Quantum impurities in 2+1 dimensional conformal field theories: application to Zn impurities in YBCO

or

A new boundary conformal field theory in 2+1 dimensions

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•C. Buragohain

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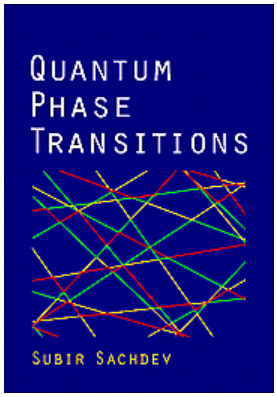
Transparencies on-line at
http://pantheon.yale.edu/~subir

Science **286**, 2479 (1999).
Phys. Rev. B **61**, 15152 (2000)

Yale University



Quantum Phase Transitions
Cambridge University Press

1. Paramagnetic and Neel ground states in two dimensions --- coupled-ladder antiferromagnet

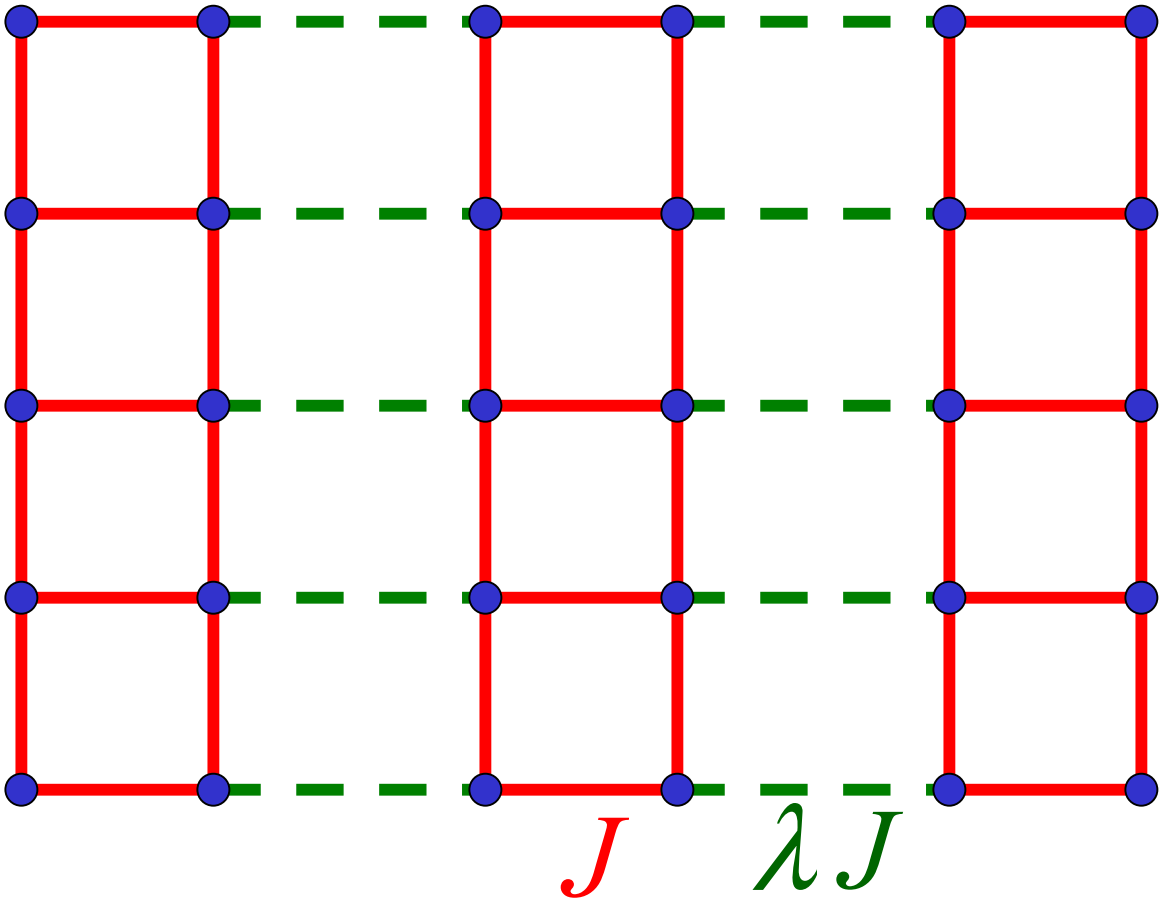
2. Nearly-critical paramagnets with
   spin gap $\Delta << J$
   Quantum field theory: low T spin dynamics is universally determined by Δ and $c = (c_x c_y)^{1/2}$

3. Non-magnetic impurities (Zn or Li) in nearly-critical paramagnets
   New boundary conformal field theory:
   T=0 damping of spin-1 collective mode - universal line-shape with
   no additional parameters needed:
   only need $n_{\rm imp}$

4. Application to d-wave superconductors.
   Comparison with, and predictions for, expts

1. Paramagnetic and Neel states

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



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

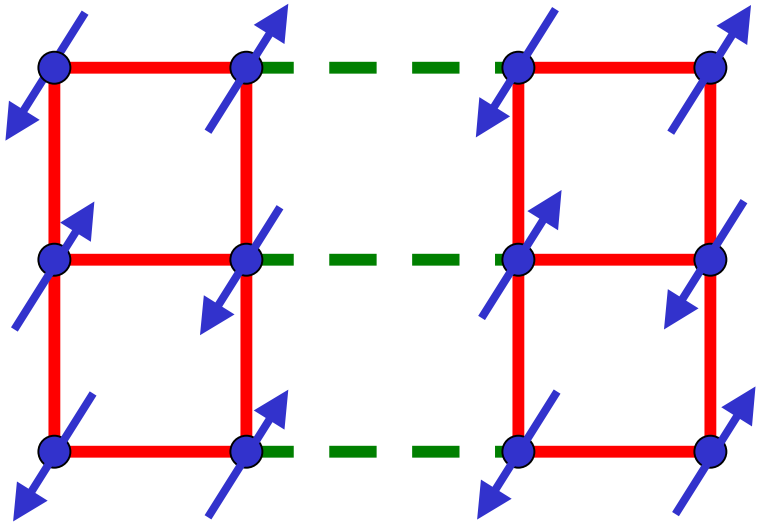
Follow ground state as a function of λ

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

$\lambda = 1$

Square lattice antiferromagnet

Experimental realization: La_2CuO_4



Ground state has long-range magnetic (Neel) order

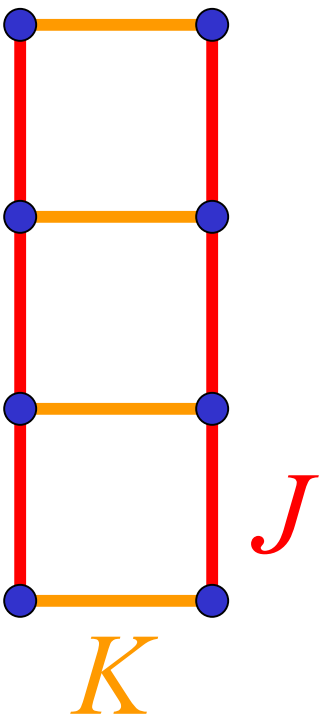
$$\left\langle \vec{S}_i \right\rangle = (-1)^{i_x + i_y} N_0 \neq 0$$

Excitations: 2 spin waves

Quasiclassical wave dynamics at low T

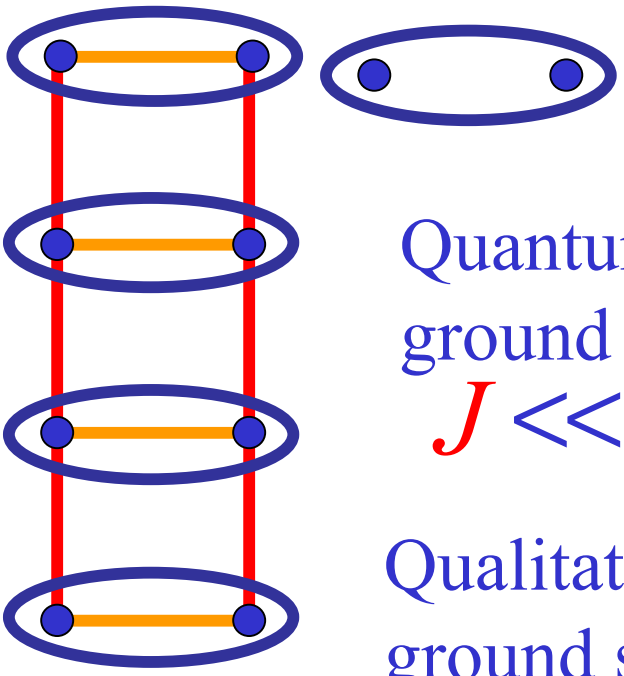
(Chakravarty et al, 1989; Tyc et al, 1989)

$\lambda = 0$



Decoupled 2-leg ladders

Allow $J \neq K$

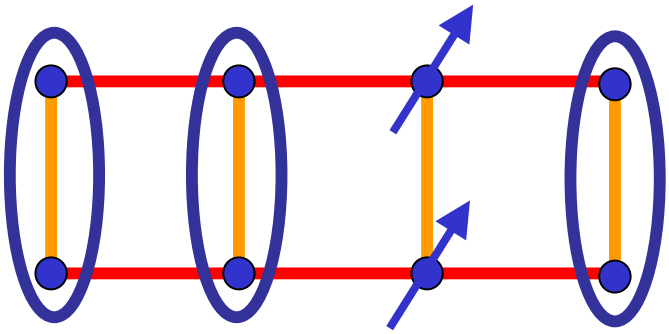


$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Quantum paramagnet ground state for $J \ll K$

Qualitatively similar ground state for all J/K

Excited states

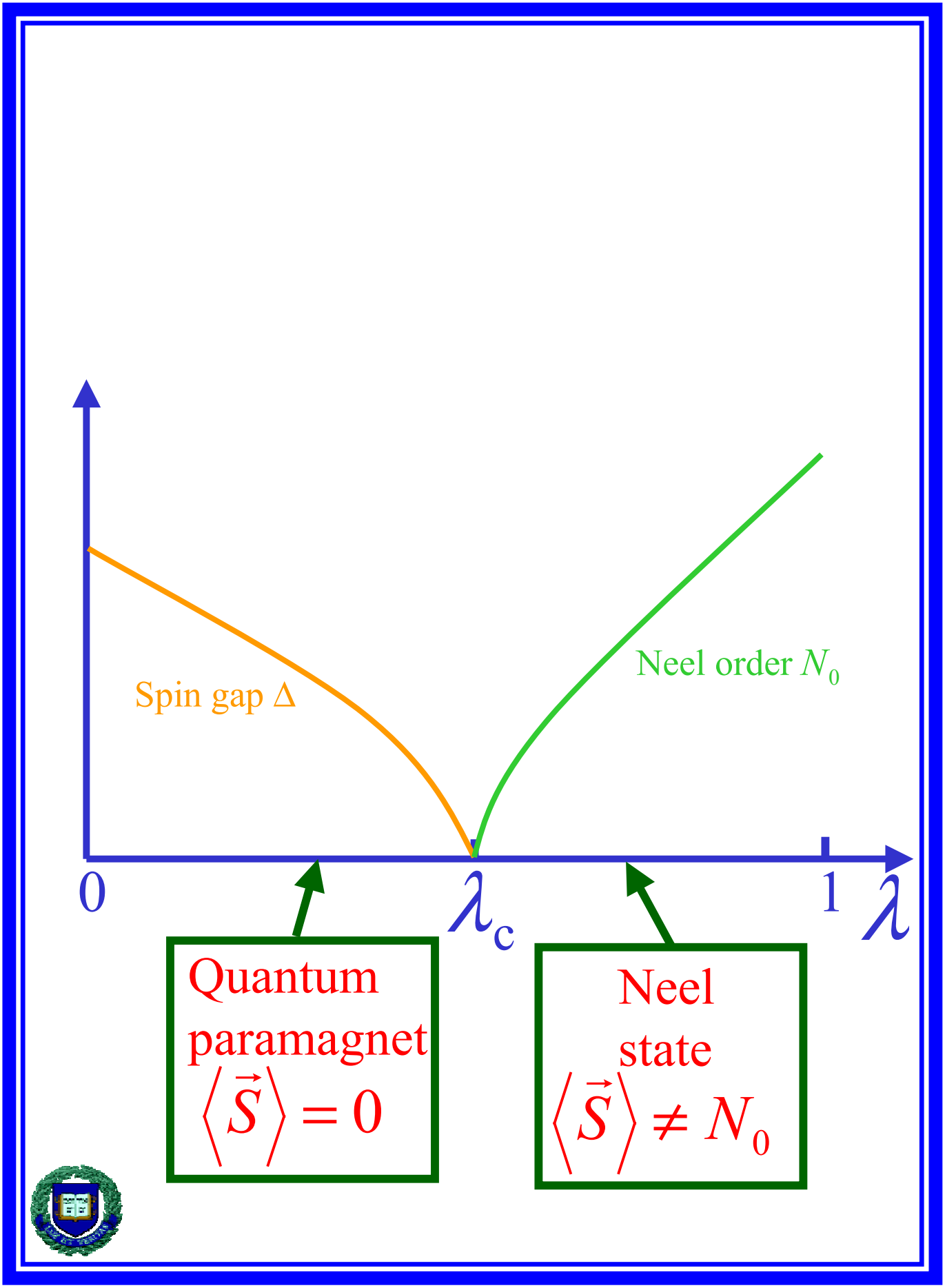


Triplet (S=1) particle (collective mode)

Energy dispersion away from antiferromagnetic wavevector

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

$\Delta \rightarrow$ Spin gap


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

2. Nearly-critical paramagnets

λ is close to λ_c

Quantum field theory:

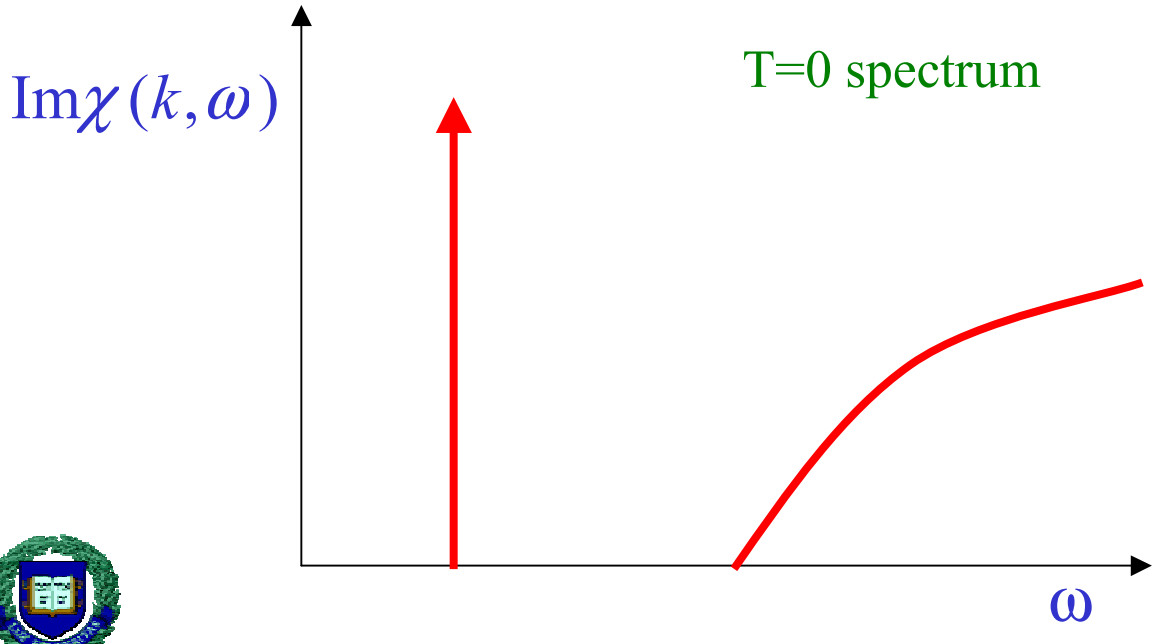
$$\mathcal{S}_b = \int d^d x d\tau \left[\frac{1}{2} \left((\nabla_x \phi_\alpha)^2 + c^2 (\partial_\tau \phi_\alpha)^2 + r \phi_\alpha^2 \right) + \frac{g}{4!} (\phi_\alpha^2)^2 \right]$$

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



Coupling g approaches fixed-point value under renormalization group flow: beta function ($\varepsilon = 3-d$) :

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

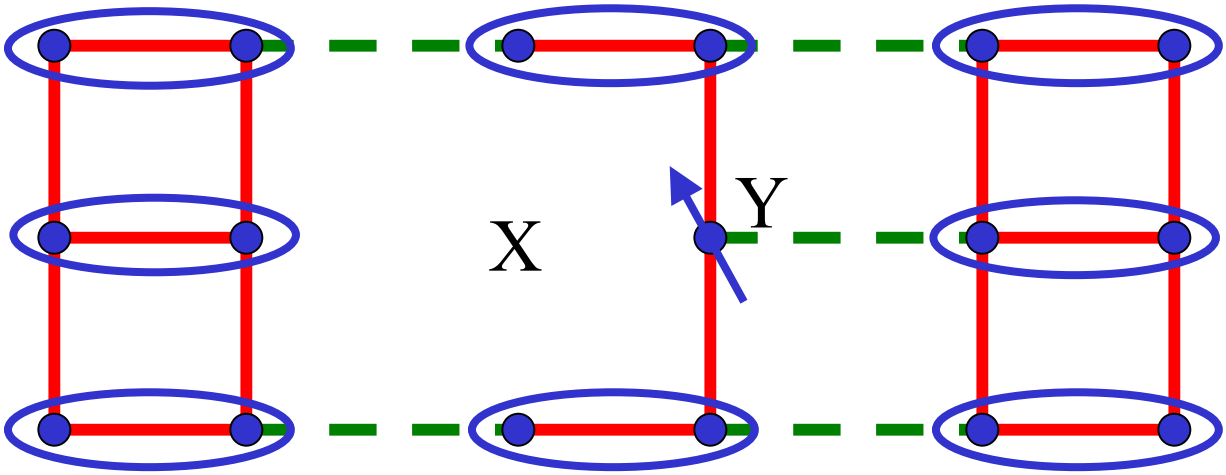
Only relevant perturbation – ***r***

strength is measured by the spin gap Δ

Δ and $c = \sqrt{c_x c_y}$ completely determine entire spectrum of quasi-particle peak and multiparticle continua, the S matrices for scattering between the excitations, and $T > 0$ modifications.

3. Quantum impurities in nearly-critical paramagnets

Make *any* localized deformation of antiferromagnet; e.g. remove a spin



Susceptibility $\chi = A\chi_b + \chi_{imp}$

(A = area of system)

In paramagnetic phase as $T \to 0$

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

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

$$\lim_{\tau\to\infty} \left\langle \vec{S}_Y(\tau) \cdot \vec{S}_Y(0) \right\rangle = m^2 \neq 0$$

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

Action of "impurity" spin

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

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

Boundary quantum field theory: $\mathcal{S}_b + \mathcal{S}_{\rm imp}$

Recall -

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

Coupling γ approaches *also* approaches a fixed-point value under the renormalization group flow

(Sengupta, 97
Sachdev+Ye, 93
Smith+Si 99)

Beta function:

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

No new relevant perturbations on the boundary;
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 !

Universal properties at the critical point $\lambda = \lambda_c$

$$\left\langle \vec{S}_Y(\tau) \cdot \vec{S}_Y(0) \right\rangle = \frac{1}{\tau^{\eta'}}$$

$$(\text{and } m = \left|\lambda - \lambda_c\right|^{\eta' \nu})$$

η' is a new boundary scaling dimension

Operator product expansion:

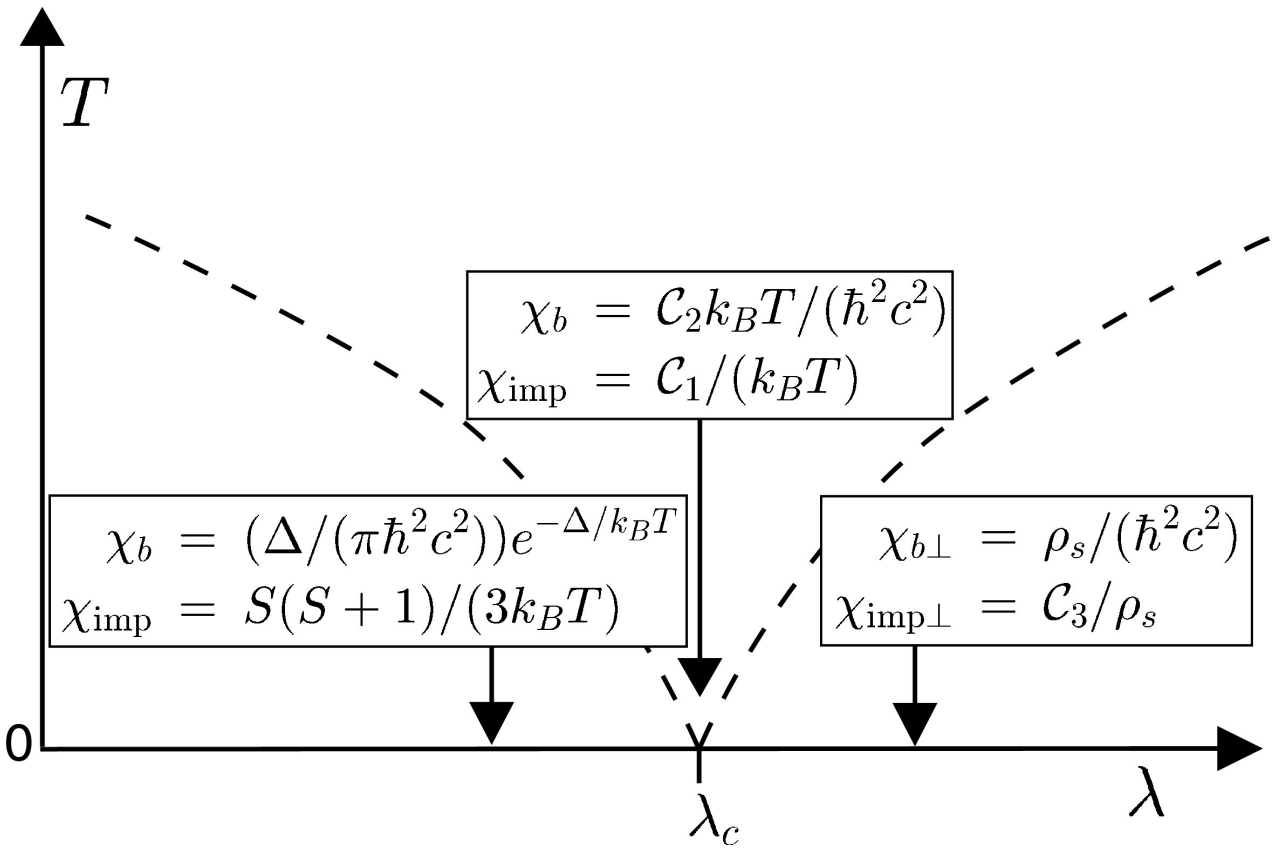
$$\lim_{x \to 0} \phi_\alpha(x, \tau) \sim \frac{n_\alpha(\tau)}{\left|x\right|^{(d-1+\eta-\eta')/2}}$$

However $$\chi_{imp} \neq \frac{1}{T^{1-\eta'}}$$

This last relationship holds in the multi-channel Kondo problem because the magnetic response of the screening cloud is negligible due to an exact "compensation" property. There is no such property here, and naïve scaling applies. This leads to

$$\chi_{imp} = \frac{\text{Universal number}}{k_B T}$$

Curie response of an irrational spin



In the Neel phase

$$\chi_{imp\perp} = \frac{\text{Universal number}}{\text{spin stiffness}}$$

$$\text{spin stiffness } \rho_s = \left(\rho_{sx}\rho_{sy}\right)^{1/2}$$

Bulk susceptibility vanishes while impurity susceptibility diverges as $\rho_s \to 0$

At $T > 0$, thermal averaging leads to

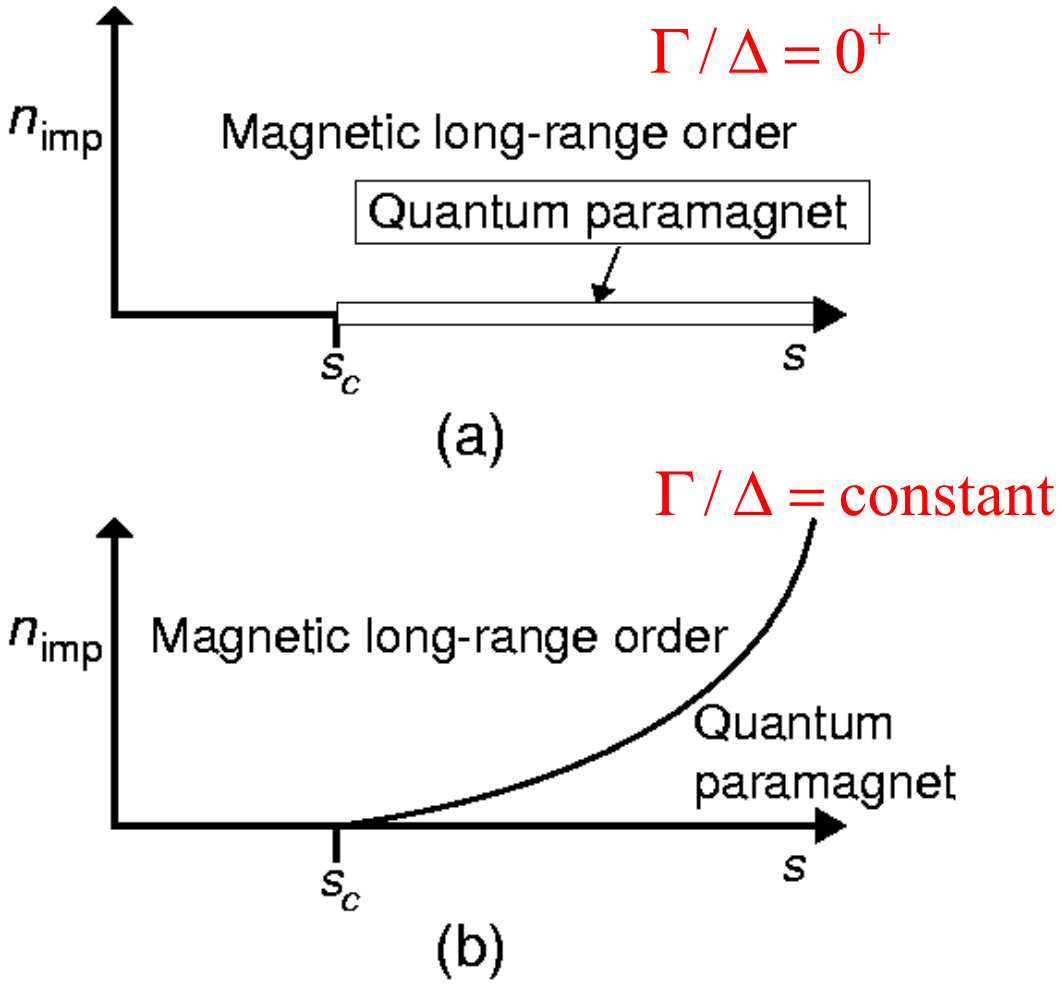
$$\chi_{\rm imp} = \frac{S^2}{3k_B T} + \frac{2}{3}\chi_{{\rm imp}\perp}$$

Finite density of impurities n_{imp}

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

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

Two possible phase diagrams

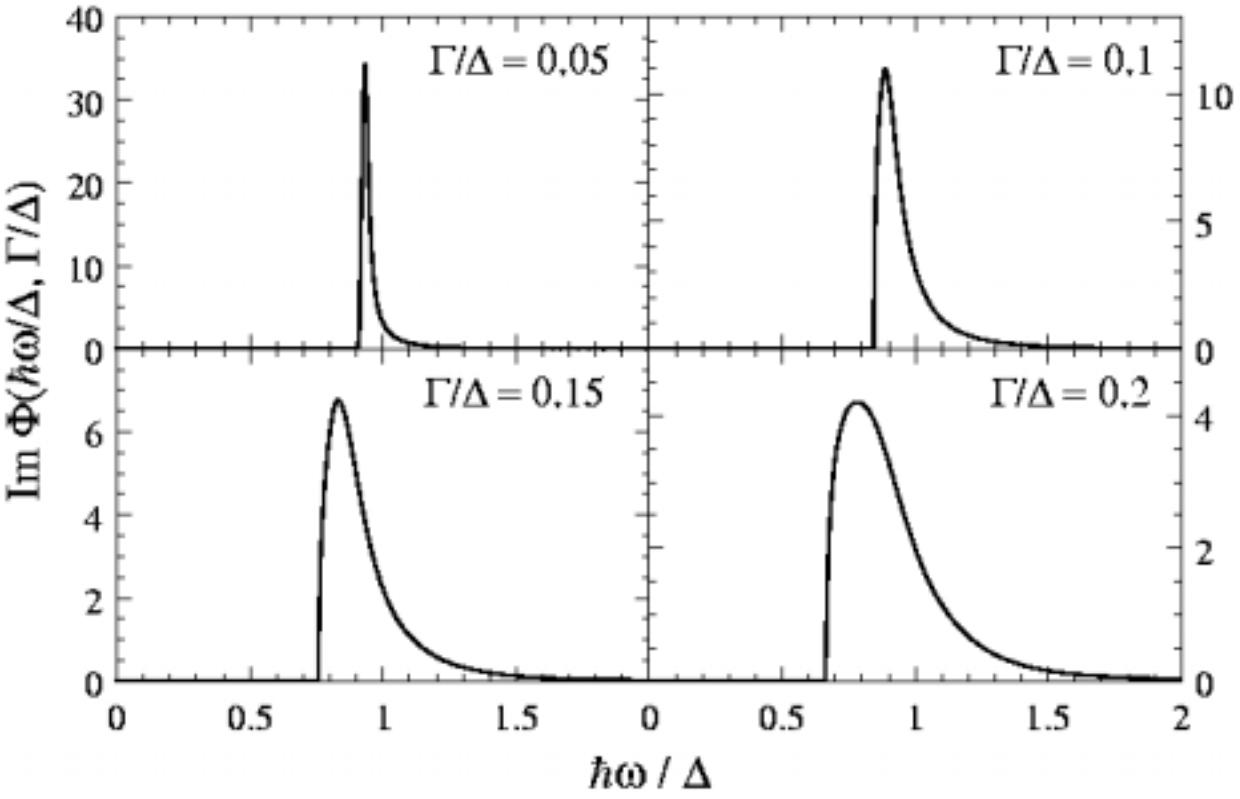


Fate of collective mode peak

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

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

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



Predictions: Half-width of line $\approx \Gamma$

Universal asymmetric lineshape

4. Application to d-wave superconductors and experiments on YBCO

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

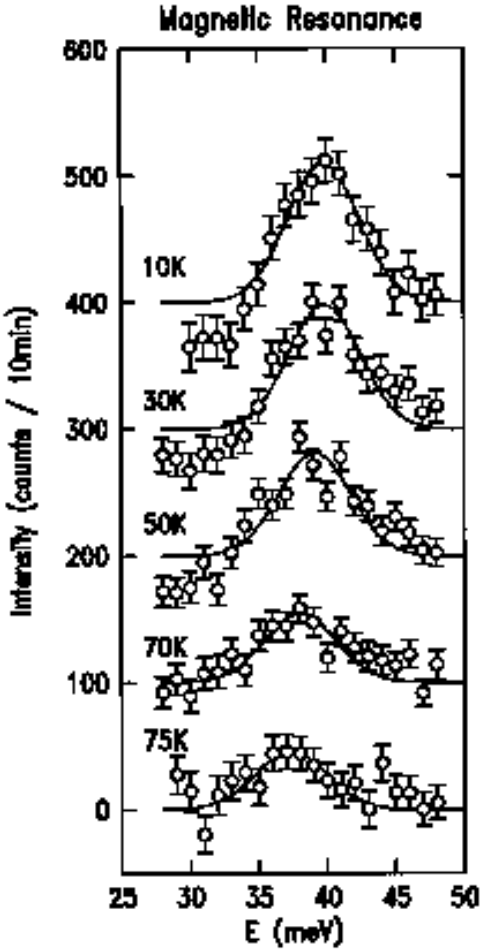
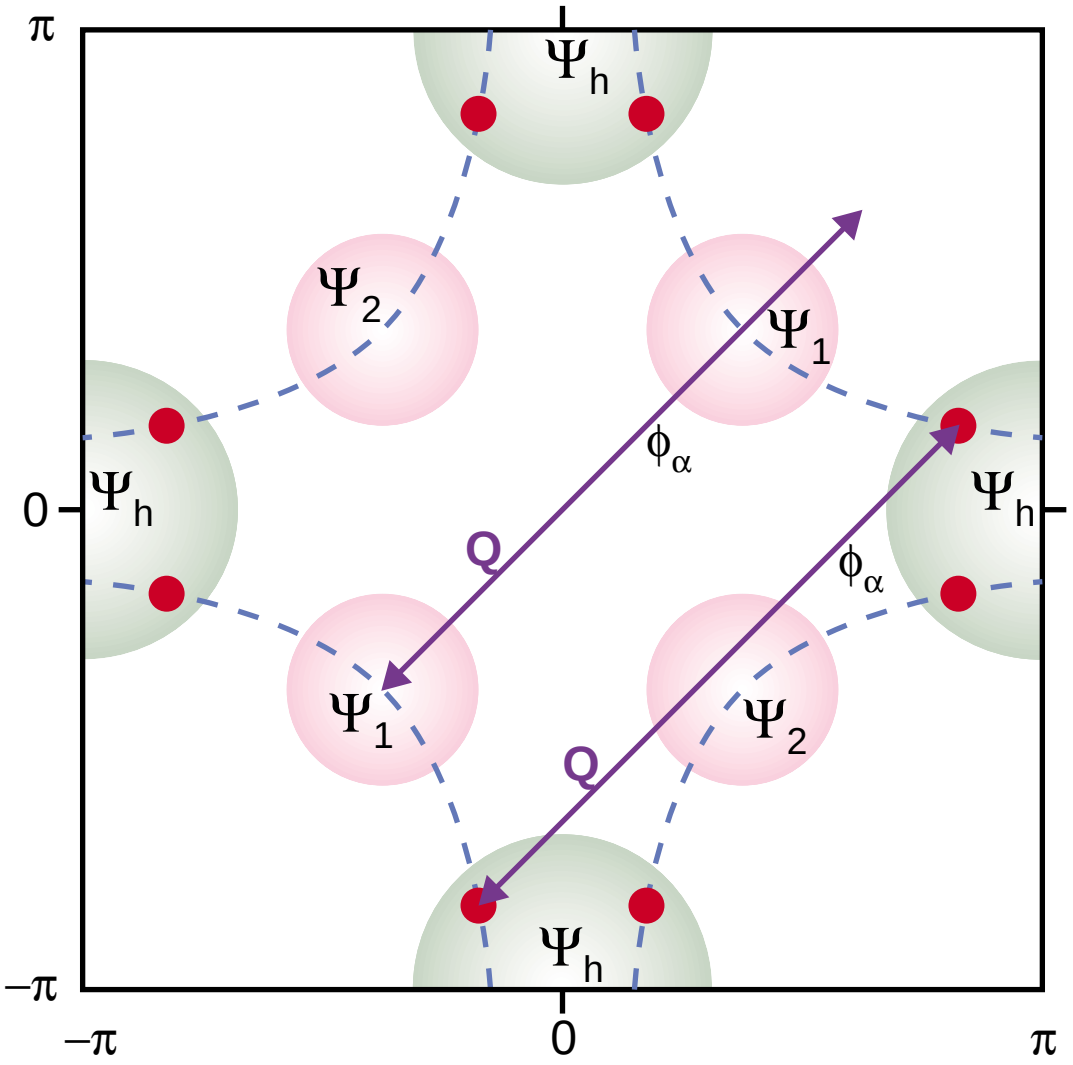


FIG. 8. Unpolarized beam, constant-Q data [Q=(3/2,1/2,−1.7)] of the 40 meV magnetic resonance obtained by subtracting the signal below T_c from the T=100 K background. The lines are fits to Gaussians, as described in the text. For clarity successive scans are offset by 100.

Spin-1 collective mode in $YBa_2Cu_3O_7$- little observable damping at low T.

coupling to superconducting quasiparticles unimportant, and spin correlations in some regions of phase space are like those of a (nearly-critical ?) paramagnet

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

As $\Delta \to 0$ there is a quantum phase transition to a magnetically ordered state

(A) Insulating Neel state (or collinear SDW at wavevector **Q**) $\Longleftrightarrow$ insulating quantum paramagnet

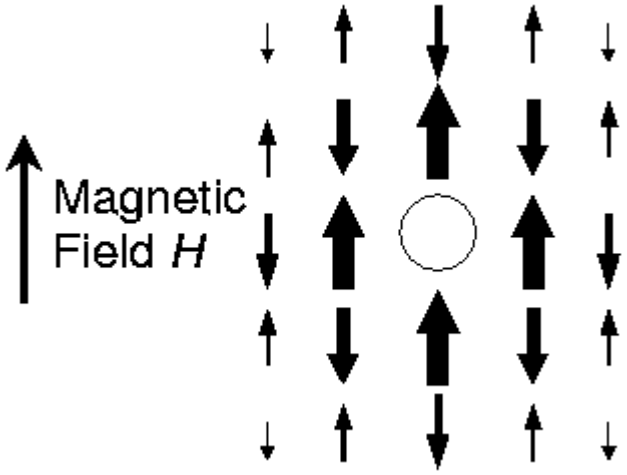
(B) *d*-wave superconductor with collinear SDW at wavevector **Q** $\Longleftrightarrow$ *d*-wave superconductor (paramagnet)

Transition (B) is in the same universality class as (A) provided Ψ_h fermions remain gapped at quantum-critical point.

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



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

Coupling of impurity to fermionic quasiparticles $\Psi_{1,2}$

$$\sum_r J_K(r) S\, n_\alpha \Psi^\dagger(r) \sigma^\alpha \Psi(r) + U \Psi^\dagger(0)\Psi(0)$$

Kondo couplings

Potential scattering

(Many works (*e.g.* Pepin and Lee, Salkola, Balatasky and Scalapino) have ignored impurity spin and treated and effective potential scattering model with $U \to \infty$; we take U finite and include Kondo resonance effects)

Because density of states vanishes linearly at the Fermi level, there is no Kondo screening for any finite J_K (below a finite J_K) with (without) particle-hole symmetry

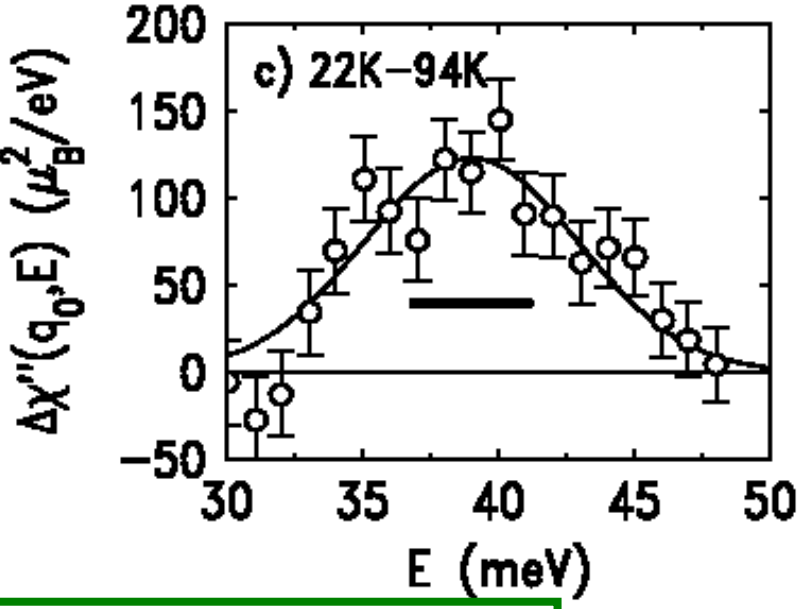
(Withoff+Fradkin, Chen+Jayaprakash, Buxton+Ingersent)

Our theory applies for $\Delta > T_K$

Implications of impurity spin for STM experiments: A. Polkovnikov, S. Sachdev and M. Vojta, to appear

$YBa_2Cu_3O_7 + 0.5\%\ Zn$

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)



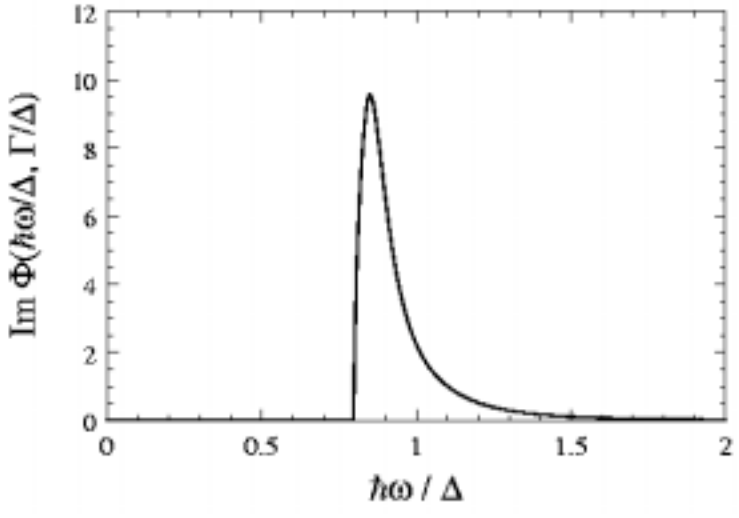
$$n_{\text{imp}} = 0.005$$

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

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

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

Quoted half-width = 4.25 meV



Conclusions

1. Universal $T=0$ damping of S=1 collective mode by non-magnetic impurities.

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

   independent of impurity parameters.

2. New interacting boundary conformal field theory in 2+1 dimensions

3. Universal irrational spin near the impurity at the critical point.