Quantum phase transitions in two-dimensional antiferromagnets and superfluids

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1. Simple model of a quantum phase transition ---
   coupled-ladder antiferromagnet

2. Collective dynamics at low temperatures
   A. Quasiclassical waves
   B. Quasiclassical particles
      Application to one-dimensional gapped antiferromagnets

3. A global phase diagram for doped antiferromagnets and application to the cuprate superconductors.
   A. Magnetic order- paramagnet transitions in insulating square lattice antiferromagnets.
   B. A phase diagram for doped antiferromagnets.

C. Quantum phase transitions

(a) Magnetic order

(b) charge order

D. Experimental implications

4. Quantum impurity in a nearly-critical antiferromagnet ---

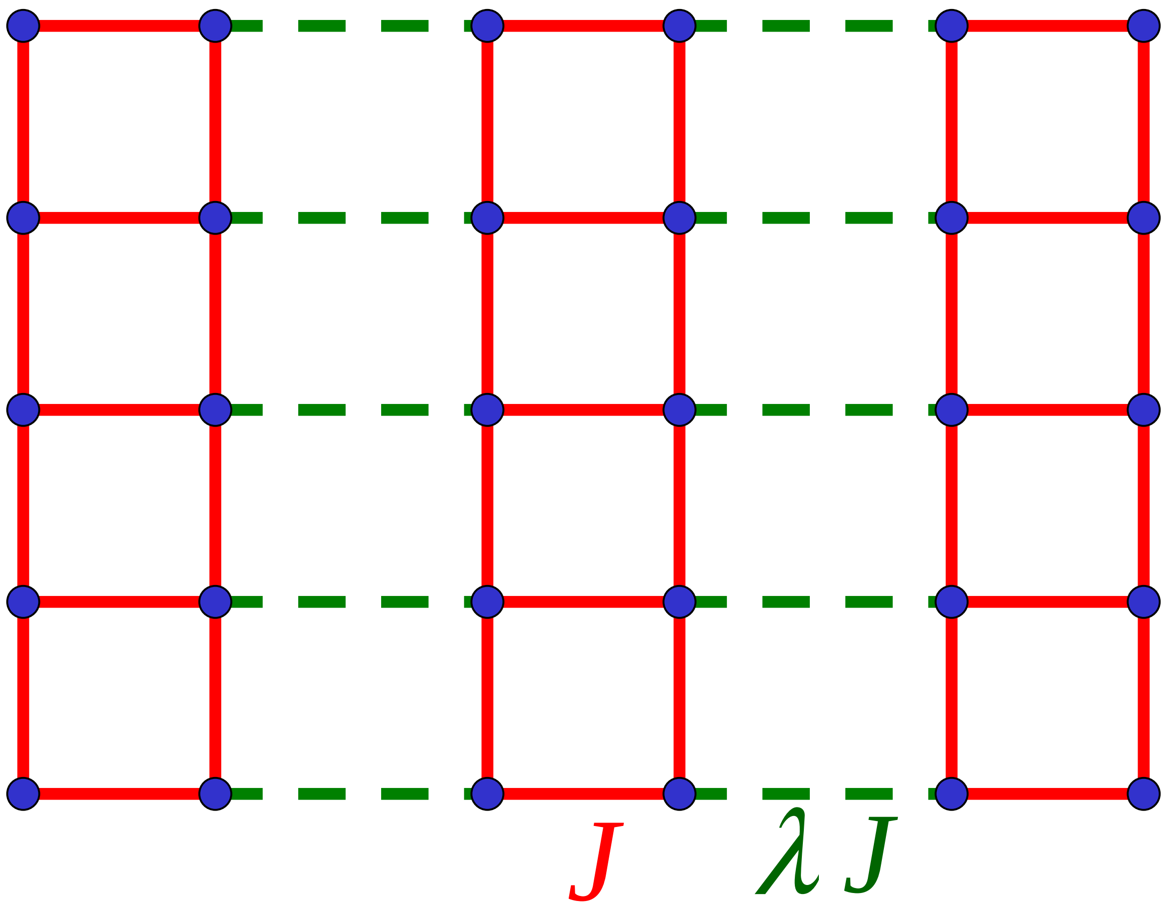
localized excitation with an

irrational spin

Applications to double-layer quantum Hall systems and the superconductor-insulator transition.

1. A simple theoretical model

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



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

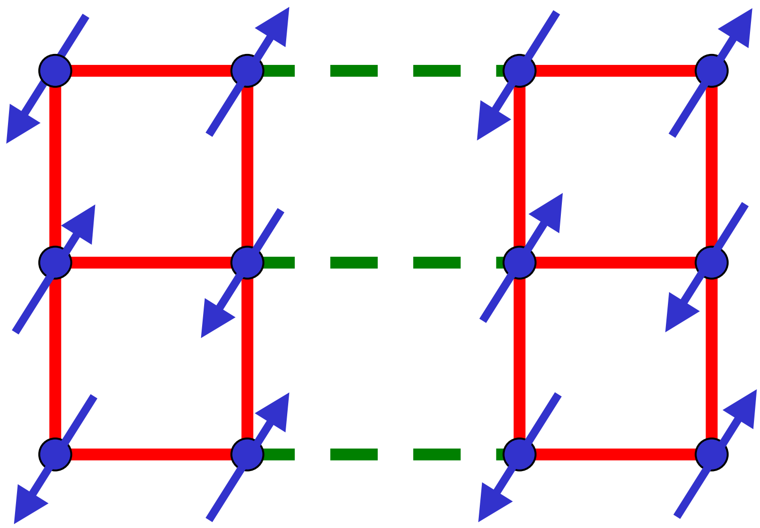
Follow ground state as a function of λ

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

$\lambda = 1$

Square lattice antiferromagnet

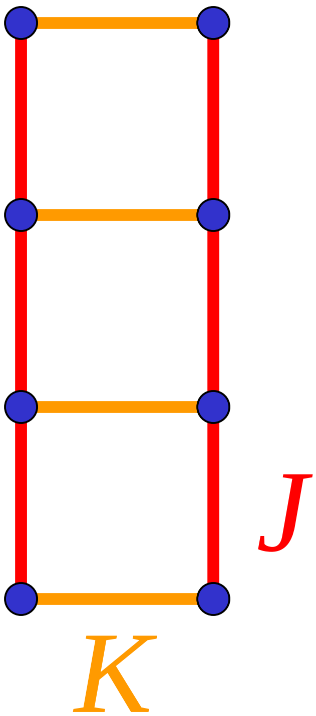
Experimental realization: La_2CuO_4



Ground state has long-range magnetic (Neel) order

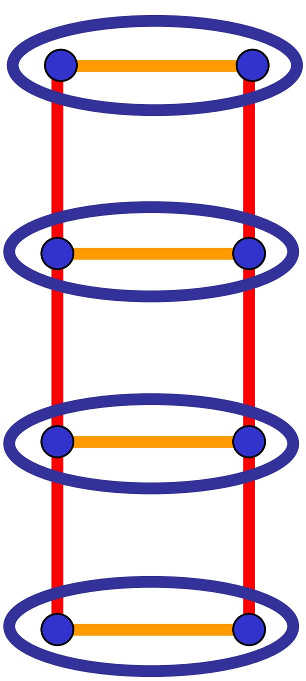
$$\left\langle \vec{S}_i \right\rangle = \left(-1\right)^{i_x + i_y} N_0 \neq 0$$

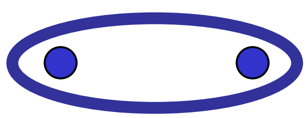
$\lambda = 0$



Decoupled 2-leg ladders

Allow $J \neq K$



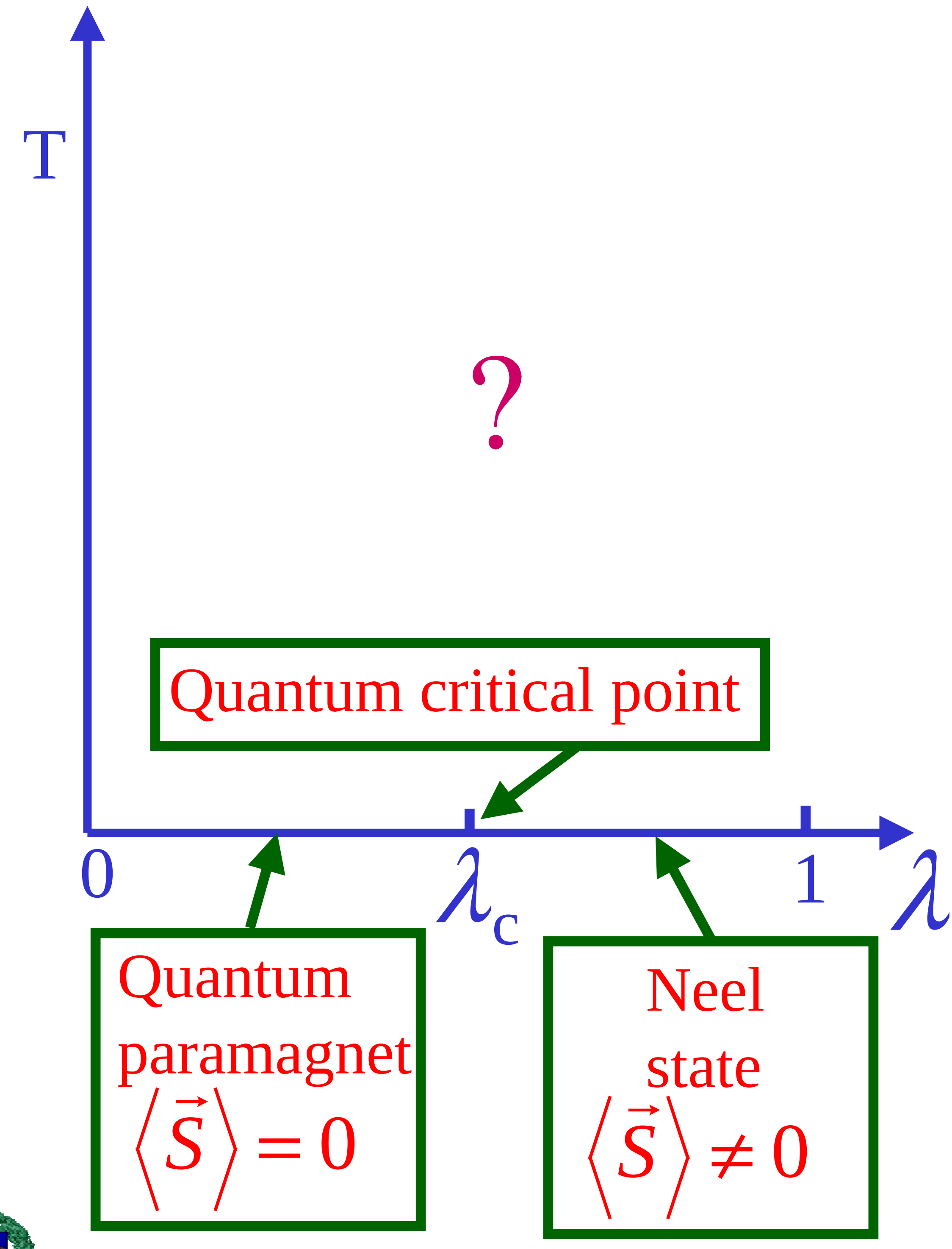
 $= \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle \right)$

Quantum paramagnet ground state for

$J \ll K$

Qualitatively similar ground state for all

J / K


T
?
Quantum critical point
0
λ_c
1
λ
Quantum paramagnet
$\langle \vec{S} \rangle = 0$
Neel state
$\langle \vec{S} \rangle \neq 0$

2. Collective dynamics for T>0

A. Neel state

Excitations: 2 spin waves

Correlation length (ξ)

~ typical spin wave wavelength

~ $\exp\left(2\pi\rho_s / k_B T\right)$

$\rho_s \rightarrow$ Spin stiffness

Typical spin wave energy

~ $\hbar c/\xi \ll k_B T$

Mode occupation number

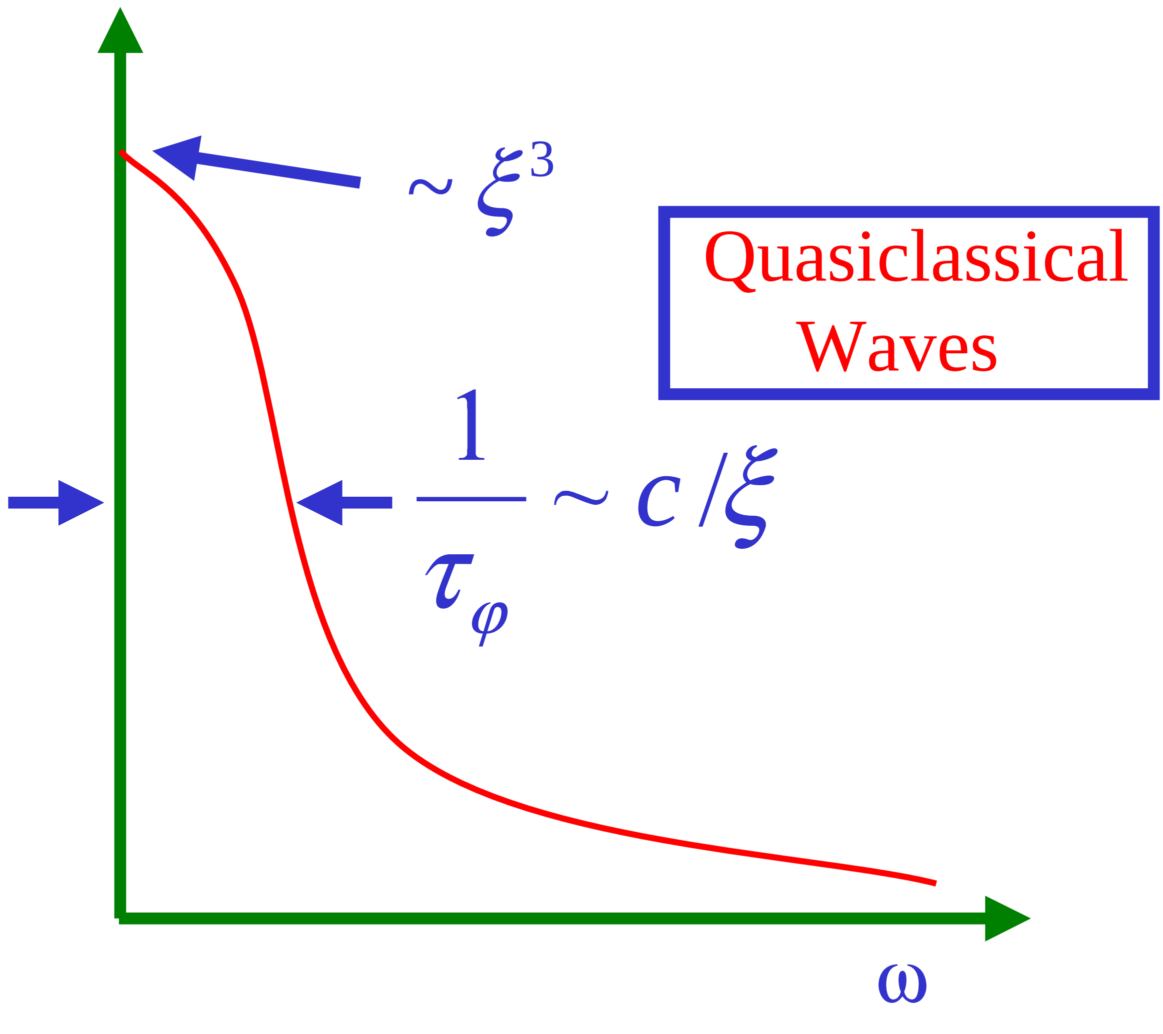
$1/\left(\exp\left(\varepsilon / k_B T\right) - 1\right) \gg 1$

→ Quasiclassical waves

(Chakravarty et al, 1989)

Dynamic Structure Factor at antiferromagnetic wavevector

$S(\pi,\omega)$

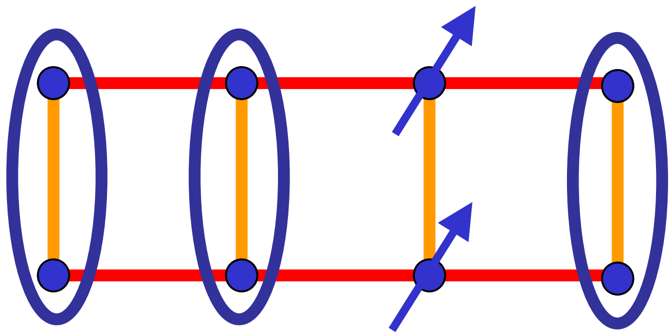


Angular or “phase” relaxation

2. Collective dynamics for T>0

B. Quantum paramagnet

Excited states



Triplet (S=1) particle

Energy dispersion away from antiferromagnetic wavevector

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

$\Delta \rightarrow$ Energy gap

All low T dynamic correlations are universal functions of Δ and c

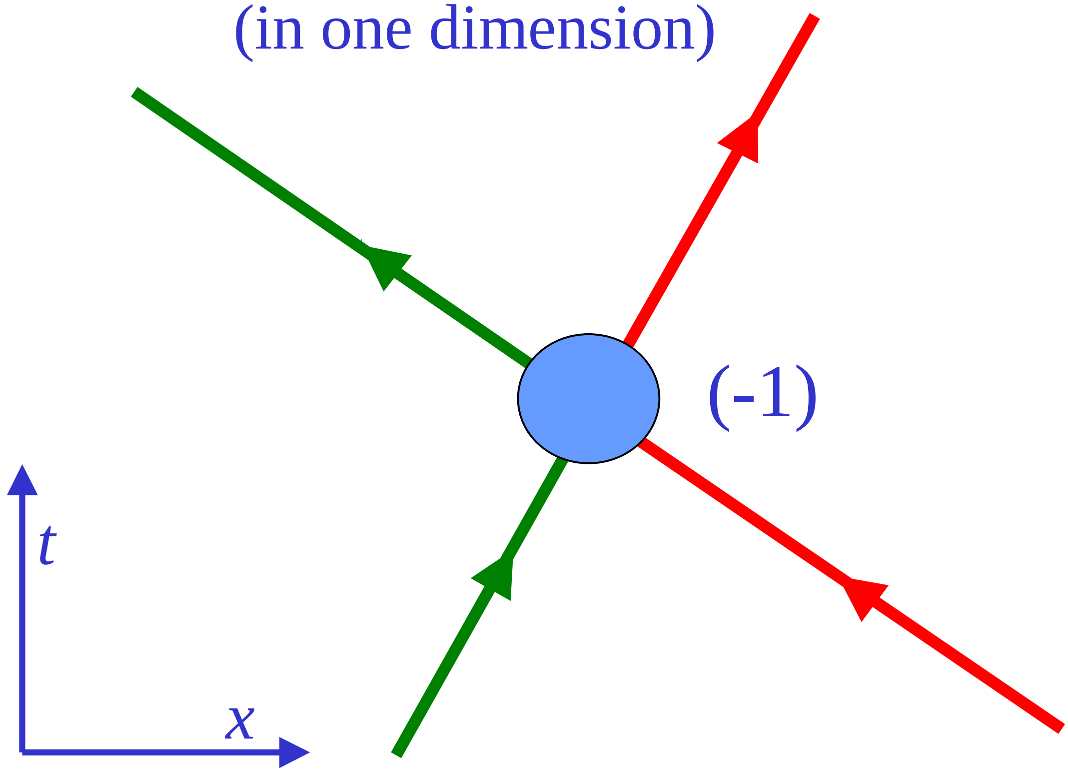
Key Observations

1. De Broglie wavelength $\sim \dfrac{\hbar c}{\sqrt{\Delta k_B T}}$

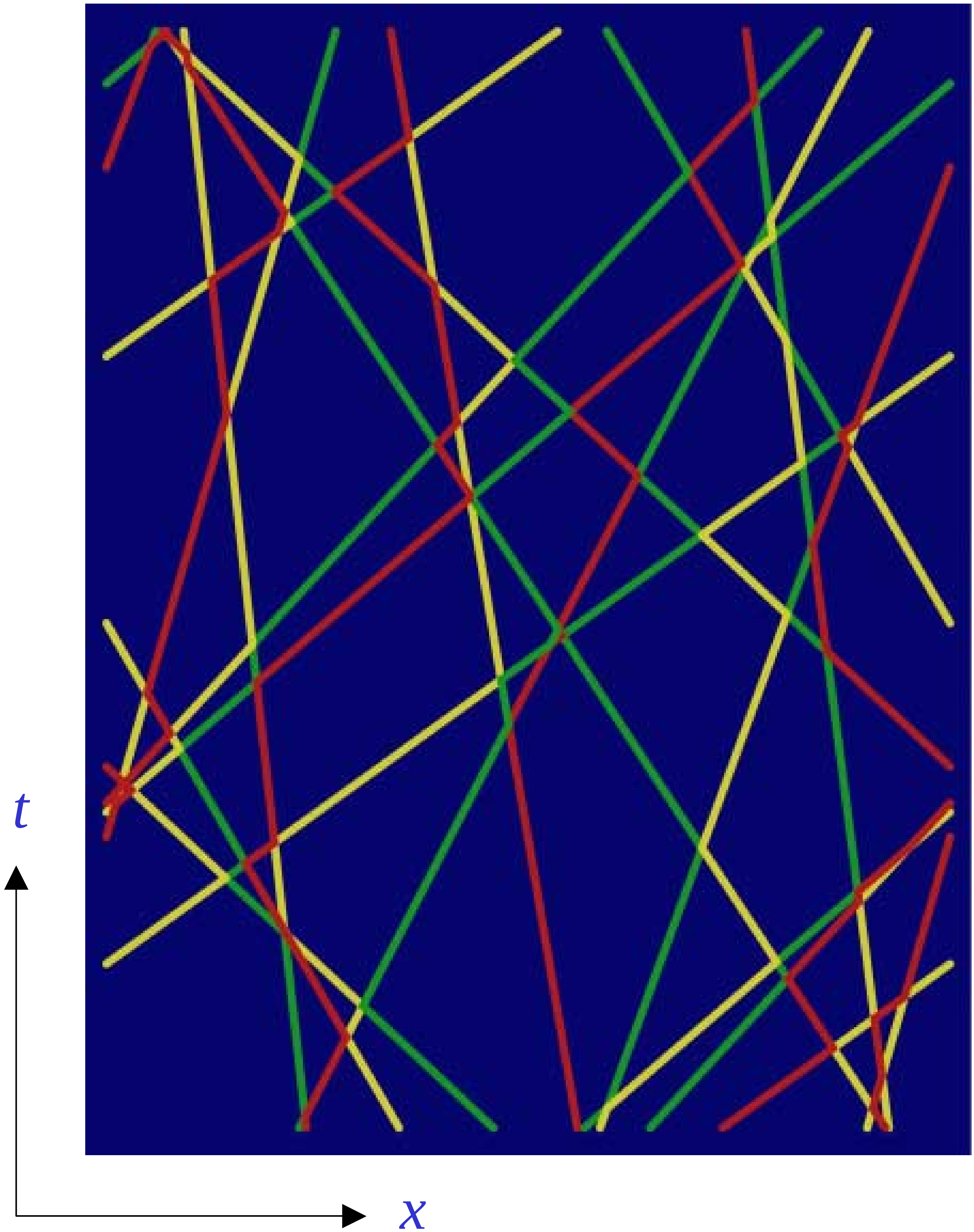
$<<$ interparticle spacing $\sim e^{\Delta / k_B T}$

(Quasiclassical particles)

2. Quantum mechanical S-matrix
has a super-universal form at low momenta
(in one dimension)

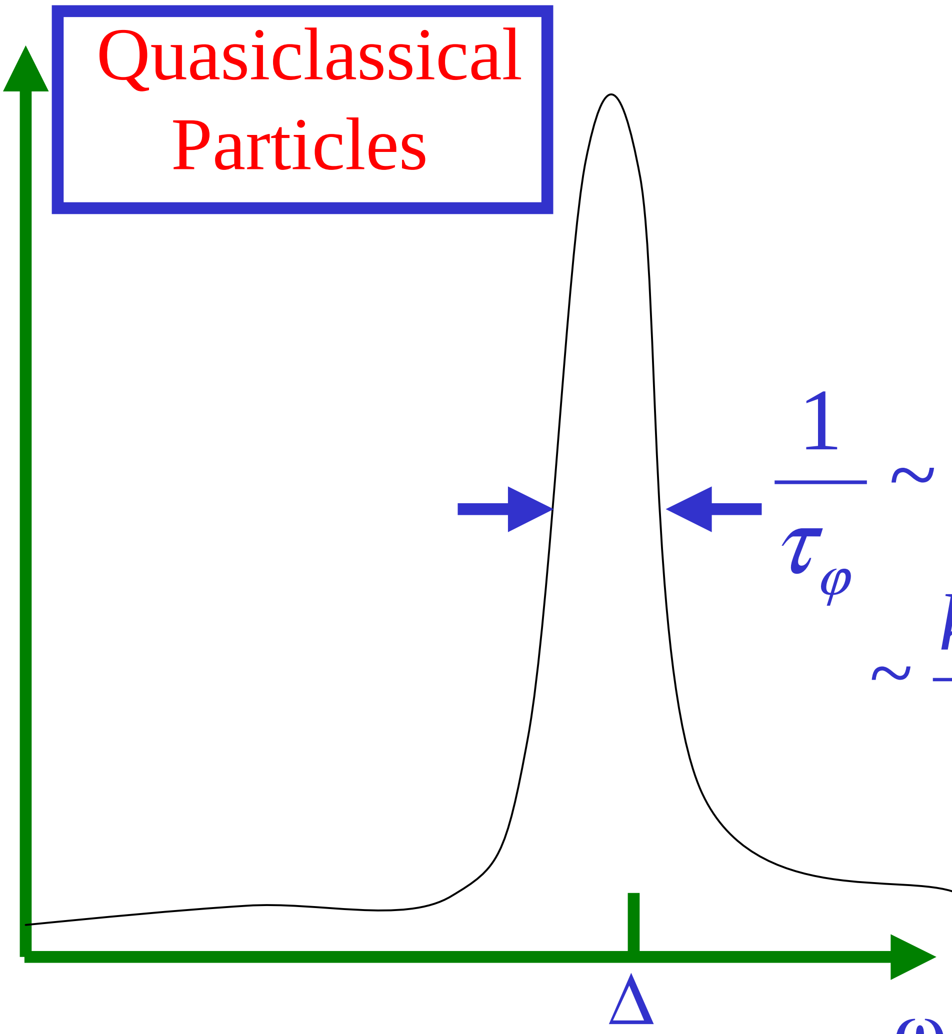


Spins bounce while
momenta exchange


t
x

Dynamic Structure Factor at antiferromagnetic wavevector

$S(\pi,\omega)$

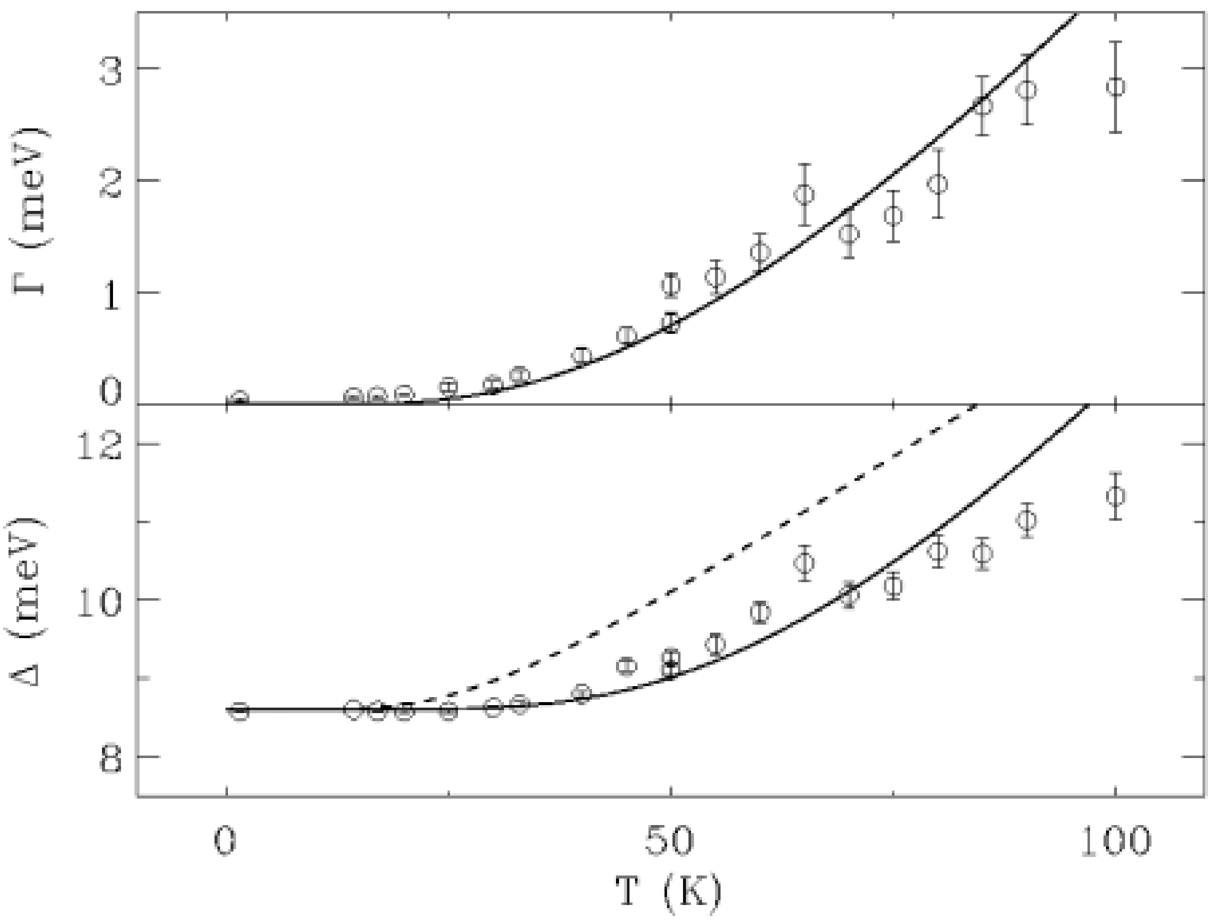


$$\frac{1}{\tau_\varphi} \sim \text{collision rate} \sim \frac{k_B T}{\hbar} e^{-\Delta / k_B T}$$

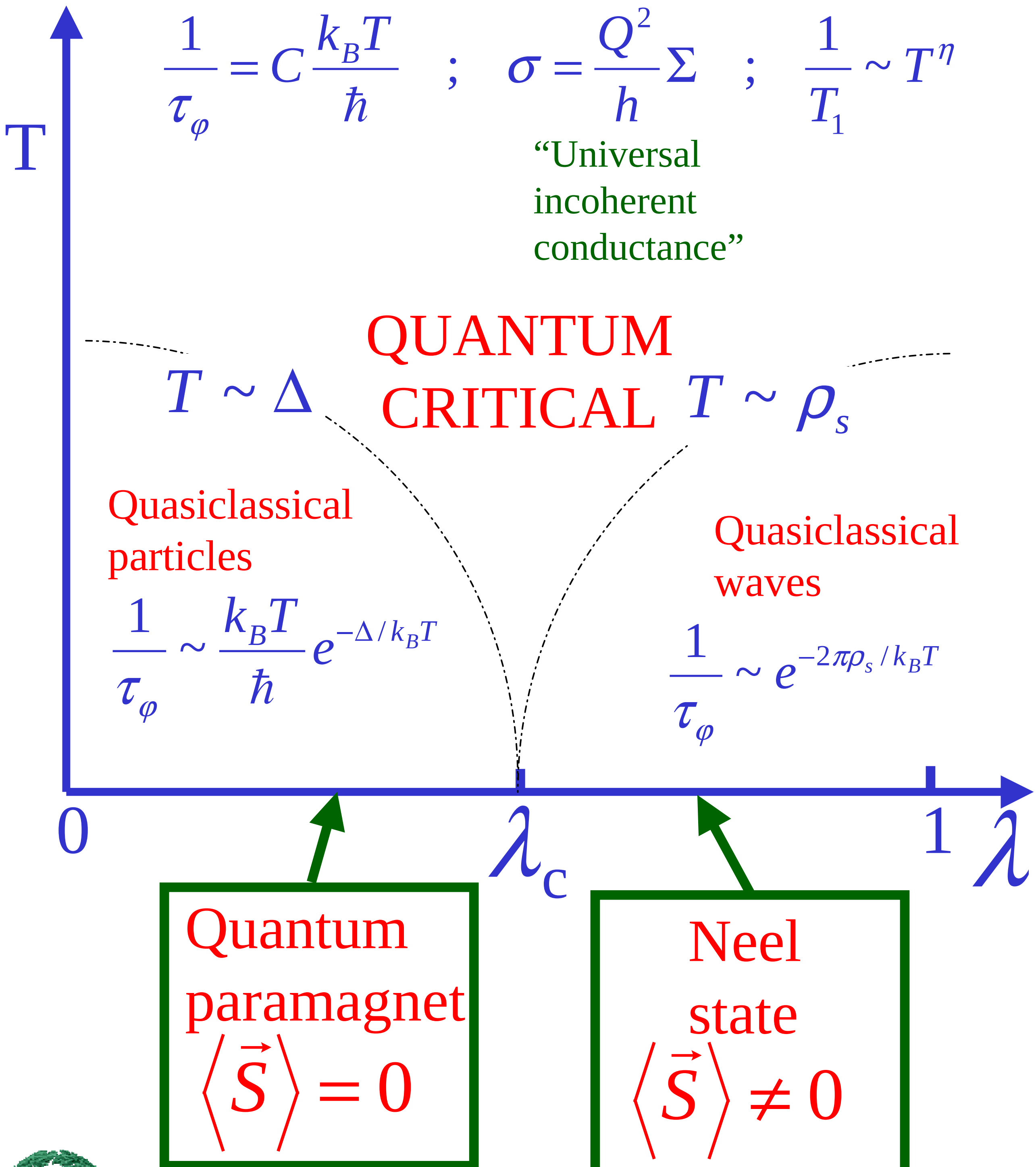
Particles are quantum lumps of "amplitude oscillation" of anti-ferromagnetic order parameter

Excitation energy Δ and linewidth Γ for Y_2BaNiO_5

C. Broholm et al. (unpublished)



Solid line for Γ – theory with no free parameters



$\frac{1}{\tau_\varphi} = C\frac{k_B T}{\hbar}$; $\sigma = \frac{Q^2}{h}\Sigma$; $\frac{1}{T_1} \sim T^\eta$
"Universal incoherent conductance"
T
QUANTUM CRITICAL
$T \sim \Delta$
$T \sim \rho_s$
Quasiclassical particles
$\frac{1}{\tau_\varphi} \sim \frac{k_B T}{\hbar} e^{-\Delta / k_B T}$
Quasiclassical waves
$\frac{1}{\tau_\varphi} \sim e^{-2\pi\rho_s / k_B T}$
0
λ_c
1
λ
Quantum paramagnet
$\langle \vec{S} \rangle = 0$
Neel state
$\langle \vec{S} \rangle \neq 0$

3. A global phase diagram for doped antiferromagnets and application to the cuprate superconductors

(M. Vojta and S.S., Phys. Rev. Lett. in press)

Extended t-J model on the square lattice

$$H = \sum_{i>j} \left[-t_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} + J_{ij} \vec{S}_i \cdot \vec{S}_j + V_{ij} n_i n_j \right]$$

Plot phase diagram of stable ground states as a function of:

(1) Doping δ

(2) Frustration $\dfrac{J_2 \text{ (second neighbor)}}{J_1 \text{(first neighbor)}}$

OR

N, where spin symmetry

$$SU(2) \rightarrow Sp(N)$$

Method and partial results on phase diagram:
S. Sachdev and N. Read, Int. J. Mod. Phys. B **5**, 219 (1991).

Ground states are fully characterized by the manner in which symmetries are broken:

1. S - electromagnetic *U(1)*

2. M – magnetic *Sp(N)*

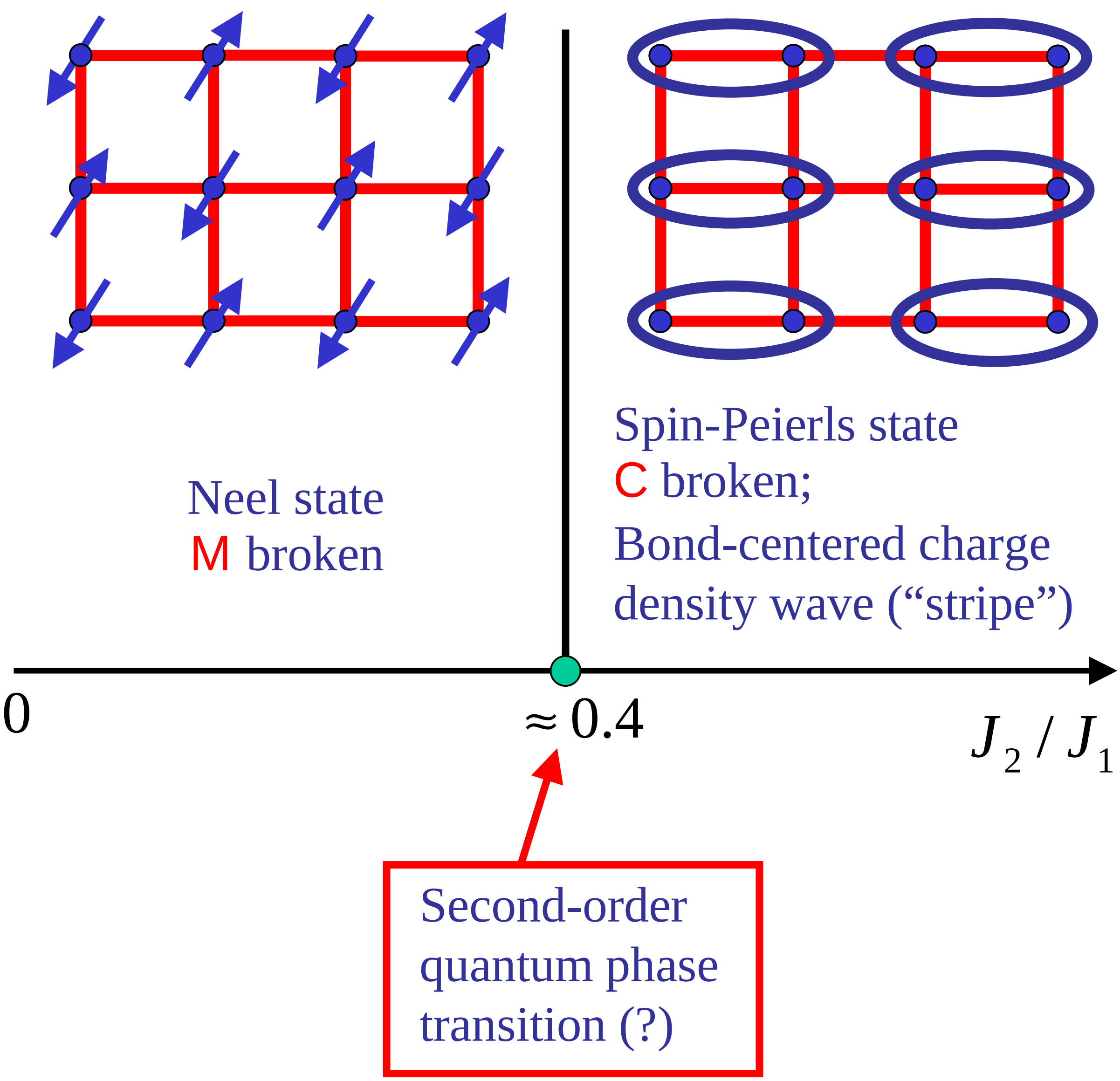
3. C – lattice translations are reflections (must be broken by observables (like charge density) which are invariant under S and M)

e.g.
Neel state - breaks only M

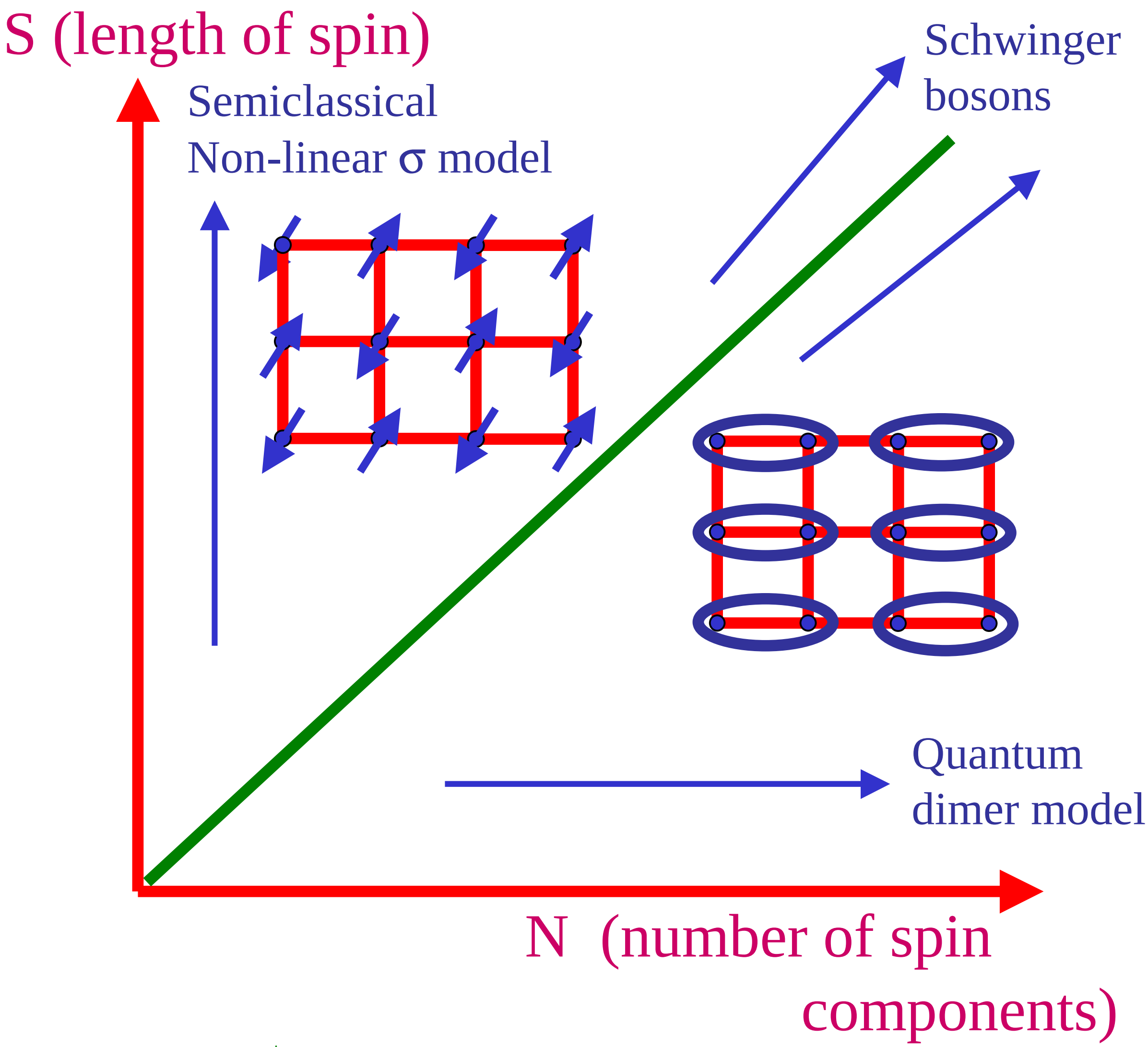
Incommensurate, collinear spin-density-wave - breaks M and C

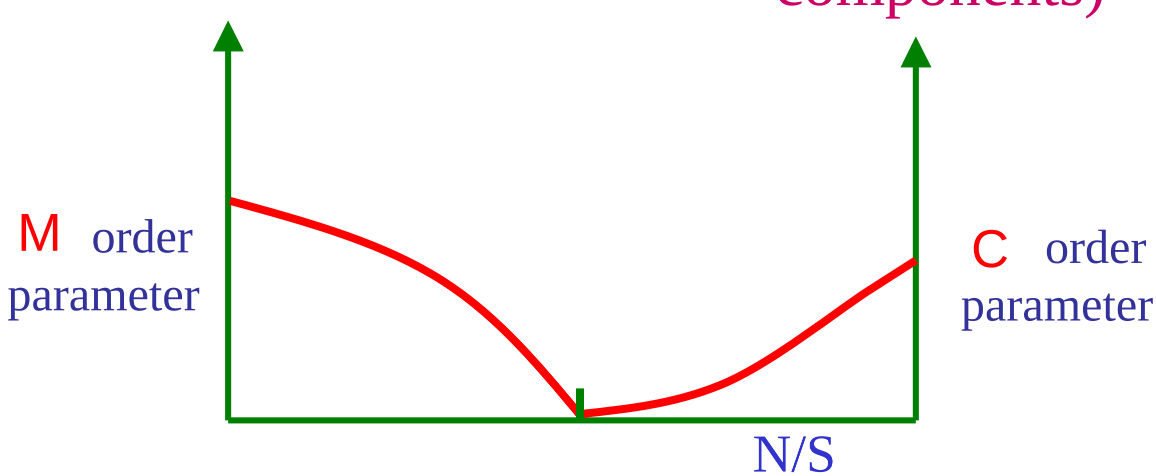
A. Magnetic order- paramagnet transitions in insulating square lattice antiferromagnets.

$\delta=0$

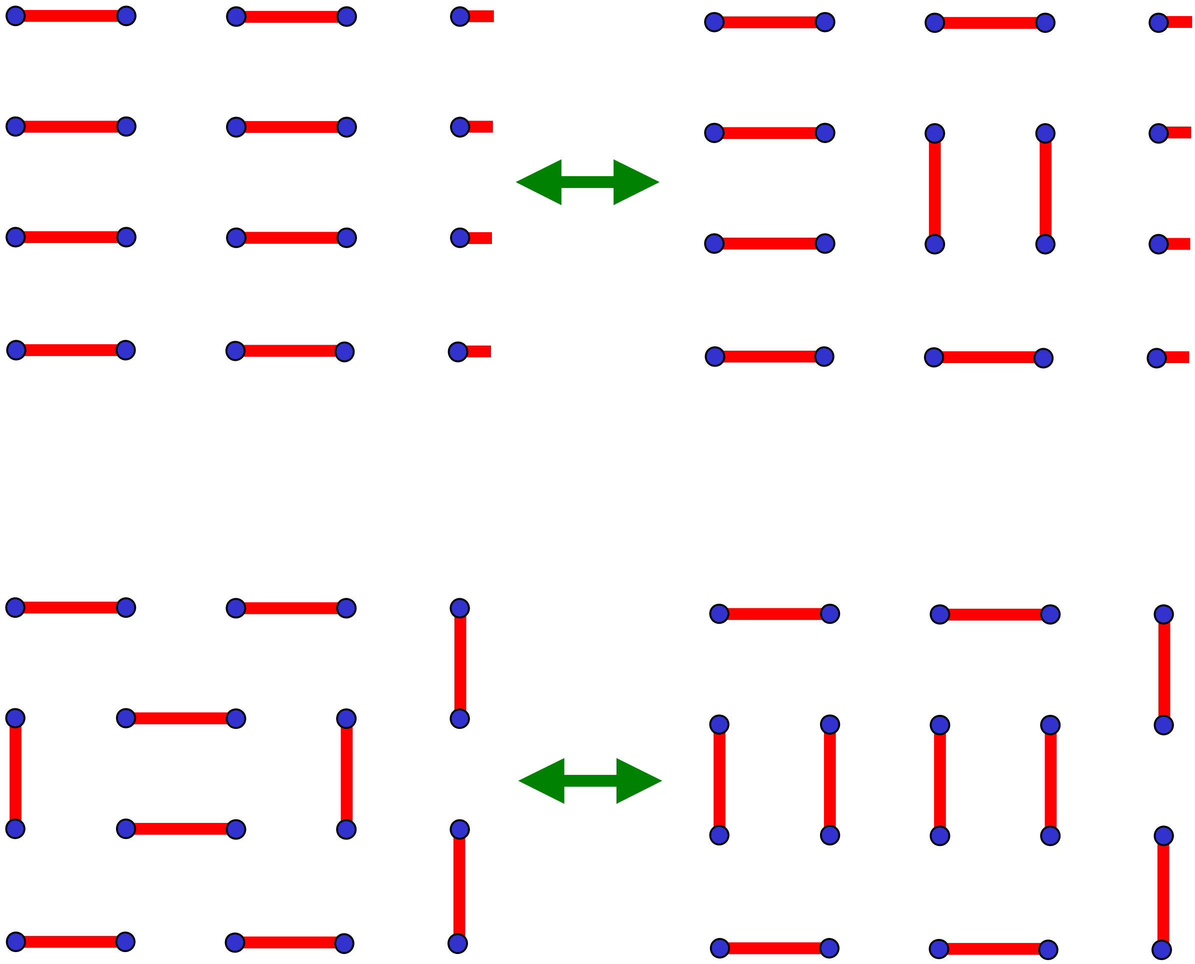


(Kotov et al cond-mat/9903154
Singh et al cond-mat/9904064)



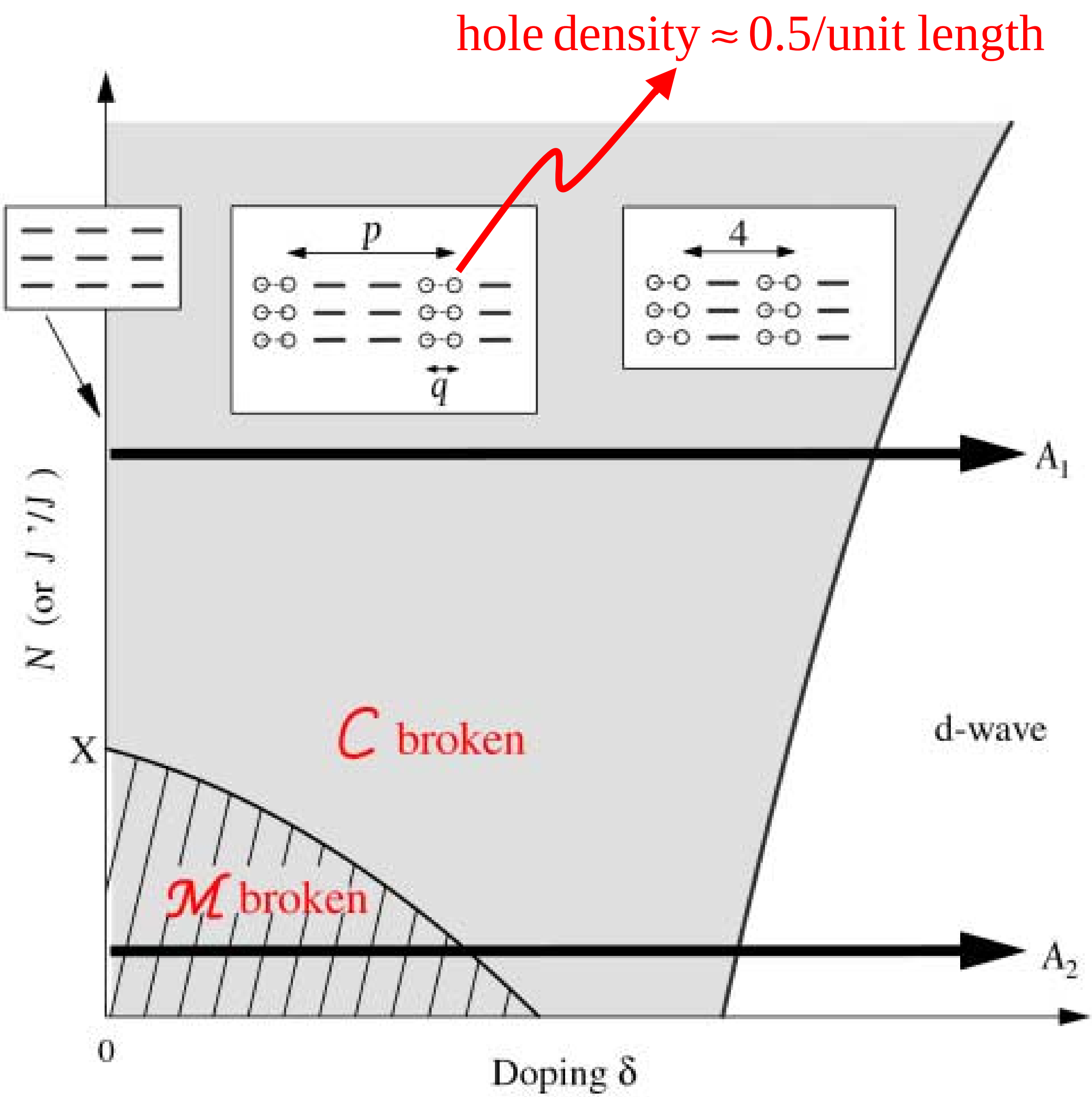


N. Read and S. Sachdev, Phys. Rev. Lett. **62**, 1694 (1989)
G. Murthy and S. Sachdev, Nucl. Phys. **B344**, 557 (1990)

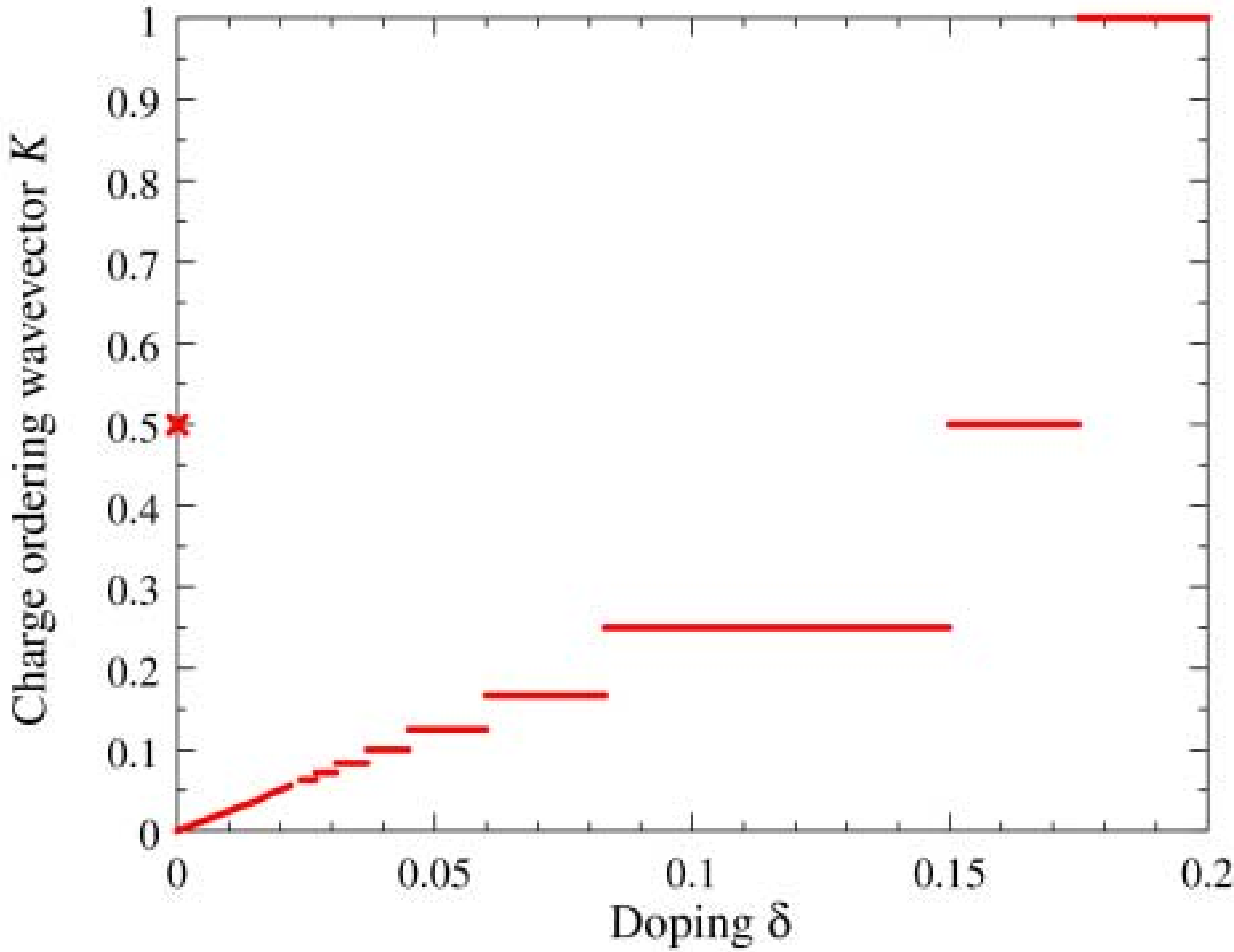


Quantum “entropic” effects prefer one-dimensional ordered structures

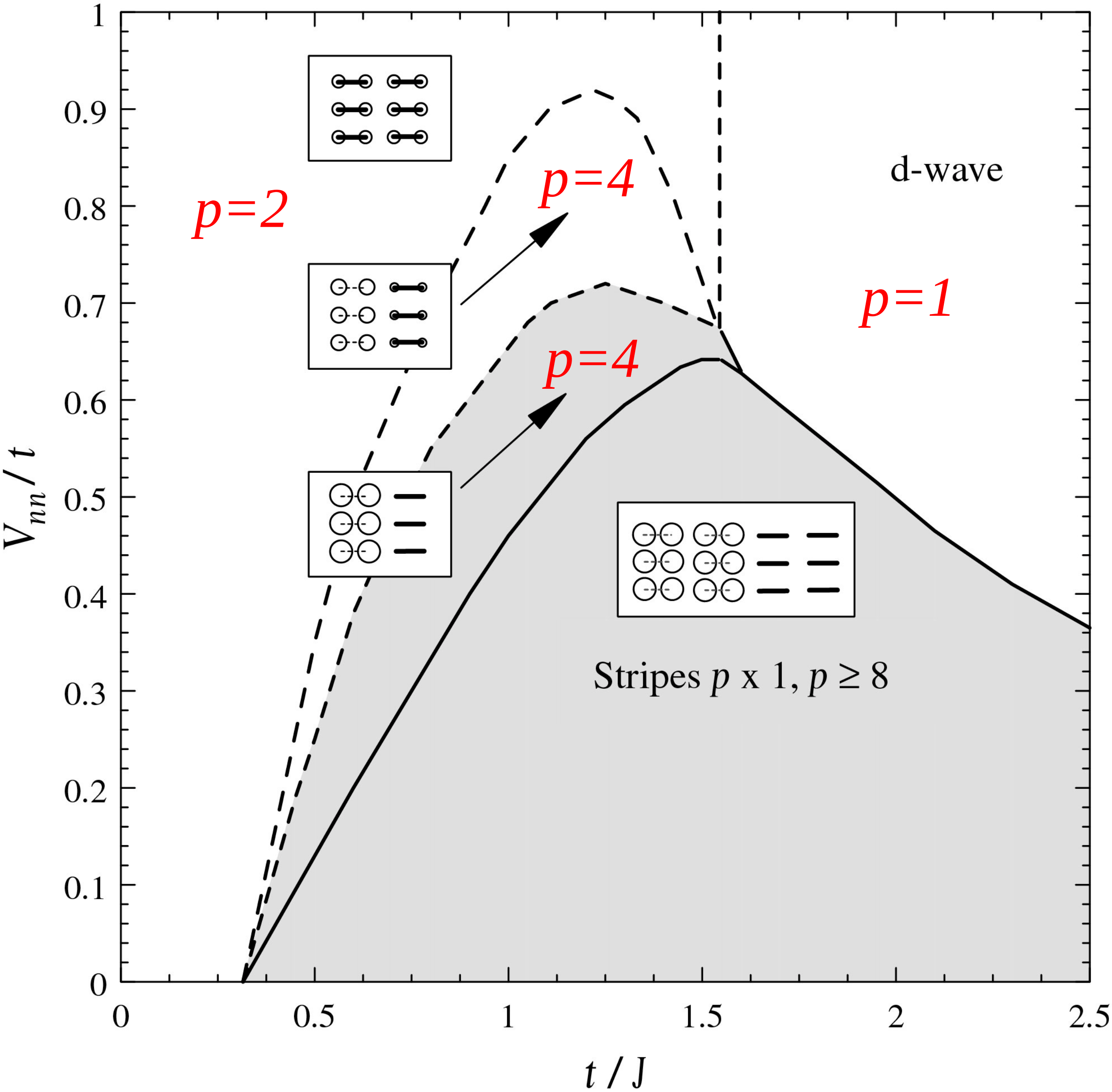
B. A phase diagram for doped antiferromagnets



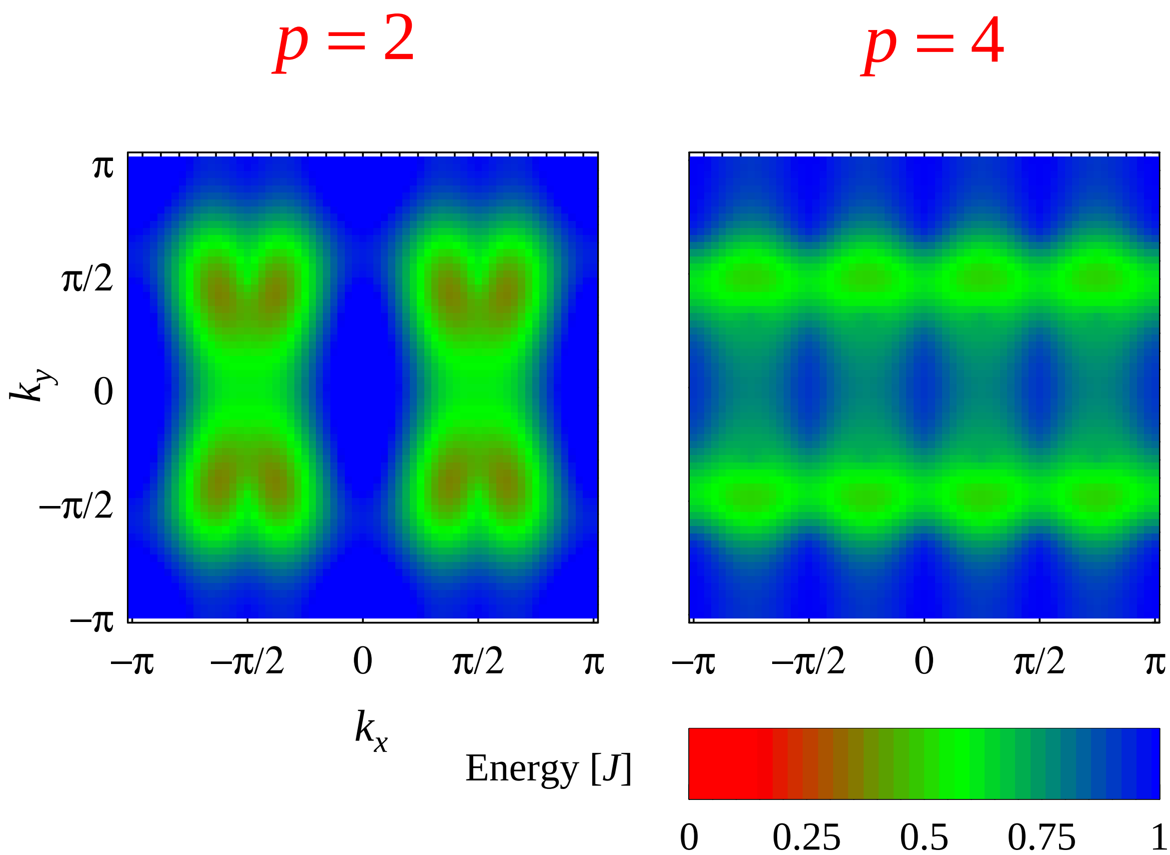
S broken for all $\delta > 0$, large N



Plateaus at 1/(even integer)



p=2
p=4
p=4
p=1
d-wave
Stripes p x 1, p ≥ 8
V_{nn} / t
t / J
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.5
1
1.5
2
2.5



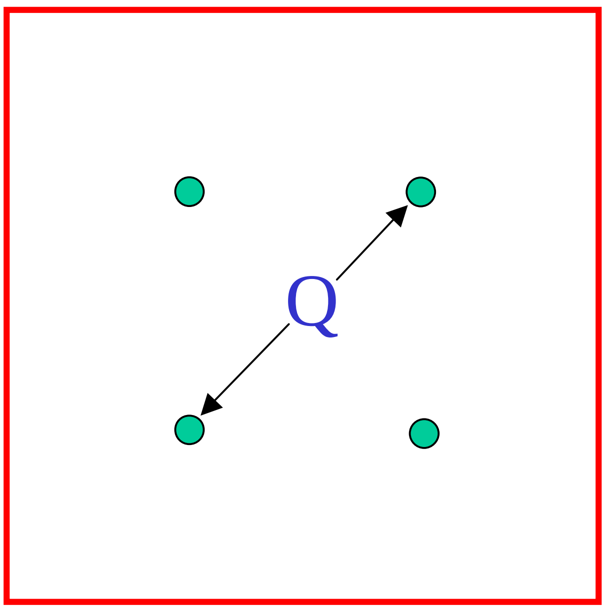
Fermion excitation energy at $\delta = 1/8$

C. Quantum phase transitions

(a) Onset of M ordering

Low energy excitations:

- Magnetic order parameter
- Gapless Fermi quasiparticles

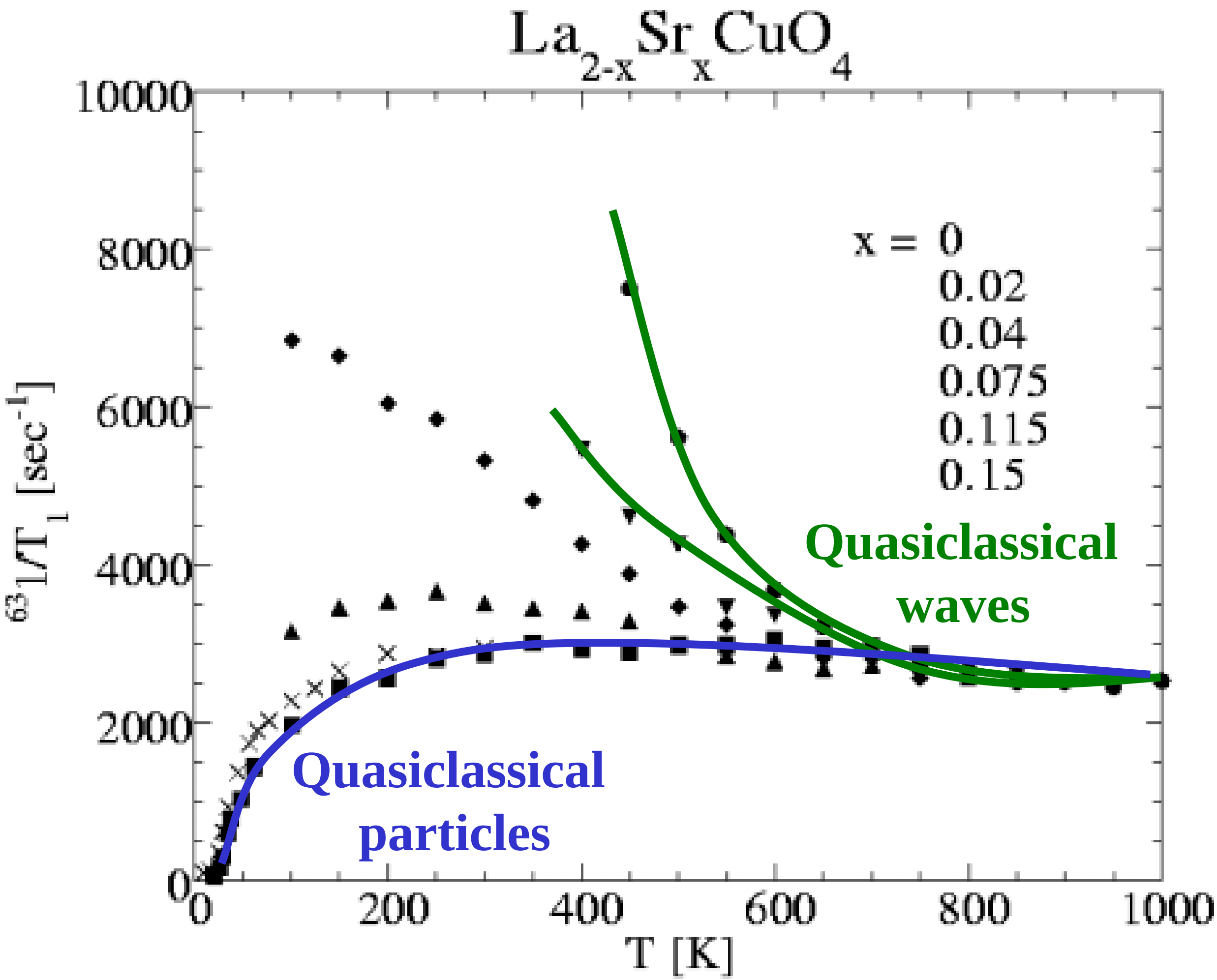


Gapless Fermi Points in a d-wave superconductor

If $Q \neq G$ (magnetic-ordering wavevector),or if fermion excitations are fully gapped, then magnetic ordering transition is identical to that at $\delta=0$, and described by the $O(3)$ non-linear σ model:

$$S = \int d^2x d\tau \left[\frac{1}{2g} \left(\partial_\mu \boldsymbol{n} \right)^2 \right] \quad ; \quad \boldsymbol{n}^2 = 1$$

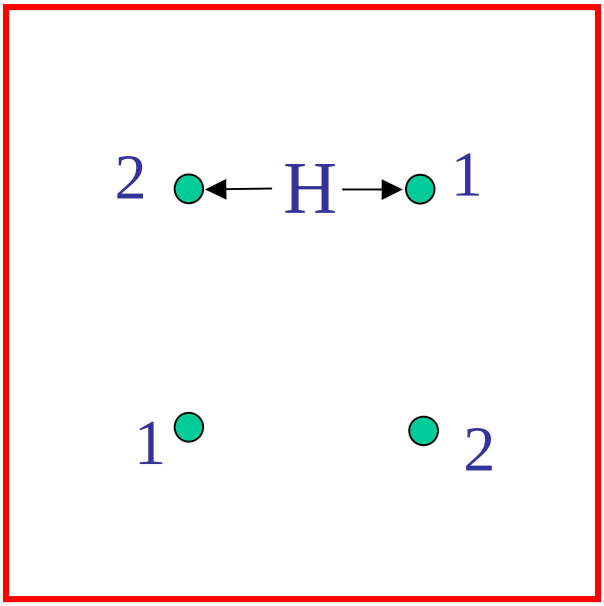
NMR measurements by Imai *et al*
Phys. Rev. Lett. **70**, 1002 (1993).



Particle ⟶ "resonance" peak in neutron scattering ?

(Rossat-Mignod, Mason, Keimer…)

(b) Onset of C ordering



Gapless Fermi Points in a d-wave superconductor

If H = K (charge-ordering wavevector), quantum transition is described by a theory of

4 “Dirac” fermions: $\psi_{1\alpha}$, $\psi_{2\alpha}$

2 complex scalars (amplitude of charge density wave at wavevector K): Φ_x , Φ_y

$$S = \int d^2x\, d\tau \Big[\overline{\psi}_{1\alpha} \partial\!\!\!/ \psi_{1\alpha} + \overline{\psi}_{2\alpha} \partial\!\!\!/ \psi_{2\alpha} + \left|\partial_\mu \Phi_x\right|^2 + \left|\partial_\mu \Phi_y\right|^2$$
$$+ i\lambda \left(\Phi_x \psi_{2\alpha}^\dagger \sigma_y \psi_{1\alpha} + \Phi_y \varepsilon_{\alpha\beta} \psi_{2\alpha} \sigma_y \psi_{1\beta} + \mathrm{H.c.} \right)$$
$$+ r\left(\left|\Phi_x\right|^2 + \left|\Phi_y\right|^2 \right) + u\left(\left|\Phi_x\right|^2 + \left|\Phi_y\right|^2 \right)^2 + v\left|\Phi_x\right|^2 \left|\Phi_y\right|^2 \Big]$$

Renormalization group analysis

Expansion in ε=3-d

(Similar to analysis by L. Balents, M.P.A. Fisher, and C. Nayak Int. J. Mod. Phys. B **12**, 1033 (1998))

$$\frac{d\lambda}{d\ell} = \frac{\varepsilon}{2}\lambda - 3\lambda^3$$

Scale-invariant, interacting fixed point with dynamic exponent $z=1$.

$T>0$ fermion Green's function:

$$G_F(k,\omega) = \frac{\Lambda^{-\eta_F}}{(k_B T)^{1-\eta_F}} \mathrm{X}_1\left(\frac{ck}{k_B T}, \frac{\hbar\omega}{k_B T}\right)$$

Anomalous exponent $\eta_F = \varepsilon/6 + \cdots$

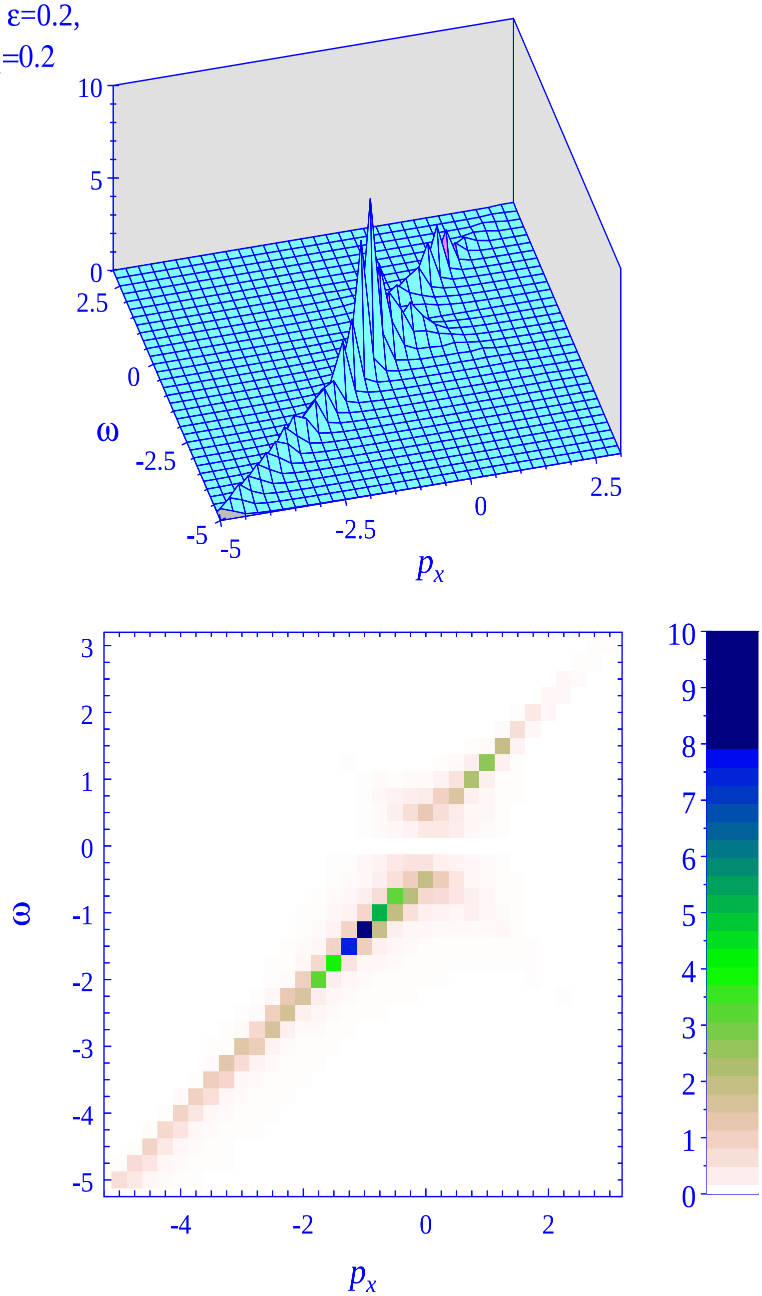
(Bare ε expansion for scaling function X_1 fails at very low momenta and frequency. Self energy has term $\Sigma(0,\omega) \sim -i\varepsilon(k_B T)^2 \delta(\hbar\omega)$. Self-consistent, quasi-classical theory is necessary to compute fermion damping)

Proposal: this quantum-criticality is the origin of photoemission line broadening observed by Valla, Fedorov,Johnson,Wells et al (Science, in press) in optimally doped $\mathrm{Bi_2Sr_2CaCu_2O_{8+\delta}}$

$$c\Delta k = k_B T\, \mathrm{X}_2\left(\frac{\hbar\omega}{k_B T}\right)$$

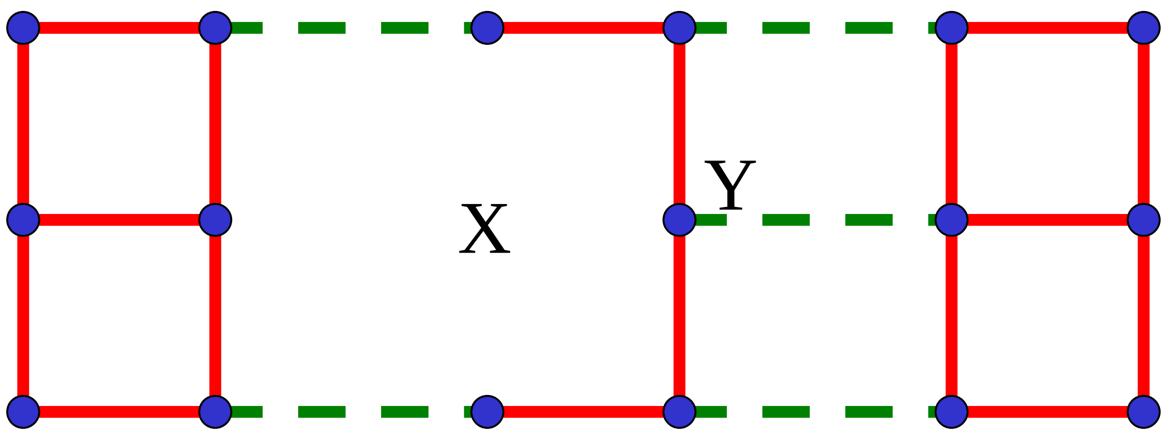
Scaling function for photoemission probability.

$\mathrm{Im}\,\Phi_f^{-1}(\omega, \boldsymbol{p}) * n_f(\omega)$
for $\boldsymbol{p}=(p_x,0,0)$, $\varepsilon=0.2$,
$\omega \rightarrow \omega + i\eta$, $\eta=0.2$



4. Quantum impurity in a nearly-critical antiferromagnet

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 $T \rightarrow 0$

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

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

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

At $\lambda = \lambda_c$

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

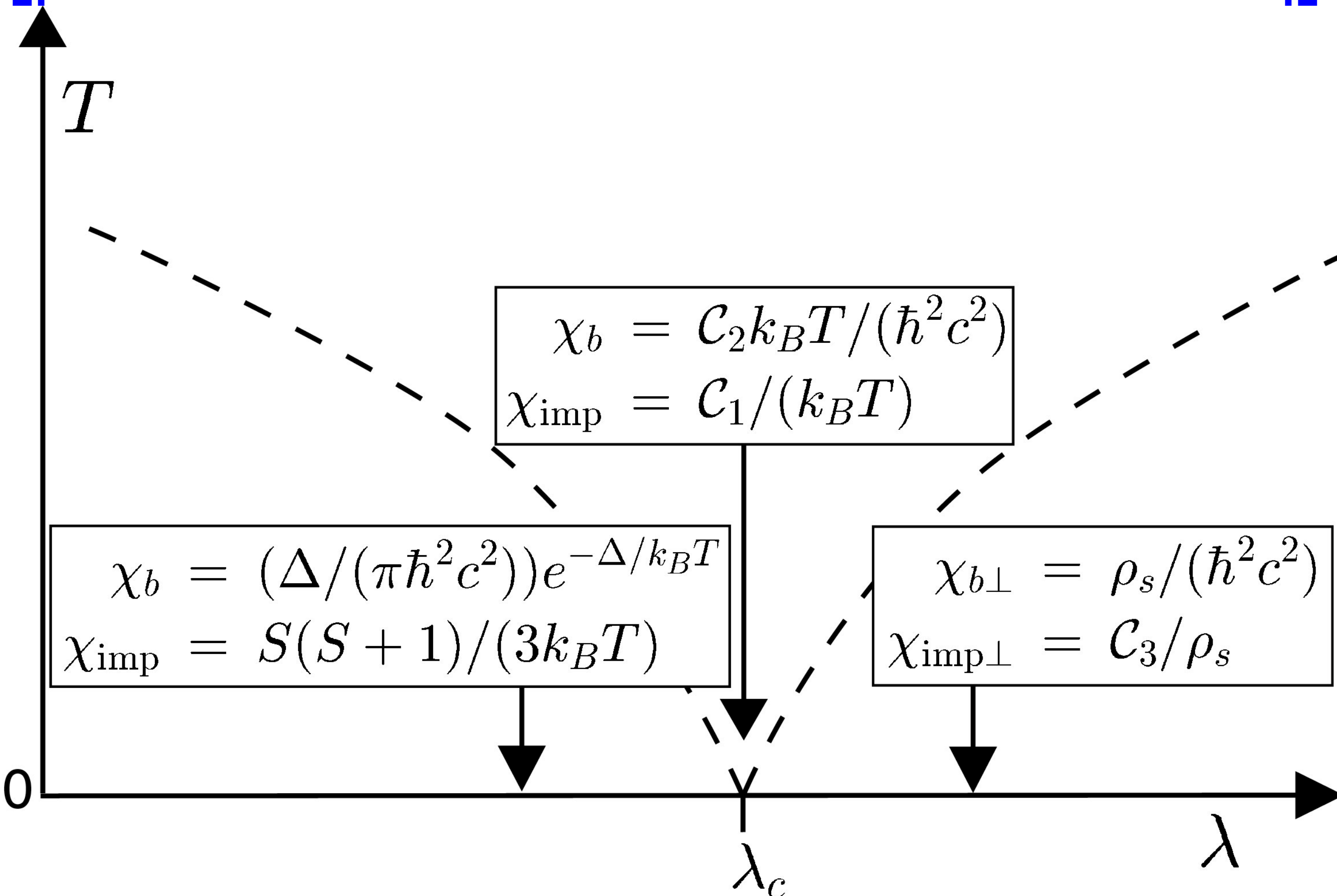
$$(\text{and } m = |\lambda - \lambda_c|^{\eta'\nu})$$

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

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

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

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

Boundary quantum field theory

$$\mathcal{S} = \int d^d x d\tau \left[\frac{1}{2}\left((\nabla_x \phi_\alpha)^2 + c^2(\partial_\tau \phi_\alpha)^2 + r\phi_\alpha^2\right) + \frac{g}{4!}(\phi_\alpha^2)^2\right] + \int d\tau \left[iSA_\alpha(n)\frac{dn_\alpha}{d\tau} - \gamma S n_\alpha(\tau)\phi_\alpha(x=0,\tau)\right]$$

$\vec{\phi}$ Neel order parameter

$\vec{n}$ Orientation of impurity spin

β functions; $\varepsilon = 3 - d$

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

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

Physics controlled by fixed points at $g = g^*$ and $\gamma = \gamma^*$.

Bulk excitations in quantum paramagnet

At *T=0* there is a magnon pole

$$S(G,\omega) = \frac{1}{\Delta - \omega}$$

Impurities broaden this to

$$S(G,\omega) = \frac{1}{\Delta - \omega - i\Gamma}$$

We obtained (exponents are exact)

$$\Gamma \approx n_i \Delta^{1-d} (\hbar c)^d$$

For experiments on Zn-doped $YBa_2Cu_3O_7$

(Fong *et al*, PRL **82**, 1939 (1999))

$$n_i = 0.005$$

$$\Delta = 41\,\text{meV}$$

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

$$\Rightarrow \quad \Gamma = 5\,\text{meV}$$

Measured value = 4.25 meV

Conclusions

1. Described T>0 crossovers near a simple magnetic quantum phase transition; found relaxation rates and transport coefficients which are universal functions of fundamental constants and thermodynamic variables ("universal incoherent conductance").

2. Theory of T>0 spin dynamics in gapped quasi-one-dimensional antiferromagnets- quantitative comparisons with experiments.

3. Global phase diagram for transitions in doped antiferromagnets compared with many experiments on the high temperature superconductors.
   A. Proposed a phase diagram for doped antiferromagnets on the square lattice. All ground states are "conventional", and their excitations can be described by electron Hartree-Fock/ BCS theory.
   B. Described quantum-critical points between phases: these control anomalous behavior in $T>0$ crossovers.

C. Experimental issues:

- Bond-centered vs. site-centered stripes
- States with 2x1 unit cells ?
- Correspondence between wavevectors of Fermi points and spin/charge fluctuations ?

D. Theoretical issues:

- Theory for $T>0$ fermion damping in quantum-critical region
- Charge transport for $T > T_c$

4. Theory of quantum impurity in a nearly critical antiferromagnet – irrational spin excitations and a new boundary quantum field theory.