Quantum impurities in Mott insulators and *d*-wave superconductors

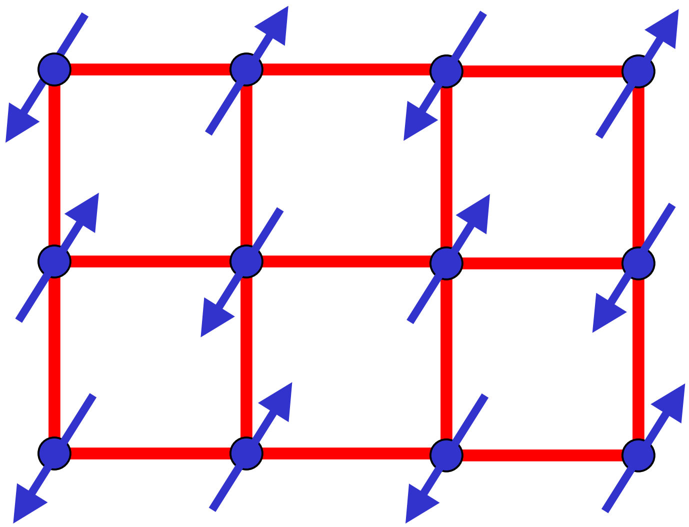
Matthias Vojta (Augsburg)
Chiranjeeb Buragohain
Anatoli Polkovnikov
Subir Sachdev

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

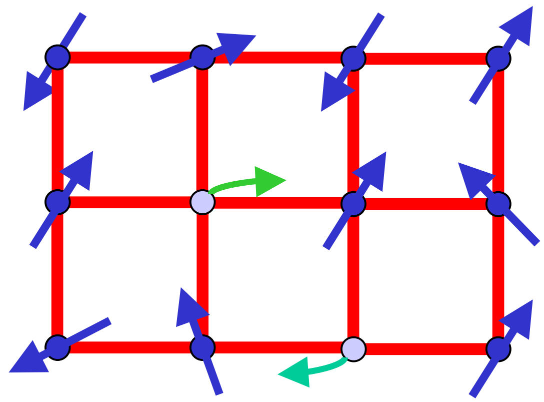


$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Ground state has long-range magnetic (Neel) order

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

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



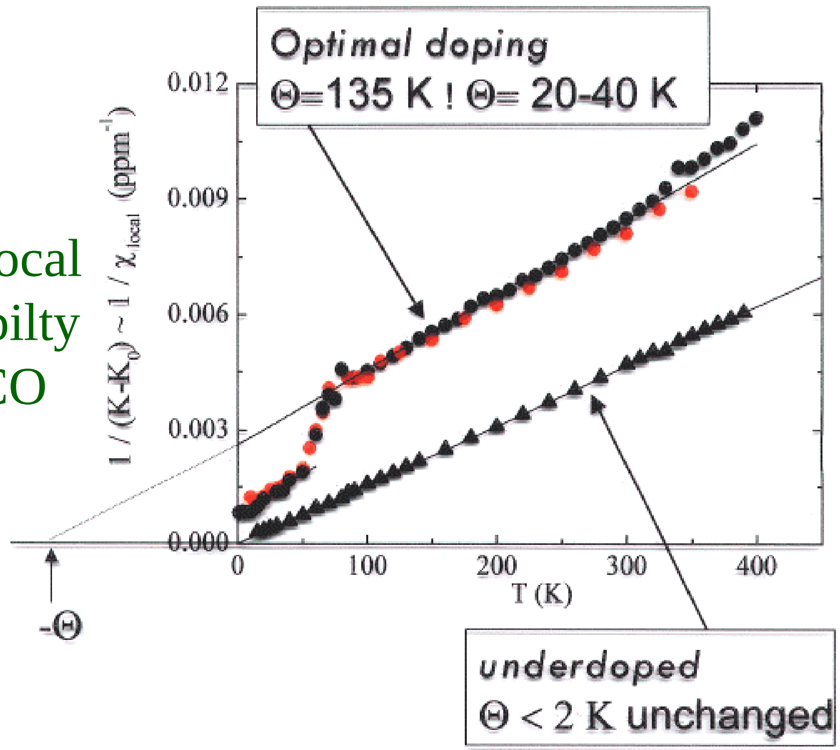
Exhibits superconductivity below a high critical temperature T_c

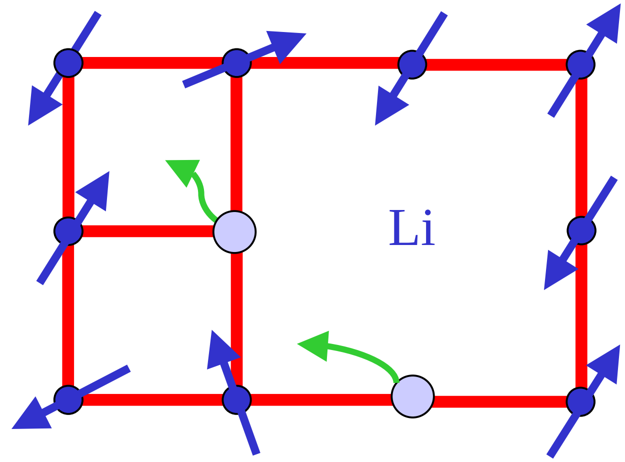
Almost all $T \rightarrow 0$ properties can be understood in the framework of a standard BCS theory in which the electrons form spin-singlet, *d*-wave Cooper pairs. However, many $T > T_c$ properties are anomalous.

$$\text{As } T \rightarrow 0, \quad \left\langle \vec{S}_i \right\rangle = 0 \quad \text{and} \quad \chi_{\text{spin}} = 0$$

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

Inverse local susceptibilty in YBCO





^{7}Li NMR below T_c

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

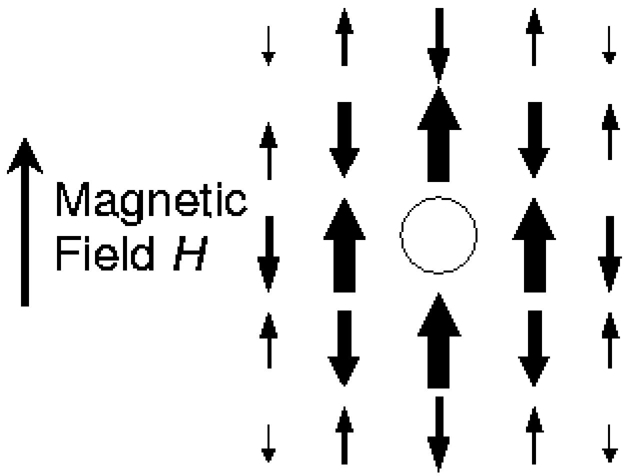
Measured $\chi_{\text{impurity}}(T \to 0) = \dfrac{S(S+1)}{3k_B T}$ with $S = 1/2$ in underdoped sample.

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

Zn impurity in $YBa_2Cu_3O_{6.7}$

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).



Total spin *S*=1/2

S=1 resonance mode in YBCO

$YBa_2Cu_3O_7$

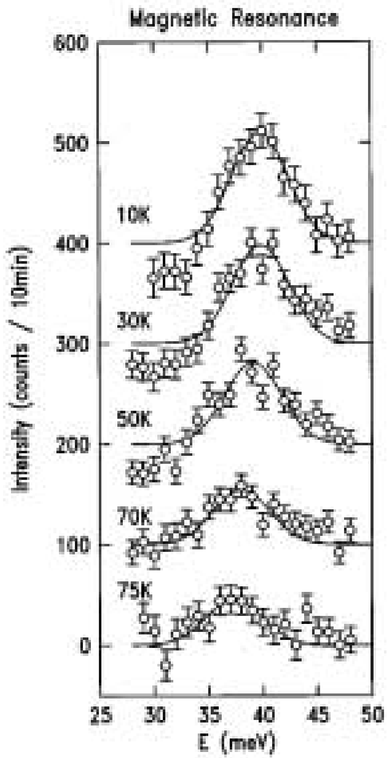
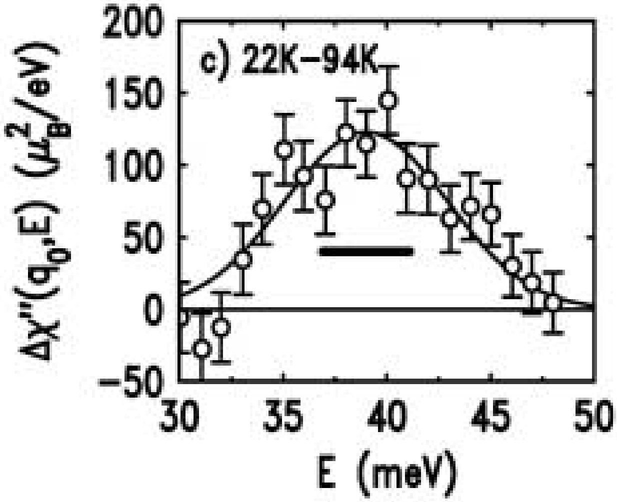


FIG. 8. Unpolarized beam, constant-**Q** data [**Q**=(3/2,1/2,−1.7)] of the 40 meV magnetic resonance obtained by subtracting the signal below T_c from the $T=100$ K background. The lines are fits to Gaussians, as described in the text. For clarity successive scans are offset by 100.

Resolution limited width

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

$YBa_2Cu_3O_7 + 0.5\%$ Zn



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

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

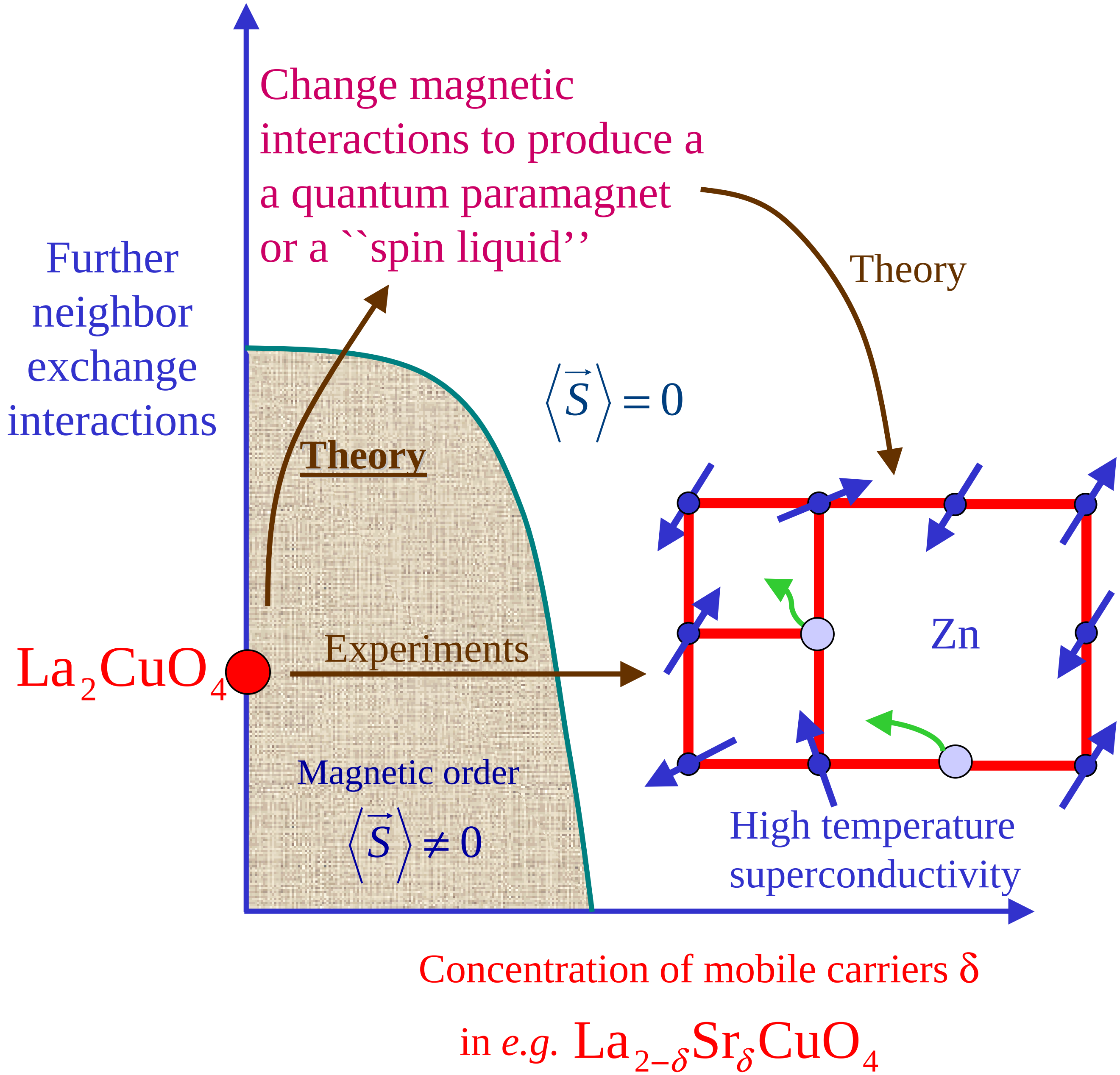
2. What is the energy scale at which the collective spin resonance is broadened by Zn impurities ?

"Swiss cheese" model

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

$$\mathcal{C} \rightarrow \text{ universal number}$$

3. Does the *S=1/2* moment near a non-magnetic impurity have any implications for STM measurements of a single Zn impurity ?


Change magnetic
interactions to produce a
a quantum paramagnet
or a ``spin liquid''
Theory
Further
neighbor
exchange
interactions
$\langle \vec{S} \rangle = 0$
Theory
Experiments
La_2CuO_4
Zn
Magnetic order
$\langle \vec{S} \rangle \neq 0$
High temperature
superconductivity
Concentration of mobile carriers δ
in *e.g.* $La_{2-\delta}Sr_\delta CuO_4$

Outline

I. Neel and paramagnetic states of the coupled ladder antiferromagnet.

A. Field theory for quantum phase transition.

B. General theory of localized defects across the quantum critical point.

II. Paramagnets and superconductors on the square lattice.

A. Confinement of spinons and breaking of translational symmetry in insulators.

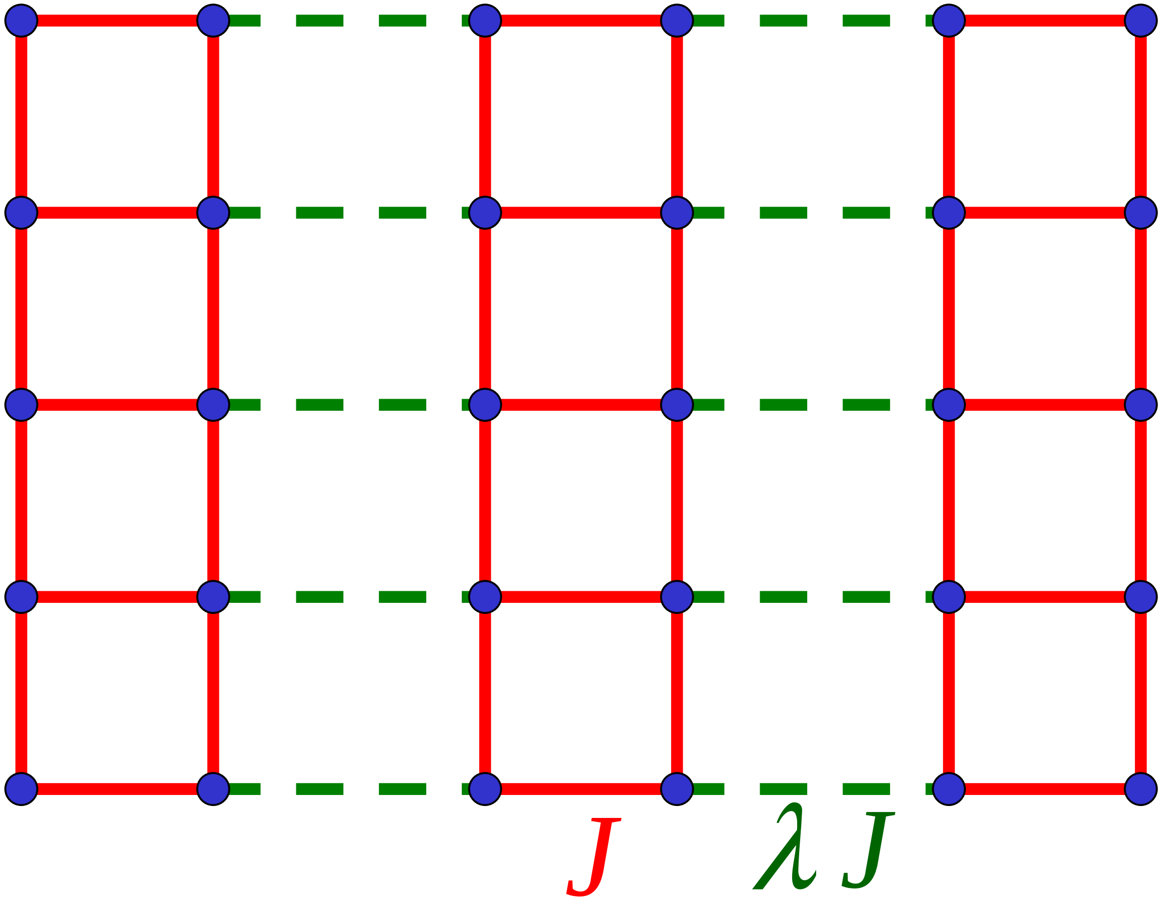
B. Generalization to magnetic transitions in *d*-wave superconductors

III. Theory for STM spectra of Zn impurities.

I. Neel and paramagnetic states of the 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).

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



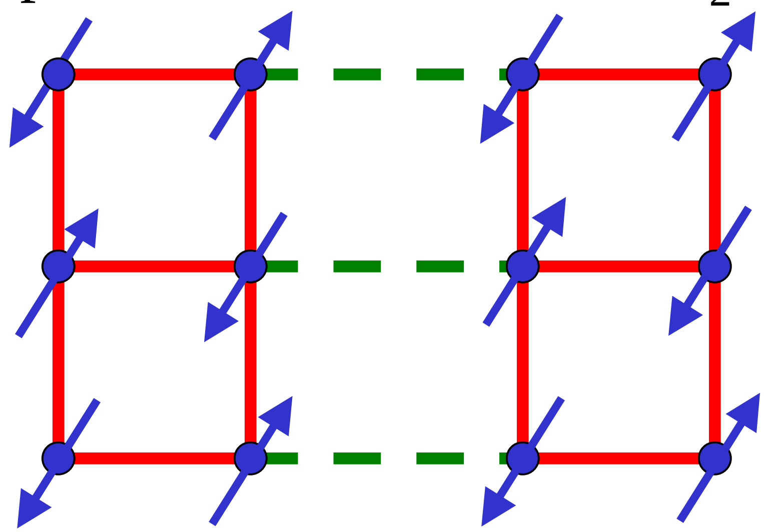
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$0 \leq \lambda \leq 1$$

λ close to 1

Square lattice antiferromagnet

Experimental realization: La_2CuO_4



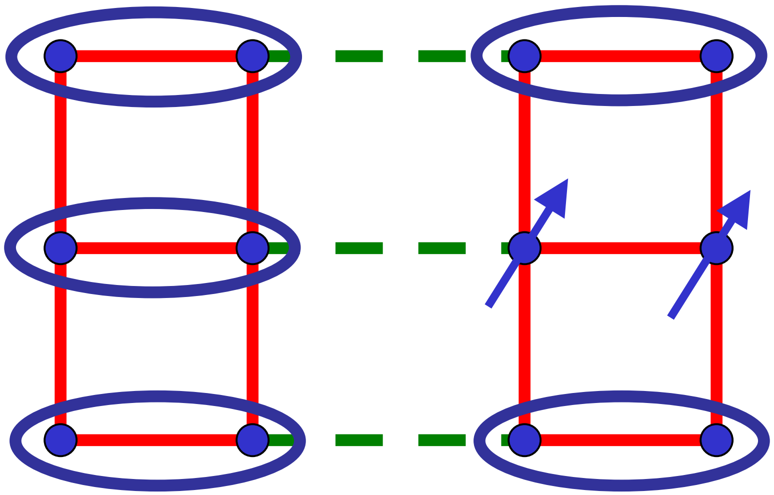
Ground state has long-range magnetic (Neel) order

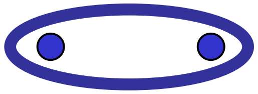
$$\left\langle \vec{S}_i \right\rangle = \left(-1\right)^{i_x+i_y} N_0 \neq 0$$

Excitations: 2 spin waves

λ close to 0

Weakly coupled ladders





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

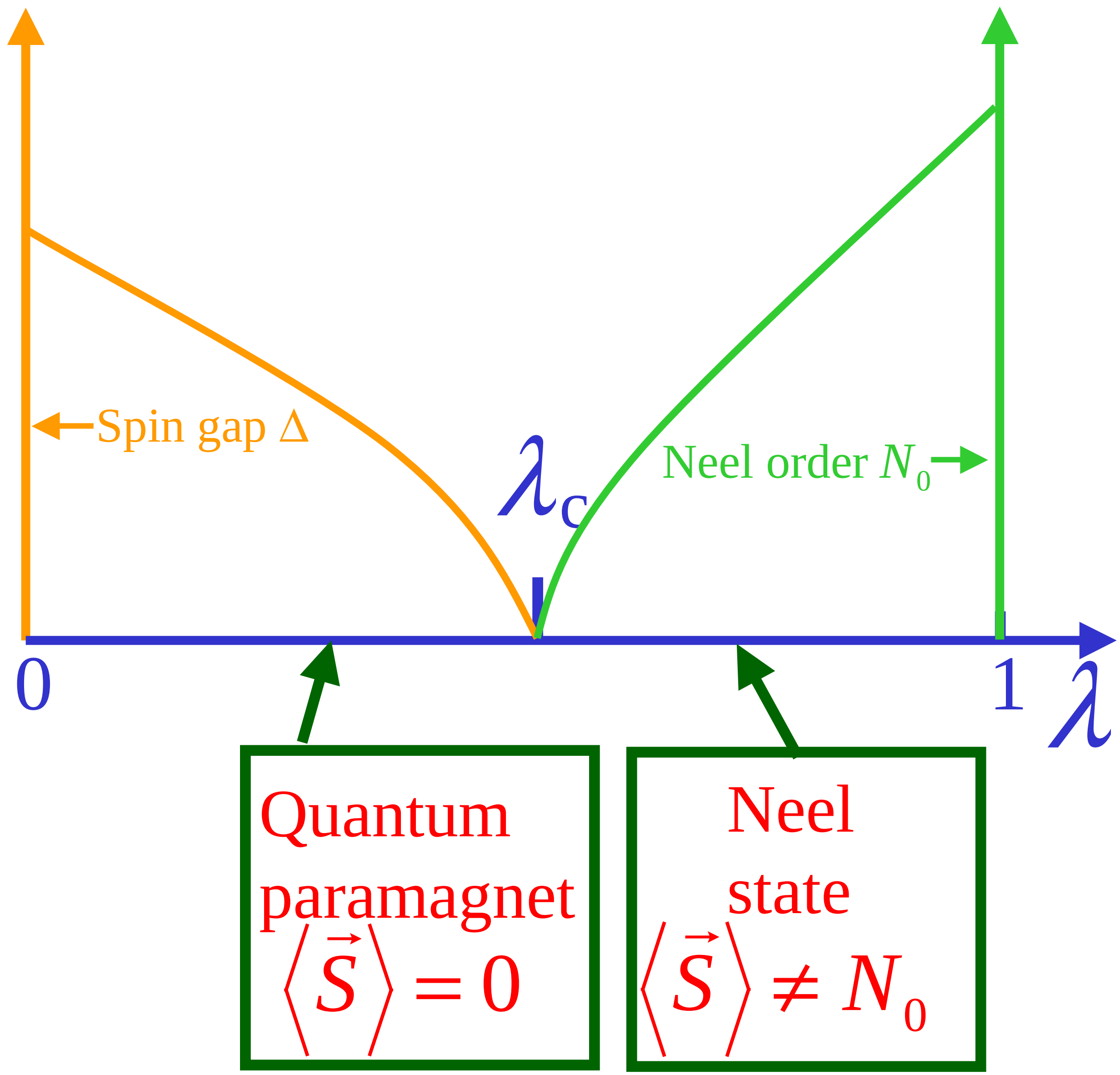
Paramagnetic ground state

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

Excitation: S=1 particle (collective mode)

Energy dispersion away from antiferromagnetic wavevector

$$\varepsilon = \Delta + \frac{c^2 k^2}{2\Delta}$$



Spin gap Δ
λ_c
Neel order N_0
0
1
λ
Quantum paramagnet
$\langle \vec{S} \rangle = 0$
Neel state
$\langle \vec{S} \rangle \neq N_0$

I.A Quantum field theory:

λ close to λ_c

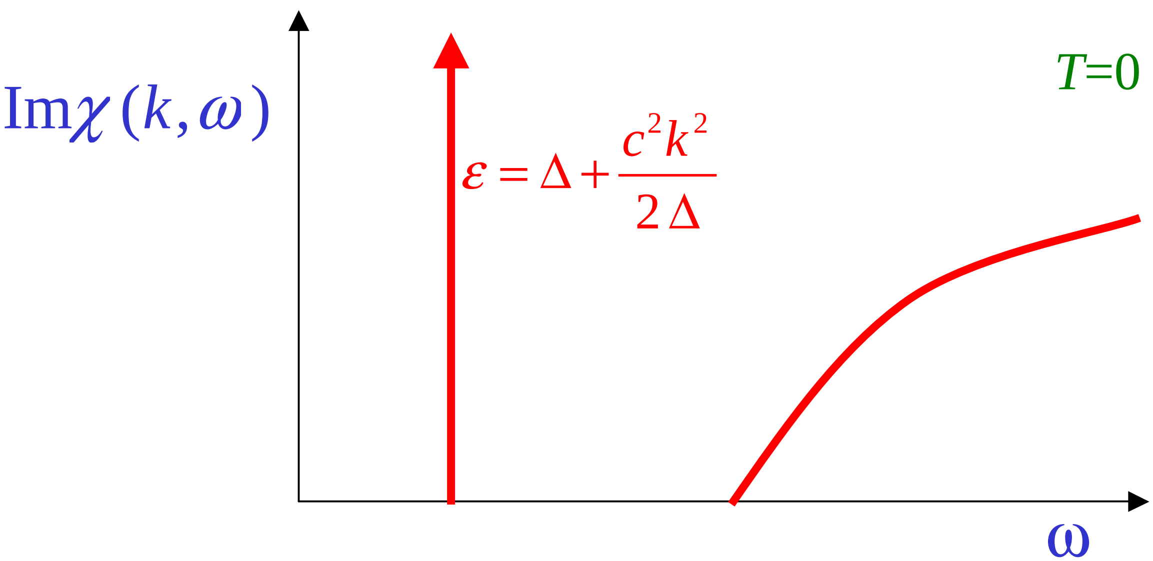
$$S_b = \int d^2x d\tau \left[\frac{1}{2}\left(\left(\nabla_x \phi_\alpha\right)^2 + c^2 \left(\partial_\tau \phi_\alpha\right)^2 + r\phi_\alpha^2 \right) + \frac{g}{4!}\left(\phi_\alpha^2\right)^2 \right]$$

ϕ_α → 3-component antiferromagnetic order parameter

$r > 0$	→	$\lambda < \lambda_c$
$r < 0$	→	$\lambda > \lambda_c$

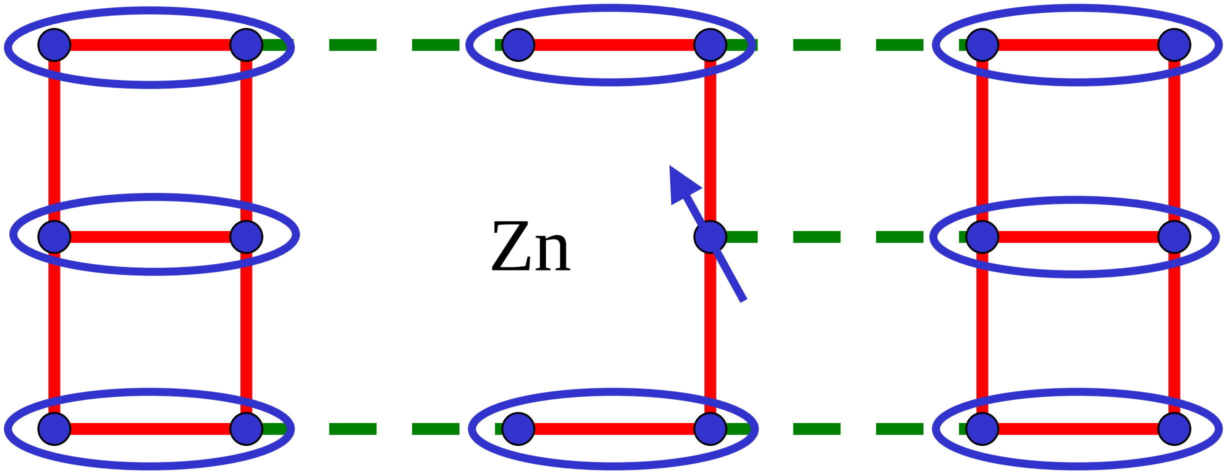
Oscillations of ϕ_α about zero (for $r > 0$)
→ spin-1 collective mode

T=0 spectrum



I.B Impurities in the coupled-ladder antiferromagnet

Make *any* localized deformation e.g. remove a spin



Susceptibility $\chi = A\chi_b + \chi_{imp}$ (A = area of system)

In paramagnetic phase as $T \to 0$

$$\chi_b = \left(\frac{\Delta}{\hbar^2 c^2 \pi}\right) e^{-\Delta / k_B T} \quad ; \chi_{imp} = \frac{S(S+1)}{3k_B T}$$

For a general impurity χ_{imp} *defines* the value of S

Quantum field theory for *S=1* resonance in the presence of a non-magnetic impurity

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

Action of "impurity" spin

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

$A_\alpha(n)$ → 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

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);

β functions (ε=3-d):

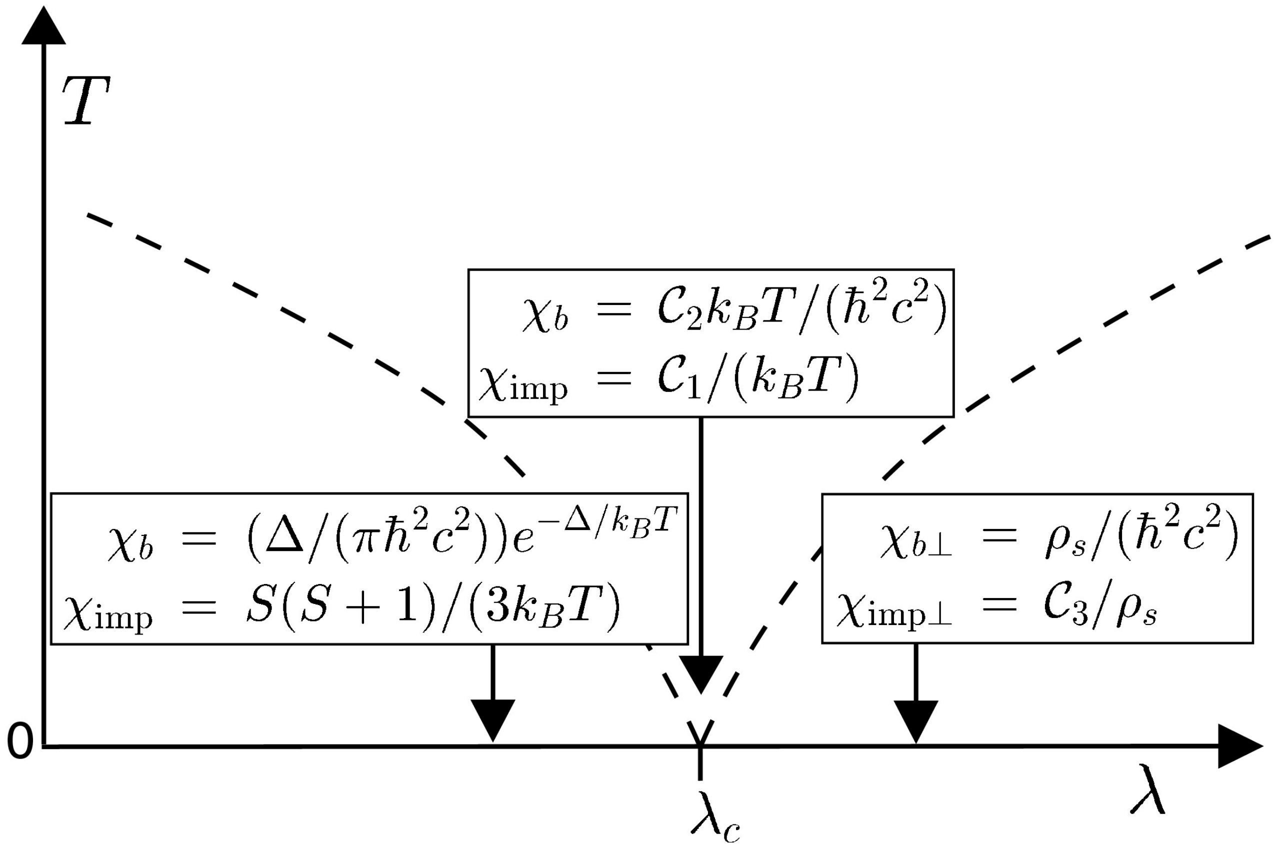
$$\beta(g) = -\varepsilon g + \frac{11g^2}{6} - \frac{23g^3}{12} + O(g^4)$$

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

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 !

Susceptibilities across the quantum critical point



C$_1$, **C**$_2$, **C**$_3$ are universal numbers which have been computed in the ε expansion.

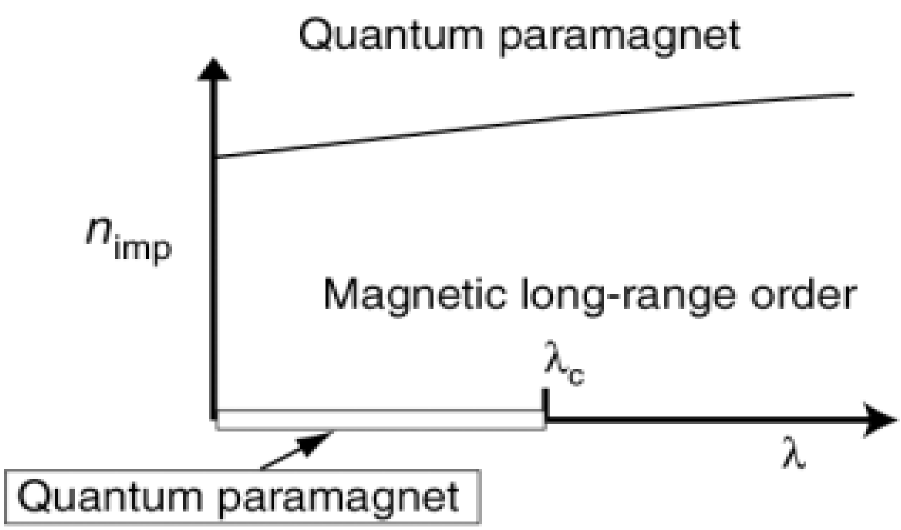
At $\lambda = \lambda_c$, impurity response is the Curie susceptibility of an irrational spin.

Finite density of impurities n_{imp}

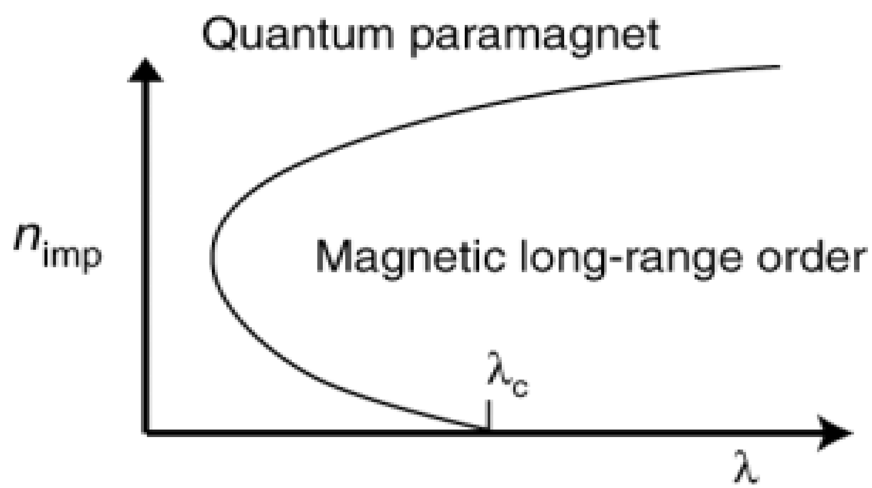
Relevant perturbation – strength determined by only energy scale Γ that is linear in n_{imp} and contains only bulk parameters

$$\Gamma \equiv \frac{n_{imp}(\hbar c)^2}{\Delta} \quad ; \quad \frac{1}{Q} \equiv \frac{\Gamma}{\Delta} = n_{imp}\left(\frac{\hbar c}{\Delta}\right)^2 = n_{imp}\xi^2$$

Two possible phase diagrams



$\Gamma_c/\Delta = 0^+$



$\Gamma_c/\Delta = \text{constant}$

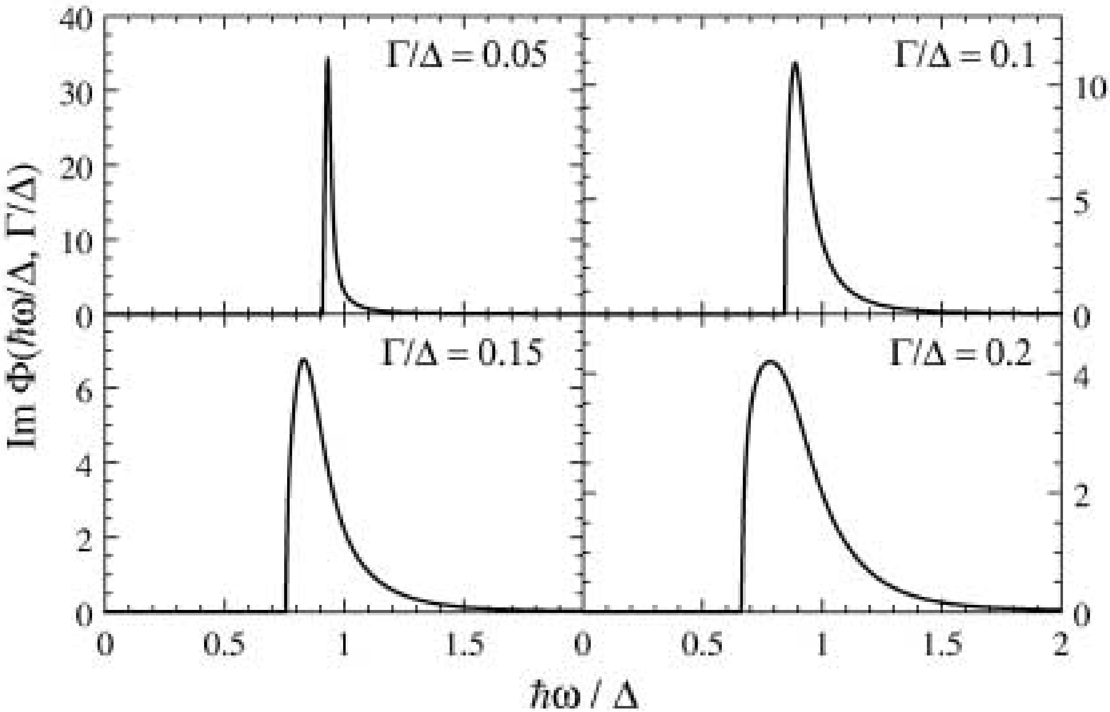
Dynamic susceptibility at ω of order Δ

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

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

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

Φ → *Universal* scaling function. We computed it in a "self-consistent, non-crossing" approximation



Predictions:
Half-width of line ≈ Γ

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).

II. Paramagnets and superconductors on the square lattice

II.A Insulators

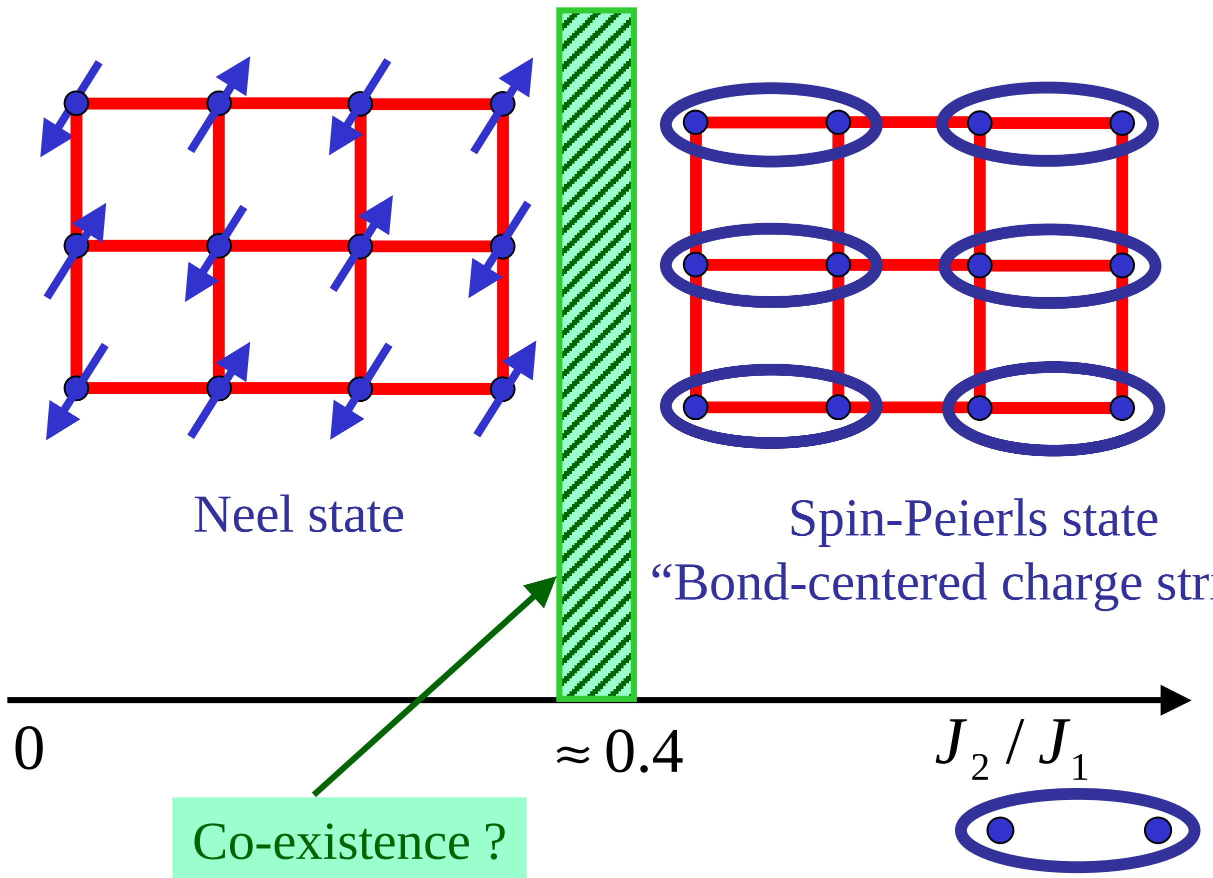
$$H = \sum_{i<j} J_{ij} \; \vec{S}_i \cdot \vec{S}_j$$

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

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

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

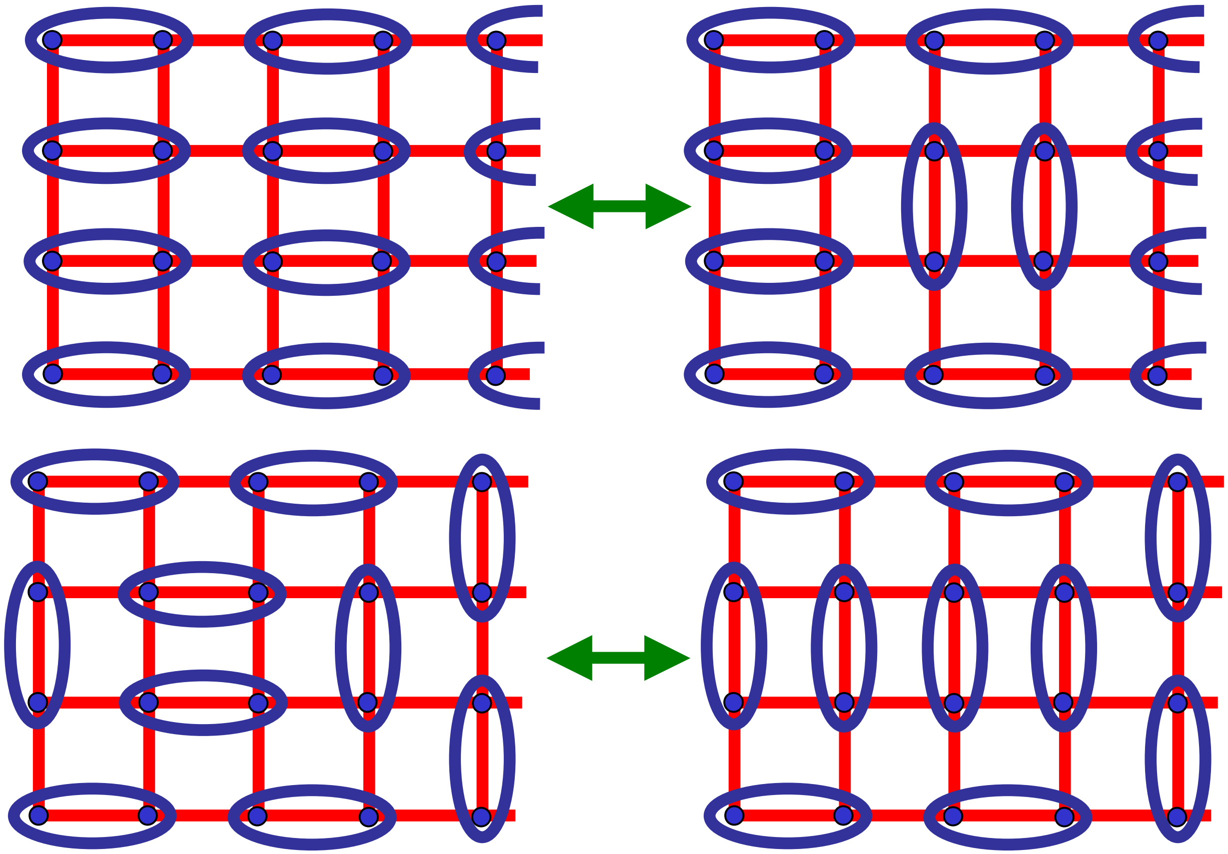
M.S.L. du Croo de Jongh, J.M.J. van Leeuwen, W. van Saarloos, cond-mat/0002116.



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

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.

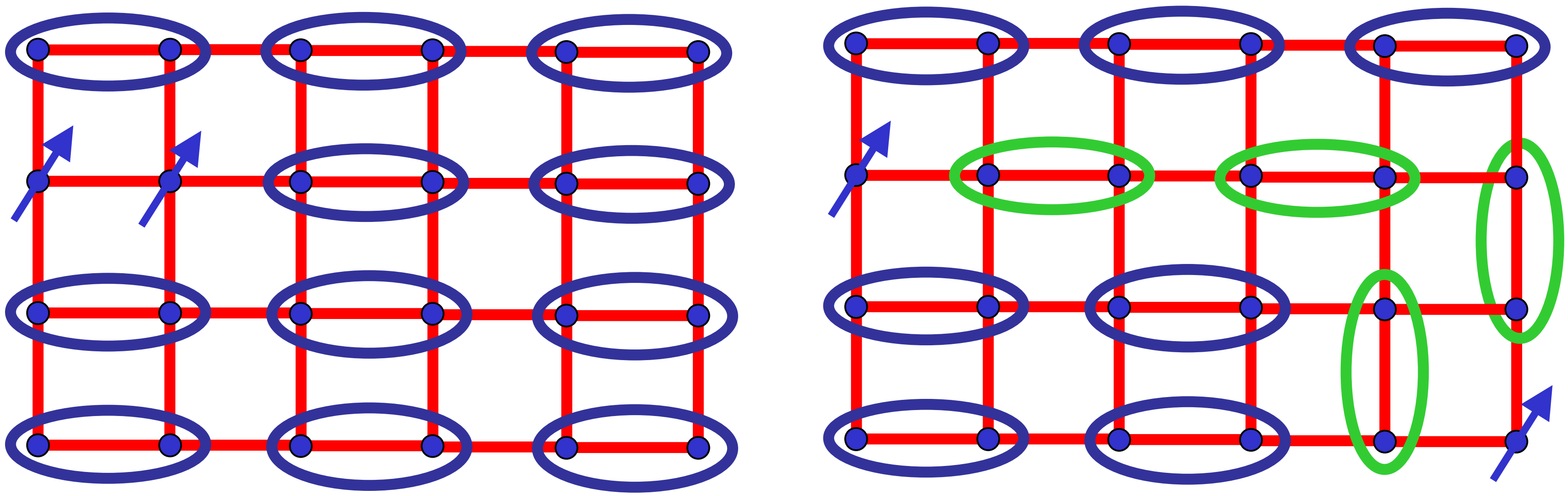
These effects always lead to a broken square lattice symmetry near the transition to the Neel state.

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

Excitations

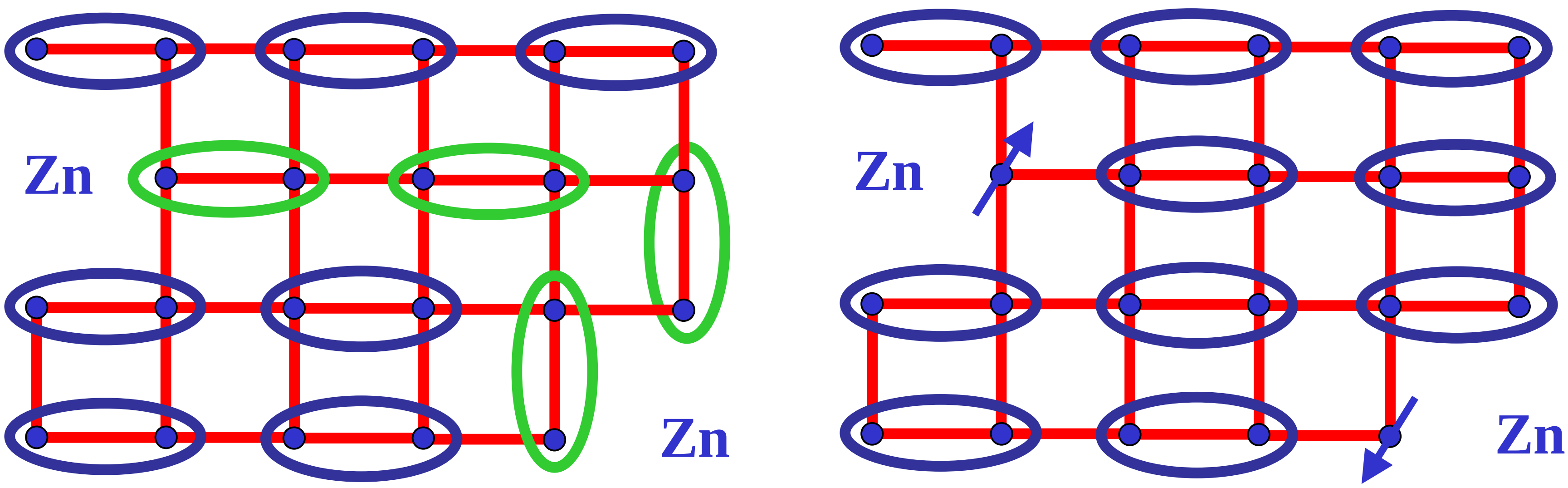
Stable S=1 particle

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

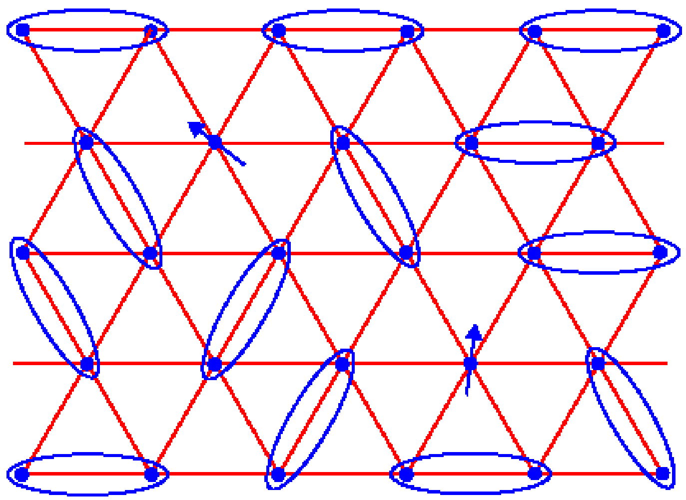
Effect of static non-magnetic impurities (Zn or Li)



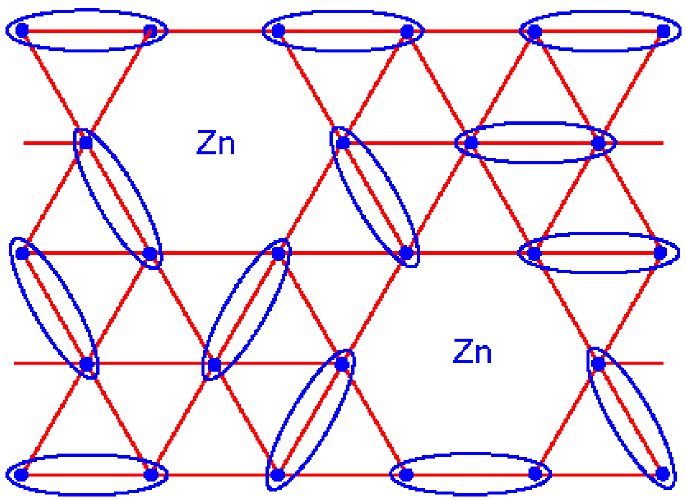
Spinon confinement implies that free S=1/2 moments **must** form near each impurity

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

Paramagnetic ground state with spinon deconfinement



Spinons are deconfined



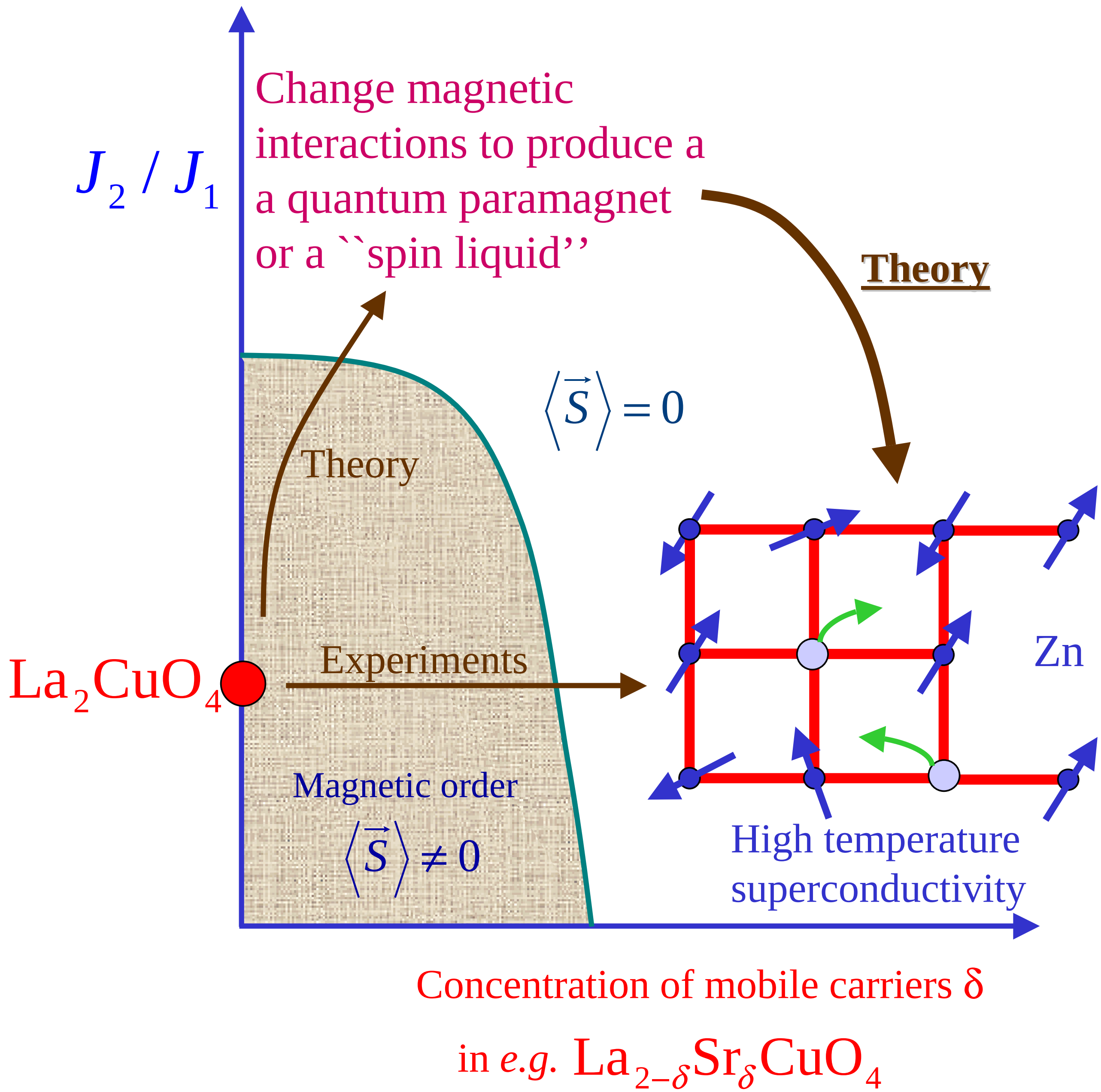
Free S=1/2 moments need not be present near the impurities

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

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

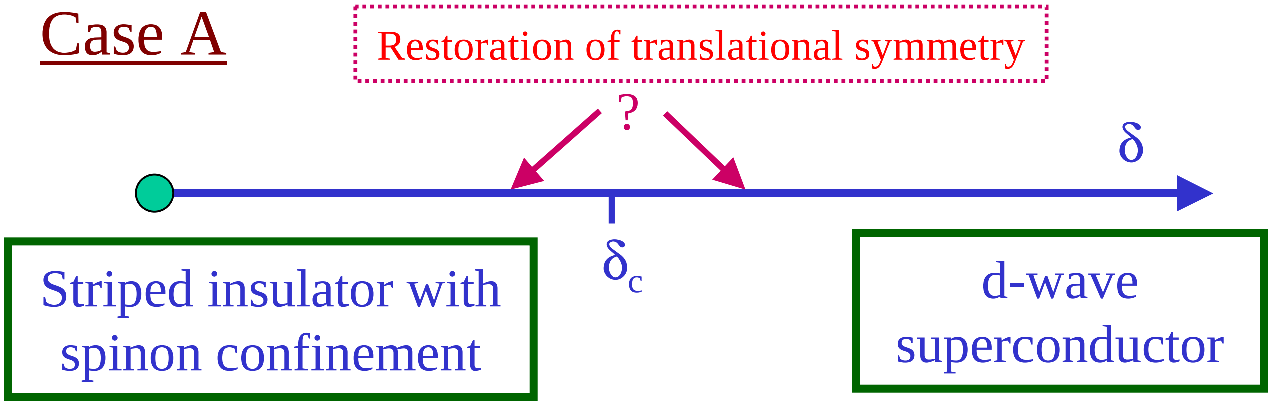
N. Read and S. Sachdev, Phys. Rev. Lett. **66**, 1773 (1991).
R. Jalabert and S. Sachdev, Phys. Rev. B **44**, 686 (1991).

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.


J_2 / J_1
Change magnetic interactions to produce a a quantum paramagnet or a ``spin liquid''
Theory
$\langle \vec{S} \rangle = 0$
Theory
La_2CuO_4
Experiments
Zn
Magnetic order
$\langle \vec{S} \rangle \neq 0$
High temperature superconductivity
Concentration of mobile carriers δ
in *e.g.* $La_{2-\delta}Sr_{\delta}CuO_4$

II.B Zn or Li impurities in doped Mott insulators

Case A



Moments form near each Zn or Li.

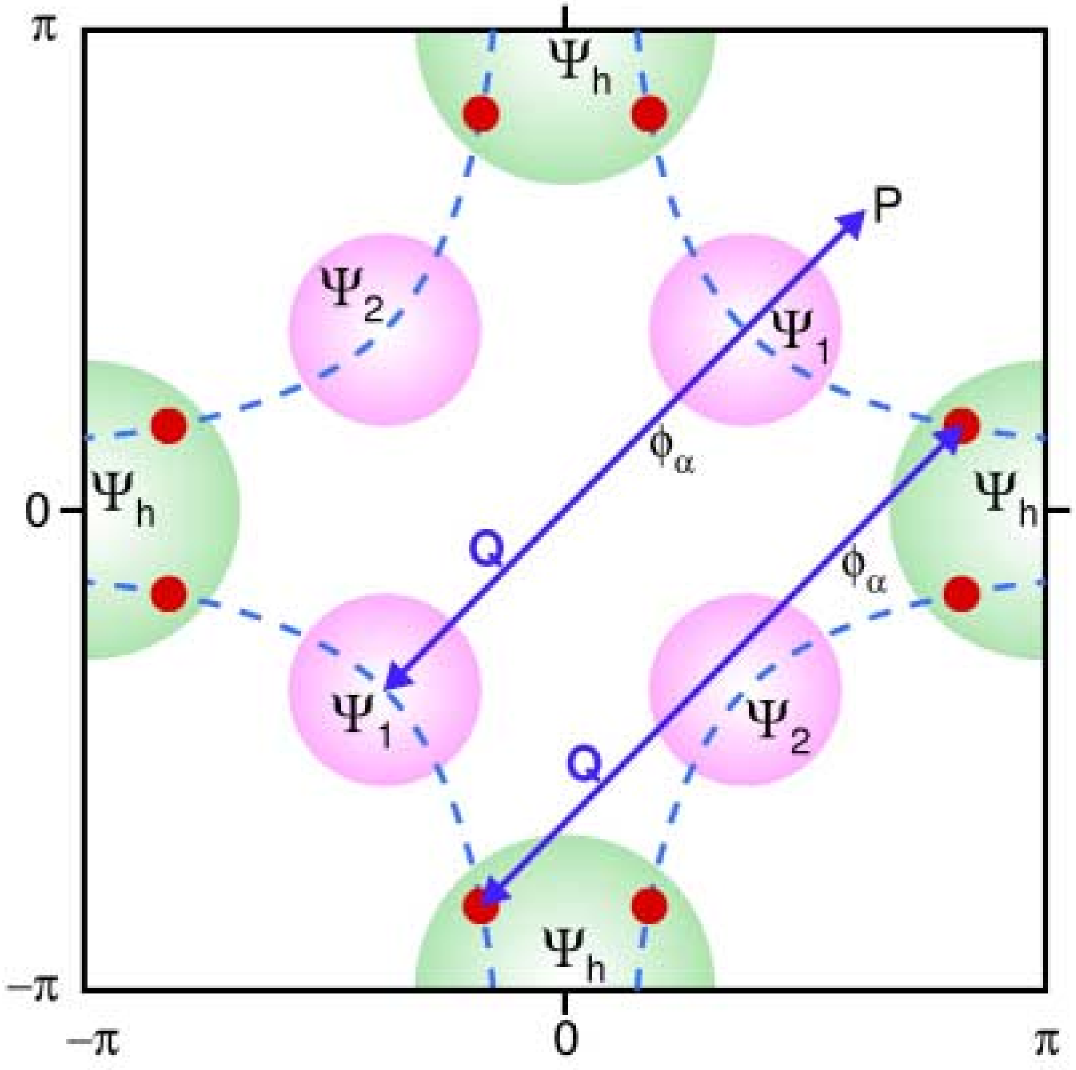
This moment is quenched by fermionic Bogoliubov quasiparticles at a quantum phase transition at $\delta=\delta_c$.

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

II.B Magnetic transition in a d-wave superconductor



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

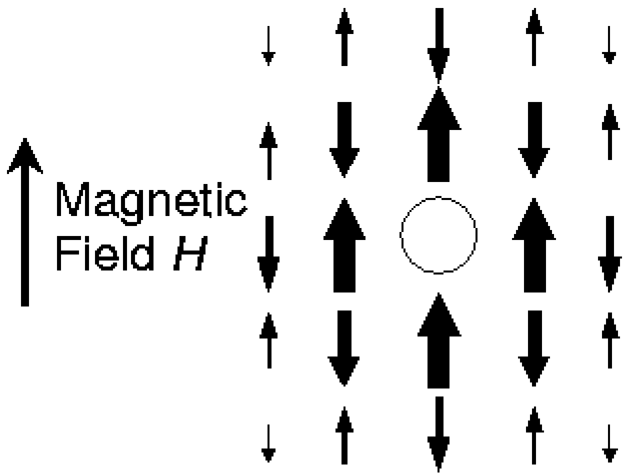
$\Psi_{1,2}$: *decoupled* from ϕ_α

Leading universal properties of transition are identical to that in an insulator

Zn impurity in $YBa_2Cu_3O_{6.7}$

Moments measured by
analysis of Knight shifts

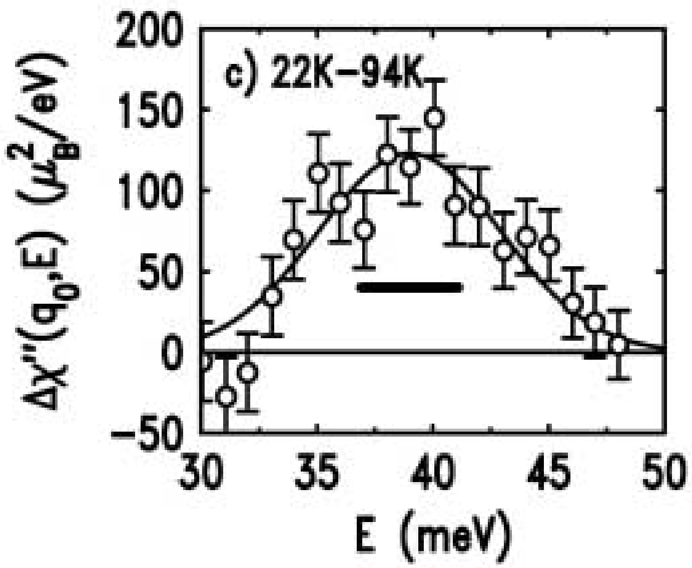
M.-H. Julien, T. Feher,
M. Horvatic, C. Berthier,
O. N. Bakharev, P. Segransan,
G. Collin, and J.-F. Marucco,
Phys. Rev. Lett. **84**, 3422
(2000); also earlier work of
the group of H. Alloul and the
original experiment of
A.M Finkelstein, V.E. Kataev,
E.F. Kukovitskii, and
G.B. Teitel'baum, Physica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



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

$YBa_2Cu_3O_7 + 0.5\%$ 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)



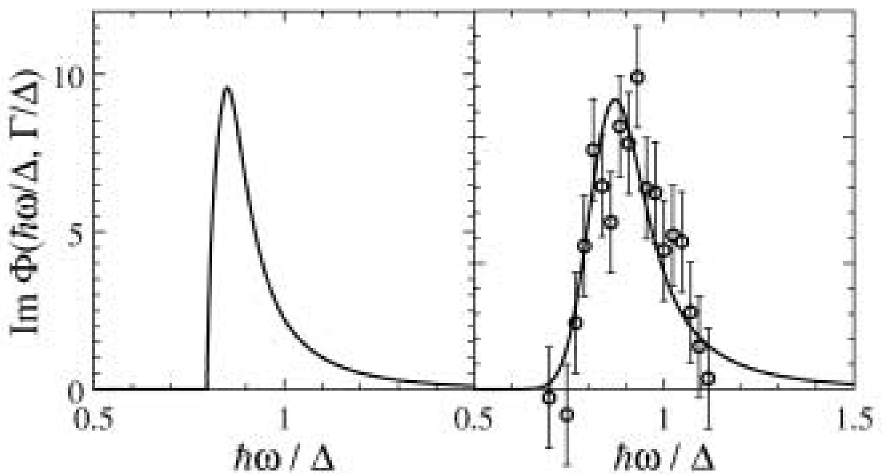
$$n_{\rm imp} = 0.005$$

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

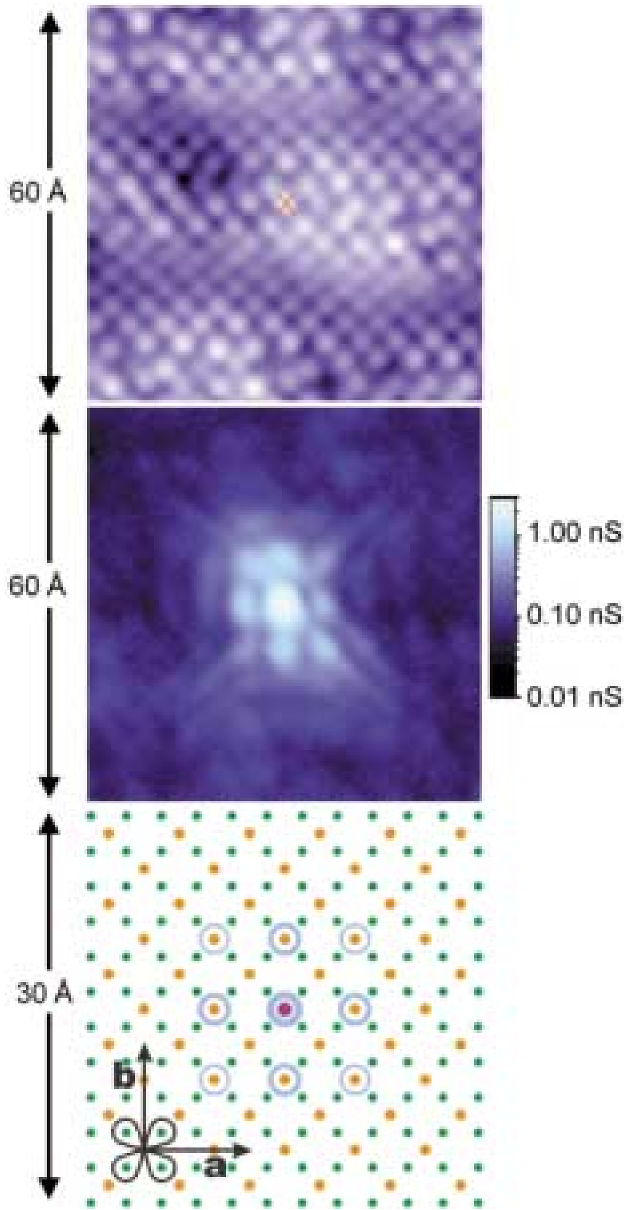
$$\hbar c = 0.2\ {\rm eV}$$

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

Quoted half-width = 4.25 meV



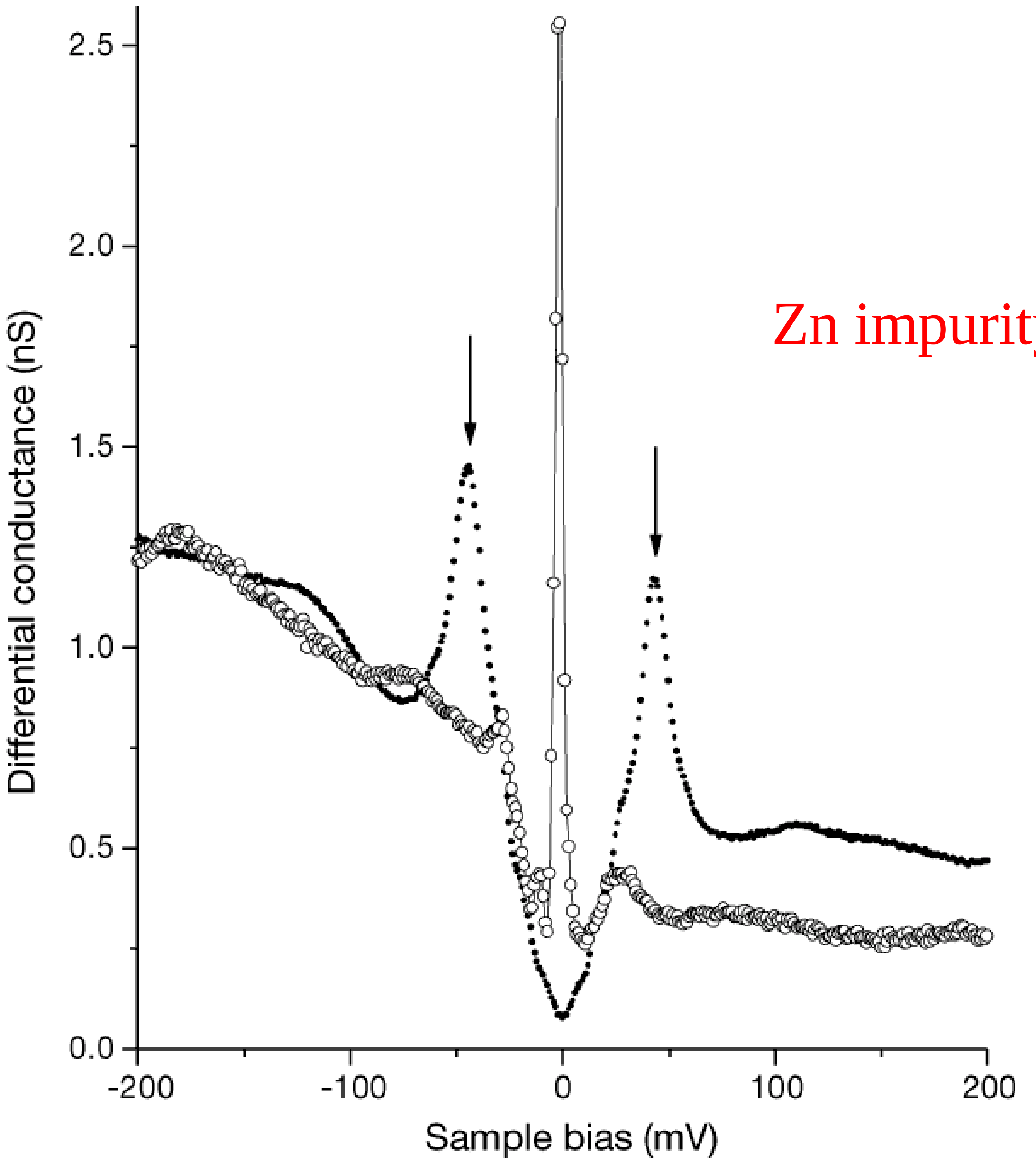
III. Implications for STM experiments



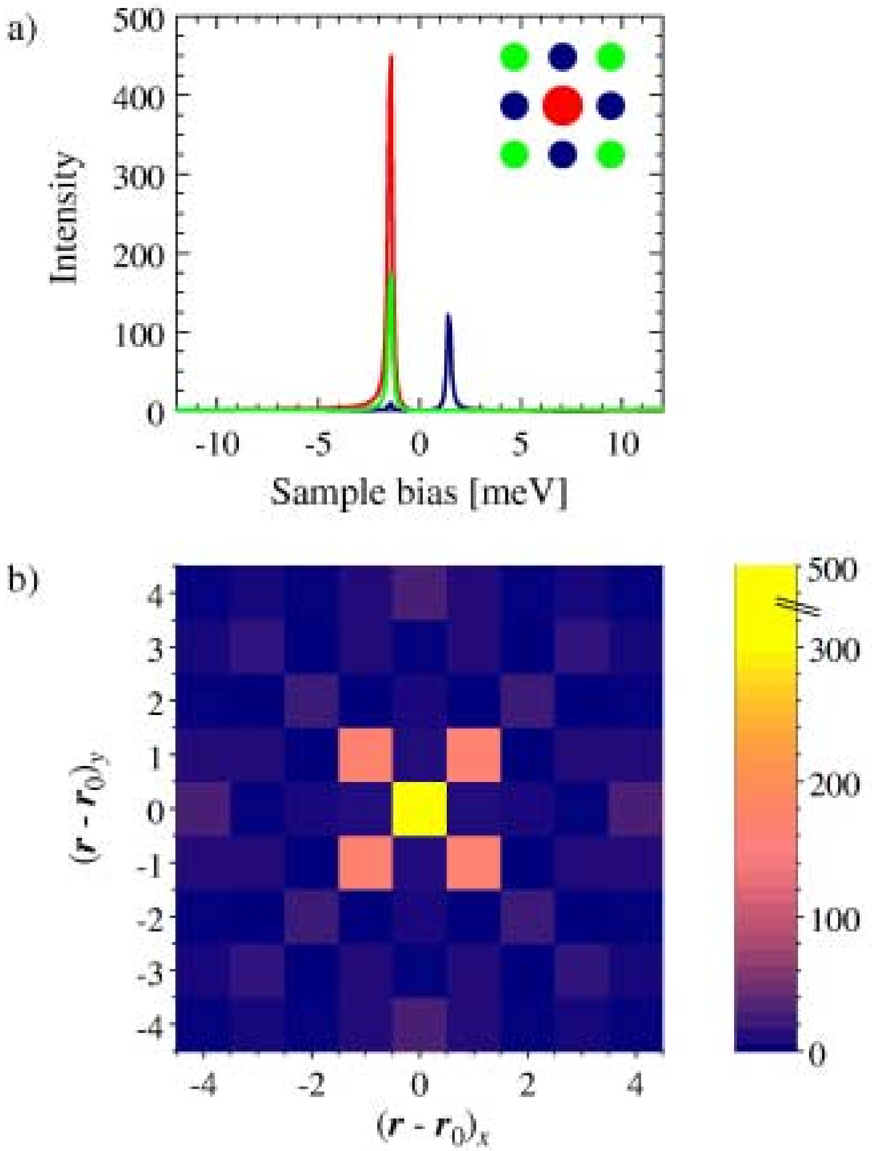
Zn impurities
in BSCCO

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

Zn impurity in BSCCO



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



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

Peak bias ~ Kondo temperature for screening of moment by fermionic Bogoluibov quasiparticles.

STM experiments imply that Kondo temperature ~ 15 K

Subsequent NMR experiments: Kondo temperature ~ 20-40 K

Alternative picture: Unitarity limit potential scattering from Zn impurities.

A.V. Balatsky, M. I. Salkola, and A. Rosengren, Phys. Rev. B **51**, 15547 (1995).
M. I. Salkola, A.V. Balatsky, and D. J. Scalapino, Phys. Rev. Lett.**77**,1841 (1996).

Conclusions

1. Strong experimental evidence for *S=1/2* moment near Zn and Li impurities in the underdoped high temperature superconductor.

2. New boundary conformal quantum field theory in 2+1 dimensions describes scattering of spin resonance mode off "non-magnetic" impurities.

3. This, and other properties of the high temperature superconductors (existence 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.

4. Energy scale of low bias peak in the STM measurements of Zn impurities = Kondo energy scale of screening of moment by fermionic quasiparticles (?)