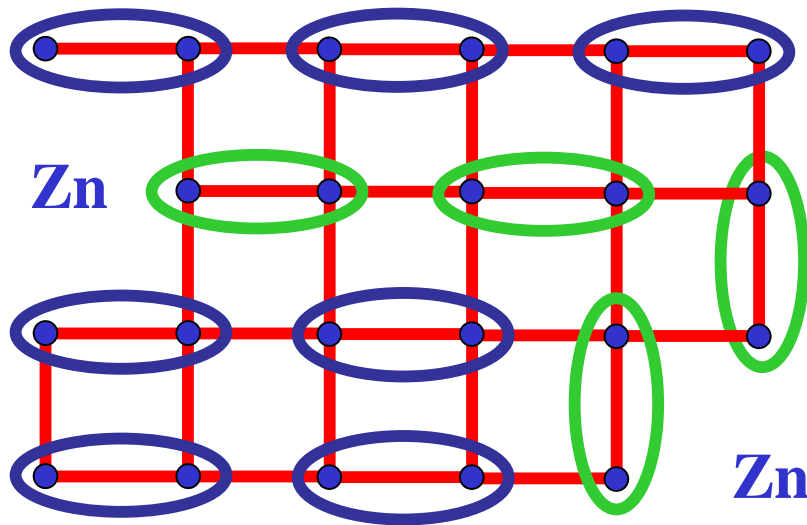
$$\varepsilon_k = \Delta + \frac{c_x^2 k_x^2 + c_y^2 k_y^2}{2\Delta}$$

$\Delta \rightarrow$ Spin gap



$S=1/2$ spinons are linearly confined by the line of “defect” singlet pairs between them

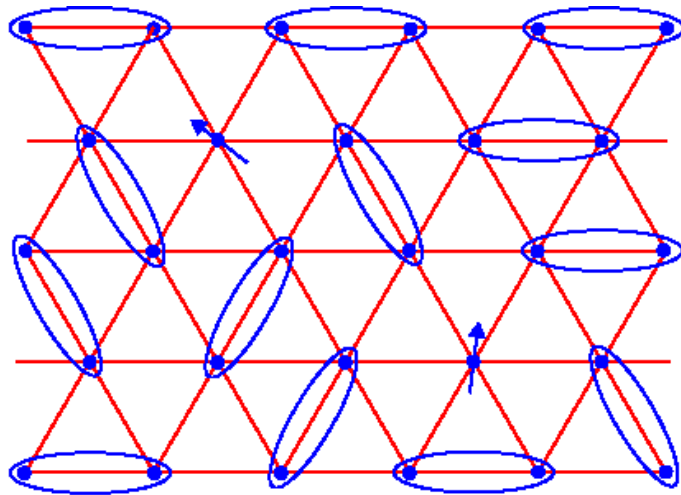
Effect of static non-magnetic impurities (Zn or Li)



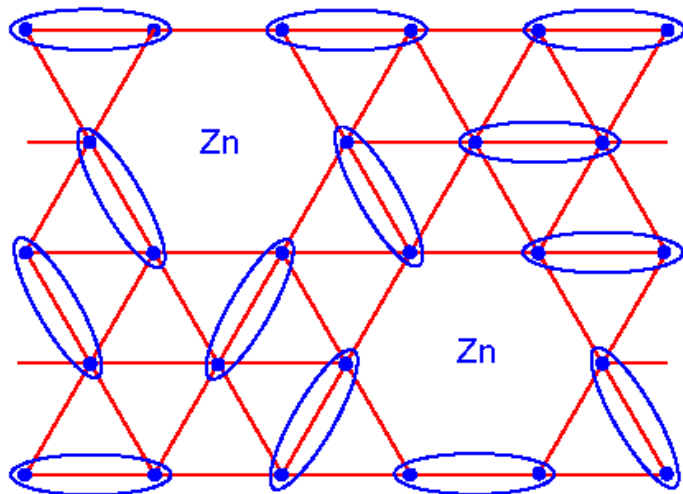
Spinon confinement implies that free $S=1/2$ moments **must** form near each impurity

$$\chi_{\text{impurity}}(T \rightarrow 0) = \frac{S(S+1)}{3k_B T}$$

Paramagnetic ground state with spinon deconfinement



Spinons are deconfined



Free S=1/2 moments need not be present near the impurities

Translationally invariant “spin liquid” state obtained by a quantum transition from a magnetically ordered state with co-planar spin polarization. Can also appear in frustrated square lattice antiferromagnets – transition to confined states is described by a Z_2 gauge theory

$$\chi_{\text{impurity}}(T \rightarrow 0) = 0$$

N. Read and S. Sachdev, Phys. Rev. Lett. **66**, 1773 (1991).

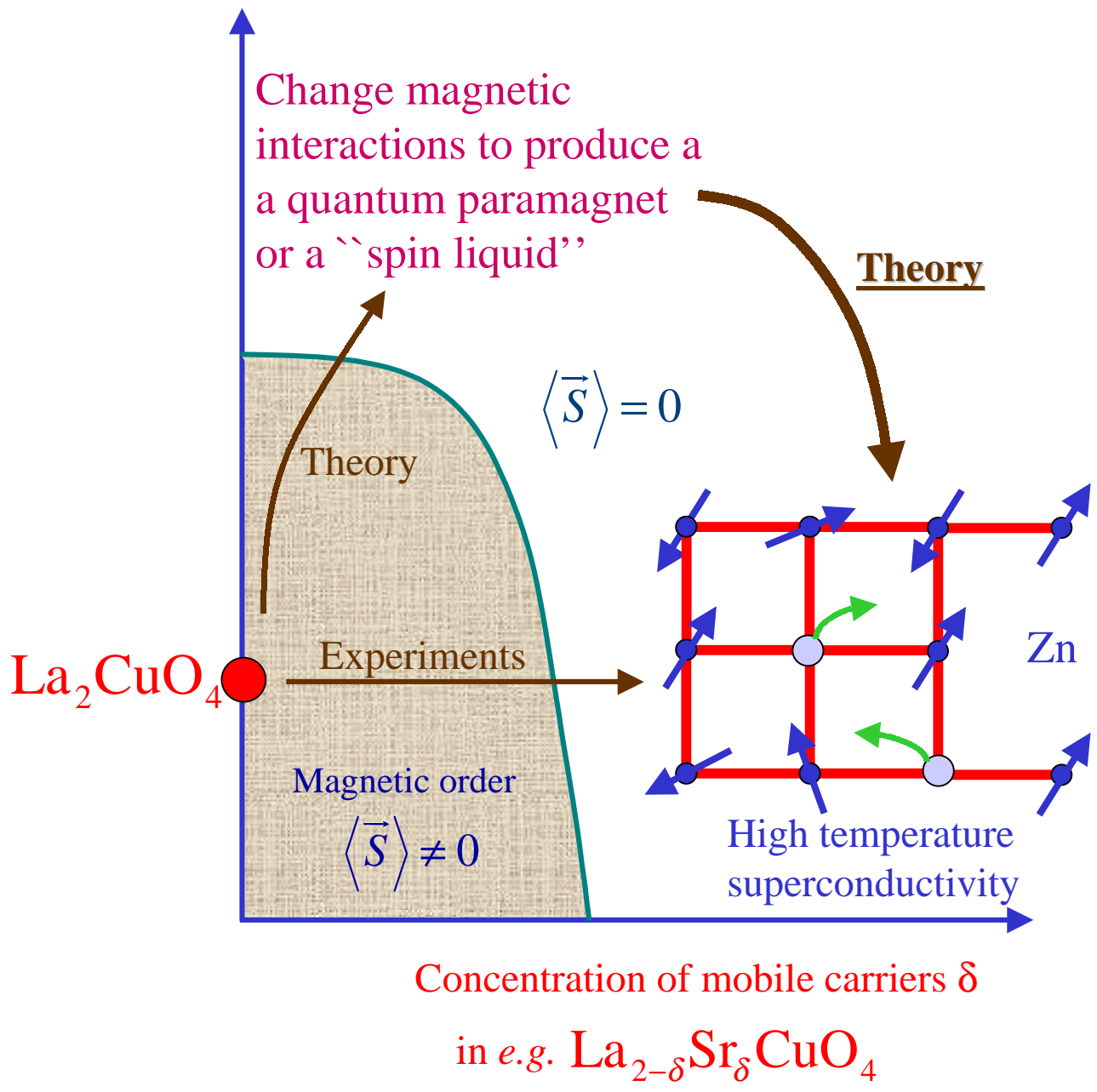
R. Jalabert and S. Sachdev, Phys. Rev. B **44**, 686 (1991).

P. Fazekas and P.W. Anderson, Phil Mag **30**, 23 (1974).

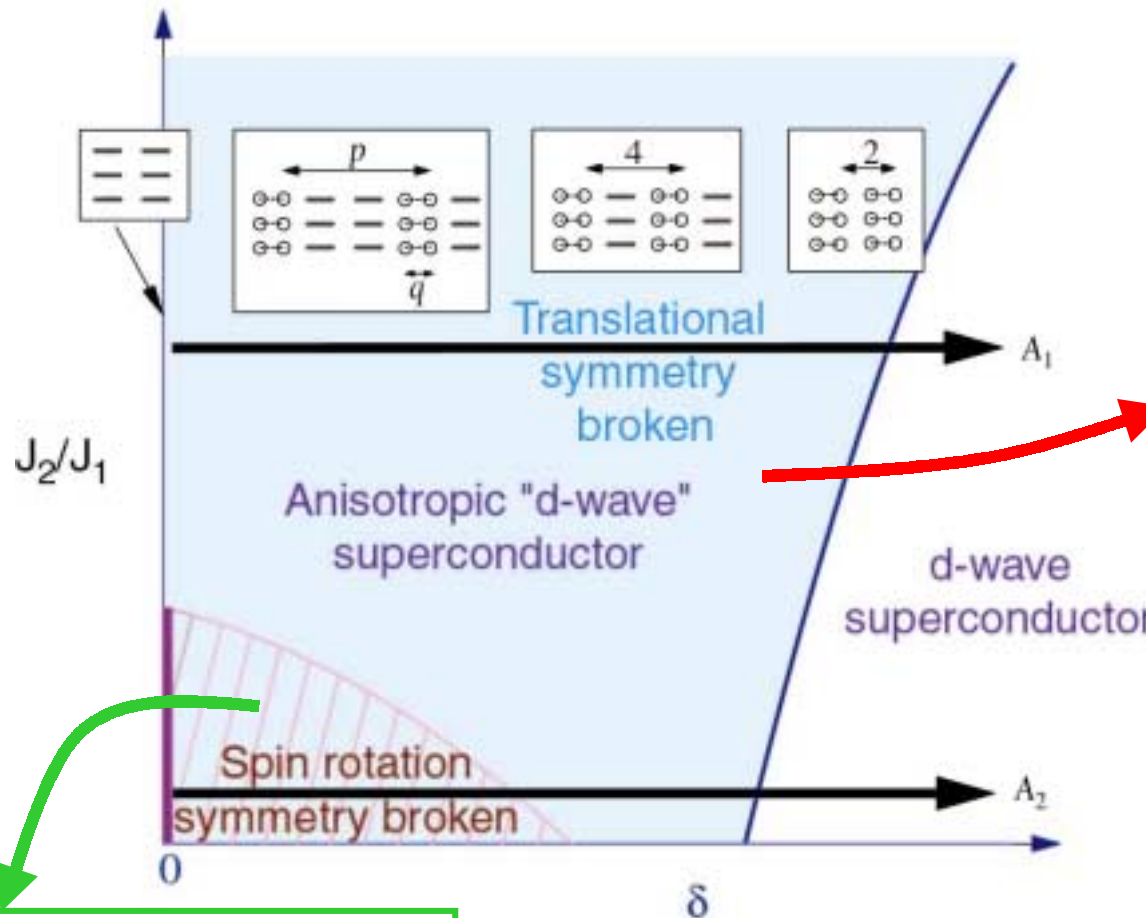
S. Sachdev, Phys. Rev. B **45**, 12377 (1992).

G. Misguich and C. Lhuillier, cond-mat/0002170.

R. Moessner and S.L. Sondhi, cond-mat/0007378.



I.B Phase diagram for doping of confined Mott insulators



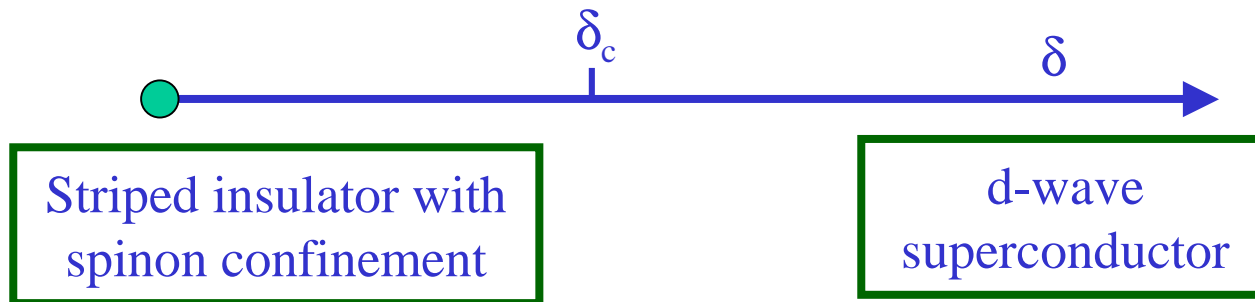
Superconductivity can coexist with bond-centered charge stripe order in region without magnetic order

Site-centered charge stripes likely in regions with magnetic order and suppressed superconductivity

- S. Sachdev and N. Read, Int. J. Mod. Phys. B **5**, 219 (1991).
 M. Vojta and S. Sachdev, Phys. Rev. Lett. **83**, 3916 (1999).
 M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. B **62**, 6721 (2000)
 See also J. Zaanen, Physica C **217**, 317 (1999),
 S. Kivelson, E. Fradkin and V. Emery, Nature **393**, 550 (1998),
 S. White and D. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998); **81**, 3227 (1998).
 C. Lannert, M.P.A. Fisher, and T. Senthil cond-mat/0007002.

Zn or Li impurities in doped Mott insulators

Case A



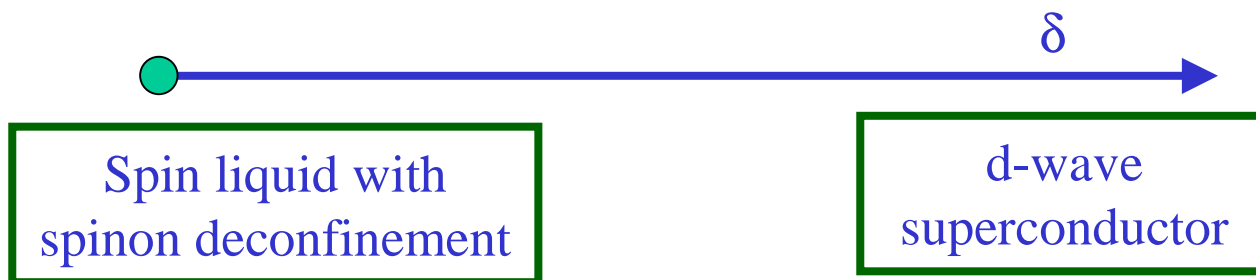
Moments form near each Zn or Li.

This moment is quenched at a quantum phase transition at $\delta = \delta_c$.

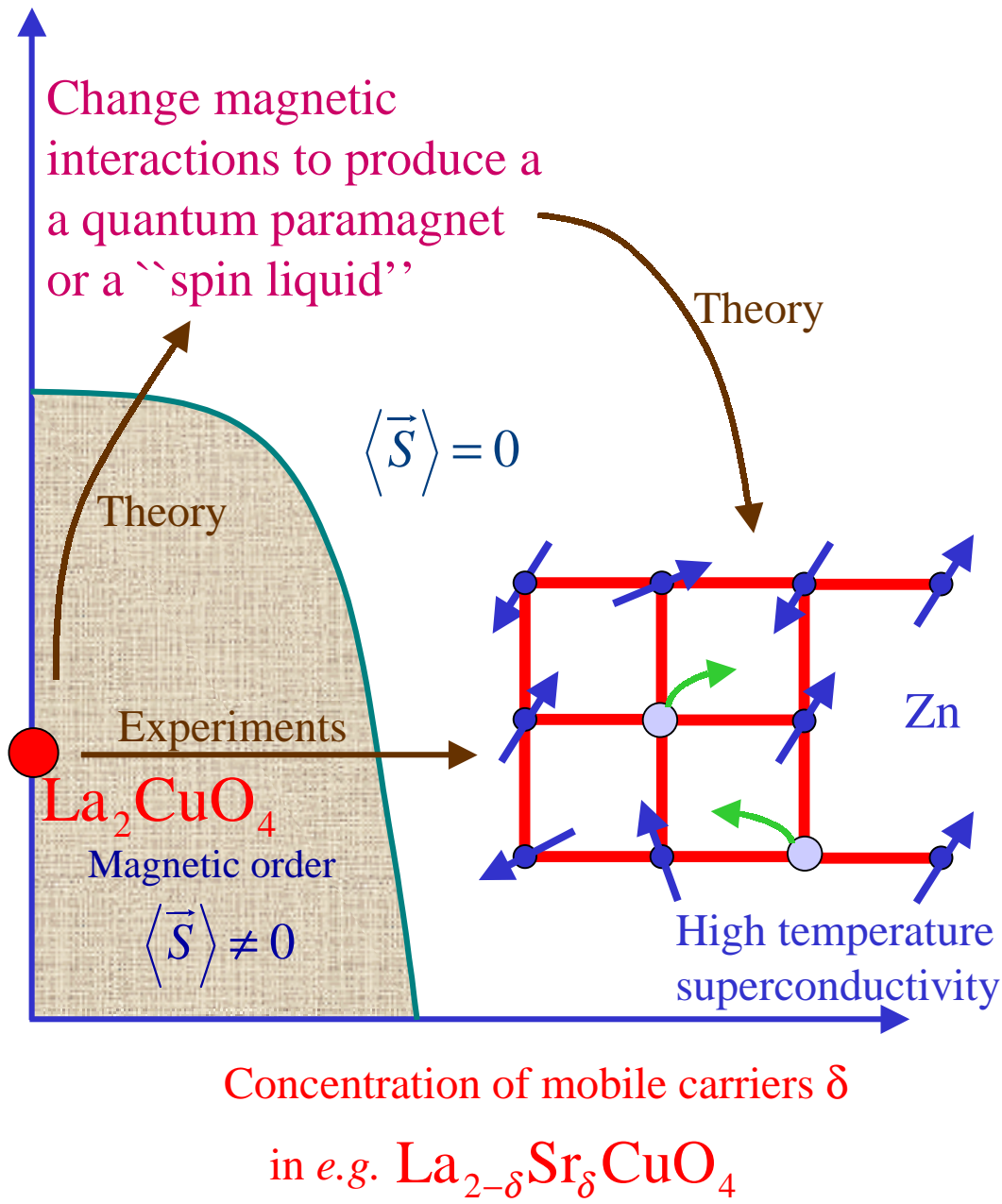
D. Withoff and E. Fradkin, Phys. Rev. Lett. **64**, 1835 (1990).

C. Gonzalez-Buxton and K. Ingersent, Phys. Rev. B **57**, 14254 (1998).

Case B



No moments form near Zn or Li ions substituted for Cu and impurity response evolves smoothly



Summary:

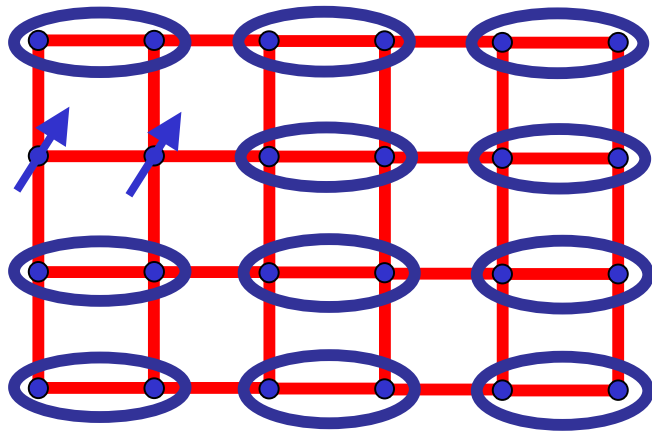
Confined, paramagnetic Mott insulator necessarily has

1. Stable $S=1$ spin collective mode.
2. Broken translational symmetry:- bond-centered charge stripe order.
3. $S=1/2$ moments near non-magnetic impurities.

These properties are expected to survive for a finite range of δ in the superconducting states

II. Effect of Zn impurities on spin resonance mode

$S=1$ resonance mode in YBCO



H.F. Fong, B. Keimer, D. Reznik,
D.L. Milius, and I.A. Aksay,
Phys. Rev. B **54**, 6708 (1996)

Spin-1 collective mode in $\text{YBa}_2\text{Cu}_3\text{O}_7$ - little
observable damping at low T.

Coupling to superconducting quasiparticles
unimportant

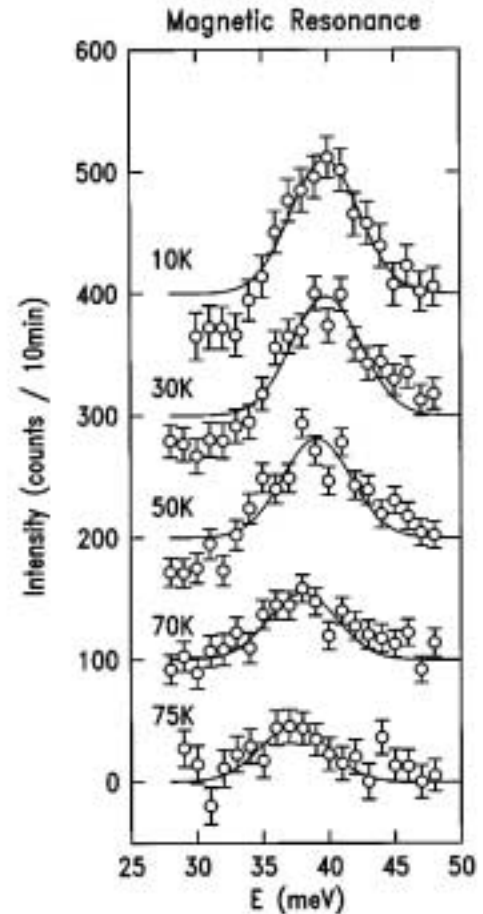


FIG. 8. Unpolarized beam, constant-Q data [$Q=(3/2, 1/2, -1.7)$] of the 40 meV magnetic resonance obtained by subtracting the signal below T_c from the $T=100$ K background. The lines are fits to Gaussians, as described in the text. For clarity successive scans are offset by 100.

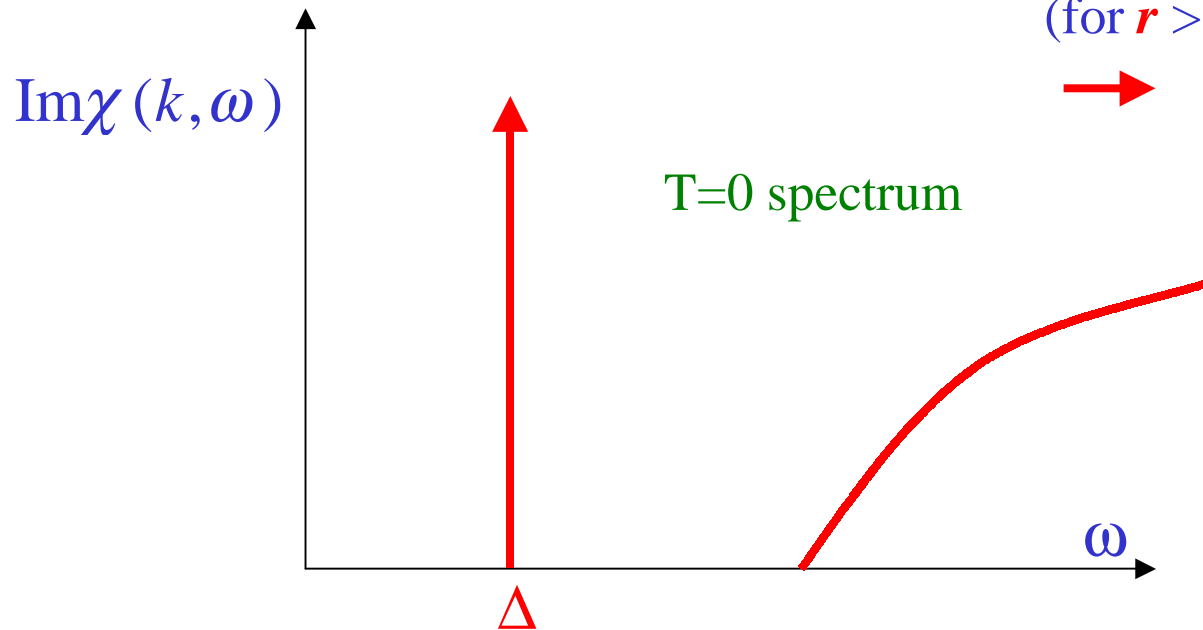
Quantum field theory for $S=1$ particle near magnetic ordering transition

$$S_b = \int d^2x d\tau \left[\frac{1}{2} \left((\nabla_x \phi_\alpha)^2 + c^2 (\partial_\tau \phi_\alpha)^2 + r \phi_\alpha^2 \right) + \frac{g}{4!} (\phi_\alpha^2)^2 \right]$$

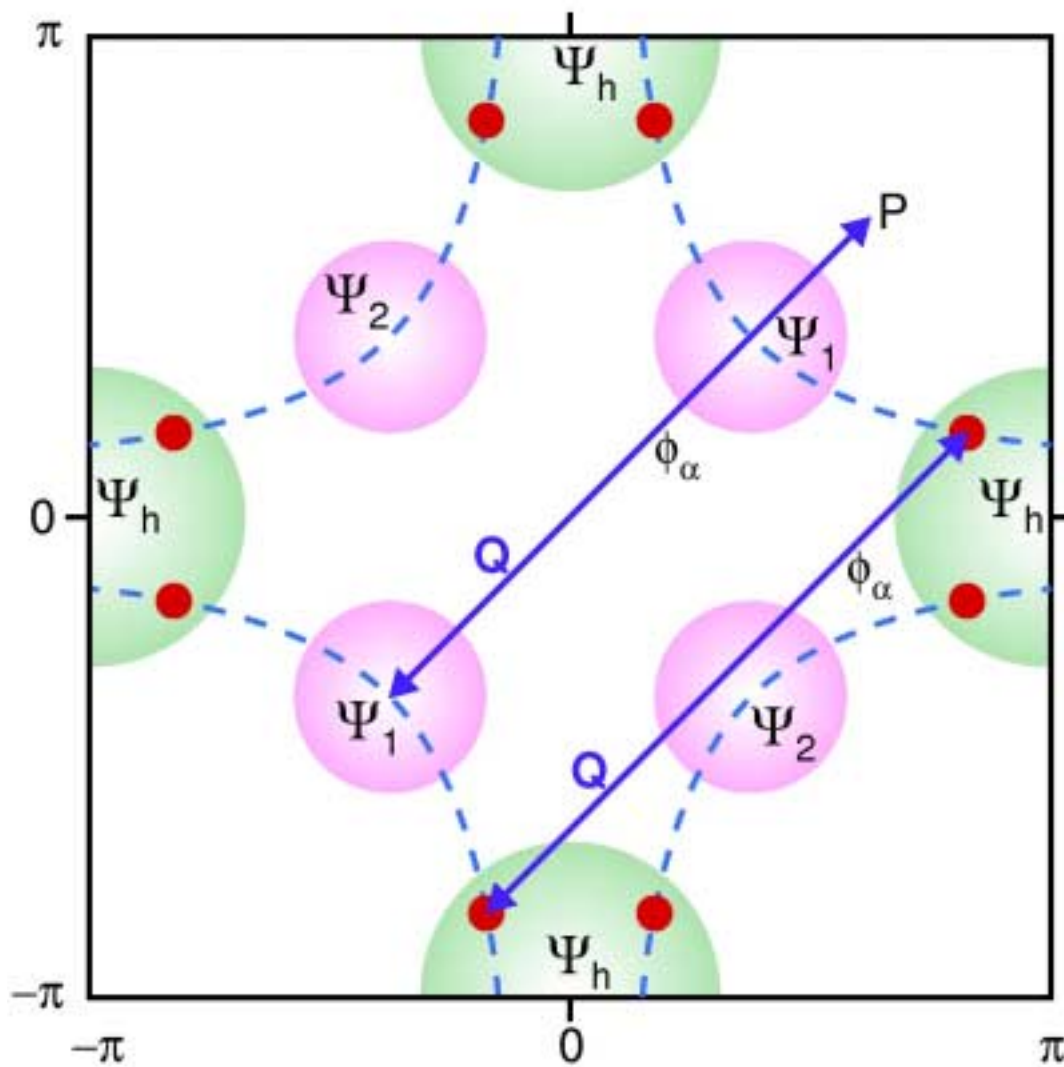
$\phi_\alpha \rightarrow$ 3-component antiferromagnetic order parameter

Oscillations of ϕ_α about zero (for $r > 0$)

\rightarrow spin-1 collective mode



Constraints from momentum conservation

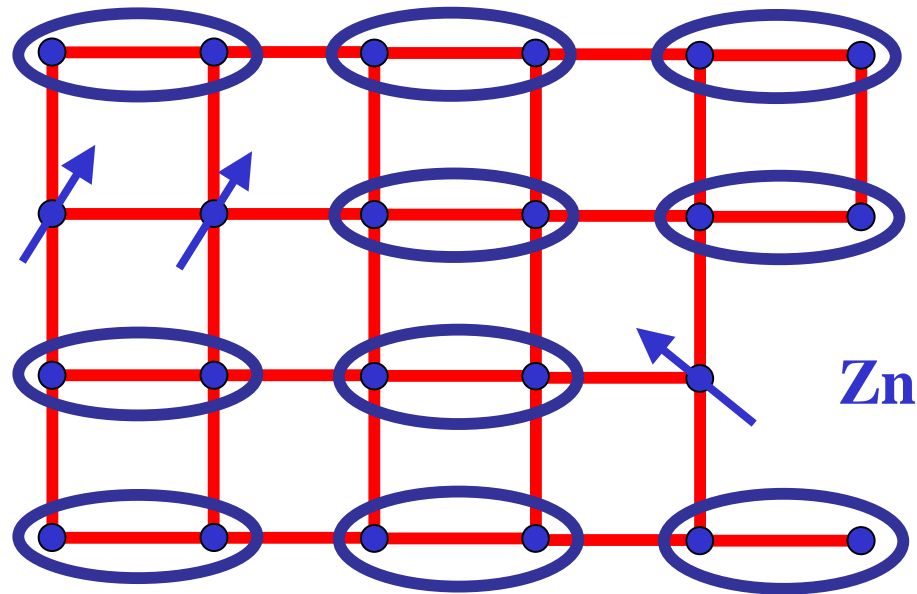
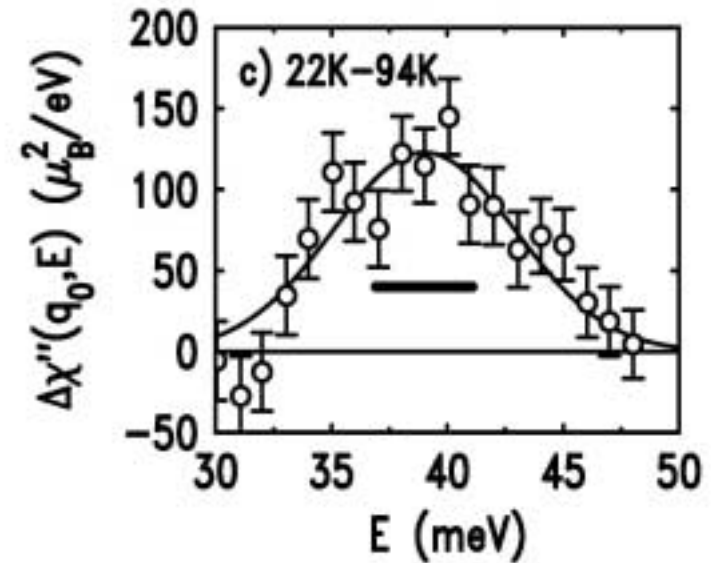


Ψ_h : strongly coupled to ϕ_α , but do not damp ϕ_α as long as $\Delta < 2 \Delta_h$

$\Psi_{1,2}$: decoupled from ϕ_α

YBa₂Cu₃O₇ + 0.5% Zn

H. F. Fong, P. Bourges,
Y. Sidis, L. P. Regnault,
J. Bossy, A. Ivanov,
D.L. Milius, I. A. Aksay,
and B. Keimer,
Phys. Rev. Lett. **82**, 1939
(1999)



Quantum field theory for $S=I$ resonance in
the presence of a non-magnetic impurity

Orientation of “impurity” spin -- $n_\alpha(\tau)$ (unit vector)

Action of “impurity” spin

$$S_{\text{imp}} = \int d\tau \left[iSA_\alpha(n) \frac{dn_\alpha}{d\tau} - \gamma S n_\alpha(\tau) \phi_\alpha(x=0, \tau) \right]$$

$A_\alpha(n) \rightarrow$ Dirac monopole function

Boundary quantum field theory: $S_b + S_{\text{imp}}$

Recall -

$$S_b = \int d^2x d\tau \left[\frac{1}{2} \left((\nabla_x \phi_\alpha)^2 + c^2 (\partial_\tau \phi_\alpha)^2 + r \phi_\alpha^2 \right) + \frac{g}{4!} (\phi_\alpha^2)^2 \right]$$

Renormalization group analysis:
 g and γ reach non-zero fixed point values

β functions:

$$\beta(g) = -\varepsilon g + \frac{11g^2}{6} - \frac{23g^3}{12} + O(g^4)$$

$$\beta(\gamma) = -\frac{\varepsilon\gamma}{2} + \gamma^3 - \gamma^5 + \frac{5g^2\gamma}{144} + \pi^2 \left(S(S+1) - \frac{1}{3} \right) g\gamma^3 + O\left((\gamma, \sqrt{g})^7 \right)$$

No new relevant perturbations near the impurity;
All other boundary perturbations are irrelevant –

e.g. $\lambda \int d\tau \phi_\alpha^2(x=0, \tau)$

Δ and c completely determine spin
dynamics near an impurity –

No new parameters are necessary !

S. Sachdev and J. Ye, Phys. Rev. Lett. **70**,
3339 (1993);

S. Sachdev, C. Buragohain, and M. Vojta,
Science, **286**, 2479 (1999).

J.L. Smith and Q. Si, Europhys. Lett. **45**,
228 (1999).

A.M. Sengupta, Phys. Rev. B **61**, 4041
(2000);

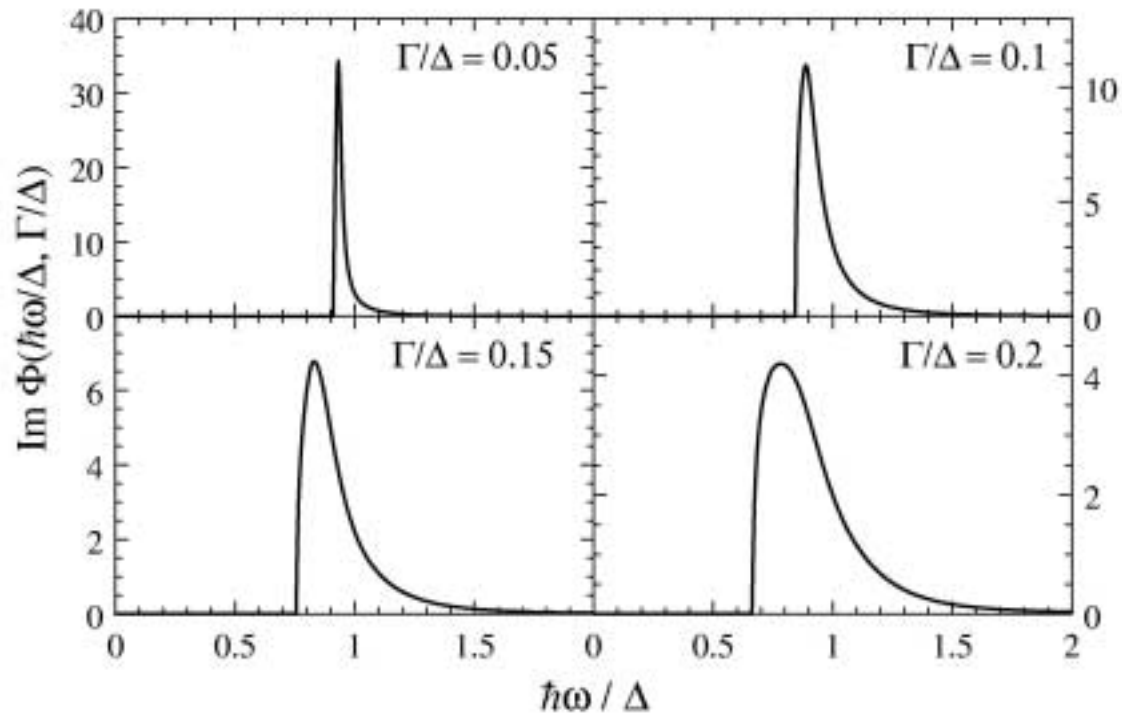
Predictions of quantum field theory

Without impurities $\chi(G, \omega) = \frac{A}{\Delta^2 - \omega^2}$

With impurities $\chi(G, \omega) = \frac{A}{\Delta^2} \Phi\left(\frac{\hbar\omega}{\Delta}, \frac{\Gamma}{\Delta}\right)$

$$\Gamma \equiv \frac{n_{\text{imp}} (\hbar c)^2}{\Delta}$$

$\Phi \rightarrow$ *Universal scaling function. We computed it in a “self-consistent, non-crossing” approximation*



Predictions:

Half-width of line $\approx \Gamma$

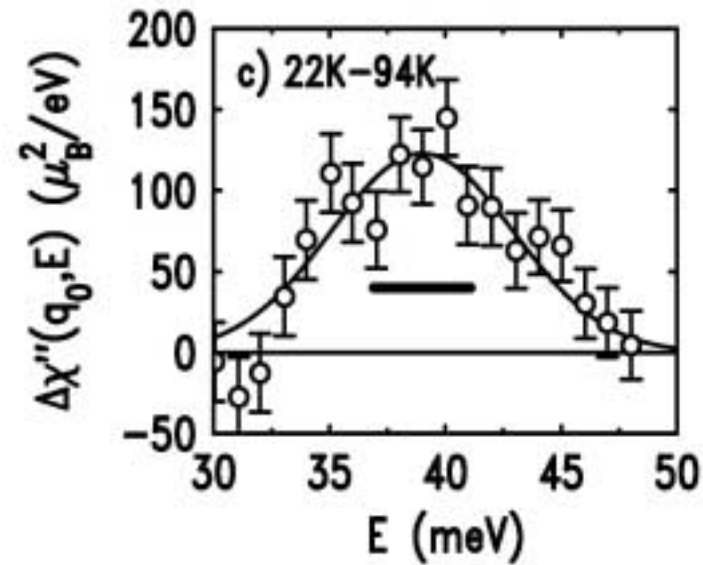
Universal asymmetric lineshape

S. Sachdev, C. Buragohain, M. Vojta, *Science* **286**, 2479 (1999).

M. Vojta, C. Buragohain, and S. Sachdev, *Phys. Rev. B* **61**, 15152 (2000).

YBa₂Cu₃O₇ + 0.5% Zn

H. F. Fong, P. Bourges,
Y. Sidis, L. P. Regnault,
J. Bossy, A. Ivanov,
D.L. Milius, I. A. Aksay,
and B. Keimer,
Phys. Rev. Lett. **82**, 1939
(1999)



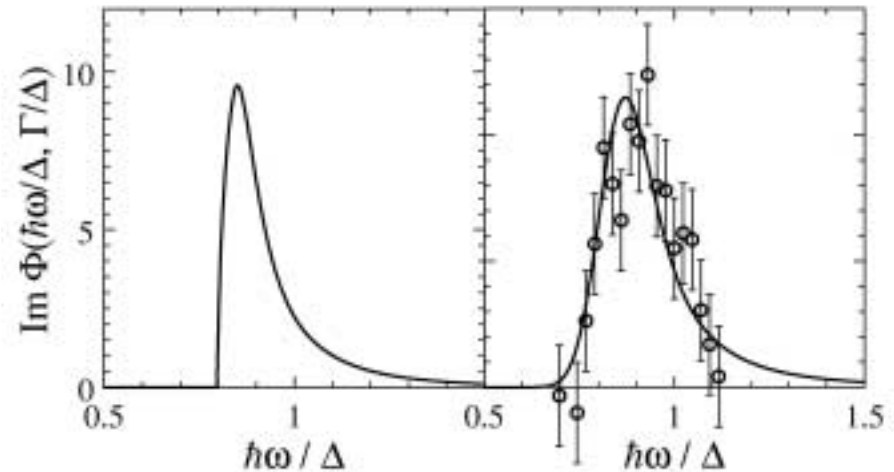
$$n_{\text{imp}} = 0.005$$

$$\Delta = 40 \text{ meV}$$

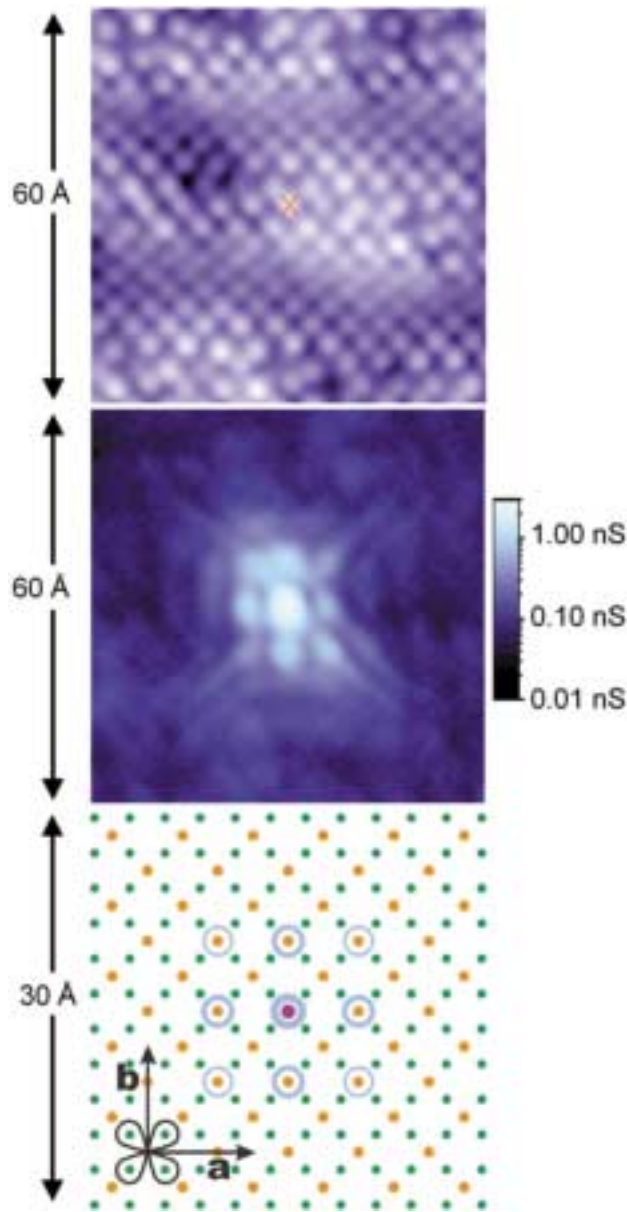
$$\hbar c = 0.2 \text{ eV}$$

$$\Rightarrow \Gamma = 5 \text{ meV}, \Gamma/\Delta = 0.125$$

Quoted half-width = 4.25 meV

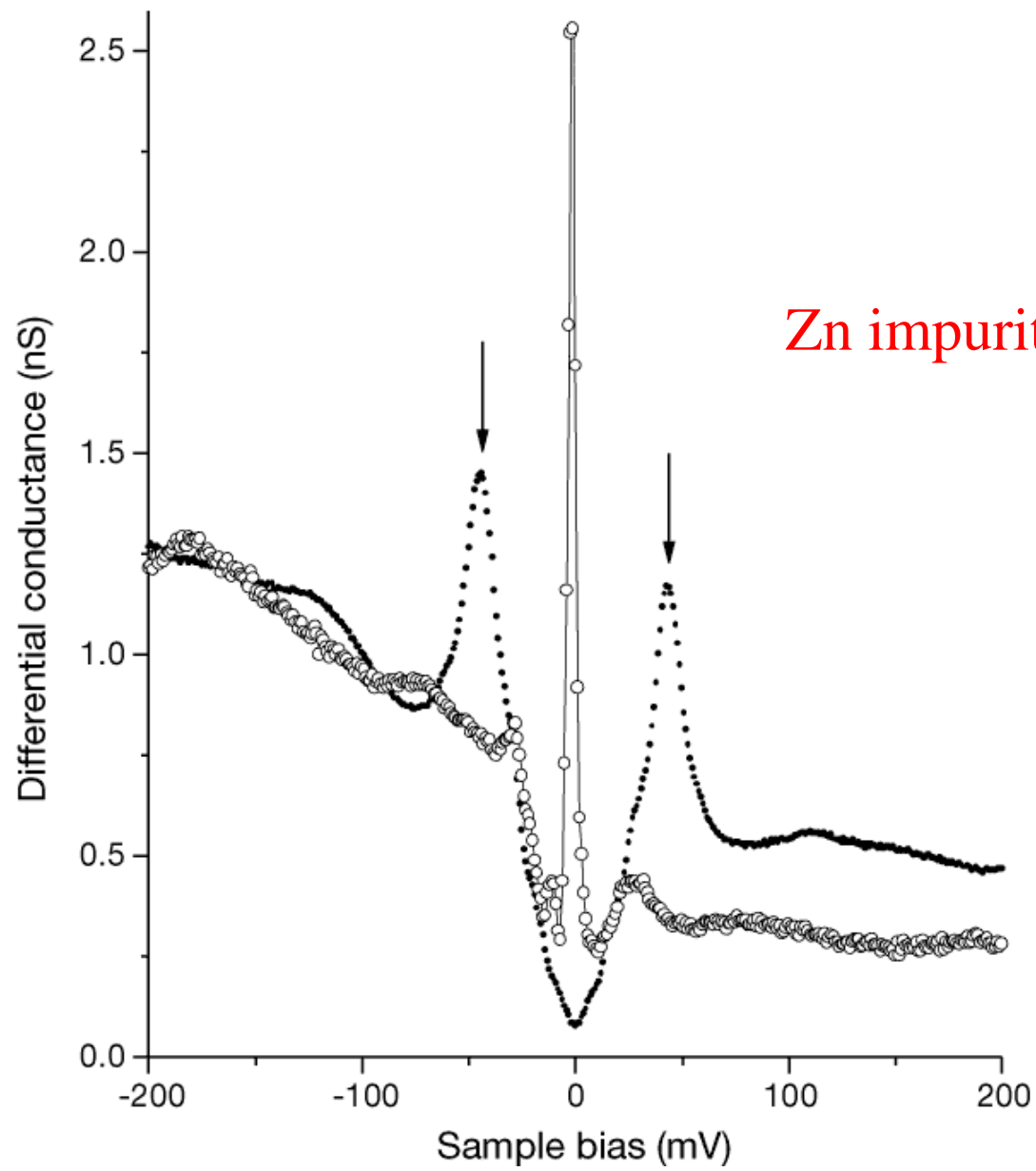


III. Implications for STM experiments



Zn impurities
in BSCCO

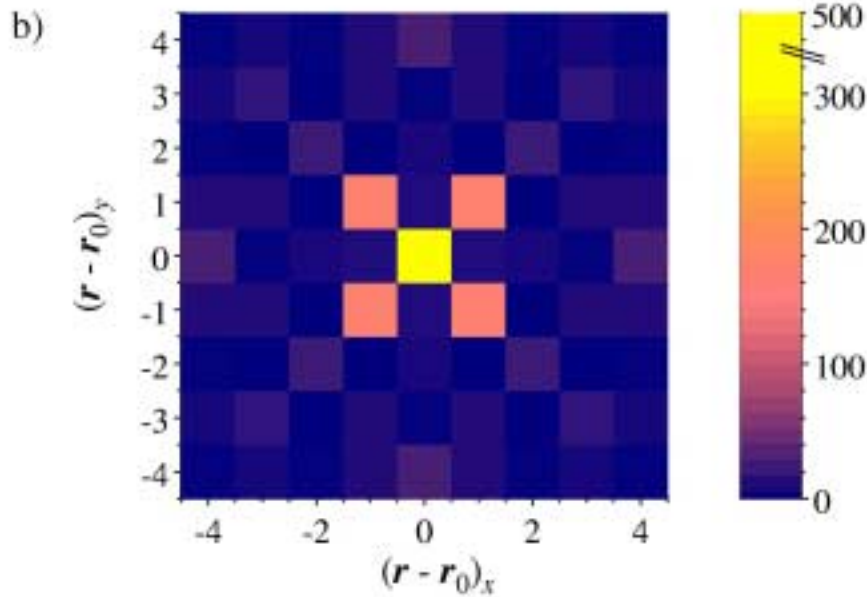
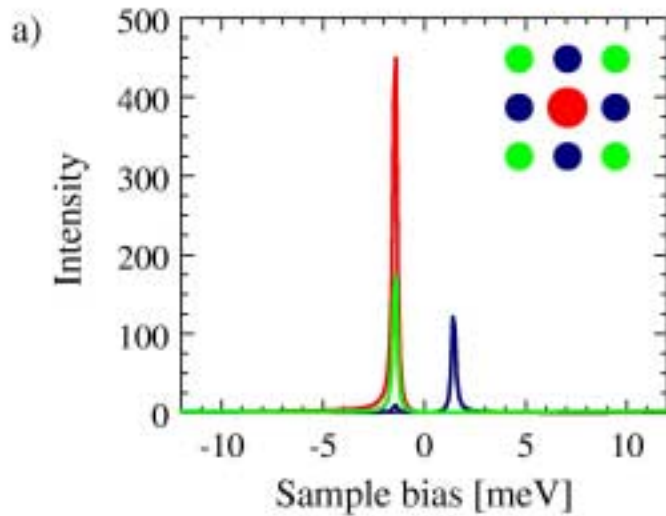
S. H. Pan *et al* Nature **403**, 746 (2000)



Zn impurity in BSCCO

Theory: $S=1/2$ local moment coupled to Bogoliubov quasiparticles of a d -wave superconductor

A. Polkovnikov, S. Sachdev, and M. Vojta,
Phys. Rev. Lett. **86**, 296 (2001)

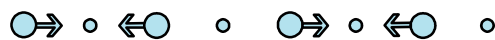
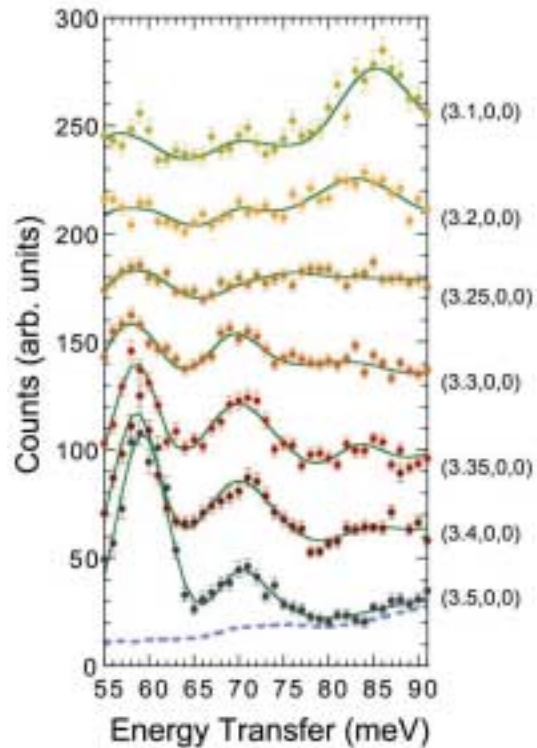


Peak bias \sim Kondo temperature
for screening of moment by
fermionic Bogoliubov
quasiparticles.

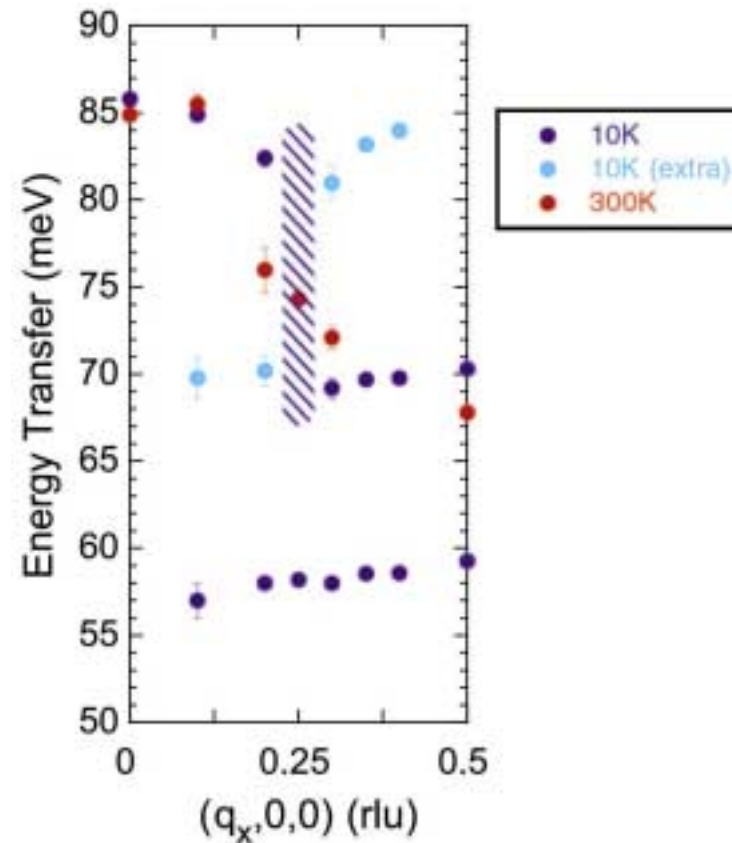
STM experiments imply that
Kondo temperature \sim 15 K

Subsequent NMR experiments:
Kondo temperature \sim 20-40 K

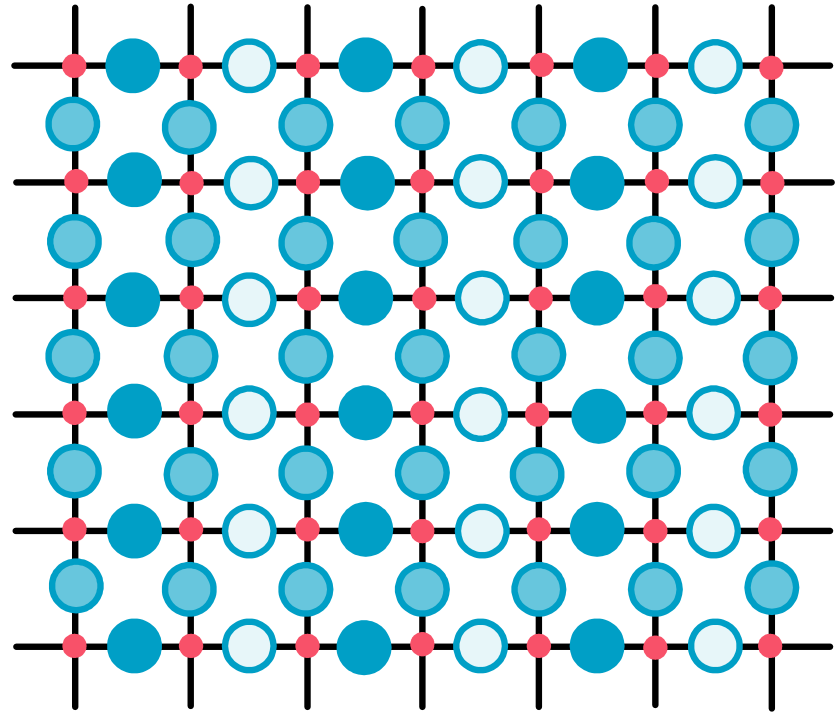
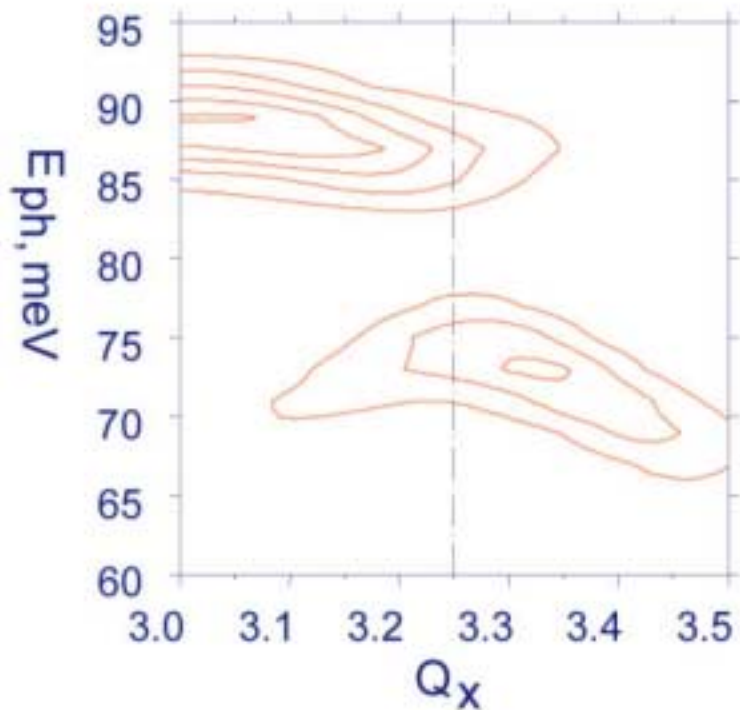
IV. Neutron scattering measurements of phonon spectra



- Oxygen
- Copper



Neutron scattering measurements of phonon spectrum of superconducting $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ by R. J. McQueeney, Y. Petrov, T. Egami, M. Yethiraj, G. Shirane, and Y. Endoh, Phys. Rev. Lett. **82**, 628 (1999)



Computation of phonon spectrum by McQueeney *et al* using a simple model based on lattice modulation on the right.

Evidence for coexistence of spin-Peierls order and “d-wave” superconductivity.

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

Conclusions

1. Strong experimental evidence for $S=1/2$ moment near Zn and Li impurities in the underdoped high temperature superconductor.
2. This, and other properties of the high temperature superconductors (existing of $S=1$ spin resonance mode, possible bond-centered charge stripe (spin-Peierls) order) are naturally understood by a theory of doping Mott insulators with confinement.
3. New boundary conformal quantum field theory in 2+1 dimensions describes scattering of spin resonance mode off “non-magnetic” impurities.