Part II
Microscopic Models for Cuprates

References

1. ``*1nteracting Electrons and Quantum Magnetism*'', **A.Auerbach**, Springer-Verlag (NY).
2. ``*Quantum Magnetism Approaches to SCES*'' , **A. Auerbach, F. Berutto and L. Capriotti** *"Field Theories in Low .. Eds. G. Morandi et. al. Springer-verlag (00), also* ***cond-mat/9801294)***

Microscopics (High Energy Physics)

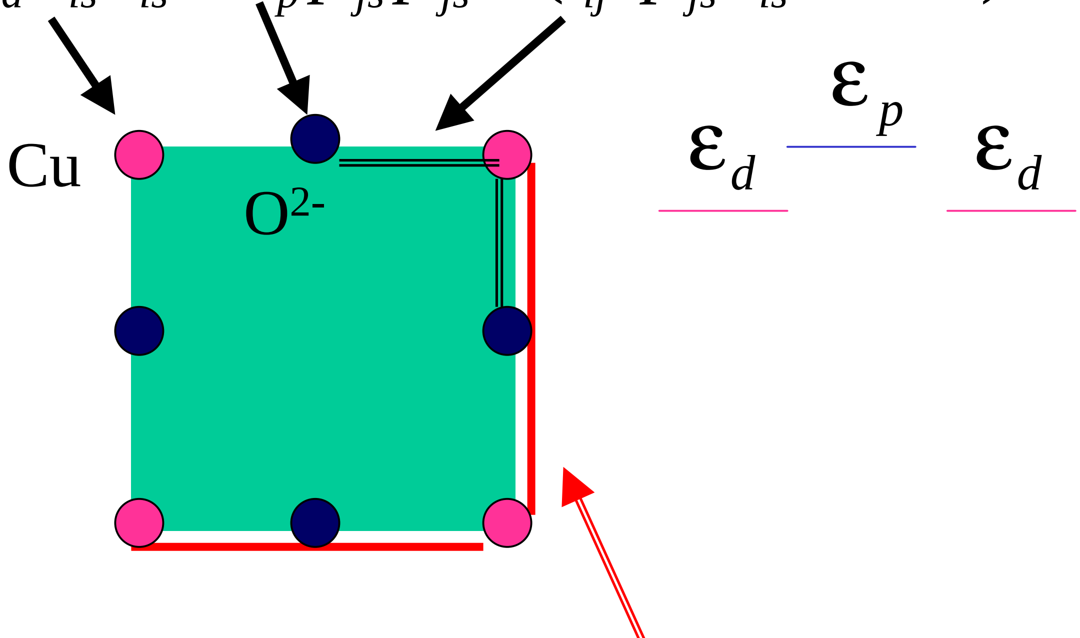
$$H = H_0^{el} + H^{el-el} + H^{el-phonon}$$

Band Structure Effective Single Electron Theory

$$H_0^{el} = \int d^3x \left[\bar{\psi}(-\frac{\nabla^2}{2m} + V^{self-cons}(x))\psi \right]$$

CuO_2 model on decorated Square Lattice *(Emery)*

$$\Rightarrow \sum_{ij} \varepsilon_d \bar{d}_{is} d_{is} + \varepsilon_p \bar{p}_{js} p_{js} + (t_{ij}^{dp} \bar{p}_{js} d_{is} + H.c.)$$



One band model $\Rightarrow \sum_{ij} t \; (\bar{d}_{is} d_{js} + H.c.)$

Interactions

$$H^{el-el} = \frac{1}{2}\iint d^3x d^3y \left(\frac{e^2}{|x-y|} \right) \overline{\psi}(x)\overline{\psi}(y)\psi(y)\psi(x)$$

Long range Coulomb interactions are screened
(*Bohm &Pines*)
 –> **Short Range Hubbard Interactions**

$$H^{el-el} = \sum_{ijklss'} U_{ijkl} \bar{d}_{is} \bar{d}_{js'} d_{ks'} d_{ls}$$

$$\omega < \omega_{plasma} \quad \Rightarrow \quad U \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + (\text{intersite})$$

Strong Coupling Regime

$$U \geq t$$

$$H^{el-phonon} = \sum_{kq} \gamma_{kq} (\bar{a}_q + a_{-q}) \overline{\psi}_k \psi_{k-q} + \sum_{qj} (n_{qj} + \frac{1}{2}) \omega_{qj}$$

Electron phonon coupling –>
effectively suppressed at large U

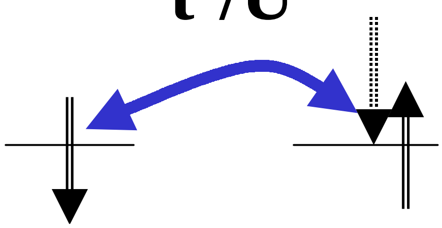
CuO_2 or One Band Model?

At large U/t ; <n> ≤ 1

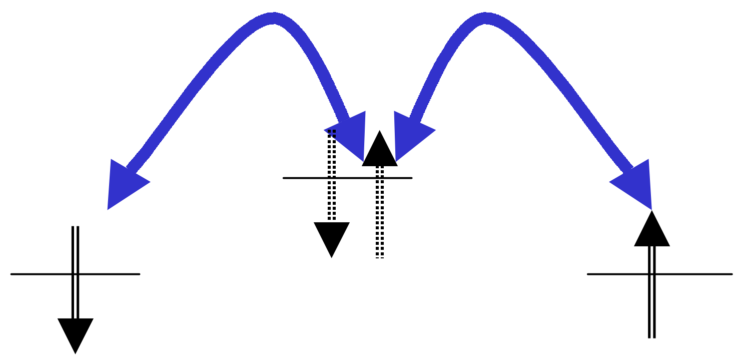
One Band Hubbard	3 band CuO_2 model

undoped: superexchange

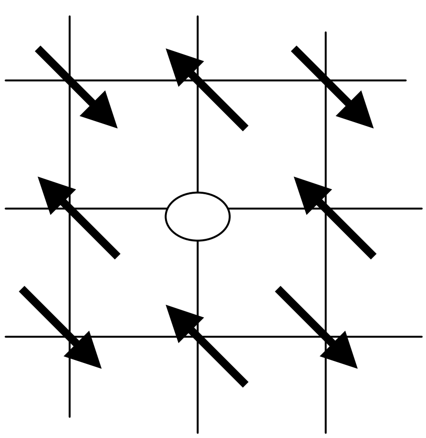
t^2/U

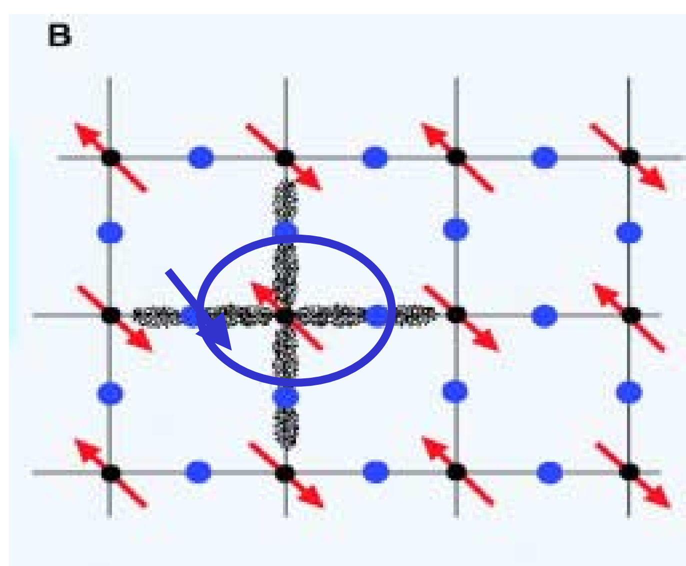


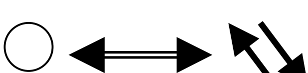
$t_{pd}^4/(\varepsilon_p - \varepsilon_d)^3$



hole state





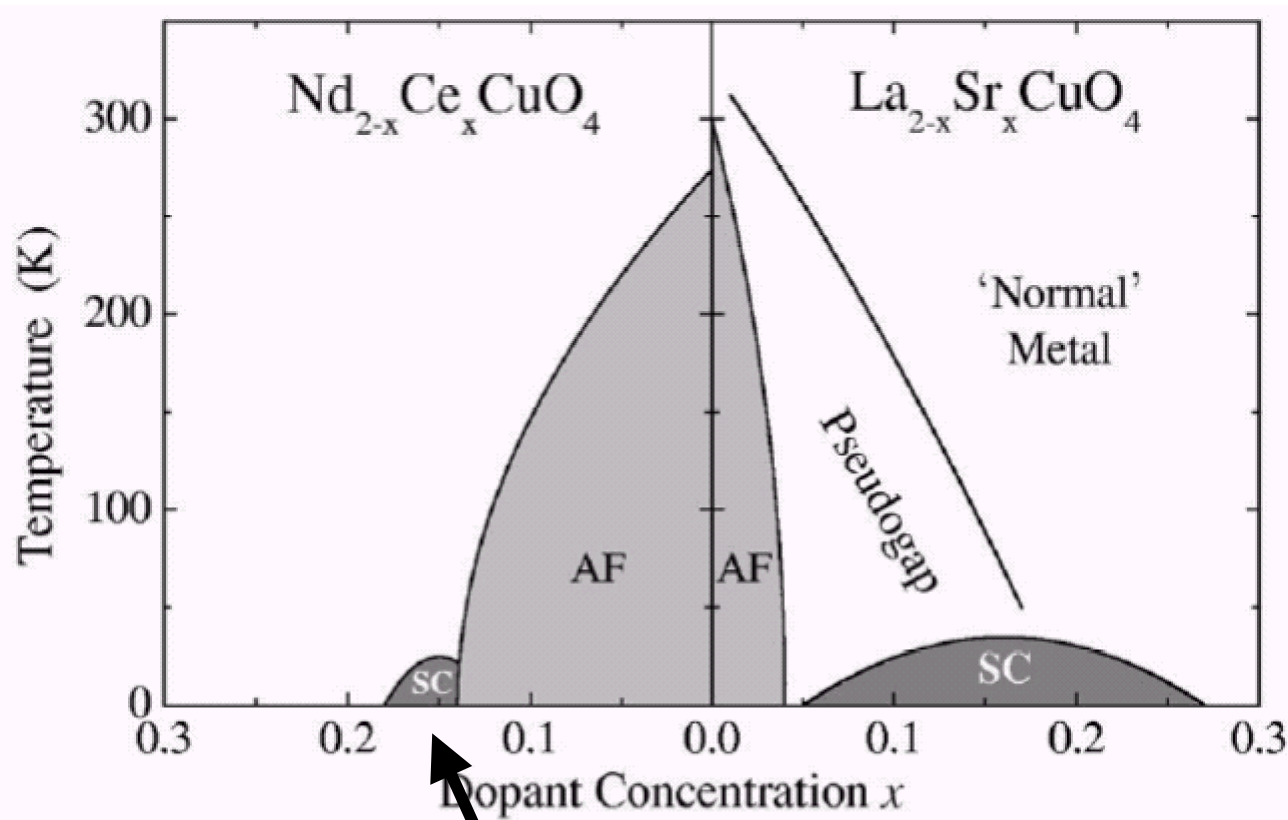


symmetry n -> 2-n

NO symmetry n -> 2-n

Electron & Hole Doping

166 *A. Damascelli et al. / Journal of Electron Spectroscopy*

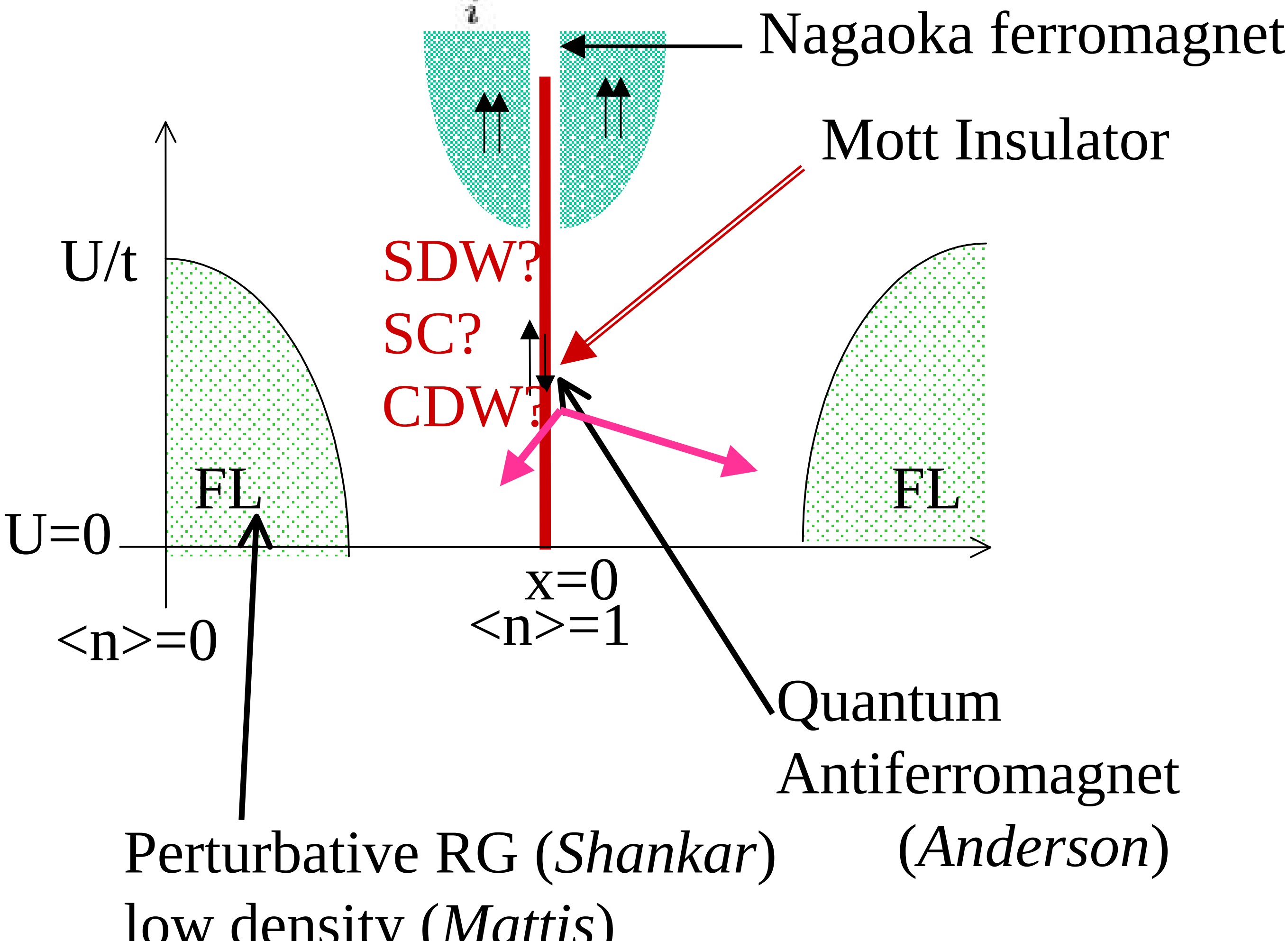


d-wave order parameter (Tsuei&Kirtley ('00))

Supporting: One Band Model

2D Hubbard Model

$$
\begin{aligned}
\mathcal{H} &= \mathcal{T} + \mathcal{U} \\
\mathcal{T} &= -t \sum_{\langle ij \rangle s=\uparrow,\downarrow} c^{\dagger}_{i,s} c_{j,s} \\
\mathcal{U} &= U \sum_{i} n_{i,\uparrow} n_{i,\downarrow},
\end{aligned}
$$



``Holes in the quantum antiferromagnet''

Renormalization Group

Wilson, Shankar

Integrate out high Fourier components

$$Z = \int D\overline{\psi}_k \psi_k \exp\left(-L[\overline{\psi},\psi]\right)$$

$$= \int_{k<\Lambda} D\overline{\psi}_{k<} \psi_{k<} \exp\left(-L^{eff}[\overline{\psi}_{k<},\psi_{k<}]\right)$$

Obtain an effective Lagrangian

$$\int_{>} D\overline{\psi}_{k>} \psi_{k>} \exp(-L) \equiv \exp\left(-L^{eff}[\overline{\psi}_{k<},\psi_{k<}]\right)$$

Perturbative RG

$$L = \overline{\psi}\hat{L}_0\psi + g\overline{\psi}\overline{\psi}\psi\psi + \ldots.$$

$$L^{eff} = \int dt dt' \, \overline{\psi}_t(t)\hat{L}_{t-t'}\psi_{t'}$$

non-Hamiltonian

$$+\int g^{eff}{}_{tt't''t'''}\overline{\psi}_t\overline{\psi}_{t'}\psi_{t''}\psi_{t'''} + \ldots.$$

RG flow :

$$g^{eff}(g,\Lambda), \quad \Lambda \to 0$$

One Step Renormalization

P_0 is a projector onto a subspace

$$P_0\begin{pmatrix} A & B \\ C & D \end{pmatrix}P_0 = A$$

A known matrix identity is:

$$P_0\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1}P_0 = \left(A - BD^{-1}C\right)^{-1}$$

Choose a decomposition of H

$$H = \begin{bmatrix} \left(H_0\right)_{00} & 0 \\ 0 & (H_0)_{11} \end{bmatrix} + \begin{bmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{bmatrix}$$

The reduced resolvent

$$P_0\left(E-H\right)^{-1}P_0 = \left(\left(E-(H_0+V)\right)_{00} - V_{01}\left[\frac{1-P_0}{E-(H_0+V)_{11}}\right]V_{10}\right)^{-1}$$

$H^{eff}(E)$

Brillouin Wigner RG

$$H^{eff} = P_0 \left\{ H_0 + V + V \sum_{n=1}^{\infty} \left[\frac{1-P_0}{E-H_0} V \right]^n \right\} P_0$$

(Not a true Hamiltonian, E dependent !)

H –> H^{eff} can be iterated by choosing successive projectors to lower eigenvalues of H_0
Explicitly, for two cutoff energies

$$E_{\Lambda'} < E_{\Lambda}$$

$$H^{eff}(\Lambda) \equiv H(\Lambda) + V(\Lambda) \rightarrow H^{eff}(\Lambda')$$

$$H^{eff}(\Lambda') = P_{\Lambda'} \left\{ H(\Lambda) - V(\Lambda) \sum_{n=1}^{\infty} \left[\frac{1-P(\Lambda')}{E-H(\Lambda)} V(\Lambda) \right]^n \right\} P_{\Lambda'}$$

Is H*(Λ')* simpler than H*(Λ)*?

Sometimes, when V effectively shrinks with ***Λ***

From Hubbard to t-J

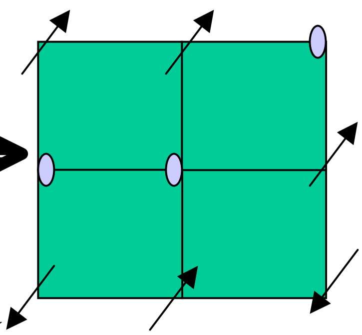
$$H_0 = U\sum_i n_{i\uparrow}n_{i\downarrow} \qquad V = -t\sum_{<ij>s} c^{\dagger}_{is}c_{js} + H.c$$

$$P_0 = \begin{cases} 1, \forall n_i < 2 \\ 0, \exists n_i = 2 \end{cases}$$

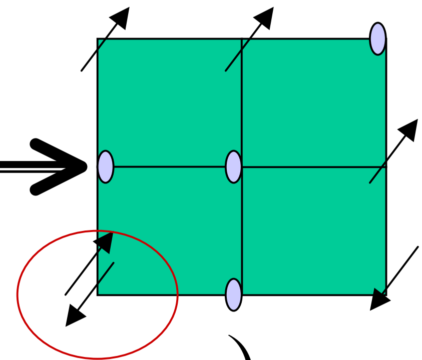
Gutzwiller projector :

Space of no double occupancies

$\mathbf{P_0}$



$\mathbf{1\text{-}P_0}$



$$H^{tJ} = P_0\left(-t\sum_{<ij>s} c^{\dagger}_{is}c_{js} - \tfrac{t^2}{U}\sum_{<ijk>ss'} c^{\dagger}_{is}c_{js}(1-P_0)c^{\dagger}_{js'}c_{ks'} + H.c.\right)P_0 + O\left(\tfrac{E}{U},\tfrac{t}{U}\right)$$

$$J = 4t^2/U$$

$$= P_0\left(-\mathrm{t}\sum_{<ij>s}\left(c^{\dagger}_{is}c_{js} + H.c.\right) + \mathrm{J}\sum_{<ij>s}\left(\vec{S}_i\cdot\vec{S}_j - n_i n_j/4\right) + \hat{J}'\right)P_0$$

$$\hat{J}' \equiv -\tfrac{t^2}{U}\sum_{<ijk>ss'} c^{\dagger}_{is}c_{ks}n_j - c^{\dagger}_{is}\vec{\sigma}_{ss'}c_{ks'}\cdot\vec{S}_j$$

Hole hopping

Heisenberg model

$$\vec{S}_i \equiv \tfrac{1}{2}\sum_{ss'} c^{\dagger}_{is}\vec{\sigma}_{ss'}c_{is'} \qquad \vec{S}_i^{\,2} = \tfrac{3}{4}$$

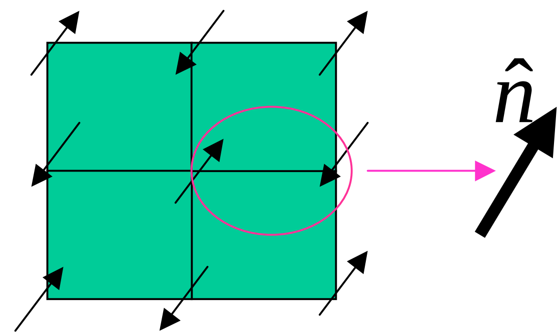
Hubbard Regime: t>J

Half Filling

No charge fluctuations: Mott Insulator

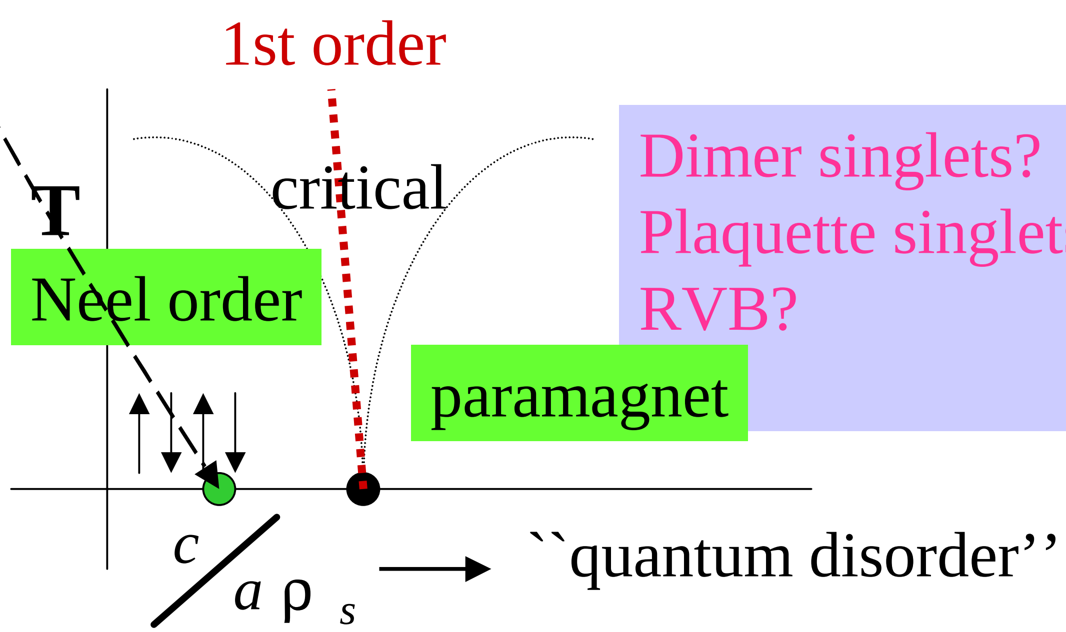
Spin ½ Quantum Heisenberg Model

$$J \sum_{<ij>s} \vec{S}_i \cdot \vec{S}_j$$



Continuum: 3D Non Linear Sigma Model

$$Z_{NLSM} \approx \int_{|\hat{n}|=1} D\,\hat{n}\;\; e^{i\Phi}\;\; \exp\left(-\frac{\rho_s}{2c} \int d^{2+1}x \sum_{\alpha=0,2} \left|\partial_\alpha \hat{n}\right|^2 \right)$$



Dimer singlets?
Plaquette singlets?
RVB?

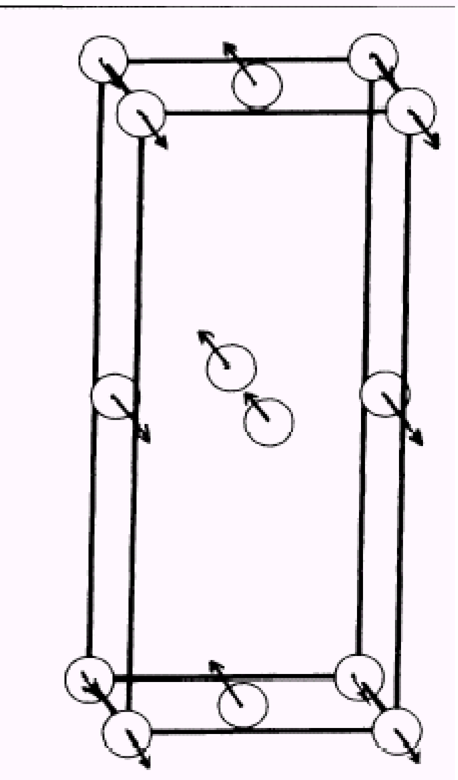
Reminder: Antiferromagnetism at x=0

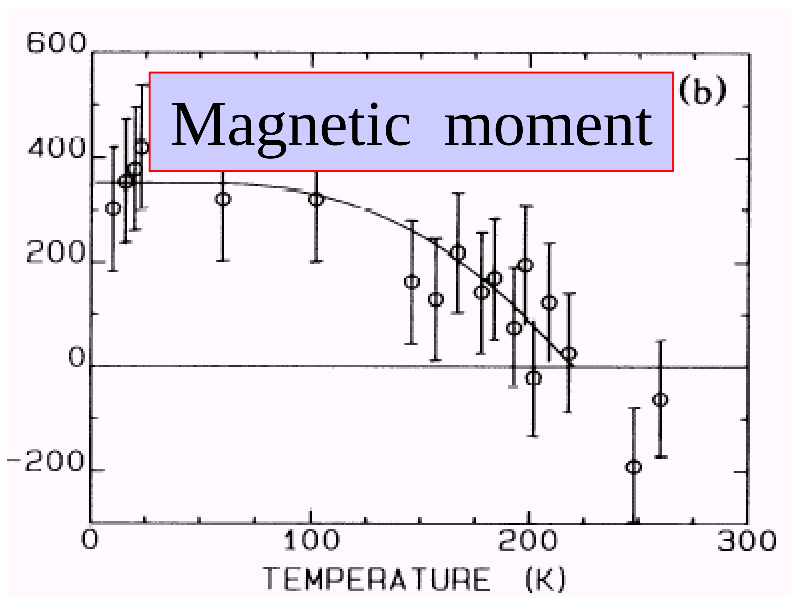
Antiferromagnetism in La_2CuO_{4-y}

D. Vaknin,[a] S. K. Sinha, D. E. Moncton, D. C. Johnston, J. M. Newsam, C. R. Safinya, and H. E. King, Jr.

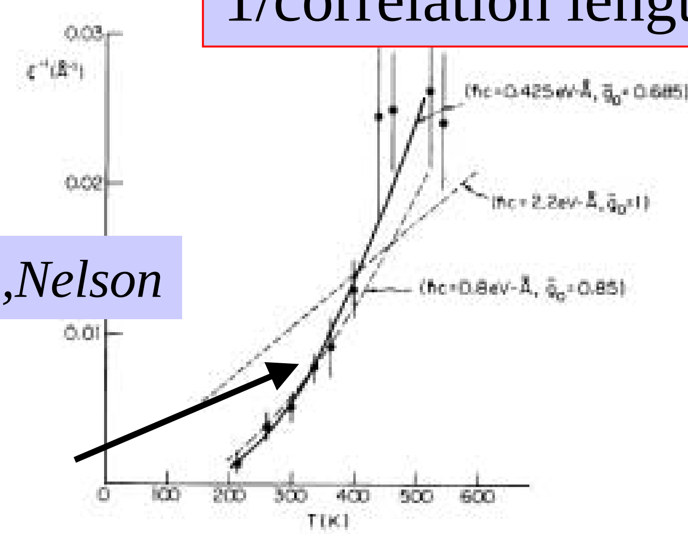
Research Laboratories, Exxon Research and Engineering Company, Annandale, New J

(Received 4 May 1987)





1/correlation length



Chakaravarty, Halperin,Nelson

Arovas, Auerbach

$$\frac{1}{\xi} \propto e^{-\pi}$$

Negative U Hubbard Model

$$H^{-U} = -t \sum_{<i,j>s} c_{is}^{\dagger} c_{js} - \frac{U}{2} \sum_{i} (n_i - 1)^2$$

$$c_{i\uparrow}^{\dagger} \rightarrow c_{i\uparrow}$$

$$c_{i\downarrow} \rightarrow c_{i\downarrow}$$

$$H^{-U} \rightarrow H^{U} = -t \sum_{<i,j>s} (c_{i\uparrow}^{\dagger} c_{j\uparrow} - c_{i\uparrow}^{\dagger} c_{j\uparrow}) + \frac{U}{2} \sum_{i} (n_i - 1)^2$$

H^{U} is a half filled positive-U Hubbard model

At large U/t, the effective Hamiltonian in the singly occupied supspace is

$$H^{-x-xz} = \sum_{<ij>} J^{z} S_i^z S_j^z - J^{x} \left(S_i^x S_j^x + S_i^y S_j^y \right) - 2\mu \sum_{i} S_i^z$$

$$S_i^z = (n_i - 1)/2 = a_i^{\dagger} a_i - \tfrac{1}{2}$$

$$S_i^{+} = c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} = a_i^{\dagger}$$

pseudospin

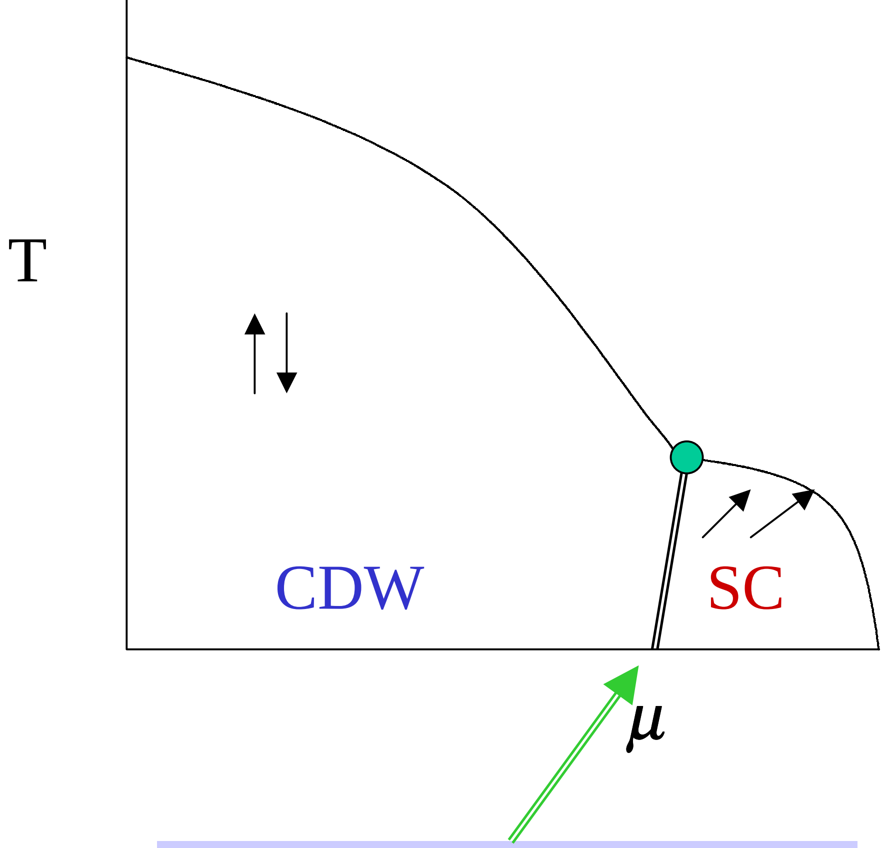
electrons

hard core boson

Solid to Superfluid transition

$$H^{cl} = \sum_{<ij>} J^z \Omega_i^z \Omega_j^z - J^x \left(\Omega_i^x \Omega_j^x + \Omega_i^y \Omega_j^y \right)$$

$$+ \sum_{nnn} K^z \Omega_i^z \Omega_k^z - 2\mu \sum_i \Omega_i^z$$

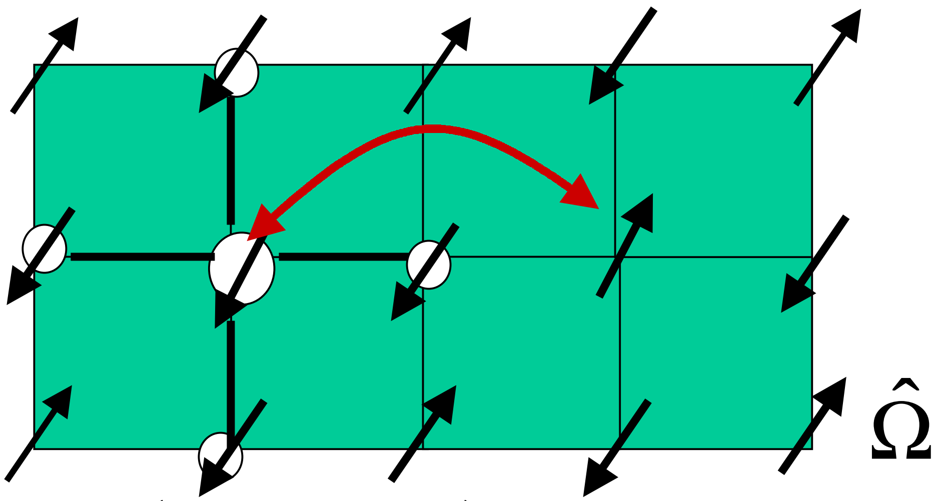


K<0: first order: spin flop

K>0: frustrated lattices: supersolid mixed phase

The Doped Antiferromagnet

Single hole



$$H^{cl} = -t\sum_{ij}\left(1+\hat{\Omega}_i\cdot\hat{\Omega}_j\right)^{1/2} e^{iAij} f_i^\dagger f_j + J\sum_{ij}\hat{\Omega}_i\cdot\hat{\Omega}_j$$

Auerbach& Larson

<u>t<J, semiclassical effective H:</u>

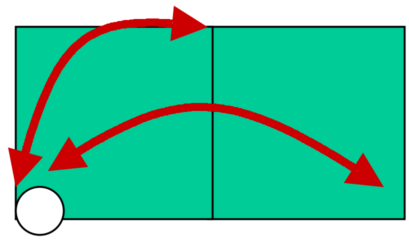
Spin polaron, hops on one sublattice, coupled to Neel gauge field. Kinematic Pairing Mechanism

$$\Rightarrow \sum_{\eta} \int d^2x \; f_\eta^\dagger\left(\partial_t + (i\nabla + \eta A)^2\right) f_\eta + L_{NLSM}(\hat{n})$$

Weigmann'88, Wen, Lee, Shankar '89

Single hole dispersion

same sublattice hopping



$$\mathcal{H}^f = \sum_{\mathbf{k}s} (\epsilon^f_{\mathbf{k}} - \mu) f^\dagger_{\mathbf{k}s} f_{\mathbf{k}s},$$

$$\epsilon^f_{\mathbf{k}} = t'(\cos(k_x a) + \cos(k_x a))^2 + t''(\cos(k_x a) - \cos(k_y a))^2$$

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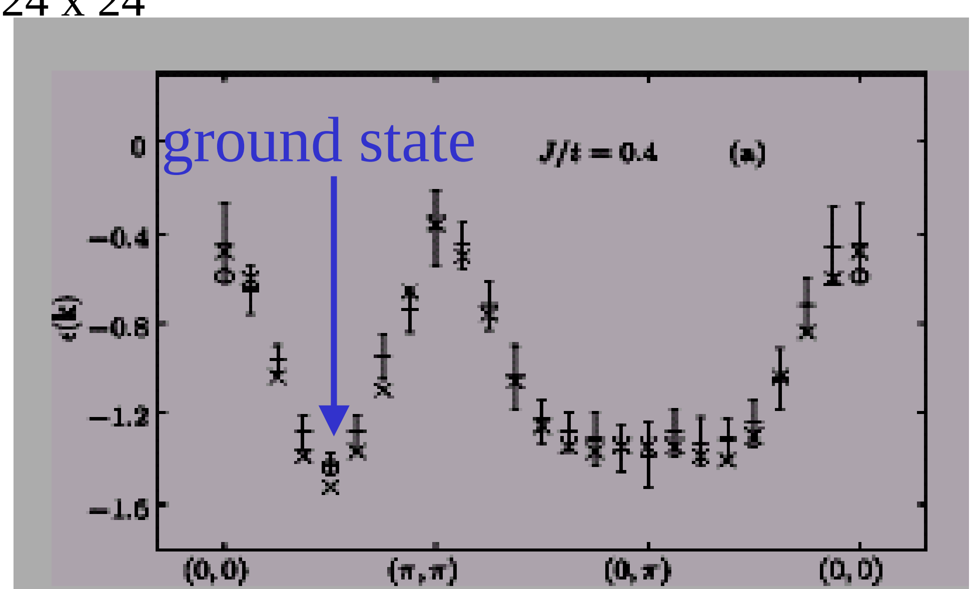
Single-hole dynamics in the t–J model on a square lattice

Michael Brunner, Fakher F. Assaad, and Alejandro Muramatsu

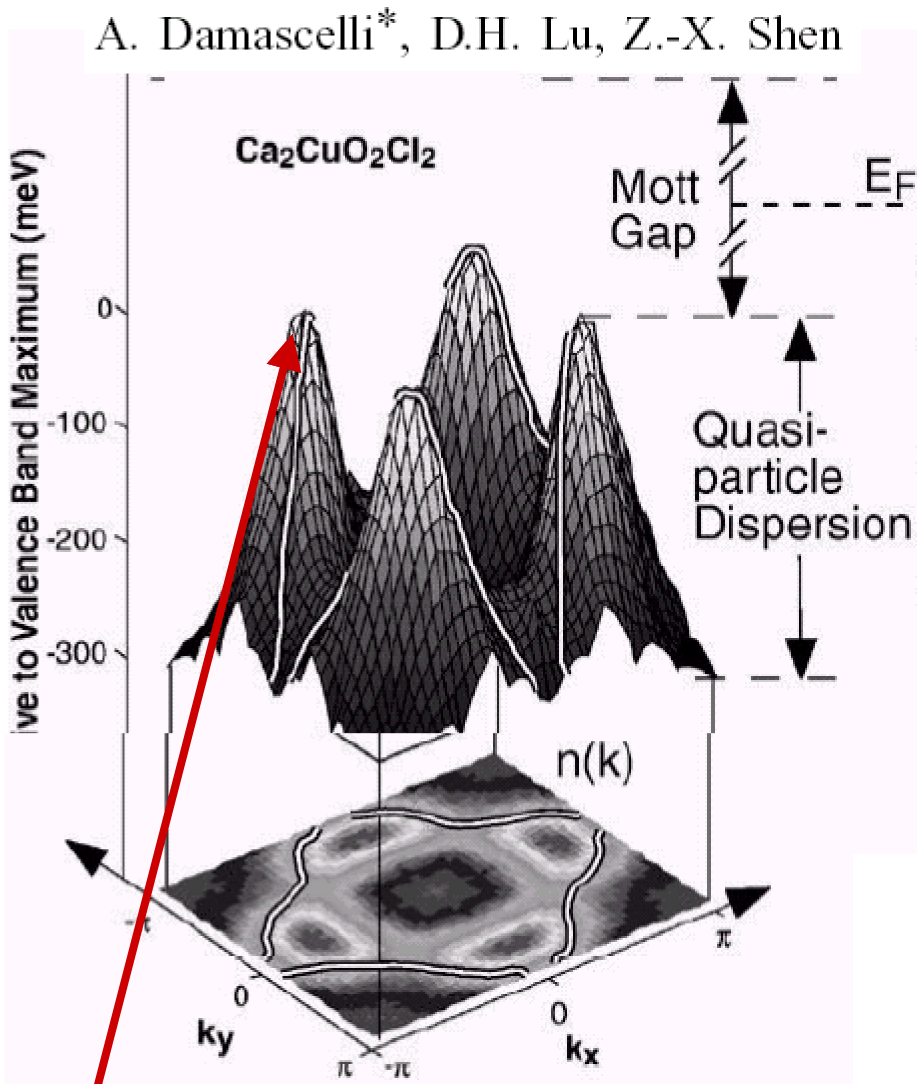
Quanmtum Monte-Carlo

24 x 24



t’’ ~ 0.1 t’
t’ ~ J

Single hole ARPES



ground state momentum

Two Holes in a Cluster

$$\Delta_N \equiv E_N - 2E_{N+1} + E_{N+2} < 0$$

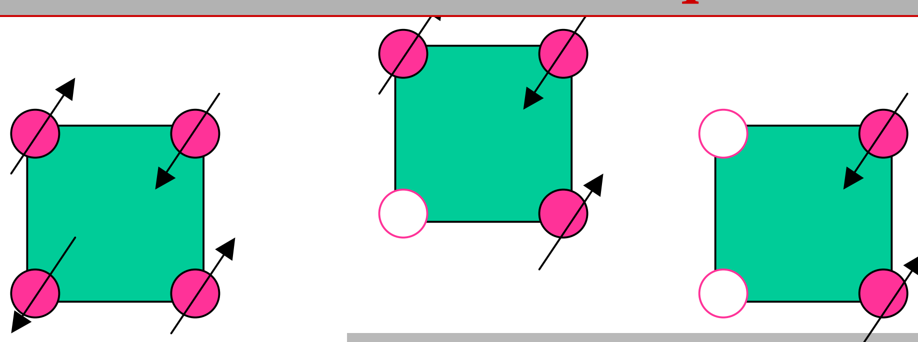
Pair binding on finite clusters LxL

Signature of pairing for L>ξ

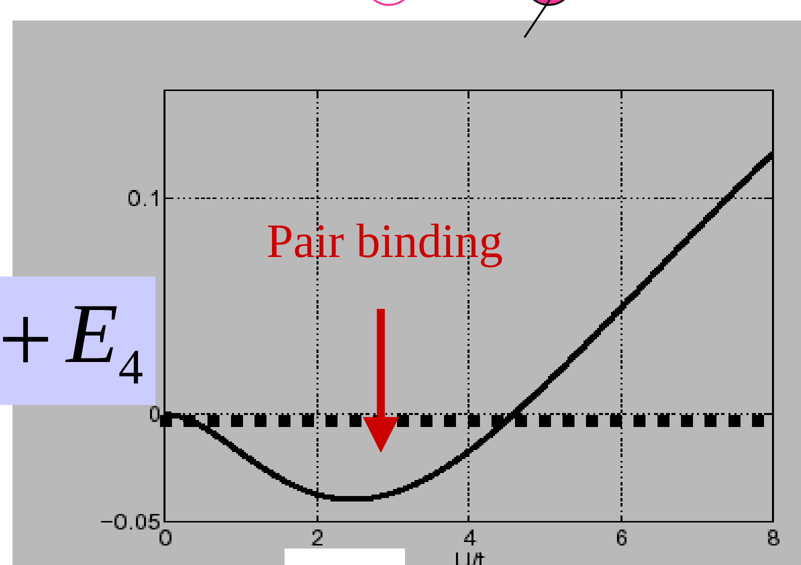
Pair binding was found for Hubbard and t-J clusters close to half filling!

(Hirsch et.al., Fye et.al 89.)

Even for the 2x2 Hubbard Plaquette:



$$\Delta \equiv E_2 - 2E_3 + E_4$$



U/t

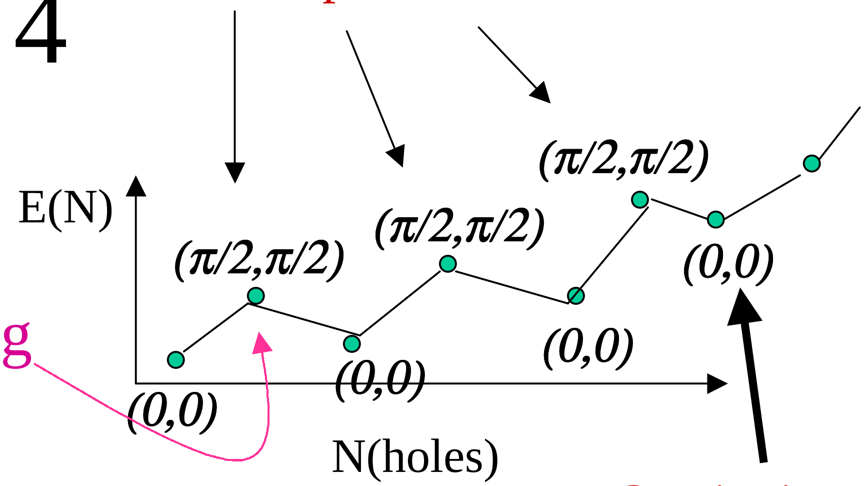
2 hole pairing

Static and dynamical properties of doped Hubbard clusters

E. Dagotto, A. Moreo, F. Ortolani,* D. Poilblanc,† and J. Riera‡

Holes in pockets

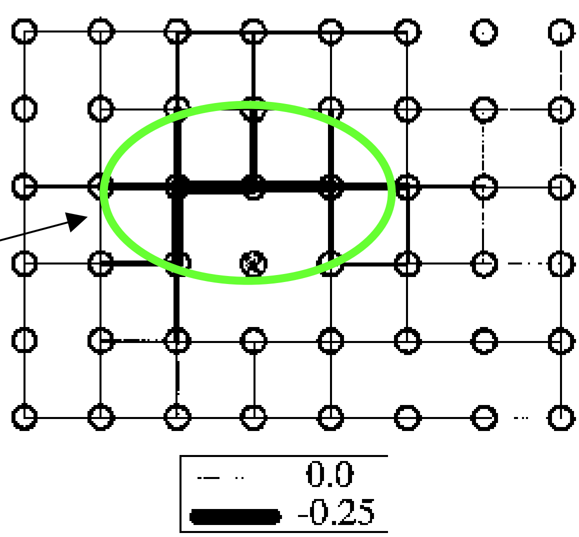
4×4



Pair binding

3 pairs in a condensate

Pair correlations in t-J model by DMRG (*White&Scalapino*)



short pair coherence length

2D Hubbard Model : Status Report

Undoped

Heisenberg model, Neel phase.

Single hole:

ground state momentum $(\pi/2,\pi/2)$, $\varepsilon(k)$.

Two holes::

Pair binding on small clusters (numerical).

Will they bind in large lattices?

Many holes:

Phase separation/stripes?

Superconductivity?

What destroys Neel order?

Conflicting mean field theories…..

t-J Model: spins and holes are strongly entangled on lattice scale.

We need to derive a lower effective H!

Part III

Derivation of Effective Hamiltonian using Contractor Renormalization