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**Group Discussion Meeting on  
NEW INSIGHTS  
INTO  
THE OLD HUBBARD MODEL**

**25 February - 1 March 1991**

**LECTURE NOTES**

**THE INSTITUTE OF MATHEMATICAL SCIENCES  
MADRAS - 600 113  
INDIA**

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## Preface

It was felt that we should have a small workshop to go into some details of the new theoretical developments in the large U one band Hubbard model. Fortunately we had sufficient expertise in our country to have this exercise at Madras. It is true that following Anderson's RVB theory of high  $T_c$  superconductors many new insights have been gained in the last 4 years and many old works have gained new importance. At the beginning, 5 days was thought to be a reasonable period to do this job. What became clear at the end of the workshop was that there are so many things to be learned and also to be done. We barely touched the problem of holes in Mott insulator, spiral phases, Nagaoka problem, Numerical approach, Gauge theory and failure of Fermi liquid theory and Luttinger liquid – and one week was already over.

Since many of the works have been published we bring out this Matscience report in a very informal fashion – collection of photo copies of transparencies and some lectures.

The success of the Workshop depended on my colleagues A. K. Mishra, R. Shankar, G. Subramonian and R. Jayaraman (Deputy Registrar) who were part of the organising committee and G. Sethuraman, our Chief Administrative Officer and his team of Administrative staff and also all the excellent lectures and the enthusiastic participants. We thank R. Ramachandran, our Director for the support and his keen interest.

G BASKARAN

MATSCIENCE

## Large U Hubbard Model and Failure of Fermi Liquid Theory

G. BASKARAN

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### Lecture - I

There has been renewed interest in the Hubbard Model ever since the discovery of high temperature superconductors<sup>1</sup>. It was Anderson<sup>2</sup> who suggested that the low energy physics of the CuO based ceramic superconductors is described by a one band Hubbard Model with large U. Historically, the Hubbard model has been discovered by several authors – by Anderson<sup>3</sup> to describe the magnetism in Mott insulators like MnO, by Pines, and Poole to describe the physics of the systems organic carbon  $p-\pi$  by Kanamori<sup>4</sup>, Gutzwiller<sup>5</sup> and Hubbard<sup>6</sup> to describe the narrow band systems with a particular aim to understand itinerant ferromagnetism. Hubbard<sup>6</sup> and much later Brinkman and Rice<sup>7</sup> used this model to understand Metal insulator or Mott transition. A lattice gas version of liquid He<sup>3</sup> also leads to a Hubbard model.

Hubbard model is a tight binding model of fermions with the only two body interaction being an onsite repulsion between fermions of opposite spins. In its simplest version it has one orbital per site - the only two parameters are  $\rho$ , the mean number of electrons per site, and  $U/t$ , the ratio between the onsite repulsion and the nearest neighbour hopping matrix element. We are going to concentrate on this one band Hubbard model, as this is most relevant for understanding the high  $T_c$  superconductors.

The phase diagram of the Hubbard model in the  $U/t - \delta$  plane is believed to be very rich, containing various phases like Mott insulator, band insulator with antiferromagnetic order, conducting spiral spin structures, itinerant ferromagnets, fermi liquid,

and a non-fermi liquid. This is the reason why the Hubbard model has been used to describe various condensed matter systems exhibiting many different properties.

Our present understanding of the Hubbard model is not satisfactory inspite of the enormous study that has gone into it – of course it depends on which region of parameter space one is in. For exactly half filled band i.e.  $\delta = 0$ , and  $U/t \gg 1$ , the Hubbard Hamiltonian reduces to the Heisenberg model, as shown by Anderson<sup>3</sup> and the low energy excitations are spin fluctuations. We understand the physics in this region to the extent we understand Heisenberg Hamiltonian. Even the Hartree-Fock approximation describes the physics very well as far as magnetic order is concerned for all values of  $U/t$  for the half filled band. Subtle questions related to any fundamental difference between a Mott antiferromagnet and band antiferromagnet, however, remain unsettled though some attempts have been made in this direction<sup>10</sup>.

Real problems arise only when we consider the doped antiferromagnet for large  $U/t$ . In this region the effective model is the  $t - J$  model<sup>2,11</sup>. All the recent attempts have been to understand this model. For  $U = \infty$  or  $J = 0$ , we have Nagaoka ferromagnet<sup>12</sup> for small  $\delta$ . In this region again the understanding is not complete even though there are some interesting recent works<sup>13</sup>.

There are a few milestones in the development in our understanding of the Hubbard model. The notion of upper Hubbard band, indications of violation of Luttinger's theorem, the notion of Gutzwiller's projection and all the recent insights that Anderson has brought in mostly single handedly. In fact my lectures will be mainly a quick review of the insights that Anderson has brought in recently together with a few of my own ideas. A good review of earlier results with critical comments are found in the

excellent book by Conyers Herring<sup>14</sup> and a good review by David Adler in the Seitz and Turnbull<sup>15</sup> series.

### Fermi Liquid Theory

Electrons in metals and many conductors are remarkably robust in the sense that their low energy properties are essentially the same as that of a free fermi gas inspite of the long range coulomb interaction. The same is true of liquid He<sup>3</sup>, which is a neutral fermi system with a hardcore type short range repulsion. Starting from Sommerfeld's free - electron theory of metals ending with Landau's formulation of Fermi liquid theory, this idea is central. The essence of Fermi liquid theory<sup>16</sup> is the one to one correspondence between the low lying spectrum of free fermi gas with the interacting fermi system.

Landau formulated the Fermi liquid theory in terms of quasi particles and their interaction in momentum space, close to the fermi surface. The quasiparticles carry spin and charge together and are "adiabatic continuation" of the non-interacting fermions. The quasiparticles are infinitely long lived at the Fermi surface and close to the Fermi surface their life time  $\tau(E) \sim (E - \epsilon_F)^2$ . The quasi particles do interact and this is parametrized by the various Landau parameters. The mass of the quasi particles is renormalized.

The Fermi surface remains intact in the sense the momentum distribution function  $n_k$  exhibits a finite discontinuity at the Fermi wave vector  $k_F$ . A neat characterization of the fermi liquid is in terms of the analytic structure of the fermion propagator.

$$G_k(\omega) = \int_0^\infty \langle 0 | T C_{k\sigma}(t) C_{k\sigma}^\dagger(0) | 0 \rangle e^{i\omega t} dt$$

For a non interacting Fermi gas

$$G_k^0(\omega) = \frac{1}{\omega - (\epsilon_k - \mu)}$$

It has a pole on the real axis. In a Fermi liquid, the pole moves into the unphysical sheet in the complex  $\omega$  plane for a general  $k$ .

$$G_k(\omega) = \frac{1}{\omega - \epsilon_k - \Sigma_k(\omega)}$$

where  $\Sigma_k(\omega)$  is the self energy. In particular the imaginary part of energy, the inverse of the fermion life time approaches zero as  $(\epsilon - \mu)^2$  as  $k \rightarrow k_F$ . And the residue of the pole at  $k = k_F$  remains finite :

$$G_{k_F}(\omega) = \frac{Z_{k_F}}{\omega - (\epsilon_{k_F} - \mu)} + \text{incoherent}$$

$$\text{where } Z_k \sim (1 - \frac{\delta \Sigma_k(\omega)}{\omega}|_{\omega=0})^{-1}$$

As long as the residue  $Z_k$ , which is the wave function renormalization constant remains finite, the interacting system remains a fermi liquid.

The wave function renormalization constant  $Z_k$  can also be expressed as

$$\sqrt{Z_k^{1/2}} = (N+1, k | C_{k\sigma}^\dagger | N, G)$$

where  $|N, G\rangle$  is the groundstate of the interacting  $N$  particle system and  $|N+1, k\rangle$  is the groundstate of the  $N+1$  particle system having a momentum  $k$ . When the state  $C_{k\sigma}^\dagger |N, G\rangle$  has evolved in time, the state  $|N+1, k\rangle$  is supposed to be the coherent part that is left behind after infinite time.

### Failure of Fermi liquid theory

It is unlikely that any interacting fermi system is a fermi liquid in its ground state. The residual weak interactions among the quasi - particles will lead to a ground state with spontaneously broken ground state. This could be a spin density wave or charge density wave or a superconducting state. This is what happens according to Kohn and Luttinger in the case of an electron gas at very low T. In the Hubbard model, we are not interested in the failure of Fermi liquid theory arising in the above sense - fundamentally a fermi liquid with a spontaneous symmetry breaking modification. What we are looking for is a fundamental modification of the "normal state". That is we do not envisage a fundamental symmetry difference between the Fermi liquid and the non - Fermi liquid. The difference arises in the behaviour and nature of the quasi - particles.

The Luttinger liquid<sup>17</sup>, which exists in several 1 - d models, including the 1 - d Hubbard model<sup>18</sup> is one such example where the Fermi liquid theory fails without any spontaneous symmetry breaking.

### Lecture - II

As mentioned in the last lecture we are looking for a correlated novel quantum liquid which has the same symmetry as the fermi liquid, but differs in the ground state correlation and the nature of the excitation spectra. Hubbard's various decoupling approximations<sup>7</sup>, the presence of the upper Hubbard band and the failure of Luttinger

theorem all pointed to the presence of a non - fermi liquid. It was Anderson's appreciation of the anomalous normal state properties and his insightful analysis of the t - J model which is revealing to us the real nature of the non fermi liquid state.

This novel correlated quantum liquid has been named as Luttinger liquid by Anderson<sup>19</sup> borrowing a terminology that Haldane<sup>17</sup> has used to describe certain classes of 1-d interacting systems with non-fermi liquid ground state. Anderson's argument is that the physics is similar in two dimensional Hubbard model. One of the important properties of this new quantum fluid is the spin-charge decoupling. There are two kinds of low energy excitations, one carrying only spin called spinons and the other carrying only charge called holons.

The above is true in the one-dimensional Hubbard model. This is essentially a new understanding of the (Lieb-Wu) exact solution<sup>8</sup> of the Hubbard model, which has existed as a mathematical solution for the last 2 decades, that Anderson has brought out. In fact in the one dimensional Hubbard model the insulating half-filled band case and the conducting non-filled band, all have fractionalization of quantum numbers. For the Heisenberg AFM, the spin 1 and spin 0 excitations are scattering states of more fundamental spin- $\frac{1}{2}$  excitations which are the spinons. Thus the fundamental excitations are neutral spin- $\frac{1}{2}$  excitations. These excitations resemble electrons to the extent of having the same spin. Unlike an electron it is neutral and has a collective solitonic (topological) character.

These spinon excitations are believed to survive after doping in the 2-d Hubbard model. Its neutral character is only an asymptotic statement: the effective charge carried by the spinons tend to zero as the energy of the spinon tends to zero. The zero

energy spinon excitations define a line in the Brillouin zone which we call as the spinon fermi surface or pseudo fermi surface. In simple mean field theories<sup>21</sup> these pseudo fermi surfaces coincide with the fermi surface of the corresponding non-interacting electron system. It is not completely clear if the spinons are fermions and whether they have a Fermi surface.

Excitations which carry only charge are also believed to occur on surfaces in the momentum space. The spins of these excitations vanish as the energy tends to zero. It is also believed that the charge fermi surface or holon fermi surface coincides with the fermi surface of the ferromagnetically polarized fermi gas (Nagaoka-fermi surface). This fermi surface has twice the volume of the normal fermi surface as this counts all the charges irrespective of their spins. The spinon and holons are non-trivial collective excitations. It is useful to think of the Luttinger liquid vacuum as

$$\zeta_{k\sigma}|0\rangle = 0 \quad k \rightarrow k_F^h$$

$$h_k|0\rangle = 0$$

$$a_k|0\rangle = 0$$

as  $k \rightarrow k_F^h$  where  $\zeta_{k\sigma}$  is the spinon annihilation operator for spinon and  $h_k$  and  $a_k$  are that for holons and antiholon respectively. Then  $k_F^S$  and  $k_F^h$  are the holon and spinon fermi surface momenta.

Having defined a Luttinger - Anderson liquid in terms of the excitation spectrum, we will briefly see characterization in terms of electron propagators. The one dimensional Hubbard model helps us in this as well. It is known<sup>19</sup> that the electron propagator

acquires a branch point in the 1 - d Hubbard model as  $k \rightarrow k_F$

$$G_k(\omega) \sim \frac{1}{(\omega - \mu)^\alpha}$$

when  $\alpha$  is a parameter which in general depends on the ratio  $U/t$  and  $\delta$ . i.e. the pole has disappeared giving rise to a branch cut. We expect this in the doped 2 - D Hubbard model. This is far from being understood. Even the vanishing of  $Z_{k_F}$  is not established satisfactorily.

It should be noted that a branch point structure does not mean a simple spin charge decoupling in the low energy excitations. Much work needs to be done in the novel departures from the conventional fermi liquid theory.

I have developed a model which exhibits spin-charge decoupling and holon, spinon excitations. Its relation to Hubbard model is being investigated. The model is called a momentum space t - J model defined as

$$H = \sum \epsilon_k C_{k\sigma}^\dagger C_{k\sigma} + h.c. - \sum J_{kk'} \vec{S}_k \cdot \vec{S}_{k'}$$

where

$$\vec{S}_k = C_{k\sigma}^\dagger \vec{\sigma}_{\alpha\beta} C_{k\beta}$$

With appropriately chosen form of  $J_{kk'}$  it exhibits some Luttinger liquid like behaviour.

### Lecture - III

In this lecture we will briefly see what is the origin of this non-fermi liquid behaviour and summarise a recent attempt to understand this using scattering theory. When the RVB theory was proposed by Anderson he emphasized the importance of Gutzwiller

projection. It is actually a statement that in the tight binding Hubbard model, for large  $U/t$ , the double occupancy is only virtual in the ground and low lying states. Thus any attempt to solve the large  $U$  Hubbard model should treat the on site repulsion  $U\sum n_{i\downarrow}n_{i\uparrow}$  as  $H_0$  and the kinetic energy should be treated as a perturbation.

This is what leads to the  $t - J$  model

$$H = -t \sum_{\langle ij \rangle} C_{i\sigma}^\dagger C_{j\sigma} + h.c. + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

with the important local constraint  $\sum_i n_{i\sigma} \neq 2$  for every site. This projection or constraint is the origin of non-fermi liquid behaviour. This greatly reduces the dimension of the Hilbert space in which low energy states participate. It also forces new correlations in the ground state.

A feeling of the importance of the reduction in Hilbert space can be gotten by studying a two particle problem in a Hubbard model. This two particle problem was studied by Hubbard<sup>7</sup> several years ago who discussed the antibound state. This antibound state was rediscovered by Hsu and myself<sup>23</sup> in the context of RVB theory while trying to understand the origin of superconducting correlations in the Hubbard model. Consider a two particle problem in the Hubbard model. We will consider only the spin singlet state, which alone is affected by the onsite repulsion term for this two particle problem. The eigen function for the orbital part is

$$\psi(n_1, n_2) = e^{\frac{iK(n_1+n_2)}{2}} \varphi(n_1 - n_2)$$

where  $K$  is the centre of mass momentum of the pair and  $\varphi(n_1 - n_2)$  is the relative coordinate wave function. The Schrodinger equation for  $\varphi(n)$  is

$$-t \sum_{\Delta=\pm 1} \varphi(n_1 - n_2 + \Delta) + U\delta_{n_1, n_2} \varphi(n_1 - n_2) = E\varphi(n_1 - n_2)$$

In the relative coordinate it is thus the Slater-Koster one impurity problem in the tight binding model :

$$-t(\varphi(n-1) + \varphi(n+1)) + U\delta_{n,0}\varphi(n) = E\varphi(n)$$

When  $U = 0$ , the case of no interaction, the spectrum is continuous and extends from  $-t + \epsilon(K)$  to  $t + \epsilon(K)$ . Where  $\epsilon(K)$  is the centre of mass energy. When  $U \neq 0$  and positive an isolated state splits off the top of the continuum. Since it exists as an isolated state with no overlap with the continuum of scattering states on the positive side of the energy axis, it is called an antibound state.

What is important is that even an infinitesimal  $U$  causes an orthogonality :

$$\sum_n \varphi_E^*(n, U=0) \varphi_E(n, U) = 0 \text{ at } E = -t + \epsilon(k) \text{ and any } U > 0$$

A way to understand the above result is in terms of a finite phase shift for the scattering states at energy  $E = -t + \epsilon(k)$ . In two dimensions also this happens for any positive  $U$ .

This means that the two particle state at the bottom of the scattering continuum is made orthogonal even by an infinitesimal  $U$ . The question is how does this two particle phenomenon manifests itself in the case of finite density of particles? Imagine adding an extra particle to a system of free fermi gas in its ground state. We will also adiabatically tune a Hubbard  $U$  but only between this particle and the rest of the particles. This test particle will be scattered by all the particles and in particular by those close to the fermi surface. It is likely that the scattering phase shift that was there for the two particle will lead to an orthogonality of the manybody wave function. This is what Anderson has demonstrated recently.

Let us consider the one dimensional problem. We can easily calculate the phase shift using the standard phase shift theorem. Following Anderson<sup>20</sup> we will consider standing waves in a given bounded domain and do the analysis (It is more like a reaction matrix). The phase shift is given by

$$\frac{\delta}{\pi} = \frac{\epsilon_0 - E_{Q=0}}{E_{Q_1} - E_{Q=0}}$$

where  $\epsilon_0$  is the lowest eigen value of the interacting two particle problem. And the sum of kinetic energies

$$E_Q = \epsilon_{K+Q} + \epsilon_{K-Q} \approx 2\epsilon_K + \frac{Q^2}{2m}$$

Here  $2K$  is the centre of mass momentum and  $Q$  is the relative momentum of the two particles and  $Q = \frac{\pi n}{L}$ . The above formula tells us that the ratio of the energy shift to the unperturbed energy level separation gives us the phase shift.

The eigen value equation for the two particle problem can be easily obtained from the Schrodinger equation

$$\frac{L}{U} = \sum \frac{1}{\epsilon - E_Q}$$

When  $L$  is the number of sites in the 1-d chain and  $E_Q = \epsilon_{k+Q} + \epsilon_{k-Q}$  and  $Q = \frac{n\pi}{L}$ . We will consider the lowest eigenvalue  $\epsilon = \epsilon_0$ . We can write the sum as the RHS as a principal integral and a singular term :

$$\begin{aligned} \frac{L}{U} &= \frac{1}{\epsilon_0 - E_{Q=0}} - \frac{L}{2\pi} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} \frac{dQ}{Q^2} \\ &\approx \frac{1}{\epsilon_0 - E_{Q=0}} - \frac{L}{2\pi} \frac{L}{\pi} \\ \frac{L}{U} &\approx \frac{1}{\epsilon_0 - E_{Q=0}} - \frac{L^2}{2\pi^2} \end{aligned}$$

And  $E_{Q_1} - E_{Q=0} \cong \frac{\pi^2}{L^2}$

$$\begin{aligned} \frac{L}{U} &= \frac{1}{\epsilon_0 - E_{Q=0}} - \frac{1}{2\epsilon_0 - E_{Q=0}} \\ \frac{\delta}{\pi} &= \frac{\epsilon_0 - E_{Q=0}}{E_{Q_1} - E_{Q=0}} = 1 \end{aligned}$$

Thus we find that the scattering phase shift is  $\pi$ . In one dimension the result is therefore independent of the centre of mass momentum  $K$ .

When we repeat the same analysis in two dimensions for zero centre of mass momentum we get

$$\frac{L^2}{U} = \frac{1}{\epsilon_0 - E_{Q=0}} - \frac{L^2}{2\pi^2} \int_{Q=(\frac{\pi}{L}, \frac{\pi}{L})}^{\Delta} \frac{2\pi Q dQ}{Q^2}$$

The principal value integral is logarithmically divergent. So we get

$$\frac{\delta}{\pi} = \frac{\epsilon_0 - E_{Q=0}}{E_{Q_1} - E_{Q=0}} = \frac{1}{\ln L}$$

Here  $L^2$  is the no of sites in the system.

The phase shift in two dimensions is finite for finite systems and tends to zero logarithmically as  $L \rightarrow 0$ . However, the scattering length diverges but only logarithmically.

This logarithmic divergence of scattering length does not cause failure of fermi liquid theory when the density of particles  $\rho$  tends to zero. However, the finite density has to be treated carefully - we have to consider at least the blocking of the fermi sphere to the two particle intermediate states in the scattering processes. Anderson shows that this blocking alone leads to a finite phase shift. The calculation is as follows.

$$\frac{L^2}{U} = \sum \frac{1}{\epsilon - E_Q}$$

where the prime in the summation indicates that the two particles do not get scattered into the fermi sea. We will also consider the centre of momentum to be  $2k_F$ . As before the summation can be separated and is :

$$\frac{L^2}{U} \approx \frac{1}{\epsilon_0 - E_{Q=0}} - \frac{1}{2\pi^2} \left[ P \int_{Q_1}^{K_F} \frac{2\pi Q dQ}{Q^2} \frac{Q^2}{\pi k_F^2} + \int_{K_F}^{\infty} \frac{2\pi Q dQ}{Q^2} \right]$$

The first term in the square bracket denotes scattering involving small momentum transfer (forward scattering). It is remarkable that this term converges. Therefore

$$\epsilon_0 - E_{Q=0} \approx \frac{\pi^2}{L^2} \frac{1}{|\ln k_F| + \frac{1}{n(0)U}}$$

where  $n(0)$  is the density of states at the fermi surface and  $k_F$  is the fermi wave vector.

Therefore

$$\frac{\delta}{\pi} = \frac{1}{\pi |\ln k_F| + \frac{1}{n(0)U}}$$

Notice that what has contributed to finite phase shift is the convergence of the principal value integral, in particular the forward scattering part. This phase shift vanishes when the particle density vanishes and also when  $U$  vanishes.

Anderson argues that this finite phase shift at the fermi surface causes an orthogonality catastrophe leading to the vanishing of  $Z_{K_F}$ . This part of Anderson's argument is not transparent to me. Basically what he says is that a phenomenon similar to Anderson's orthogonality catastrophe that occurs when we add a local static one-body potential to a free fermi sea happen in this case as well.

Below I summarise some of Anderson's results.

- 1) Manybody theory should be done in a meaningful way not losing track of what

is our aim. Infact he beautifully demonstrates that naive analysis will lead to a wrong statement that the phase shift is zero in two dimensions.

2) The finite phase shift leads to a long range interaction between electrons close to the fermi surface. i.e. the  $K$  space is responding in an incompressible way to the fact that  $Q = K - K'$ , the relative momentum of the two injected particles, cannot be zero. No two opposite spin particles may occupy exactly the same momentum state close to the fermi surface.

3)  $Z_{K_F}$  vanishes as

$$Z_{K_F} \sim N^{-\left(\frac{1}{2}\right)^2}$$

4) Both  $\frac{\delta\Omega}{\delta\omega}$  and  $\frac{\delta\Gamma}{\delta K}$  are anomalous at the fermi surface, and  $\frac{\delta\Omega}{\delta\omega} \sim -\omega^{-\left(\frac{1}{2}\right)^2}$ .

I wish to close the summary of Anderson's work by saying that the singular forward scattering leads to a long range exchange interaction between particles in momentum space. However, it is not clear how this failure of fermi liquid will lead to spin charge decoupling. Infact, a model that I have constructed, (reprinted as an appendix to this lecture) which I briefly mentioned in the second lecture leads to spin-charge decoupling arising from a specific long range interaction in momentum space. The best place to read Anderson's work is the Anderson-Ren paper and chapter VI of the Princeton Book.

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## AN EXACTLY SOLVABLE FERMION MODEL: SPINONS, HOLONS AND A NON-FERMI LIQUID PHASE

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An interacting fermion model in  $d$ -dimensions is introduced and solved exactly. Low energy excitations have complete spin-charge decoupling. The holon spectrum is gapless and exhibits a pseudo-Fermi surface. Spinons have a gap and, as in the 1-D Hubbard model, the spinons exist only in a limited region of the Brillouin Zone. As a function of electron concentration the system exhibits metal insulator transition.

The low energy physics of high- $T_c$  superconductors<sup>1</sup> is well-described by the  $t$ - $J$  model. Anderson<sup>2</sup> introduced this model as an essential part of the RVB theory of the normal and superconducting properties of ceramic superconductors. While a satisfactory, systematic and quantitative many-body theory is still lacking, Anderson and collaborators and others<sup>2-11</sup> have gained qualitative insights through some novel approximation methods and also largely from the anomalous normal state properties. More recently Anderson<sup>8</sup> has brought in more insights and some quantitative progress inspired by the high resolution photo-emission experiments, tunnelling and also the Lieb-Wu spectrum of the 1-D Hubbard Model. The emerging physical picture of the normal state is a novel quantum fluid, where Fermi liquid theory fails. The simple pole of the electron propagator close to  $k_F$  is converted into a branch point resulting from spin-charge decoupling. The resulting spinons and holons have their own "Fermi surfaces".

The  $t$ - $J$  model seems very difficult to solve at the present moment and the anticipated spin-charge decoupling has not been shown to exist in a satisfying and quantitative fashion. The aim of the present letter is to construct a model which has a non-Fermi liquid phase exhibiting spin-charge decoupling. It is not at all obvious that our present model is an "adiabatic continuation" of some aspects of the  $t$ - $J$  model. It may perhaps teach us something about the mechanism underlying spin-charge decoupling and the emergence of holon pseudo-Fermi surface in strongly correlated systems.

Ours is a modified  $t$ - $J$  model. Instead of the absence of double occupancy in real space, it has absence of double occupancy in momentum space for low energy states. Electrons in momentum space have an infinite-range exchange interaction.

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The basic idea is to concentrate on momentum space rather than real space. Recall that one of the attractive features of the BCS reduced Hamiltonian is its simplicity in momentum space which leads to its exact solvability and also to the non-trivial BCS condensed state. Interestingly, we find that a simple two-body interaction can be added in momentum space to the free particle problem which *modifies* the ground state *qualitatively*, leading to single occupancy in some region of momentum space resulting in spin-charge decoupling. We are also motivated by the fact that real-space double occupancy constraint leads to somewhat similar constraint in momentum space. This is explicit in the split band picture that comes in Hubbard's decoupling approximation<sup>10</sup> as a reduction in the Fermi surface volume by two. This is also an *explicit* assumption in the RVB transport theory of Anderson and Zou.<sup>11</sup>

In this letter we present a simple version of our model, find the ground and excited states, and discuss the thermodynamic and transport properties. Our model is

$$H = \sum_k C_{ka}^\dagger C_{ka} + \sum_{kk'} S_k \cdot S_{k'}$$
 (1)

where

$$S_k = C_{ka}^\dagger \sigma_{aa} C_{ka}$$
 (2)

is the spin operator in momentum space and is *not* the Fourier transform of  $S_i = C_{ia}^\dagger \sigma_{ii} C_{ia}$ . Let me point out that for simple choices of  $J_{kk'}$  it is possible to get spinons, holons and the desired shapes of their pseudo-Fermi surfaces. To make the dramatic effect of exchange interaction in momentum space clear, we will concentrate on a simple choice:

$$J_{kk'} = J(1 - \delta_{kk'}) \quad \text{and} \quad J > 0.$$
 (3)

Again for simplicity we will assume  $\epsilon_k = h^2 k^2 / 2m$  instead of the tight binding dispersion. The Hamiltonian is

$$H_0 = \sum_k (\epsilon_k - \mu) C_{ka}^\dagger C_{ka} + J \sum_k S_k \cdot S_{k'}$$
 (4)

$$= \sum_k (\epsilon_k - \mu) C_{ka}^\dagger C_{ka} + J(\sum_k S_k)^2 - J \sum_k S_k^2.$$
 (5)

For  $J=0$ , the ground state is a free Fermi sea. As we increase  $J$  from 0, the Fermi sea gets rearranged close to the Fermi surface as explained below. The first term of Eq. (5) favours double occupancy in momentum state. The second term does not mind single occupancy — it only favours total singlet in momentum space. The third term minimises the energy if the  $k$  states are singly occupied. It is very

easy to see that this competition results in a ground state

$$|G\rangle = P_s \prod_{k_1 < |k| < k_2} C_{k\sigma}^\dagger \prod_{|k| < k_1} C_{k\sigma}^\dagger C_{k\sigma}|0\rangle, \quad (6)$$

where  $P_s$  is a singlet projection operator,  $\sigma_k$  is any  $k$ -dependent spin configuration in the momentum space in the singly occupied annulus  $\Omega$  of radii  $k_1$  and  $k_2$  such that  $\sum k_1 < |k| < k_2 S_k^z = 0$ .

The radii  $k_1$  and  $k_2$  are determined by the two equations

$$(\epsilon_{k_1} - \epsilon_{k_2}) = J \quad (7)$$

and

$$\sum_{k_1 < |k| < k_2} = \sum_{k_1 > |k| > k_2}, \quad (8)$$

where  $k_F$  is the Fermi wavevector of the non-interacting Fermi sea. The above state is a filled doubly occupied Fermi sea upto a radius  $k_1$ ; between the radii  $k_1$  and  $k_2$  it is *singly occupied* and all the electrons in this annulus form a momentum space singlet (Fig. 1). The energy lost by the kinetic energy term in this new ground state is exactly compensated by the energy gain coming from the exchange term.

As is obvious the ground state has a large degeneracy equal to the total number of singlets that can be formed with  $N_\Omega$  spins, where  $N_\Omega$  is the number of  $k$ -points

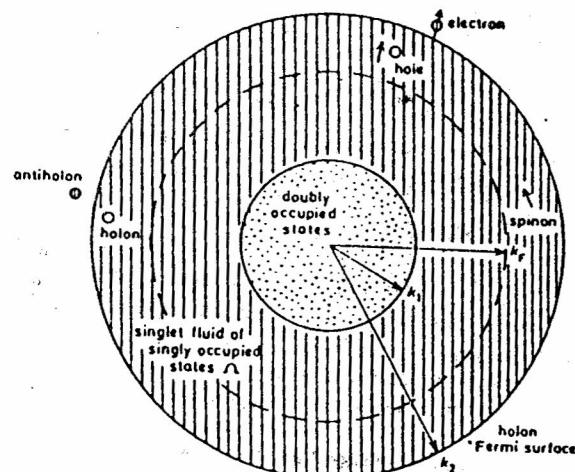


Fig. 1. The modified Fermi sea in momentum space containing a holon, an antiholon, a spinon, an electron and a hole.

in the singly occupied annulus  $\Omega$ . This enormous degeneracy can be easily shown to be lifted by an appropriate choice of  $J_{kk'}$ . The resulting ground states will be called momentum-space RVB states.

Electrons in the annulus represent singly occupied but singlet paired states. Holon-antiholon pairs can be created out of this state as follows. Consider the state

$$P_s C_{k'\sigma}^\dagger C_{k\sigma}|G\rangle$$

where  $k' > k_2$  and  $k_1 < k < k_2$ . The energy of this state is  $\epsilon_{k'} - \epsilon_k$ . The electron that is in a state  $k'$  outside the annulus is singlet paired to all the electrons in the annulus. Thus this particle does not have any definite spin: This is the antiholon. Similarly the hole created in the annulus at momentum state  $k$  does not have a spin and it is in an environment of singlet paired electrons in  $k$ -space: This is a holon: As  $|k|, |k'| \rightarrow k_2$  the excitation energy goes to zero. Thus  $|k| = k_2$  defines the holon pseudo-Fermi surface. Note that even though we have used the word pseudo-Fermi surface for holons, we do not claim that holons are fermions. Work is in progress to find out the statistics of holons.

The importance of the singlet projection in defining the holon-antiholon pair state is seen if we consider the following triplet state, which incidentally produces an electron-hole pair:

$$P_T C_{k'\sigma}^\dagger C_{k\sigma}|G\rangle,$$

where  $P_T$  is the triplet projection operator, and assume that  $k_1 < |k| < k_2$  and  $|k'| > k_2$ . The energy of this state is  $\epsilon_{k'} - \epsilon_k + 2J$ . This state has an unpaired up spin electron with momentum  $k'$  and a holon with momentum state  $k$  with an unpaired spinon uniformly distributed in the shell  $\Omega$ . This is an electron-hole pair excitation. As  $k, k' \rightarrow k_2$  the energy  $\rightarrow 2J$ . Therefore we have a gap for physical electron-hole pair excitation spectrum.

Apart from the holon pseudo-Fermi surface, there exists a charge carrying spectrum which is also gapless:

$$P_s C_{k'\sigma}^\dagger C_{k\sigma}|G\rangle$$

where  $|k| < k_1$  and  $|k'| > k_2$ . The energy of this excitation goes to zero as  $k' \rightarrow k_2$  and  $k \rightarrow k_1$ . This defines the Fermi surface for this excitation. Notice that as  $J$  exceeds  $4\epsilon_F$ ,  $k_1$  shrinks to zero and  $k_2$  expands to  $2^{1/d} k_F$ , where  $d$  is the dimensionality. In such a situation we have only the holon pseudo-Fermi surface and all the filled states are singly occupied.

Spinon excitations can also be easily created. They have an energy gap. Consider the following state:

$$P_s^{kk'} C_{k'\sigma}^\dagger C_{k\sigma} C_{k\sigma}^\dagger C_{k\sigma}|G\rangle,$$

where  $k, k' \in \Omega$ . The above state contains an electron in state  $k_1$  and an electron in state  $k'_1$ . The singlet operator  $P_{\sigma}^{kk'}$  singlet projects the rest of the  $N_{\Omega} - 2$  electrons. Thus the above state contains two up spinons with momenta  $k$  and  $k'$  and energy  $2J$ . For our simple choice  $J_{kk'}$ , the spinons have a gap and have no dispersion. Since the spinons have a gap the ground state is more like a short-range RVB in real space. At the moment we think of the momentum  $k$  of the spinon more as a label rather than the actual crystal momentum carried by the spinon. There are some subtleties associated with the actual momentum carried by the spinon which we will not discuss here. Also it is possible to collapse the spinon gap along a desired pseudo-Fermi surface by a suitable choice of  $J_{kk'}$  without affecting the holon pseudo-Fermi surface. When  $J > 4\varepsilon_F$ , the region  $\Omega$  expands and we have only a singly occupied holon Fermi sea. It is easy to see that the allowed momentum of the spinons is within this Fermi sea only. Spinons with momenta outside  $\Omega$  simply do not exist! Analogous phenomena are known to happen in 1-D Hubbard model and XXZ Heisenberg model.

The electron propagator  $G_k(\omega)$  has an interesting structure for  $k \sim k_F$  implying a gap in the electron spectrum. When we inject an electron at  $k = k_F$ , we get a doubly occupied singlet at  $k = k_F$  leaving an electron somewhere else unpaired (depending on whether we have even or odd number of total electrons). It is easy to show that the enormous degeneracy of the ground state makes the wavefunction renormalization  $Z_k$  vanish for all  $k$  lying in the annulus. To understand this let us consider the definition of  $Z_k$ :

$$\sqrt{Z}_k = (N+1; k | N+1; k, \text{exact}) ,$$

where

$$|N+1, k\rangle = C_{k\sigma}^{\dagger} |0\rangle$$

and the state  $|N+1; k, \text{exact}\rangle$  is a "relaxed" state which contains definitely one electron at state  $k\sigma$  with the rest of the electrons relaxed to obtain minimum energy consistent with the quantum numbers of  $|N+1, k\rangle$ . If the relaxation is a qualitative rearrangement,  $Z_k$  goes to zero. In the present case the rearrangement happens for the simple reason that there is a large ground state degeneracy. It is possible to remove the degeneracy and still have  $Z_k$  zero. It is also easily seen that  $Z_k$  is zero for all  $k$  in the region  $\Omega$ . In the actual  $t-J$  model  $Z_k$  goes to zero because of a qualitative rearrangement arising from some kind of orthogonality catastrophe.<sup>8</sup> The momentum distribution function is constant:

$$n_k = 1 \quad \text{for } k \in \Omega .$$

In this region the particle and hole Green's functions have identical structure.

The holons and spinons do not scatter against each other. This, together with the presence of low energy current-carrying excitations, makes the resistance zero

at  $T = 0$ . However, the ground state is not superconducting since there is no phase rigidity of any kind associated with the change in the ground state. The formal expression for the partition function can be written as a finite-dimensional integral owing to the infinite range of the integration. The expression for the partition function of this model is

$$Z = \int \prod_k D m_k(\tau) e^{-\beta \sum f[m_k]} ,$$

where  $f[m_k]$  is the free-energy functional corresponding to one momentum  $k$  in an external time-dependent imaginary magnetic field  $\bar{m}(\tau)$ :

$$f_k[m] = -\beta^{-1} \ln \left\{ \text{Tr } T \exp - \int_0^\beta [(\varepsilon_k - \mu)(n_k + n_{k'}) + JS_k^2] dt \right. \\ \left. \times \exp i \int_0^\beta 2\sqrt{n} \bar{m}(\tau) \cdot S_k(\tau) d\tau - \pi \int_0^\beta m^2(\tau) dt \right\} .$$

Thus the partition function is a functional integral corresponding to one vector degree of freedom  $m_k(\tau)$ . Without evaluating this explicitly or even numerically, the low- $T$  specific heat and susceptibility follow from the low-lying excited states we have found. The specific heat at small  $T$  is

$$C_v = \text{const.} T$$

due to the existence of the pseudo-Fermi surface. One of the peculiar features of our model is that in spite of the presence of finite gap for spin excitation it has zero spin susceptibility. This is due to the fact if we polarize a fraction  $\alpha N$  of spins by external uniform magnetic field then the energy change coming from the term  $(\sum S_k)^2$  is proportional to  $\alpha^2 N^2$ . Thus the low- $T$  susceptibility is identically zero.

The metal insulator transition in the tight binding version of this model is very easily seen when we choose  $J > 2dt$ . In this case, the region  $\Omega$  expands and all the occupied states are only singly occupied. When we have one electron per site (half-filled band) this singly occupied band fills the entire momentum space leading to an insulator. The gap for charge excitation is  $3J/2$ . This is the analogue of Mott-Hubbard gap in the sense that there is no spontaneous symmetry breaking in this Mott insulator. It is a paramagnetic insulator — it cannot be expressed easily as a single Slater determinant (even though it can be written as a singlet projection of a single Slater determinant for simple choice of  $J_{kk'}$ ). All the insulating and conducting states that we have discussed so far have the character that they have no long-range magnetic or CDW order.

Our model has a long-range force in momentum space and this is responsible for the interesting spin-charge decoupling. The infinite  $U$  Hubbard model, believed to be at the heart of understanding the normal state properties of high- $T_c$  superconductors, has long-range gauge forces<sup>6,7</sup> owing to the double occupancy

constraint. Perhaps our long-range forces may be explained as arising from the constraint in the infinite  $U$  Hubbard model. In this sense the  $J$  of our model may not be directly related to the  $J$  of the  $t$ - $J$  model.

It is easy to incorporate an additional BCS-like attraction between electrons which leads to *pairing of holons* rather than of electrons. Details of this will be published elsewhere. It will be interesting to see if the recently studied infinite-range or infinite-dimensional Hubbard model<sup>12</sup> has any of the properties exhibited by our model.

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## Structure of holes in a Mott insulator

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The electronically relevant structural feature common to all the high-T<sub>c</sub> cuprate superconductors is the square-planar CuO<sub>2</sub> sheets with relatively weak inter-planar coupling, separated by the spacer layers of other oxides that act merely as charge reservoirs. The electronic structure of the CuO<sub>2</sub> sheets involves the crystal-field split copper 3d<sub>x<sup>2</sup>-y<sup>2</sup></sub> orbital hybridized with the oxygen 2px and 2py ligand orbitals. It is known now that in the limit of strong hybridization this can be reduced effectively to a 2-dimensional one-band tight-binding Hubbard Hamiltonian, parametrized by the on-site repulsion U, the hopping matrix element t and the deviation from half-filling  $\delta$  (controlled by cation doping or oxygen stoichio-metry). This is the minimum model, presumably generic to all cuprates-- this is consistent with the fact that all cuprate superconductors have similar phase diagrams, and indeed their T<sub>c</sub>'s, normalized with respect to their respective T<sub>c</sub> max, when plotted against the carries concentration  $\delta$  (more precisely  $\delta^{*}$  determined by the London penetration depth) do superpose.

The 2D Hubbard model has been studied intensively in the context of a purely electronic mechanism of superconductivity in

these novel cuprates. It is now realized, however, that the normal state electrical resistivity ( $\rho$ ) of these cuprates is highly anomalous in that it is linear in temperature from the highest temperature ( $>600$  K) down to  $T_c$ , which can be made much smaller than the transport Debye temperature as in "BL 2201". Purely phenomenologically, such a temperature dependence of resistivity would imply a marginal Fermi-liquid which in turn correctly implies not only the other normal-state behaviour observed experimentally, but also attractive interaction (through dielectric function) necessary for superconductivity. This connection between normal state resistivity and superconductivity is also suggested by the near equality of the transport relaxation time and the pair-breaking time associated with the superconducting fluctuations close to  $T_c$ . Superconductivity must be  $\rho$ -compatible!

It is proposed that the normal state resistivity arises as the diffusive motion of charge carriers (quantum vacancies) resulting from "dephasing by orthogonality".

Thus, for  $U = \infty$  (or  $J=0$  in the tJ model which is equivalent to the Hubbard model in the strong coupling limit  $U/t \gg 1$ ) the quantum vacancy moves in the paramagnetic background of spins that have no dynamics of their own. It is clear then that the partial amplitudes for the propagation of the quantum vacancy between two given points, along the alternative paths must add incoherently because these alternative paths leave the background spins in orthogonal configurations. This would yield a diffusion constant typically of magnitude  $\hbar/a^*$ . The latter would imply via Einsteins' relation a T-linear resistivity if the vacancy-gas could be treated as non-degenerate. It should be possible to relate

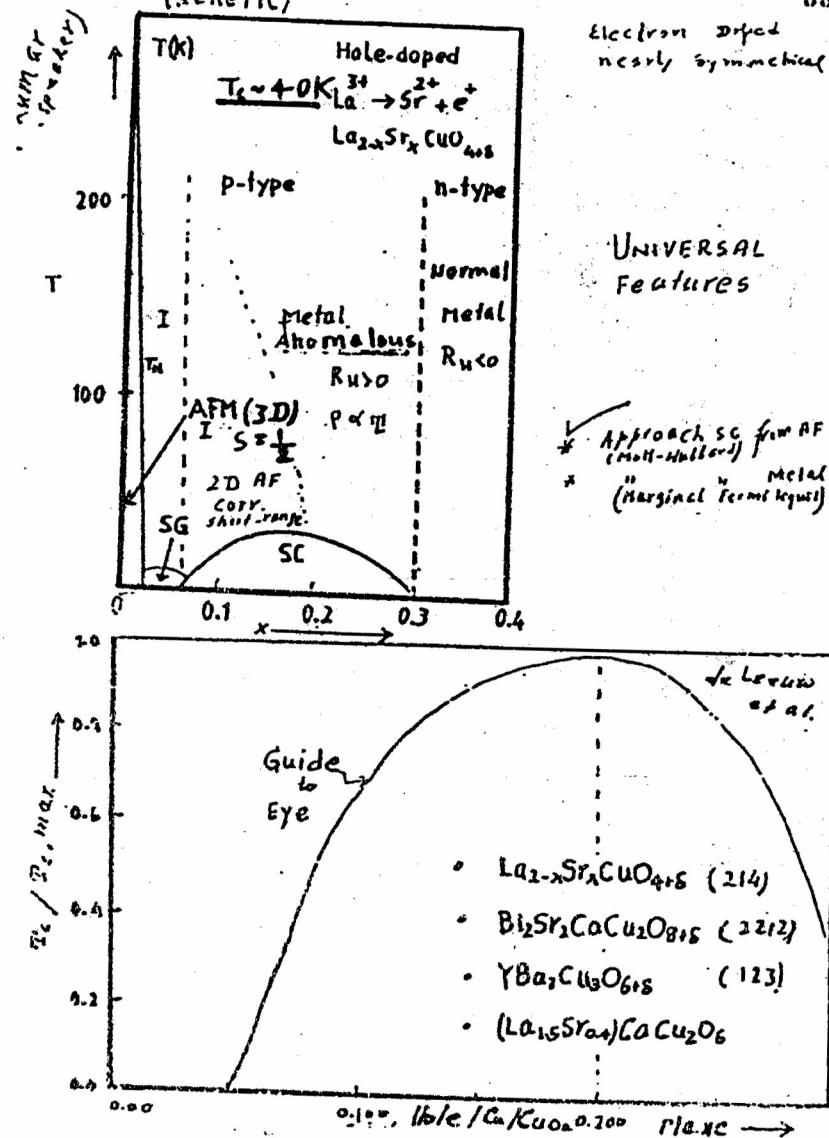
this simple physical picture of 'dephasing' to the gauge-theoretic treatment of the Nagaoka problem ( $U = \infty$ ) where the longitudinal gauge-field representing the non-double-occupancy-constraint should cause dephasing.

It is not clear at the moment if  $U = \infty$  limit has superconductivity at all. On the other hand, finite  $U$  ( $J \neq 0$ ) can lead to pairing (local) of these vacancies through the 'magnetic string' mechanism. The Autolocalization of a quantum vacancy and its delocalization by pairing leads to a phase diagram generally consistent with observations.

#### References (Author's Work)

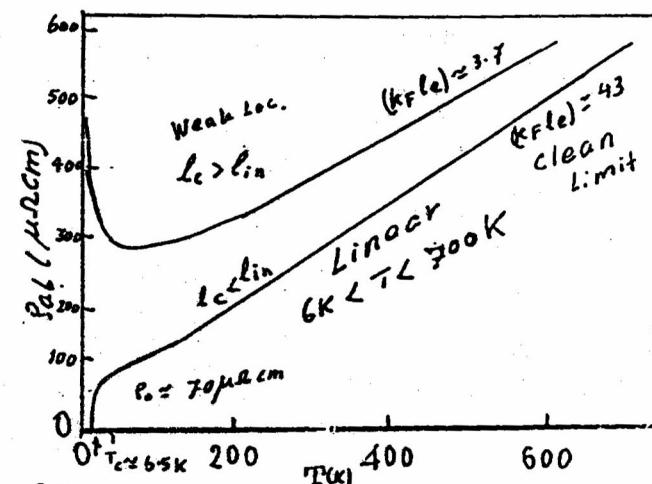
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PHASE DIAGRAM (Layered HSC)  
(generic)

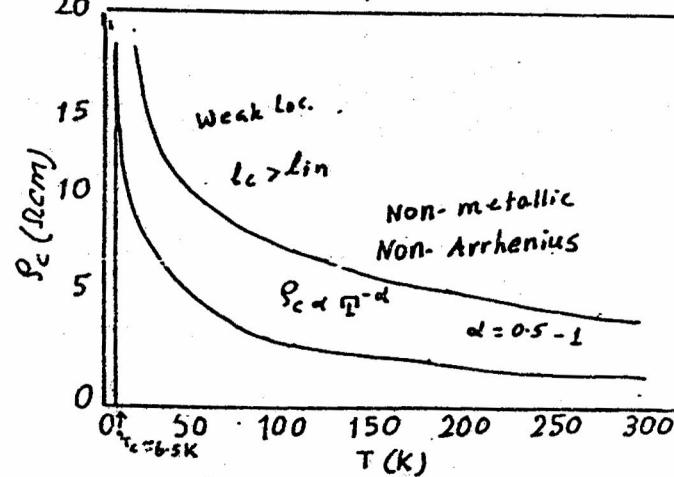


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$\overline{\rho}_c$ -Linear  $\rho_{ab}$   
non-Arrhenius  $\rho_c$  }  $Bi_{2+x}Sr_{2-y}CuO_{6+\delta}$   
Anisotropy at  $T_c$ :  $\frac{\rho_c}{\rho_{ab}} \sim 10^4-10^5$  "2201"



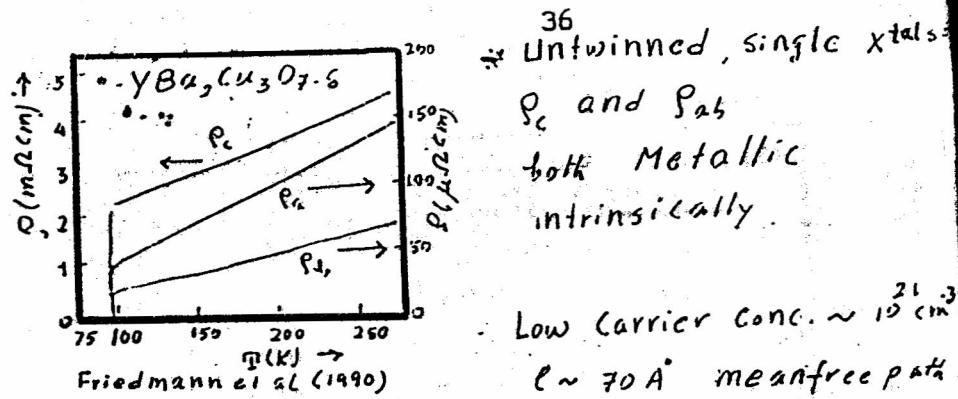
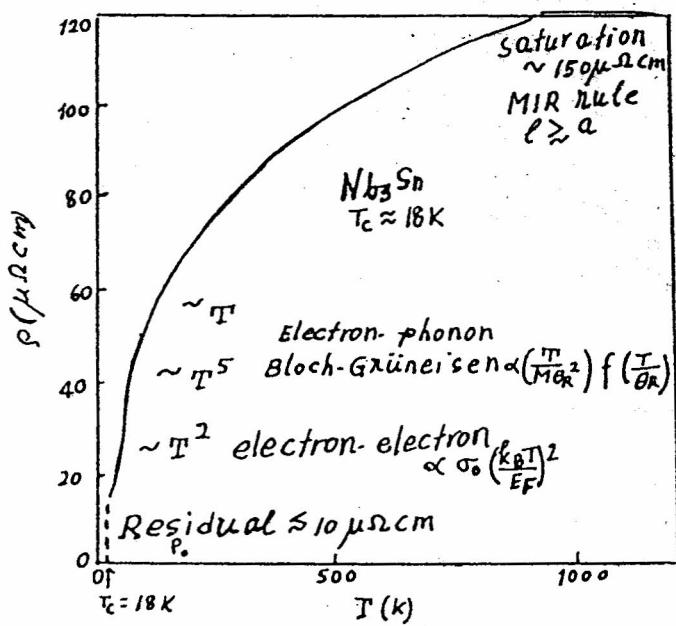
often  
 $\Rightarrow \rho_{ab} \cdot \rho_c \approx \text{const.}$



S. Martin et al.  
(1989)

Anisotropy:  
 "214"  $\sim 10^1-10^2$   
 "123"  $\sim 10^2-10^4$  (also dichalcogenides,  
graphite etc.)  
 "2201", "2212"  $\sim 10^4-10^5$

## Fermi-Liquid (clean Limit)



# mfp  $\ell \sim 70 \text{ Å} \gg \xi_0$  : Affects Flux Flow

$$\text{core} \xleftrightarrow{2\xi_0} \xrightarrow[\text{motion}]{v} (\mu H_{c2})^2 \propto \xi_0^2 = \eta v^2$$

Induced E field (Lorentz)  $\downarrow$

$\therefore \eta = \Phi_0 H_{c2} \sigma \propto \sigma$   
you can study  $\sigma(T)$  at  $T < T_c$ !

# but  $\ell \gg \xi_0 \Rightarrow$  ballistic transport across core  
Must use Landauer Resistance expression  $\rightarrow$

$$\eta = \left( \frac{3^{2/3}}{\pi^{3/2}} \right) \left( \frac{\hbar}{\xi_0} \right) \left( \frac{1}{e^{\Delta/k_B T_1}} \right) n^{2/3}; \quad \text{typically } \sim 10^9 \text{ (cgs)}$$

$\eta \downarrow$  as  $T \downarrow$   
strongly temp. dependent.

(NK 14/95 unpublished)

At Low Temp we will be  
in the Low Friction Kramers  
regime. T dependence of  $\eta$   
will dominate flow of flux.

- Hubbard = Gutzwiller = PPP Model < Anderson Model  
(MOTION OF HOLE IN HOLE-Y MOTT-INSULATOR)

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma}$$

[M-I transition  
magnetism]

- Hubbard Hamiltonian by Gutzwiller
- 1-Band Tight Binding, dimensionality D
- # Sites = N,  $\omega_i$ : band-width, U: on-site repulsion.
- # Electrons = n, D=2
- $\delta = 1 - \frac{n}{N}$  = deviation from  $\frac{1}{2}$ -filling (stoichiometry)
- Can describe spin- $\frac{1}{2}$  Fermions with short range Repulsion ( $U > 0$ ), e.g. Strongly Correlated Electrons in  $CuO_2$  sheets of HTSC, or  $^3He$ .
- Extendable: (i) Finite range of U (ii) # of bands  $> 1$   
(iii) Anderson Hamiltonian, via PPP model, e.g. 3 in Bond-chirality  $CuO_2$  repulsion
- Dimensionless parameters:

$U/t \gg 1$  Strong Coupling Limit  
 $\ll 1$  Weak Coupling Limit

$\delta \rightarrow 1$  Empty Lattice Limit (dilute electrons Wigner Latt.)  
 $\rightarrow 0$   $\frac{1}{2}$ -filled Band Limit (dilute holes)  
Doped Mott-Insulator

- Hamiltonian  $H$  is competition between
  - Lowering of K.E. by delocalization ( $t$ ) and the confining Potential barrier ( $U$ ) for  $\delta \rightarrow 0$ . (free volume  $\rightarrow 0$ ).
  - Nesting of FS as  $\delta \rightarrow 0$  giving SDW  $\rightarrow$  gapping at FS (Peierls instability) in Polyacetylene ( $c_{11}n$ )
- Hence: (Equilibrium) Thermodynamics and carrier mobility (transport) get correlated just as in metal-harmonics.

### Dilute Electron limit $S = 1 - \frac{n}{N} \rightarrow 1, \frac{1}{2}$

$\delta = 1 \Rightarrow$  empty electron band. No problem

$\delta = 1 - \frac{1}{N} \Rightarrow$  one electron  $\rightarrow$  free motion

$\delta = 1 - \frac{2}{N} \Rightarrow$  two electrons with repulsion  $U$   
Even if  $U/t \rightarrow \infty$  the T-matrix remains finite ( $= 4\pi h^2 a/m\epsilon_0$ )

$\delta = 1 - \frac{n}{N} \approx 1$  { Two electrons repelling in excitable Fermi-Surface background

$$V(q, \omega) = \frac{U}{1 + \chi(q, \omega)U}, \quad \chi = \frac{1}{1 + \frac{U}{\omega}}$$

$$\chi(q, \omega) = \frac{1}{1 + \frac{U}{\omega}}$$

polarisation irreo.

- Fermi-Liquid
- Paramag. Metal  $R_h < 0$  ( $\therefore$  Less than  $\frac{1}{2}$  full)  
No SWAVE supercond.  
No Diagonal Order (CDW, SDW)

- But p-wave supercond. possible:

$$V(r-r') = -\Gamma \hat{\chi}_{dp}(z-z') \underbrace{S_d(z) S_p(z')}_{\text{paramas. } \chi} \quad \Gamma > 0$$

$$\tilde{V}(z) \rightarrow -\Gamma \hat{\chi}_{dp}(z) S_d(z) S_p(z)$$

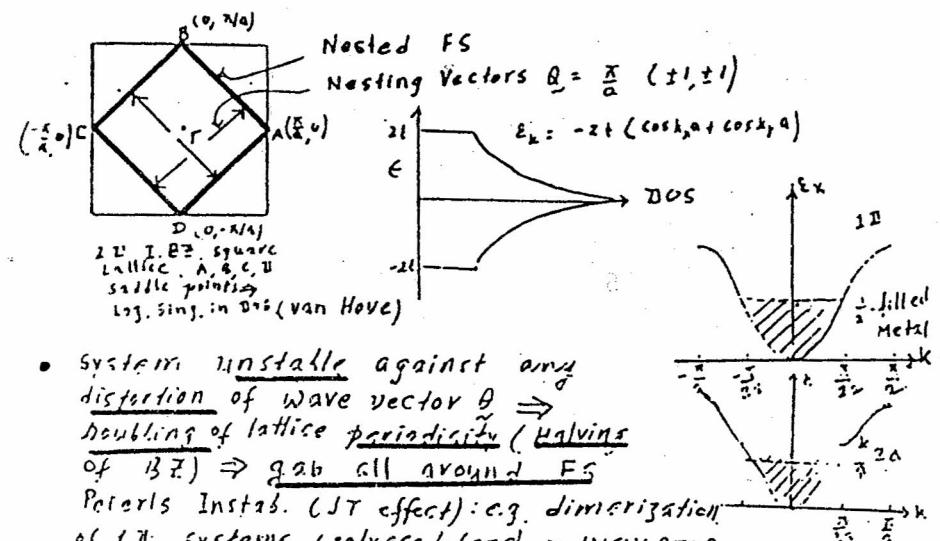
Always +ve definite ( $\therefore$  stability)  
 $\therefore$  only the parallel spin (triplet) we have binding

- (In fact  $\tilde{V}(q, \omega)$  remains repulsive for  $\omega < \omega(q)$ , the paramagnon frequency for anti-parallel  $(q, \omega)$ )  
e.g.  $^3He$

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- Half-Filled (Stoichiometric) Limit  $\delta = 0$   
and  $S = 0(\frac{1}{N})$
- $\delta = n$ 
  - Weak coupling,  $U/t \ll 1$ , Nesting of FS is important;
  - Strong coupling,  $U/t \gg 1$ , Nesting Not Important;

### • Weak Coupling Limit

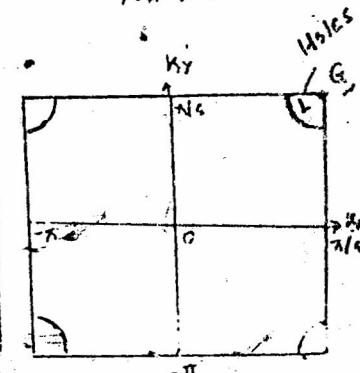
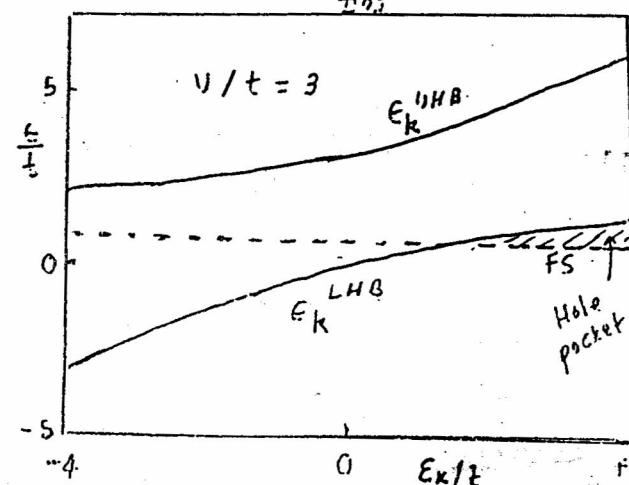
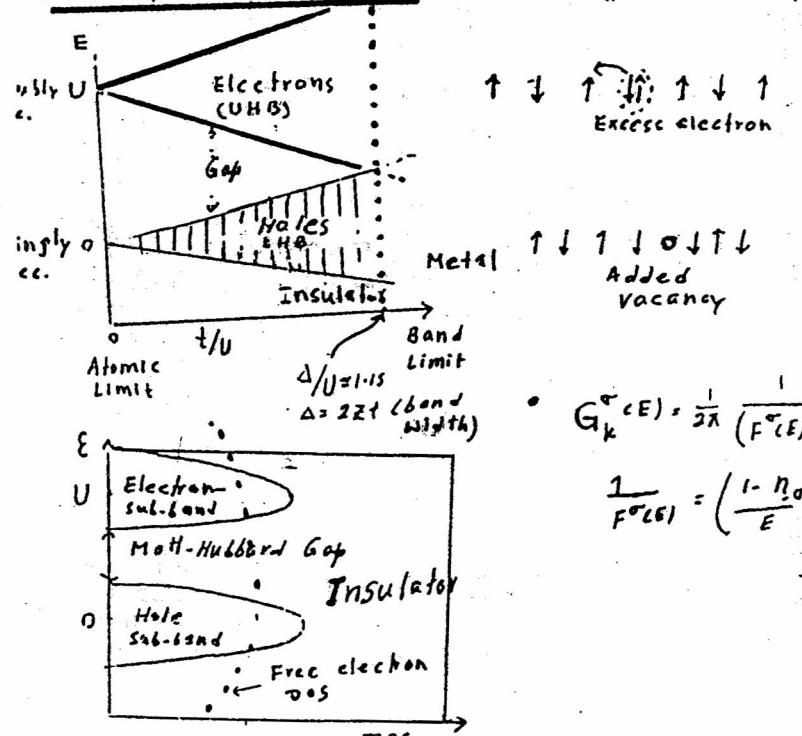


- For  $U > 0$  SDW condenses (commensurate)
 

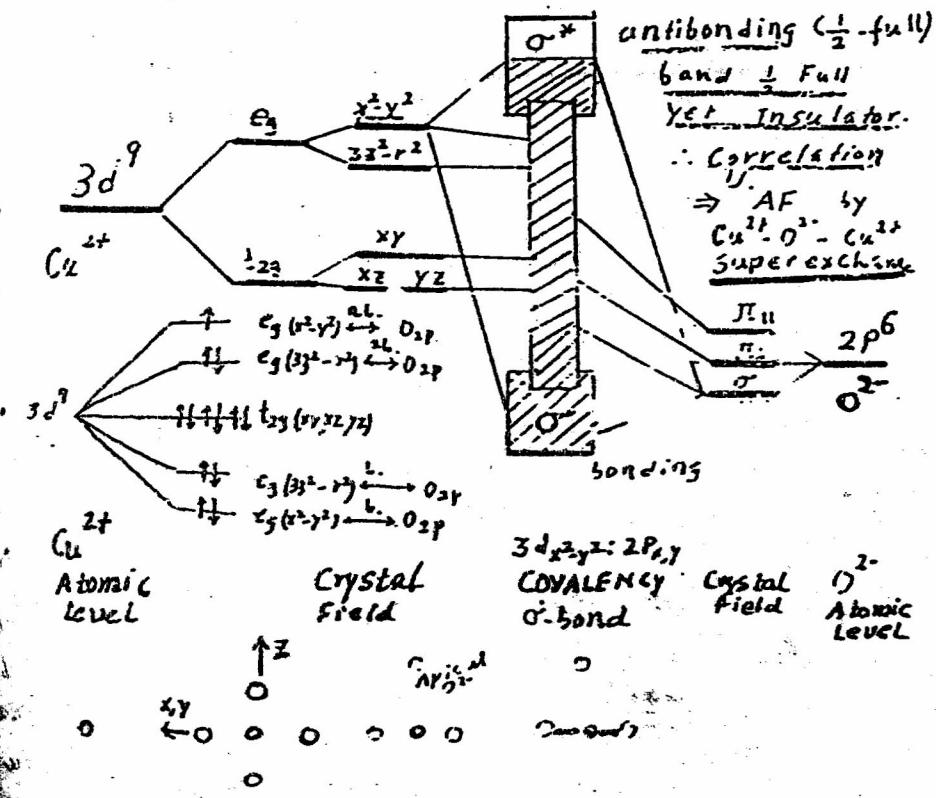
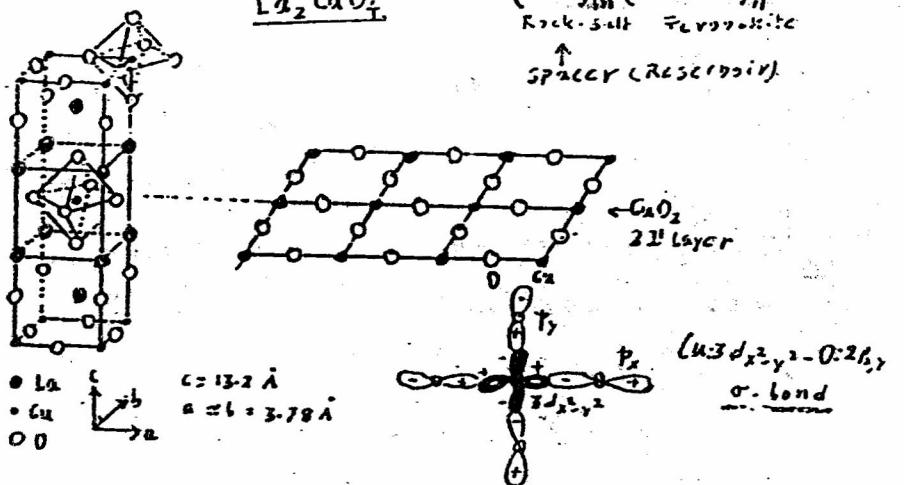
Doping destroys nesting  $\rightarrow S \neq 0$ , locally SDW gap lowered, two holes share deformation to give lower energy than separated holes  $\rightarrow$  SPIN BAG.
- BUT: Above critical temp  $T_0 = 0 \Rightarrow$  metal! Not consistent with observations, one hole. We are not in weak coupling regime.

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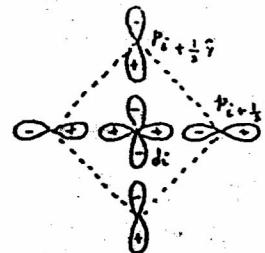
### • Strong Coupling: $U/t \gg 1$ , $S = 0$ and $S = 0(\frac{1}{N})$



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Multi-band vs one-band

Hole Rep.

$H = - \sum_{i,j,k,l} (t_{ij} d_i^{\dagger} d_j + h.c.) + E_p \sum_i n_i^{\dagger} n_i + U_d \sum_i n_{di}^{\dagger} n_{di}$

$t_{ij} = (-1)^{m_{ij}}$  metal for  $d_i, d_j = \frac{1}{2}$   
 $m_{ij} = 0$  for  $d_i, d_j = \frac{1}{2}$ .

$E_p \sim 1 \text{ eV}$   
 $U_d = 8-10 \text{ eV} > \Delta$   
 $E_p - E_d = 3 \text{ eV} \approx \Delta$   
 $\therefore$  Hole added on Oxygen.

For  $\text{CuO}_4$  cluster:  
 Bonding Ligand ( $\text{O}^-$ ) forms Singlet  $\Phi_i = \frac{1}{\sqrt{2}} (p_{i\downarrow}^{\dagger} d_{i\downarrow} - p_{i\uparrow}^{\dagger} d_{i\uparrow})$

$E_{\text{singlets}} = -8 \left( \frac{t_{ii}^2}{\Delta} + \frac{E_p^2}{U_d - \Delta} \right)$  Coherence effect.  
 here  $p_{i\sigma} = \frac{1}{\sqrt{2}} \sum_{\ell} (-1)^{m_{i\ell}} t_{i\ell\sigma}$  (bonding-ligand)

(Orthonormalization causes slight charge hopping of composite hole:

$$\sum_{i \neq j} \frac{1}{\sqrt{2}} (d_{i\downarrow}^{\dagger} d_{j\downarrow}) \rightarrow \sum_{i \neq j} \frac{1}{\sqrt{2}} (d_{i\downarrow}^{\dagger} d_{j\downarrow})$$

$\uparrow$  Spin Reversal

$$\sum_{i \neq j} t_{ij}^{\text{eff}} (\gamma_j^{\dagger} d_{i\downarrow}) (\gamma_i^{\dagger} d_{j\downarrow})$$

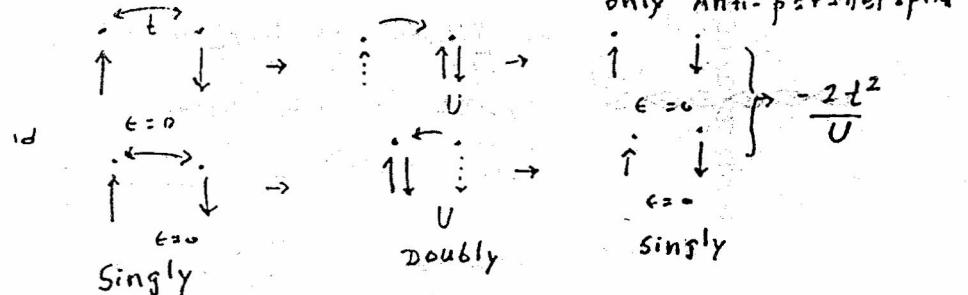
$$= \sum_{i \neq j} t_{ij}^{\text{eff}} (1 - \eta_{ij} - \sigma) d_{i\downarrow}^{\dagger} d_{j\downarrow} (1 - \eta_{ji} - \sigma)$$

→ creation of Ca-hole at site i: the Singlet is destroyed  
 $\eta_i \equiv$  empty state of the d-hole at site i

### AFM : kinetic Exchange

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virtual occ. of  
double occupancy  
only Anti-parallel spins

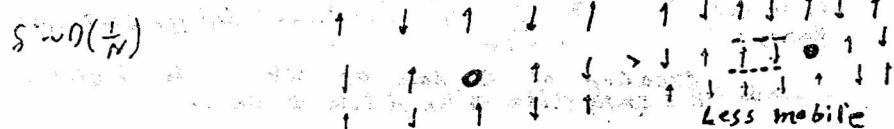


$$\Rightarrow J(S_i \cdot S_j - \frac{1}{4}) \text{, } J = \frac{4t^2}{U} > 0 \quad \text{AFM Ins.}$$

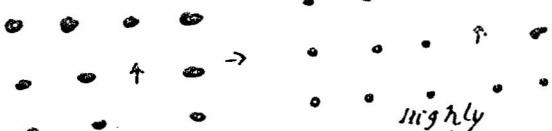
Exchange

A Vacancy (hole) in hole-doped Mott-Hubbard Insulator moves in AFM background : A many-body problem even for a single Hole. The background spins are scrambled, at least in the Ising limit

ASYMMETRY : between  $S=0$  and  $S=1$



$$S \sim 1 - 0(\frac{1}{n})$$



when  $\delta \ll p_c$ ,  $R_F$  must change sign

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HOLE Vacuum :  $[Cu:3d^{10}; O:2p^6]$   
 $Cu^{1+} \quad O^{2-}$

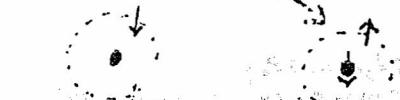
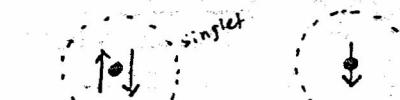
$Cu^{3+}$  2 copper holes  
 $U_{dd}$

$O^{1-}$  1 oxygen hole  
 $\Delta$

$Cu^{2+}$  1 copper hole

Only  $Cu^{1+}$ ,  $Cu^{2+}$ ,  $O^{1-}$ ,  $O^{2-}$   
are energetically admitted.  $Cu^{2+} - O^{2-} - Cu^{2+}$  superexchange  
Doped holes in Oxygen σ-orbitals (photoemission, x-ray absorption)

TWO POSSIBILITIES WITH ADDED HOLE



Strong Hybridisation

Singlet Modes  
Leaving wake of REVERSE  $Cu^{2+}$ -spins ( $\downarrow$ -bar)

Weak Hybridisation  
Interlacing of two bands  
Again Wake of  $Cu^{2+}$ -spins reverse

A. direct overlap of Oxygen p-orbit overlap  $\rightarrow$  alternate channel without wake

Charge Transfer Insulator

### hole in AFM Background : t-J Model

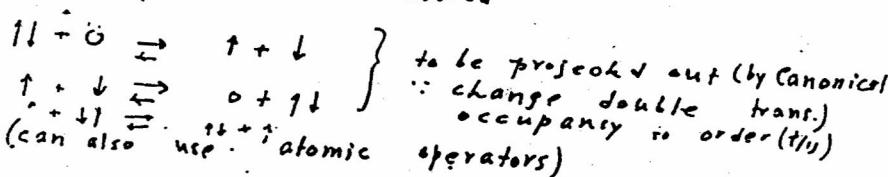
- $U \gg t \Rightarrow$  double occupancy disfavoured

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Forbid double occupancy to first order in  $t/U$ ,  
and keep effect of high-energy double occupancy  
as virtual process giving kinetic exchange

$$\rightarrow H_{eff} = -t \sum_{\langle i,j \rangle} (1 - n_{i\sigma}) c_{i\sigma}^{\dagger} c_{j\sigma} (1 - n_{j\sigma}) + \frac{4t^2}{U} \sum_{\langle i,j \rangle} (s_i \cdot s_j - \frac{1}{4})$$

- [∴ kinetic energy term can connect :



$$\rightarrow H_{eff}^{MFA} = -tS \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + \left(\frac{4t^2}{J}\right)(1-2S) \sum_{\langle i,j \rangle} (s_i \cdot s_j - \frac{1}{4})$$

Treat all the electrons as heavy

Alternatively,

$$H_{eff} = -t \sum_{\langle i,j \rangle} h_{i\sigma}^{\dagger} h_{j\sigma} + (1-2S) J \sum_{\langle i,j \rangle} (s_i \cdot s_j - \frac{1}{4})$$

This is convenient  
for motion of a single hole

$$T = -t \sum_{\langle i,j \rangle \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}$$

Multiply from left and from right by

$$I = n_{i,-\sigma} + h_{i,-\sigma} \quad \text{and} \quad I = n_{j,-\sigma} + h_{j,-\sigma} \quad \text{respectively}$$

$$(h_{i,-\sigma} = I - n_{i,-\sigma})$$

$$T_0 = -t \sum_{\langle i,j \rangle \sigma} (n_{i,-\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} n_{j,-\sigma} + h_{i,-\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} h_{j,-\sigma})$$

$$T_1 = -t \sum_{\langle i,j \rangle \sigma} n_{i,-\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} h_{j,-\sigma}$$

$$T_{-1} = -t \sum_{\langle i,j \rangle \sigma} h_{i,-\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} n_{j,-\sigma} \quad \begin{array}{l} \text{increase # of doubly} \\ \text{occupied by } I \end{array}$$

canonical transformation to eliminate  $T_0$  and  $T_1$ :  
in leading order of  $t/U$ :

$$H \rightarrow e^{iS} H e^{-iS} \quad , \quad iS = \frac{1}{U} (T_0 - T_{-1})$$

$$H_{eff} = -t \sum_{\langle i,j \rangle \sigma} h_{i\sigma}^{\dagger} h_{j\sigma} + \frac{4t^2}{U} \sum_{\langle i,j \rangle} (s_i \cdot s_j - \frac{1}{4}) + \dots$$

On use:

$$c_{i\sigma} = e_i^+ \alpha_{i\sigma} + \sigma \beta_{i\sigma}^+ d_i$$

$$c_{i\sigma}^{\dagger} = \alpha_{i\sigma}^+ e_i + \sigma d_i^+ \beta_{i\sigma}$$

$$e_i^+ e_i + \sum_{\sigma} \beta_{i\sigma}^+ \alpha_{i\sigma} + d_i^+ d_i = 1$$

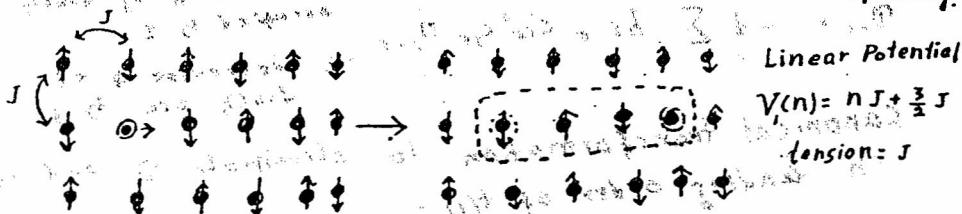
## Magnetic String

Idea is old

- \* In AF Semiconductors ( $\text{CuO}_2$ )
  - Buluevsky (1968)
  - Nagaev
  - Khomskii
  - Nagaev (1974)
- In doped RE + AF ( $\text{EuS}$ )

- \* In high- $T_c$  Cuprate Superconductors ( $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ )
  - Hirsch (1987)
  - Emery (1987)
  - Mohan and NK (1987)
  - NK (1989)
  - NK (1990)

- \* The Idea : Single Vacancy in AF displaced  $n$  lattice spacings



$J_x = J_y$  in Ising formalism  
 $J_x \neq J_y$  in 3D state  
 But Actually  $J_x = J_y = J_z$ ?  
 AF fluctuations?  
 Time scale Argument  
 $\tau_{\text{AF}} \sim k_B T_{\text{AF}} > \tau_{\text{transl.}} \sim \hbar/k$

- \* Pair of Vacancies - moved  $n$  lattice spacings Apart

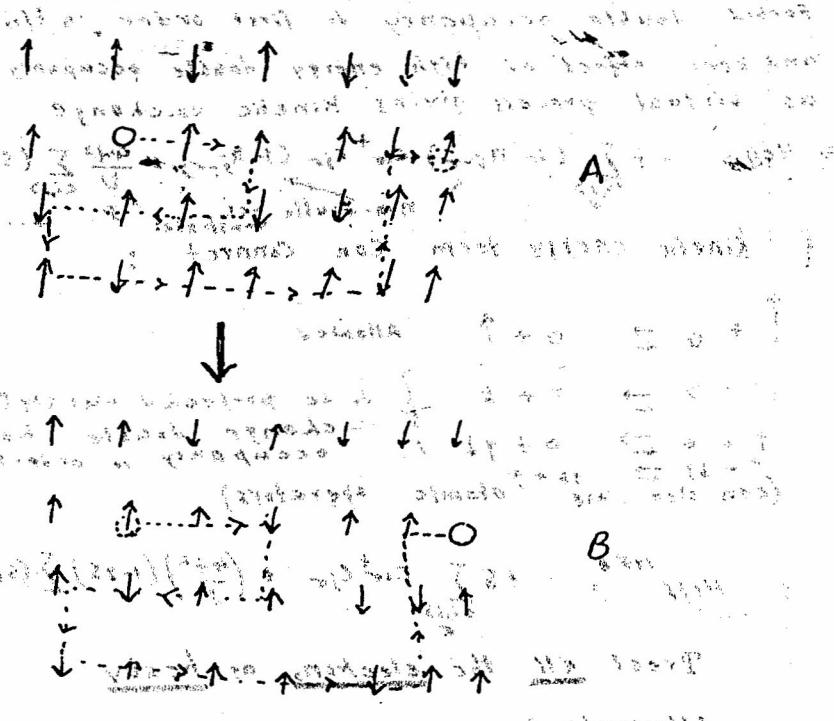


But the pair can translate freely: one Vacancy falls down the string, the other "hoovers" it up.

But  $V(n)$  in general is not Local, it is path dependent, e.g. going round a square 3 times returning the system to initial state. Energetically favoured paths are "Retraceable"  $\rightarrow$  Retraceable PATH Approximation

## Interaction between Charge Carrier (hole) and Background Spin Configurations (Path Dependent)

and Background Spin Configurations



As the hole moves from A to B

the background spins along the path are scrambled concomitantly. This is a non-perturbative effect  $\Rightarrow$  Dephasing by orthogonality of background spin states.

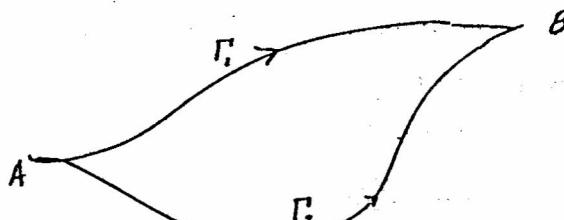
\* Incoherence by Unhgoldianity  $\leftrightarrow$

Strong coupling of carrier to

Spin configuration  $\rightarrow$  Incoherent motion (diffusion)  
rather than ballistic motion

- \* Single 'hole' in Mott-Insulator with  $J = \frac{4t^2}{U} \rightarrow 0$   
 $\Rightarrow$  background spins have no dynamics  $\Rightarrow$  'hole'  
motion scrambles spin configurations (degenerate)  
 $N \times 2^{N-1}$

- \* Propagation  $A \xrightarrow{\Gamma} B$  in a typical background



- \* Amplitudes for paths for trajectories  $\Gamma_1$  and  $\Gamma_2$  must add incoherently  $\because$  background spins are left in orthogonal states.

But all trajectories obtained from  $\Gamma$  by self-retracing insertions must be added coherently:

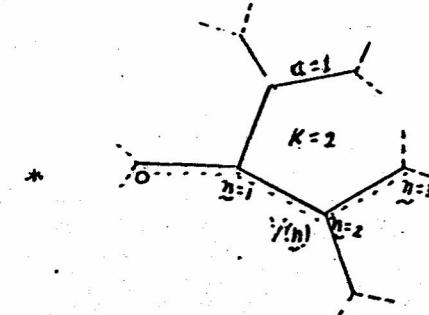
$$\overrightarrow{\Gamma} = \overrightarrow{\Gamma}_1 + \overrightarrow{\Gamma}_2$$

- \* Also some special closed-loop trajectories that return the spin systems to initial config.

The above propagator  $\rightarrow$  diffusion  $\propto t^2$ , temp.  
independent  $\Rightarrow \sigma = \frac{e^2}{\text{Volume}} \left( \frac{D}{k_B T} \right) \therefore \rho \propto T$ .

- \* Single Vacancy - A localization

- \* Retraceable Path Approximation  $\Rightarrow$  Bethe Lattice  
NO CLOSED LOOPS



$$K = Z-1 \text{ (Connectivity)} = 3$$

$$Z = \text{Coordination number} = 4$$

n = lattice site

$$V(n) = nJ + \frac{3}{2}J, J = \frac{4t^2}{U}$$

= Magnetic String Linear Potential

n = SAW distance  $\rightarrow$  n

- \* In RPA potential  $V(n)$  and state  $|n\rangle$  are both labelled locally n

\* Effective Tight Binding Hamiltonian

$$H = -t \sum_{\langle m,n \rangle} (|m\rangle \langle n| + \text{h.c.}) + \sum_n V(n) |n\rangle \langle n|$$

$$|\Psi\rangle = \sum_n \phi_n |n\rangle, \text{ For } S\text{-wave } \phi_n = \phi_{mn} = \phi_n$$

$$-t\phi_n - K\phi_{n+1} + V_n \phi_n = E\phi_n, n = 1, 2, \dots$$

\* Boundary condition

$$-t(K+1)\phi_0 = \phi_0$$

- \* Analytically solvable for eigen-value/function

- \* Simpler in continuum limit, verifiable to be good approximation

### VACANCY PAIRING

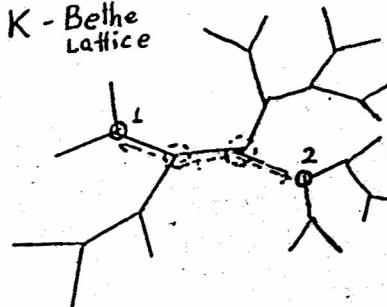
RPA  $\Rightarrow$   
K-Bethe lattice

Hard Core

$$V_{12} = J |\beta_1 - \beta_2| + J$$

Relative SAW distance

C.m. motion and  
rel. motion get  
coupled.



- To maximize energy gain by delocalization without much cost of potential energy  $\Rightarrow$

Rel. motion must be Parallel  
to C.m. motion  $\Rightarrow$

- C.m. motion free with  $t \rightarrow t/2$  and  $K=K$
- rel. motion under  $V(n)$  with  $t \rightarrow 2t$ ,  $K=1$ , hard core

$$E = E_{\text{c.m.}} + E_{\text{rel}}$$

$$E_{\text{c.m.}} = -2 \cdot \frac{t}{2} \cdot \sqrt{K} \quad \text{Bethe Lattice Band Edge.}$$

E<sub>rel.</sub> given by

$$\phi_{\text{rel.}} \equiv A_i \left( \frac{-\frac{(E-J)}{2t} + \frac{J}{2t} x}{(\frac{J}{2t})^{2/3}} \right) \Big|_{x=0} = 0$$

$$\xi_{\text{rel.}} = 2 \cdot 3 \left( \frac{U}{2t} \right)^{1/3},$$

2-4 lattice spacings

$$\Rightarrow 51 \quad \Rightarrow \frac{1}{2}(K+1)t \frac{d^2\phi}{dx^2} + (K-1)t \frac{d\phi}{dx} + (E - V(x) + (K+1)t)\phi = 0$$

$$\text{with } \left( \frac{d\phi}{dx} \right)_{x=0} = 0$$

\* Solution

$$\phi(x) = e^{-\frac{(K-1)}{(K+1)t} x} A_i(y)$$

$$y = \left( \frac{-\frac{(E-J)}{2t} + \frac{J}{2t} x + \left( \frac{K-1}{K+1} \right)^2 - 2}{\left( \frac{J}{2t} \right)^{2/3}} \right)$$

\* Eigenvalues from the Boundary Condition:

Comparison of ground state energy with the numerical results ('Exact') on 4x4 lattice Dagotto et al. (1989).

\* Size of Wavefunction:

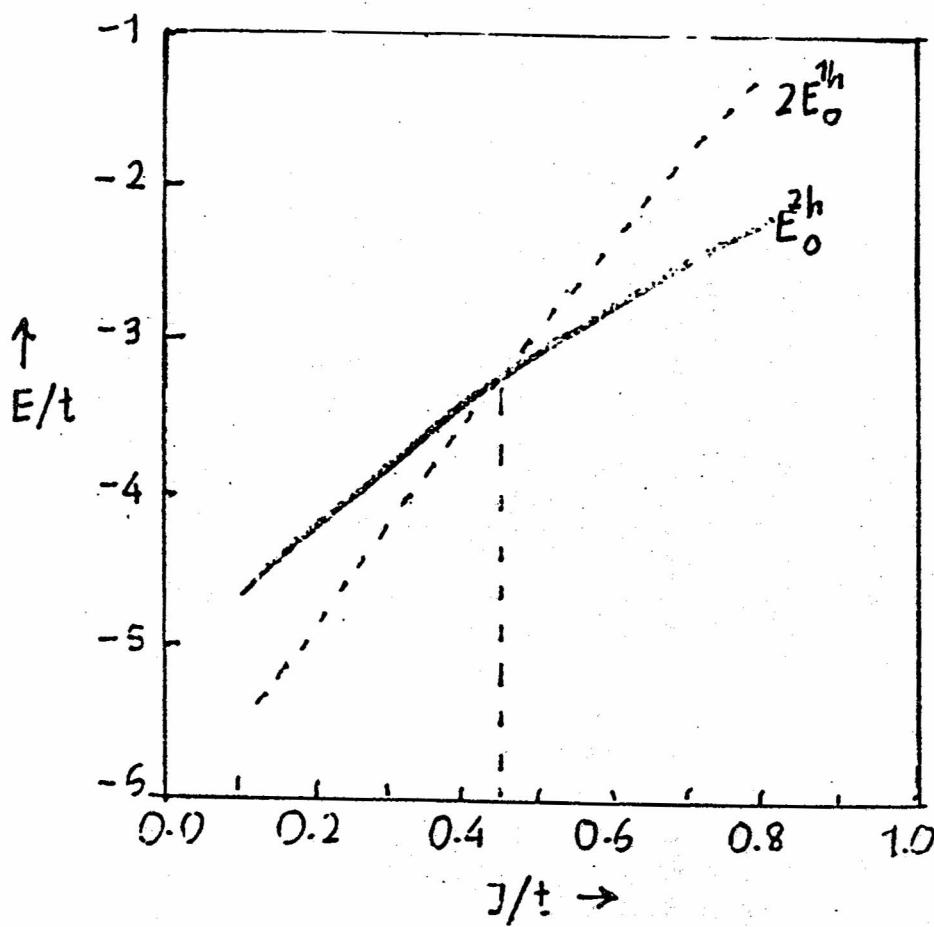
$$\xi = \alpha \left( (1+K) \frac{U}{t} \right)^{1/3}, \quad \alpha \leq 1$$

2-4 lattice spacings for  $t/U = 0.1$ ,  $(J/t = 0.4)$

\* This extended defect can propagate coherently with resonance matrix element

$\sim J \times$  overlap of  $\phi$  on neighbouring sites  
 $\ll J$

$\Rightarrow$  narrow band of Gutzwiller



For  $J/t \geq 0.42$  Holes bind

\* Zero-Point and Spin Fluctuations  
AND THE

STRING

Approximate Argument

- †  $\hat{A} \hat{B}$  String tension  $J \rightarrow 2J (\langle S_A \cdot S_c \rangle - \langle S_B \cdot S_c \rangle)$
- †  $\hat{C}$  Conn. length  $\gtrsim nnn$ ,  $nn$  will do.
- †  $\hat{D}$  The reduction factors do not multiply

\* Dimensionality: 2D is optimal (within RPA)

- \* 1D is best (except that there is no string). i.e. if AF is 2 Dimensional but  $t$  is non-zero along only 1 direction  $\Rightarrow$  strongest pairing
- \* 3D gives no pairing at all ( $k_{\perp} = 1 = 5$ ) even for  $J/t \gtrsim 1$

\* Reason  $\rightarrow$  Correlation of c.m. and rel. motion

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### Some Consequences (Plausible)

\* Low Conc. of Vacancies / site  $\delta \ll 1$

\* Size of Vacancy Wavefunction  $\xi \sim$  disordered region size  
No. of spins spanned  $\sim \xi^2$

$$* \text{Loss of LRO} \quad \text{for } (1 - \delta \xi^2) \leq p_c \quad \xi \approx \left( (1 + K) \frac{U}{t} \right)^{1/3}$$

$$p_c (2D) = 0.59 \\ \text{site dilution}$$

$$* \text{For } J/t = 0.4 \quad (t/U = 0.1), \text{ we get } \delta c_1 \approx 0.025$$

Also, a Magnetic form factor from  $\phi$

\* Metallic State: due to incipient or real pairing

For  $\delta > \delta c_2$  when  $\phi$ 's begin to physically overlap

$$\therefore \delta c_2 \xi^2 = p_c$$

$$\therefore \frac{\delta c_2}{\delta c_1} = \left( \frac{p_c}{1 - p_c} \right) \quad \therefore \delta c_2 \approx 0.04$$

\* For  $\delta > \delta c_3$ , in the normal state the Vacancies should form a non-degenerate gas with self-diffusion  $D$  caused by other Vacancies moving (hence temp. independent but  $\delta$  dependent weakly)

$$\therefore \mu = \frac{eD}{k_B T} \Rightarrow \rho_{11} \propto T$$

## Spiral Mean Field Theories, Nagaoka Theorem

H.R.KRISHNAMURTHY

Indian Institute of Science, Bangalore

## NEW MEAN FIELD THEORIES (INCL SPIRAL STATES) FOR STRONGLY CORRELATED FERMIONS:

H.R. KRISHNAMURTHY

I.I.Sc., Bangalore, India

in collaboration with C.Jayaprakash [O.S.U.; Columbus, Ohio]

S.Sarkar [U.of Alabama, Tuscaloosa], U.Wenzel [O.S.U.]

Acknowledges: P.W.Anderson, T.V.Ramakrishnan

(1) Hubbard Model in terms of holons & doublons  
(+), (-)

Dose condensation

$\Rightarrow$  Long range magnetic order

[in general Spiral Order

esp away from half filling or on  
non bipartite lattices at large  $U$ ]

Novel results on Metal Insulator Tr. in  
non bipartite lattices:

(2) t-J Model in terms of holon fermions,  
& spinon bosons:

$c_{i\sigma}^{\dagger} = b_{i\sigma}^{\dagger} f_i$   
Similarly Hubbard model with add. doublet form.  
m.f. theory, snusses and limitations:

III Work Also by: D. Yoshioka

B. Chakraborty, N. Read, C. Kane

[P. A. Lee]: K. Feinsberg, P. Hedegeard &  
Michael Brin Pedersen.

### Hubbard Model in Terms of Doublons & Holons:

$$H = -\sum t_{ij} c_{i\sigma}^+ c_{j\sigma}^- + U \sum n_i n_j$$

Make Particle-Hole Transformation on up spin:

$$\Rightarrow |0\rangle = |\uparrow\uparrow\dots\uparrow\rangle : "Vacuum" \text{ or Ref. State.}$$

$c_{ii}^+ \equiv h_i^+$  creates a "holon" at  $i$  (+ charge)

$c_{ii}^+ \equiv d_i^+$  creates a "doublon" at  $i$  (- charge)

$d_i^+ h_i^+ \equiv s_i^-$  creates a ↓ spin at  $i$

$$H = +\sum t_{ij} h_i^+ h_j^- - \sum_{ij} t_{ij} d_i^+ d_j^- + U \sum_i d_i^+ d_i^-$$

$$- U \sum_i d_i^+ d_i^- h_i^+ h_i^-$$

#### Conserved Quantities:

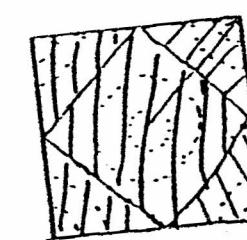
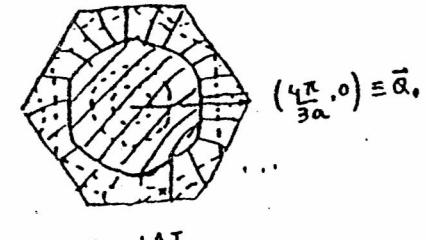
$$N\delta = \sum_i (h_i^+ h_i^- - d_i^+ d_i^-) = N(\bar{n}_0 - \bar{n}_2)$$

$$N - 2S_z = \sum_i (h_i^+ h_i^- + d_i^+ d_i^-) = N(\bar{n}_0 + \bar{n}_2)$$

$$S^z = \sum_i d_i^+ h_i^+ \quad S^{\pm} = \sum_i h_i^+ d_i^-$$

$$\text{Hole filling} \Leftrightarrow \bar{n}_0 = \bar{n}_2; \boxed{S_z = 0 \Leftrightarrow \bar{n}_0 + \bar{n}_2 = 1}$$

#### Non Interacting Case:

$$\epsilon_{0k} = \mu_0 + \epsilon_k \quad \epsilon_{2k} = -\mu_0 - \epsilon_k = -\epsilon_{0k}$$



SQ. LAT  $(n, k)$   $\in \vec{\Omega}_c$       Δ LAT  $(4\pi/3a, 0)$   $\in \vec{\Omega}_c$

Attractive Interaction  $U$  between doublons & holons must lead to

$$\text{pairing: } \langle d_i^+ h_i^+ \rangle = b_0 e^{i\vec{q} \cdot \vec{r}_i} = \langle s_i^z \rangle = \text{SPIRAL SDW}$$

$\vec{\Omega}_c$  [SDW]

$$\times \left[ \text{CDW: } \langle 1 - (d_i^+ d_i^- h_i^+ h_i^-) \rangle = \langle s_i^z \rangle \right]$$

$\vec{\Omega}_c$ : Nonzero Centre of mass momentum of pairs.

Pairing Instability when  $1 = U / \mu_{\text{pair}}(\vec{q})$

$$\mu_{\text{pair}}(\vec{q}) = -\frac{1}{N} \sum_k \frac{1 - f(\epsilon_{0k}) - f(\epsilon_{2k})}{E_{0k} + E_{2k}} = \mu_{\text{spin}}(\vec{q})$$

BCS Theory  
for Pairing

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H-F Theory  
for SPIRAL SDW.

Get Quasiparticles with energies :

$$E_{0k} = \sqrt{\left(\frac{t_{q-k}-t_k}{2}\right)^2 + U^2 b_0^2} + \left[\mu_0 + \frac{t_{q-k}+t_k}{2}\right]$$

$$E_{2k} = \sqrt{\left(\frac{t_{q-k}-t_k}{2}\right)^2 + U^2 b_0^2} - \left[\mu_0 + \frac{t_{q-k}+t_k}{2}\right]$$

Self consistent eqns for  $b_0, \mu_0$ :

$$b_0 = \frac{1}{2N} \sum_k \sin 2\theta_k [1 - f(E_{0k}) - f(E_{2k})]$$

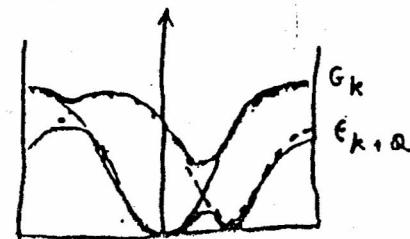
$$\delta = \frac{1}{N} \sum_k [f(E_{0k}) - f(E_{2k})]$$

$$\tan 2\theta_k = Ub_0 / \left( \frac{t_{q-k}-t_k}{2} \right)$$

$\vec{Q}$  to be determined so as to  
minimise (free) energy:

$$\begin{aligned} E_F &= \sum_k [E_{0k} f(E_{0k}) + E_{2k} f(E_{2k})] + \sum_k R_A \\ &\quad + N U \left[ b_0^2 + \left(\frac{1-\delta}{2}\right)^2 \right] - N \mu_0 \delta \end{aligned}$$

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Holons and doublons move freely in  
Ferromagnetic environment of spin bosons

Spins like to align antiferromagnetically  
because of large correlations & resulting  
exchange energies.

Spiral Phase is a good\* compromise.  
(coll. Neel AF is a special case)

[\* is it the best?

Must compare linear spin density wave/  
domain wall solutions]

### All the Qualitative Aspects of the Mott-Hubbard

Metal-Insulator transition are at once clear

$$\bar{n}_0 = \bar{n}_2 \Rightarrow \text{all particles can pair up.}$$

Pairs are charge neutral.

If binding energy  $\Leftrightarrow$  gap for charge excitations is nonzero for pairs.  $t_k^+ f_{k-k}^+$  for all  $k \Leftrightarrow$  insulator.

I : On Bipartite lattices,  $\mu(Q_0) = \infty$  at  $T=0$

Ia:  $\Rightarrow$  Pairing Instability if  $\bar{Q} = \bar{Q}_0$  for arbitrarily small  $U$  at  $T=0$ .

Pairing Theory gives  $\bar{Q} = \bar{Q}_0$  for all  $U$

$$\Rightarrow \mu_0 = 0 \quad \& \quad E_{0k} = E_{2k} = \sqrt{(t_k)^2 + (Ub_0)^2}$$

$\Rightarrow$  charge gap for any  $U$

$\Rightarrow$  2-sublattice Antiferromagnetic (Neel) Insulator for any  $U$ .

$$\Rightarrow b_0 \rightarrow y_2 - 2\left(\sum_k t_k^2\right)/2U^2$$

$$\Rightarrow \langle n_{i\downarrow} n_{j\uparrow} \rangle = \left(\frac{1}{4} - b_0^2\right) \rightarrow 2 \frac{\sum_k t_k^2}{U^2} \quad \left. \begin{array}{l} \text{as} \\ U \rightarrow \infty \end{array} \right\}$$

$\Rightarrow E_Q =$  Neel G.state energy for Supraexchange Hamiltonian

i. At finite, small temperatures  $T \ll zt$ ,

$$\chi(Q_0) \approx \frac{11}{zt} \ln\left(\frac{I}{zt}\right). \text{ is still the largest } [\ln^2 n(z)]$$

$\Rightarrow$  Pairing Instability at  $U_c(T)$  or  $T_c(U)$

$$T_c(U) = zt \exp[-zt/U]$$

Pairing theory (in 3d)

$\Rightarrow$  2 sublattice (Neel) Antiferromagnetic insulator for  $T < T_c(U)$ .

$\Rightarrow$  One transition from Para Metal to Antiferro insulator at  $T_c(U)$ .

$\Rightarrow$  Good meanfield transition if  $T_c(U) \ll zt \sim T_F$ .

Above not valid for large  $U$ !

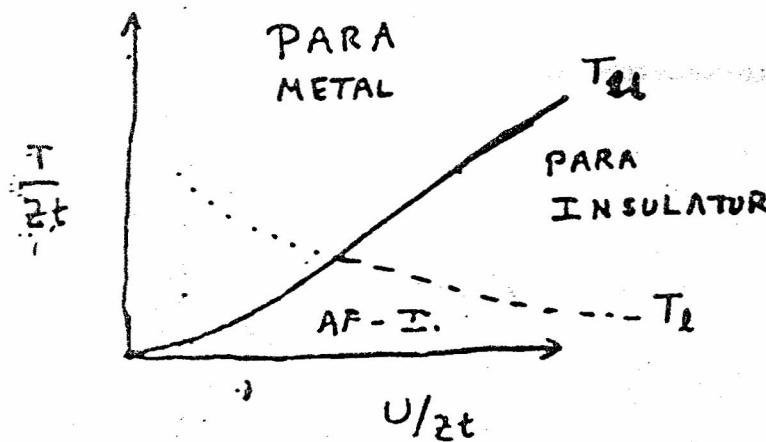
large  $U \Leftrightarrow$  Real Space Pairing.

Real Space Pairs first form at  $T_u (\sim L)$

Then Pairs bose condense at  $T_l (\sim \frac{t^2}{U})$

For  $T_c < T < T_u$  : Paramagnetic Insulator.

for  $T < T_c$  : 2 sublattice AF Insulator.



3d.

Pairing Theory always gives  $T_u$ .

[for small  $U/2t$ , " $T_e$ "  $> T_u$ , hence  
only one transition]

in 2d {  $T_e = 0$  for all  $U$ .  
⇒ AF I phase only at  $T=0$ .

[Portion of  $T_u$  above  $T_e$  may not  
be a real phase transition!]

## II. Non Bipartite lattice [eg. $\Delta$ ] $\xi = 0$

IIa:  $\chi(Q)$  finite for all  $Q$  at  $T>0$ .  
⇒ No pairing instability unless  $U > U_{c1}$ .

$$\chi_{\max}(\bar{Q}) \equiv \frac{1.52}{2t} \text{ at } \bar{Q}_1 = \left( \frac{73\pi}{a}, 0 \right)$$

⇒ Incommensurate SPIRAL at  $\frac{U_{c1}}{2t} = .66$ .

### Pairing Theory

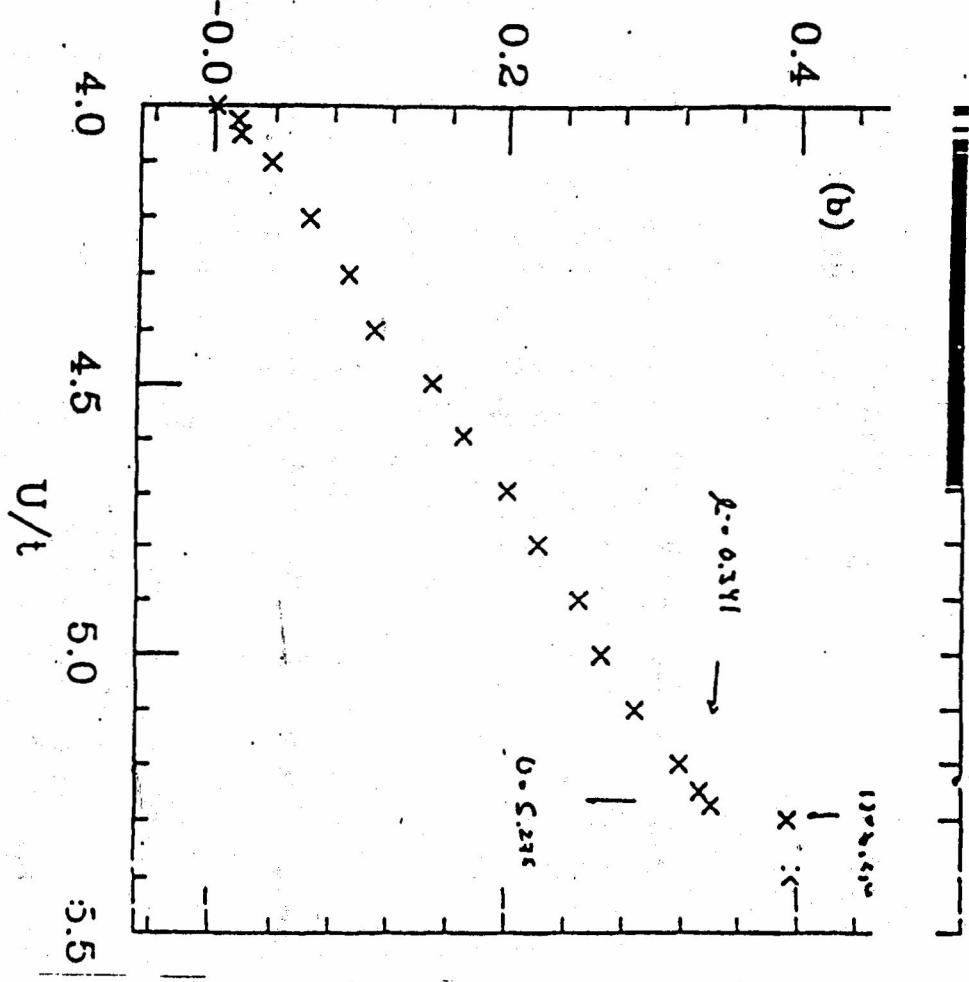
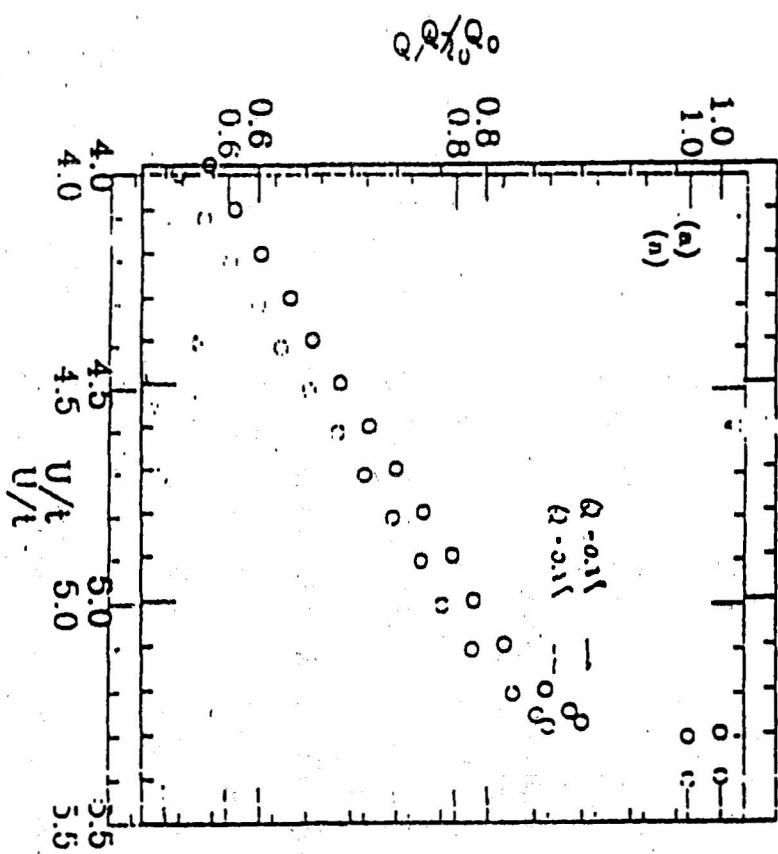
⇒  $Q$  tunes continuously from  $\bar{Q}_1$  at  $\frac{U}{2t} = \frac{U_{c1}}{2t}$   
to  $Q_0 = \left( \frac{4\pi}{3a}, 0 \right)$  at  $\frac{U}{2t} = \frac{U_{c0}}{2t} = .88$

⇒ For  $U_{c1} < U < U_{c0}$ , there are some  
 $k$  values where  $E_{0k} < 0$  or  $E_{2k} < 0$ .  
∴ Some gapless charge excitations possible  
⇒ system is metallic.

⇒ For  $U > U_{c0}$ ,  $Q = \bar{Q}_0 = \left( \frac{4\pi}{3a}, 0 \right)$  &  
 $E_{0k} > 0$ ,  $E_{2k} > 0$  for all  $k$ :

  
∴ system is 3-sublattice ( $120^\circ$  twist)  
Antiferromagnetic Insulator.

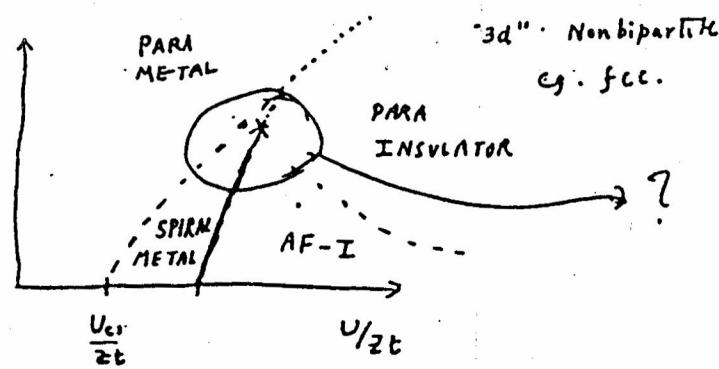
⇒ For large  $U/2t$ ,



$$\left\{ \begin{aligned} b_0 &\approx \frac{1}{2} - \frac{1}{2} \sum_k (t_{a-k} - t_k)^2 / U^2 \\ \Rightarrow \langle n_{it} n_{is} \rangle &= \frac{1}{4} - b_0^2 \approx \frac{1}{U^2} \end{aligned} \right.$$

$E_g$  = Niel G. state energy for Superexchange Hamiltonian.

IIb: Schematic finite Temp. phase-diagram:  $\rightarrow$



in 2d ( $\Delta$  lattice) SPIRAL METAL &

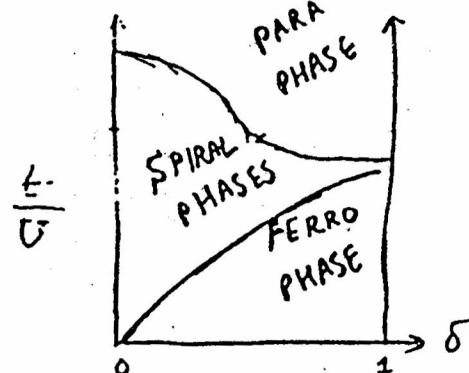
AF-I phases only at  $T=0$ .

COMPETITION FROM LINEAR SDW STATES IN  $\Delta$  LATTICE DISCUSSED IN C. Jayaprakash et.al  
"Metal-Insulator Transition in the Half-filled Hubbard Model on the  $\Delta$  lattice", Phys Rev B (to be published)

MFT also gives "sensible" results for  $\delta \neq 0$

Typical Phase diagram ( $T=0$ ,  $d=2$ )

NONBIPARTITE



DETAILS INSIDE  
"SPIRAL" REGION  
DEPEND ON  
LATTICE &  
BAND STRUCTURE

SPIRAL METALLIC for  $t/U \gtrsim \delta$

FERRO  $\rightarrow$  for  $t/U \lesssim \delta$

ALWAYS METALLIC for  $\delta \neq 0$ .

(Spin)  
SAME Results from Schwinger-Boson

Slave fermion Mean Field Theory  
(Holon)  
(doublet)

Large U limit: can be done analytically

$$E_{0k} \approx (Ub_0 + \mu_0) + \underbrace{2t\left(\gamma_k + \gamma_{Q-k}\right)}_{2} + \frac{(2t)^2}{2Ub_0} (\gamma_k^2 - \gamma_{Q-k}^2)$$

$$b_0 \approx \frac{1-\delta}{2} - \frac{1}{2} \frac{(2t)^2}{2Ub_0} \int_k \left( \gamma_k - \gamma_{Q-k} \right)^2 (1-f_k)$$

$$\frac{\xi}{N} \equiv U \left\{ b_0 - \left( \frac{1-\delta}{2} \right) \right\}^2 - \frac{(2t)^2}{16Ub_0} (1-f_Q) + \int_k f_k \tilde{E}_k$$

$$\text{Fermi: } \frac{\xi_F}{N} = -4\delta t + 2\pi\delta^2 t$$

$$\text{Anti-fermi: } \frac{\xi_{AF}}{N} = -\frac{(2t)^2}{8Ub_0} + \frac{(2t)^2}{Ub_0} \left\{ \frac{4\gamma_F^3}{3\pi^2} \ln \left( \frac{U}{\gamma_F} + 1 \right) \right\}$$

$$\delta = \frac{4\gamma_F}{\pi^2} \left[ \ln \frac{U}{\gamma_F} + \frac{\gamma_F^2}{12} \ln \frac{U}{\gamma_F} + 1 - \frac{\gamma_F^2}{18} \right]$$

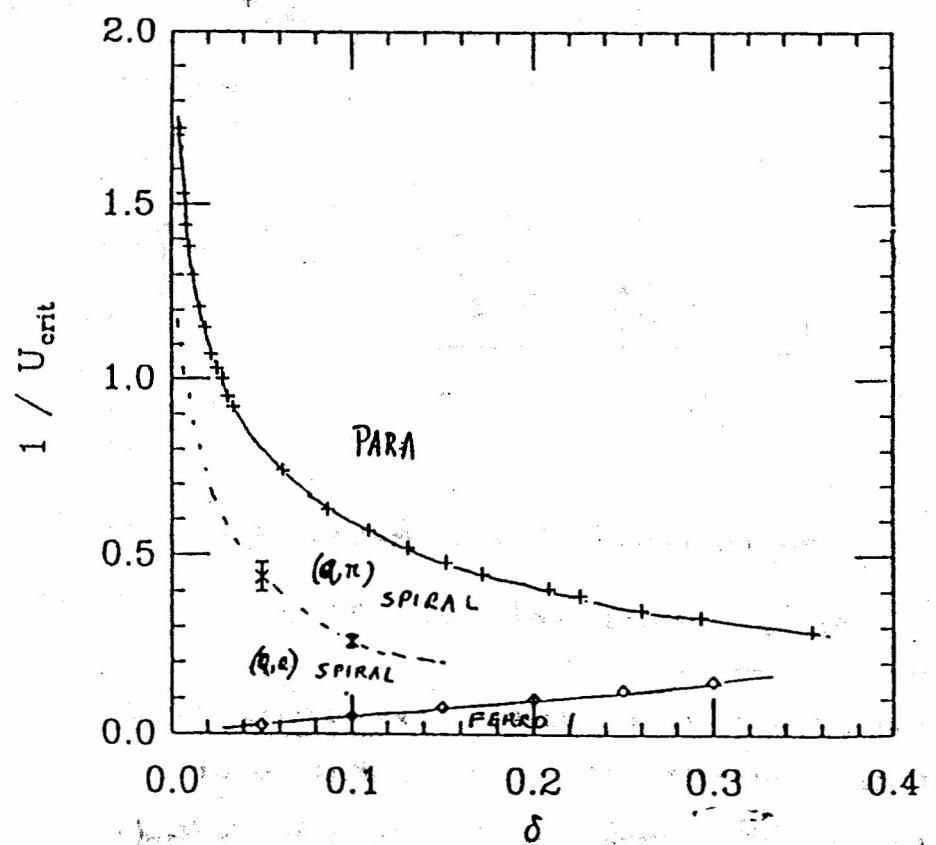
$$\text{Spiral } \frac{\xi_Q}{N} = -\frac{(2t)^2}{16Ub_0} (1-f_Q) - t \pm \delta \gamma_{Q/2}$$

$$+ 2\pi\delta^2 \sqrt{a_x a_y}$$

$$\sqrt{a_x a_y} = \frac{t^2}{4} \left[ \cos \frac{Q_x}{2} \cos \frac{Q_y}{2} + \frac{t^2}{2Ub_0} \cos Q_x \sin^2 \frac{Q_y}{2} + \cos \frac{Q_y}{2} \sin^2 \frac{Q_x}{2} \right]^{\frac{1}{2}}$$

Eg. N.N. SQUARE LATTICE

PHASE DIAGRAM : "Spiral States in the Hubbard Model", Phys Rev. B (Rapid Communications) by S. Sarker et al to be published.



### t-J Model Using SPIN-BOSONS & HOLE-FERMIONS

$$\mathcal{H} = -t \sum_{ij} \langle P C_{i\sigma}^{\dagger} C_{j\sigma} \rangle P - J \sum_i \langle \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \rangle P$$

P projects out DOUBLE OCCUPANCY.

Use the representation:

$$C_{i\mu}^{\dagger} = b_{i\mu}^{\dagger} h_i$$

$b_{i\mu}^{\dagger}$  creates spinon (Schwinger) bosons :  $\vec{S}_i = \frac{1}{2} b_i^{\dagger} \vec{\sigma} b_i$

$h_i^{\dagger}$  creates hole fermion

$$\text{constraint: } b_{i\mu}^{\dagger} b_{i\mu} + h_i^{\dagger} h_i = 1.$$

$$\mathcal{H} = t \sum (B_{ij}^+ h_j^{\dagger} h_i + \text{h.c.})$$

$$- J \sum (-h_i^{\dagger} h_i) A_{ij}^+ A_{ij}^- (-h_j^{\dagger} h_i)$$

$A_{ij}^{\pm} = \frac{1}{2} [b_{i\uparrow}^{\dagger} b_{j\downarrow}^{\pm} - b_{i\downarrow}^{\dagger} b_{j\uparrow}^{\pm}]$  : creates spin singlet pair on bond i-j

$B_{ij}^{\pm} = \frac{1}{2} [b_{i\sigma}^{\dagger} b_{j\sigma}^{\pm}]$  : hops spin bosons.

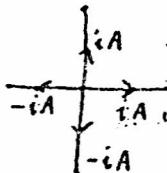
Local gauge symmetry:  $b_{i\sigma} \rightarrow b_{i\sigma} e^{i\theta_i}$   
 $h_i \rightarrow h_i e^{i\phi_i}$

Claim:

Simple mean-field theory with

$$\langle B_{ij} \rangle = B$$

$$\& \langle A_{ij} \rangle = D$$



& constraints treated on average takes into account the crucial competing spin correlations and how they affect and are affected by hole motion.

What do these amplitudes mean?

Think of  $b_i$  as classical variables:  $b_{i\mu} \propto \begin{pmatrix} \cos \theta_i e^{-i\phi_i} \\ \sin \theta_i e^{-i\phi_i} \end{pmatrix}$

gives  $\vec{S}_i = b_{i\mu}^{\dagger} \vec{\sigma} b_{i\mu}$  has polar angles  $\theta_i, \phi_i$

Then  $A_{ij} = 0, B_{ij} \neq 0 \Rightarrow \theta_i = \theta_j, \phi_i = \phi_j$  FERRO

$A_{ij} \neq 0, B_{ij} = 0 \Rightarrow \theta_i = \pi - \theta_j, \phi_i = \pi + \phi_j$  ANTI-FERRO

$A_{ij} \neq 0 \& B_{ij} \neq 0 \Rightarrow$  TWISTED OR CANTED

QH  $\Leftrightarrow$  THESE ARE SHORT RANGE SPIN CORRELATIONS.  
 LONG RANGE SPIN ORDER  $\Leftrightarrow$  BOSE CONDENSATION  
 OF THE SPIN BOSONS.

Consequences of simple mean field theory:

Propagating Fermionic & Bosonic Modes:

$$\text{Holons: } E_k = [2tB + 2JRD] z \gamma_k - \mu$$

$$\text{Spinons: } \omega_k = \sqrt{(\lambda + d\gamma_k)^2 - (\alpha \phi_k)^2}$$

$z$ : coordination #,

$$\gamma_k = \frac{2}{z} \sum \cos \vec{k} \cdot \vec{\delta}, \quad \phi_k = \frac{2}{z} \sum \frac{1}{6} \sin \vec{k} \cdot \vec{\delta}.$$

$$d = [tD + JPB/2] z$$

$$a = JAPz$$

$$R = \langle A_{ij}^+ A_{ij} \rangle$$

$$P = \langle (1 - h_i^+ h_i) (1 - h_j^+ h_j) \rangle$$

$$\begin{cases} \lambda \\ \mu \end{cases} \text{ chemical potentials:}$$

$A, B, D, \lambda \propto \mu$  self consistently determined in terms of

$$t/J, \quad \delta = \langle h_i^+ h_i \rangle \propto T.$$

|                             |  |
|-----------------------------|--|
| Simpler version             |  |
| $\Rightarrow [tD + JB/2] z$ |  |
| $\rightarrow zJ A$          |  |
| $\Rightarrow 0$             |  |
| $\Rightarrow 1$             |  |

Some Details (simple version)

$$H_B = \begin{pmatrix} b_{k\uparrow}^+ & b_{-k\downarrow}^- \\ b_{k\downarrow}^- & b_{-k\uparrow}^+ \end{pmatrix} \begin{pmatrix} \lambda + d\gamma_k & -\alpha\phi_k \\ -\alpha\phi_k & \lambda + d\gamma_k \end{pmatrix} \begin{pmatrix} b_{k\uparrow} \\ b_{-k\downarrow} \end{pmatrix}$$

$$a = zJ\lambda = zJ \langle (b_{i\uparrow}^+ b_{j\downarrow}^- - b_{i\downarrow}^- b_{j\uparrow}^+) \rangle / 2$$

$$\begin{aligned} d &= z(tD + JB/2) & D &= \langle h_i^+ h_j \rangle \\ B &= \langle b_{i\sigma}^+ b_{j\sigma}^- \rangle / 2. \end{aligned}$$

$$\begin{aligned} \gamma_k &= \frac{2}{z} \sum \cos \vec{k} \cdot \vec{\delta} & \phi_k &= \frac{2}{z} \sum \frac{1}{6} \sin \vec{k} \cdot \vec{\delta} \\ &\equiv \left( \frac{\cos k_x + \cos k_y}{2} \right) && \equiv \left( \frac{\sin k_x + \sin k_y}{2} \right) \end{aligned}$$

$$\text{Diagonalized by: } \begin{pmatrix} b_{k\uparrow} \\ b_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} c_k & s_k \\ s_k & c_k \end{pmatrix} \begin{pmatrix} d\phi_k \\ \omega_k \end{pmatrix}$$

$$c_k^2 = \cosh^2 \theta_k = \frac{\cosh 2\theta_k + 1}{2} = \frac{1}{2} \left[ \frac{\lambda + d\gamma_k + i}{\omega_k} \right]$$

$$s_k^2 = \sinh^2 \theta_k = \frac{\cosh 2\theta_k - 1}{2} = \frac{1}{2} \left[ \frac{\lambda + d\gamma_k - i}{\omega_k} \right]$$

$$\omega_k = \sqrt{(\lambda + d\gamma_k)^2 - \alpha^2 \phi_k^2}$$

$$\cosh 2\theta_k = \frac{\lambda + d\gamma_k}{\omega_k}, \quad \sinh 2\theta_k = \frac{\alpha \phi_k}{\omega_k}$$

$$\epsilon_F = \sum_k (2tBz\gamma_k - \mu) h_k^+ h_k^- = \sum_k \epsilon_k h_k^+ h_k^-$$

Self Consistent Equations:

$$\delta = \sum_k f(\epsilon_k)$$

$$D = \sum_k \gamma_k f(\epsilon_k)$$

$$A = \sum_k \left( \frac{g}{\omega_k} \sinh 2\theta_k [n(u_k) + \frac{1}{2}] \right) = 2J\lambda \sum_k \frac{\eta_k^2}{\omega_k} [n(u_k) + \frac{1}{2}]$$

$$B = \sum_k \gamma_k \cosh 2\theta_k [n(u_k) + \frac{1}{2}] = \sum_k \frac{(\lambda + d\gamma_k)}{\omega_k} [n(u_k) + \frac{1}{2}]$$

$$2-\delta = 2 \sum_k \cosh 2\theta_k [n(u_k) + \frac{1}{2}] = \sum_k \frac{\lambda + d\gamma_k}{\omega_k} [2n(u_k) + 1]$$

$\omega_k$  had min at  $\vec{k}(k_0, k_0)$  with

$$\text{at } k_0 = -\frac{d\lambda}{d^2 + a^2}$$

$$\omega_g = a \left\{ \frac{\lambda^2}{d^2 + a^2} - 1 \right\}^{1/2}$$

at  $T \rightarrow 0$ ,  $\lambda \rightarrow \sqrt{d^2 + a^2}$  and  $\omega_g \rightarrow 0 \dots$  as

$$\omega_g \approx k_0 T \exp \left[ -\frac{E_c}{k_B T} \right]$$

$$E_c = \frac{\pi}{2} \sqrt{d^2 + a^2} \left\{ 2 - \delta - \sum_k \frac{\lambda + d\gamma_k}{\omega_k} \right\}$$

$$k_c \approx \frac{\pi}{2} + 1.25 \pm \delta \quad \text{for large } t/J$$

Look at Spin-Spin Correlation Functions:

$$\langle S_i^+ S_j^- \rangle = f(r_{ij}) f^*(r_{ij}) + g(r_{ij}) g^*(r_{ij})$$

$$\begin{pmatrix} f(r_{ij}) \\ g(r_{ij}) \end{pmatrix} = \sum_k e^{-ik \cdot r_{ij}} \begin{pmatrix} \cosh 2\theta_k \\ \sinh 2\theta_k \end{pmatrix} \left[ \frac{1}{e^{\beta \omega_k} - 1} + \frac{1}{2} \right]$$

$$\tanh 2\theta_k = -a\phi_k / (\lambda + d\gamma_k)$$

AT HIGH TEMPERATURES ( $T > T_c$  in 3d,  $T > 0$  in 2d)

$\omega_k$  has GAP  $\Rightarrow$  NO BOSE CONDENSATION:

$\Rightarrow$  NO LONG RANGE SPIN ORDER

$$\langle S_i^+ S_j^- \rangle \sim \exp[-|r_{ij}|/\xi(T)] \quad \text{as } |r_{ij}| \rightarrow \infty$$

$$\xi(T) \sim \omega_g(T) \sim \frac{1}{T} \exp[E_c(k_B T)]$$

AT LOW TEMPERATURES ( $T < T_c$  in 3d,  $T=0$  in 2d)

$\omega_k$  develops zero mode  $\Rightarrow$  BOSE CONDENSATION

$\Rightarrow$  LONG RANGE SPIN ORDER!

Happens when  $\lambda = \lambda_c = \sqrt{d^2 + a^2}$

$$\Rightarrow \omega_k = 0 \quad \text{when } \vec{k} = \pm k_0 (1, 1, \dots)$$

$$\cos k_0 = -d/\lambda_c \quad \sin k_0 = a/\lambda_c$$

$$\Rightarrow \langle S_i^+ S_j^- \rangle_{(r_{ij}) \rightarrow \infty} = \rho_0^2 \cos(2\vec{k}_0 \cdot \vec{r}_{ij}) \quad \rho_0: \text{Condensate Density}$$

$$\langle S_i^+ S_j^- \rangle_{r_i \rightarrow \infty} = \rho_0^2 \cos(2\vec{k}_0 \cdot \vec{r}_{ij})$$

- $\Rightarrow$  SPIRAL ORDER when  $k_0 \neq 0, \eta_2$  with  
wavevector  $2k_0 \rightarrow$  magnetisation  $\rho_0$  }  $A \neq 0$   
 $B \neq 0$        $D \neq 0$
- $\rightarrow$  FERRO ORDER when  $k_0 \rightarrow 0$        $A=0, B \neq 0$
- $\rightarrow$  NEEL ANTIFERRO ORDER when  $k_0 \rightarrow \pi/2$ .  $A \neq 0, B=0$ ,  
 $D=0$ .

in FERRO phase :

$$J_p = -tD \sim t\delta(1-\delta),$$

$\rho_0^F = (1-\delta)/2$  : Max Alignment of Spins

Holon bandwidth =  $tB = t(1-\delta)/2$ .

in ANTIFERRO phase :

$$J_A = J(1-\delta)^2$$

$$\rho_0^A = \frac{1-\delta}{2} - \frac{1}{2} \int_k \left[ \frac{1}{(1-\gamma_k^2)} - 1 \right] = \frac{1-\delta}{2} - 0.195$$

Holon Bandwidth = 0

in SPIRAL phase

$$\rho_0^S = \frac{1-\delta}{2} - \frac{1}{2} \int_k \left[ \frac{1 - \coth k_0/\hbar}{\lambda \left[ (1 - \coth k_0/\hbar)^2 - (\sinh \phi_k)^2 \right] \gamma_k} - 1 \right]$$

Holon Bandwidth  $\neq 0$

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MEAN-FIELD THEORY FOR THE  $t-J$  MODEL

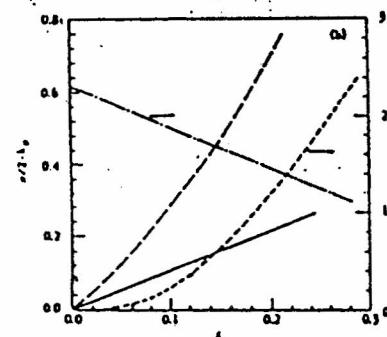
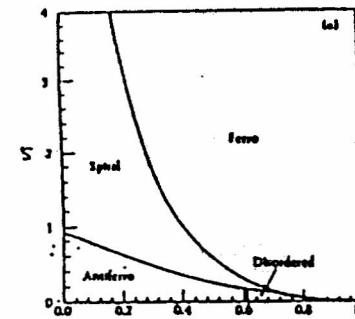


FIG. 1. (a) Phase diagram of the  $t-J$  model on a square lattice at  $T=0$  in our mean-field theory showing the antiferro, ferro, disordered spin liquid, and spiral phases. See text for discussion. (b) Variation of  $1/(a/2 - \lambda)$  as a function of  $\delta$  along the antiferro-spiral phase boundary (solid line) and at  $t/J = 1.76$  (long-dashed line). Also shown are the boson bandwidth (dash-dotted line) and 100-fermion bandwidth (short-dashed line) along the antiferro-spiral phase boundary, in units of  $J$ .

spectrum. This is different from the results obtained in the fermionic representation, and hence we favor the bosonic representation of spins over the fermions. Furthermore, the mean-field decomposition of the hole hopping term  $t$  ties together hole mobility and short-range ferromagnetic correlations, which is the physics discussed by Nagoya<sup>10</sup> for the  $U=0$  Hubbard model.

Specifically, we do a simple Hartree-Fock factorization of (2) using  $(\Lambda_\mu, B_\mu)$ , and  $(f_i/f_j)$  as the mean-field amplitudes. [This is equivalent to doing a Peierls variational calculation or to the  $n \rightarrow \infty$  limit of an appropriate large  $n$  generalization of (2).] We take into account the (average) constraint  $(\langle \sum_i b_i^\dagger b_i + f_i/f_j \rangle) = 1$  and the filling fac-

tor  $(f_i/f_j) = \delta$  via (Lagrange multiplier) chemical potentials  $\lambda$  and  $\mu$ , respectively. We find that the following simple choice for the mean-field amplitudes,

$$(A_\mu) = \lambda \sin(\vec{Q} \cdot \vec{r}_\mu/2), \quad (B_\mu) = B, \quad (f_i/f_j) = D, \quad (4)$$

where  $\vec{Q}$  denotes the zone-corner wave vector, captures the essential physics of competing spin correlations and hole motion. In particular, as we show below, a nonzero value for  $\lambda$  corresponds to short-range antiferromagnetic correlations, and for  $B$  to ferromagnetic correlations; a nonzero value of  $D$  implies hole mobility.<sup>11</sup>

The resulting mean-field Hamiltonian is quadratic in the Bose and Fermi operators and can be easily diagonalized (the Bose part by a Bogoliubov transformation). We find propagating fermionic and bosonic quasiparticles with dispersions

$$\epsilon_k = (t/2 + 2JR\delta) \gamma_k - \mu, \quad (5)$$

$$\omega_k = \{(\lambda + d\gamma_k)^2 - (g\gamma_k)^2\}^{1/2}. \quad (6)$$

respectively. Here  $x$  is the coordination number,  $d = (2J + 4PB)/t$ ,  $\gamma_k = (2/x) \sum_l \cos(k_l \cdot \vec{r}_l)$ , and  $g_k = (2/x) \sum_l \sin(k_l \cdot \vec{r}_l)$ .  $R$  and  $P$  are expectation values given by  $R = \langle \Lambda_\mu \Lambda_\mu \rangle$  and  $P = \langle (1-f_i/f_j)(1-f_j/f_i) \rangle$ . Using these we derive self-consistent equations for  $\lambda$ ,  $D$ ,  $\lambda$ , and  $\mu$ , and solve them numerically for the lowest frequency solution for various values of  $t/J$ ,  $\delta$ , and  $T$ . In this paper for the most part we discuss  $T=0$  results for the square lattice.

One important component of the physics contained in our mean-field theory is brought out by the spin-spin correlation function, which is given by (for  $r_i \neq r_j$ )

$$\langle S_i^+ S_j^- \rangle = f(r_{ij}) f^*(r_{ij}) + g(r_{ij}) g^*(r_{ij}), \quad (7)$$

$$\begin{pmatrix} f(r_{ij}) \\ g(r_{ij}) \end{pmatrix} = \sum_k e^{-i\vec{k} \cdot \vec{r}_{ij}} \begin{pmatrix} \cosh 2\theta_k \\ \sinh 2\theta_k \end{pmatrix} [n(\omega_k) + \frac{1}{2}], \quad (8)$$

where  $n(\omega_k) = (e^{\beta \omega_k} - 1)^{-1}$  is the Bose-distribution function and  $\tanh 2\theta_k = -\alpha_k/(\lambda + d\gamma_k)$  is the Bogoliubov parameter. When  $i$  and  $j$  are nearest neighbors it is easy to show that  $f(r_{ij}) = f^*(r_{ij}) = B$  and  $g(r_{ij}) = -g^*(r_{ij}) = A$ , and thus  $\langle S_i^+ S_j^- \rangle = (B^2 - A^2)/4$ . Hence the result that  $\lambda$  promotes short-range antiferromagnetic correlations and  $B$  short-range ferromagnetic correlations. From our self-consistent mean-field equations we find that a nonzero value of  $B$  implies a nonzero value of  $D$  and vice versa. Thus the correlation of hole motion with ferromagnetic correlations discovered by Nagoya is automatically included in our simple mean-field theory.

The short-range correlations determined by  $\lambda$  and  $\beta$  set in at high temperatures, governed by  $t$  and  $\beta$ . At these temperatures our self-consistent equations show that  $\lambda$  is such that  $\omega_k$  has a gap. Hence from (7) and (8) it follows that the spin correlations decay exponentially at long distances and the system has no long-range spin order.

However, at low temperatures ( $T$  less than a critical temperature  $T_c$  in three dimensions, and at  $T=0$  in two dimensions) the physics is dominated by Bose condensation of the Schwinger bosons, which leads to long-range spin order. This arises because the chemical potential  $\lambda$ , and hence, the minimum of  $\omega_k$  given by (6) decrease as

B1

### SPIN BOSON - "SLAVE" FERMION MFT for HUBBARD MODEL

$$\mathcal{H} = -t \sum_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Use the representation

$$c_{i\sigma}^{\dagger} : b_{i\sigma}^{\dagger} h_i + \text{sgn}(\sigma) d_i^{\dagger} b_{i-\sigma}$$

$b_{i\sigma}^{\dagger}$  : creates spin-boson  $\vec{S}_i = \frac{1}{2} b_i^{\dagger} \vec{\sigma} b_i$

$h_i^{\dagger}$  : creates hole-fermion  $\rightarrow$  "holon"

$d_i^{\dagger}$  : creates doubly-occupied site  $\rightarrow$  "doublet fermion".

constraint:  $b_{i\sigma}^{\dagger} b_{i\sigma} + h_i^{\dagger} h_i + d_i^{\dagger} d_i = 1$ .

$$\mathcal{H} = -t \sum_{ij} [A_{ij}^{\dagger} C_{ij} - B_{ij}^{\dagger} D_{ij} + \text{h.c.}] + U \sum_i d_i^{\dagger} d_i$$

$A_{ij}^{\dagger} \equiv \frac{1}{2} (b_{i\uparrow}^{\dagger} b_{j\downarrow}^{\dagger} - b_{i\downarrow}^{\dagger} b_{j\uparrow}^{\dagger})$  creates singlet spin pair

$B_{ij}^{\dagger} \equiv \frac{i}{2} (b_{i\sigma}^{\dagger} b_{j\sigma}^{\dagger})$  hops spin bosons.

$C_{ij}^{\dagger} \equiv d_i^{\dagger} h_j^{\dagger} - d_i^{\dagger} h_j^{\dagger}$  Pairs doublets & holons

$D_{ij}^{\dagger} \equiv h_i^{\dagger} h_j^{\dagger} - d_i^{\dagger} d_j^{\dagger}$  hops doublets & holons.

B2

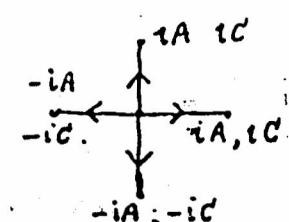
### Simple Minded Mean Field Theory:

$$\langle B_{ij} \rangle = B$$

$$\langle D_{ij} \rangle = D$$

$$\langle A_{ij} \rangle$$

$$\langle C_{ij} \rangle$$



### Consequences:

$$\text{SPINONS: } \omega_k = \sqrt{(\lambda + t \pm D \gamma_k)^2 - (t \pm C \phi_k)^2}$$

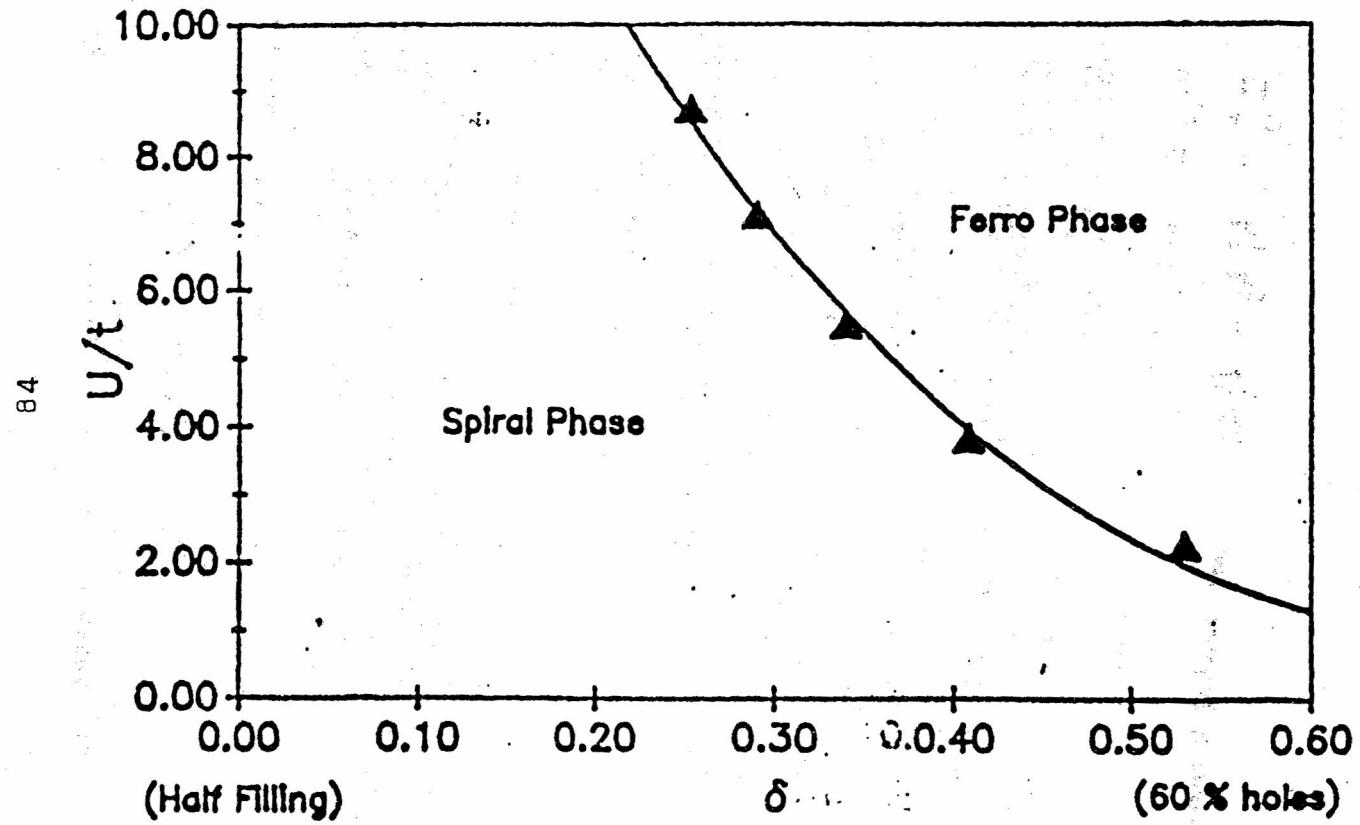
$$\left. \begin{array}{l} \text{FERMION} \\ \text{QUASI PARTICLES} \end{array} \right\} : \begin{pmatrix} E_{0k} \\ E_{2k} \end{pmatrix} = R_k \pm \left\{ \mu + 2t \pm B \gamma_k \right\}$$

$$R_k = \sqrt{\left(\lambda + \frac{U}{2}\right)^2 + (2t \pm A \phi_k)^2}$$

$A, B, C, D, \lambda, \mu$  self consistently determined in terms of

$$\frac{zt}{U}, \delta = \langle h_i^{\dagger} h_i - d_i^{\dagger} d_i \rangle \approx T$$

## Hubbard Model – Phase Diagram



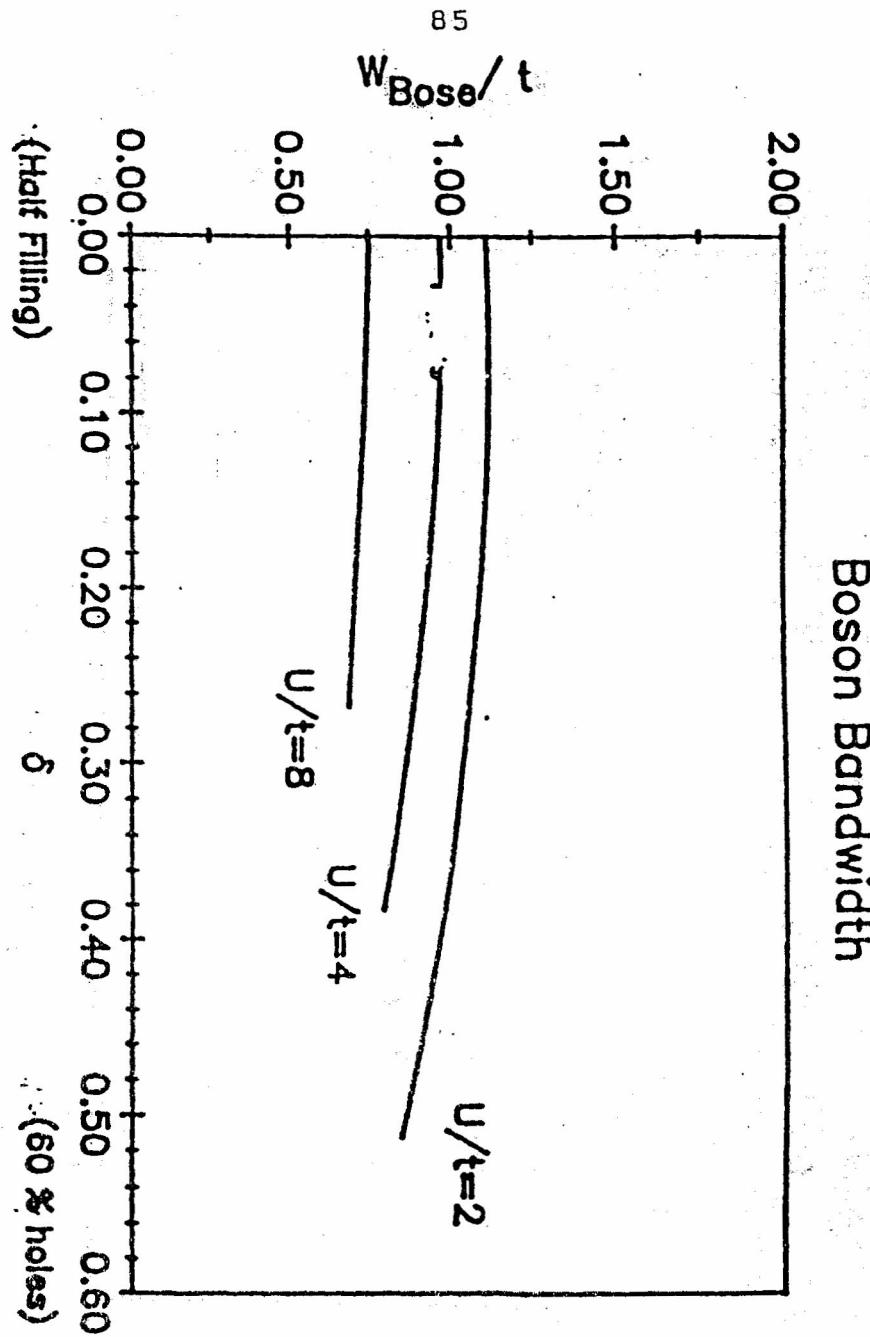
At Half filling ( $\delta = 0$ ) on square lattice  
Always find  $D = 0 = B$ .

At  $T=0$  in  $2d$  &  $T < T_c$  in  $3d$ ,  
Bose condensation at  $k_0 = \pi/2$ .

& Gap in  $E_{0k}$  &  $E_{2k}$  :  
 $\Rightarrow$  2 Sublattice Neel AF - Insulator for  
all  $U$ .

SPIRAL order for  $\delta \neq 0$ .

Agrees with t-J model results  
for large  $U/zt$   
But not so good at small  $U$ , where,  
in general, charge-spin separation breaks  
down.



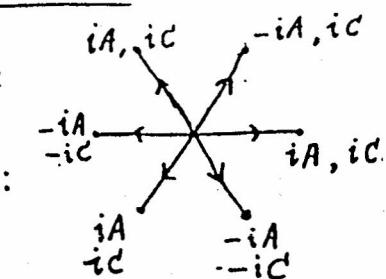
Mean Field Theory for  $\Delta$  lattice:

$$\langle B_{ij} \rangle = B$$

$$\langle D_{ij} \rangle = D.$$

$$\langle A_{ij} \rangle :$$

$$\langle C_{ij} \rangle :$$



$\Rightarrow$  SPIRAL phase for  $\delta \neq 0$ :  
METALLIC

$\Rightarrow$  for  $\delta = 0$ , large  $U$ ,  $D = 0$ , Gaps in  $E_{0k}, E_{2k}$   
3 sublattice,  $120^\circ$  twist AF I lator  
 $\vec{k}_0 = \vec{Q}_1 \left( \frac{4\pi}{3a}, 0 \right)$

$$P_0^A = .33$$

| $P_0^A$   | Huse & Elser | Series (Huse) | Our Work |
|-----------|--------------|---------------|----------|
| $\square$ | .35          | .31           | .305     |
| $\Delta$  | .38          |               | .33      |

$\Rightarrow$  At  $\delta = U < U_{co}$ , Gaps in  $E_{0k} \& E_{2k}$  disappear

$D \neq 0$ ,  $\vec{k}_0$  deviates from  $\vec{Q}_0$ :

$\Rightarrow$  Incommensurate SPIRAL METAL  
at half filling!  $\rightarrow$  as in HF mft

Pro's & Con's of Holon-Fermion, Spinon-Bolon approach:

Pros:

(#1) For  $\delta \rightarrow 0$ , theory reduces to Schwinger-Brown meanfield theory of Arrovás & Auerbach:

PRB 38, 316 (88), PRL 61, 617 (88)

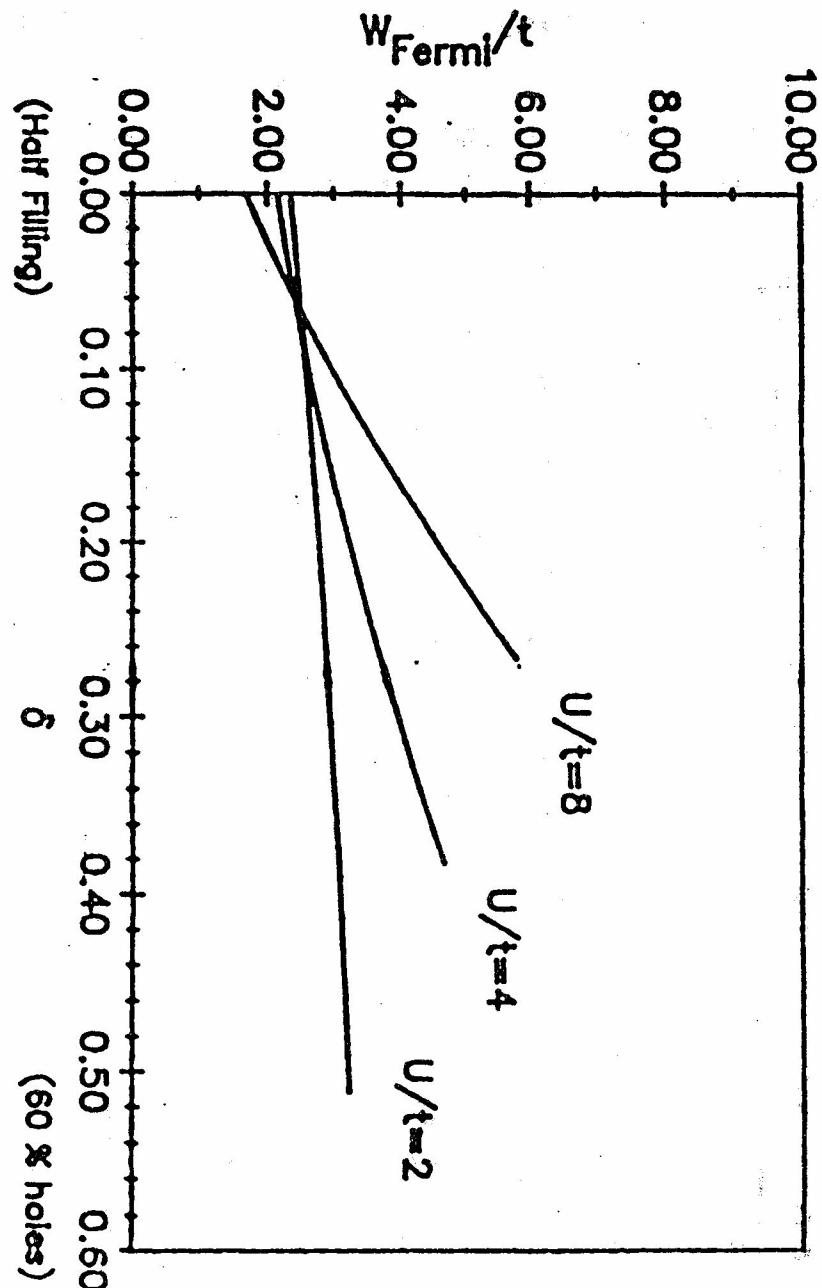
which gives an excellent description of the neutron scattering data in  $\text{La}_2\text{CuO}_4$ .

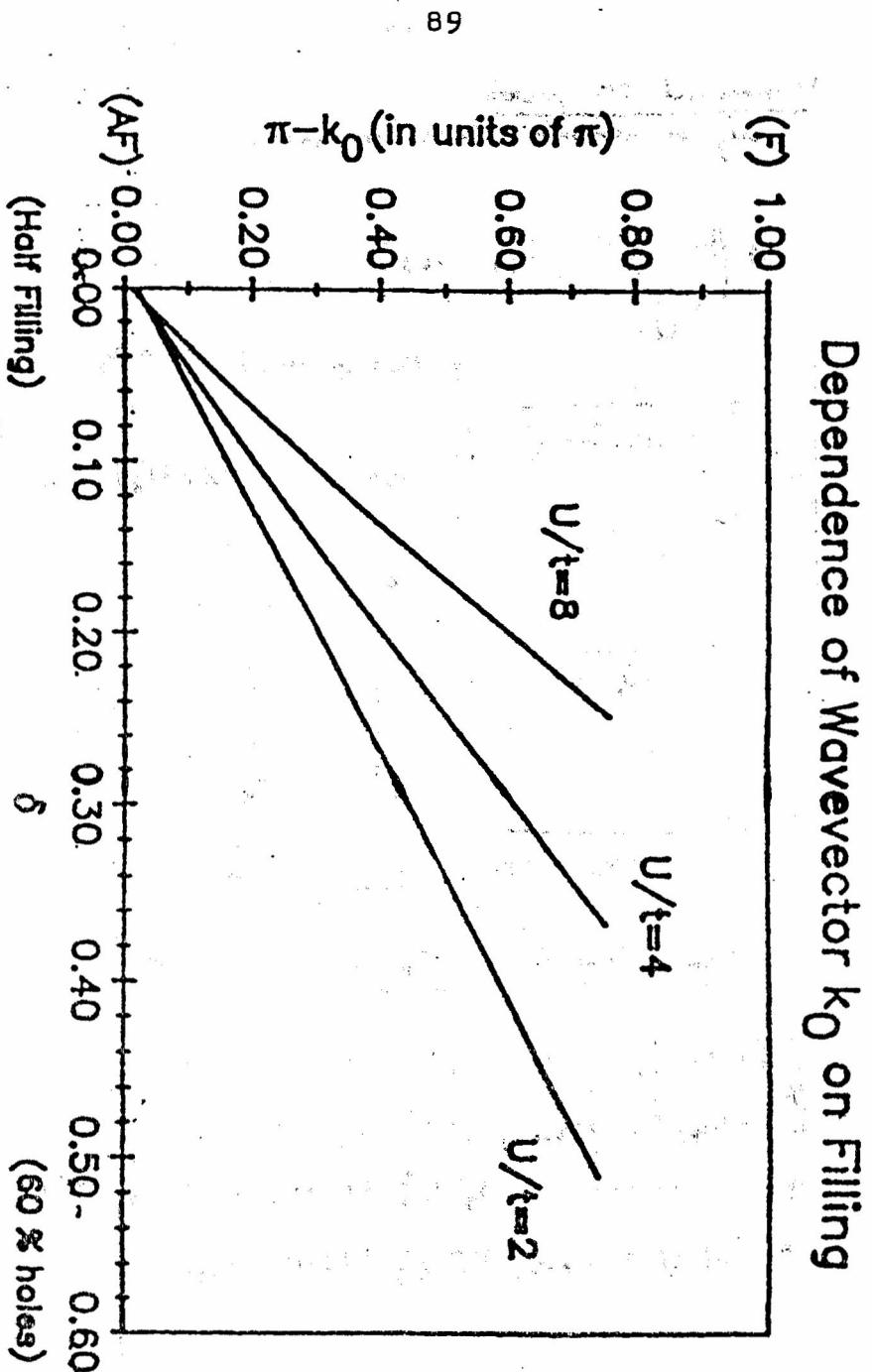
Results for  $\delta \neq 0$  in qualitative agreement with data on  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . [Detailed calculations & comparisons done by

Per Hedegård & M. Brix Pedersen (preprint)]

[Extension of Arrovás & Auerbach to include description of ordered phase at a base concentration of Schwinger-Brown in Sarker et al PRB 40, 5028 (89)]

& Yoshioka





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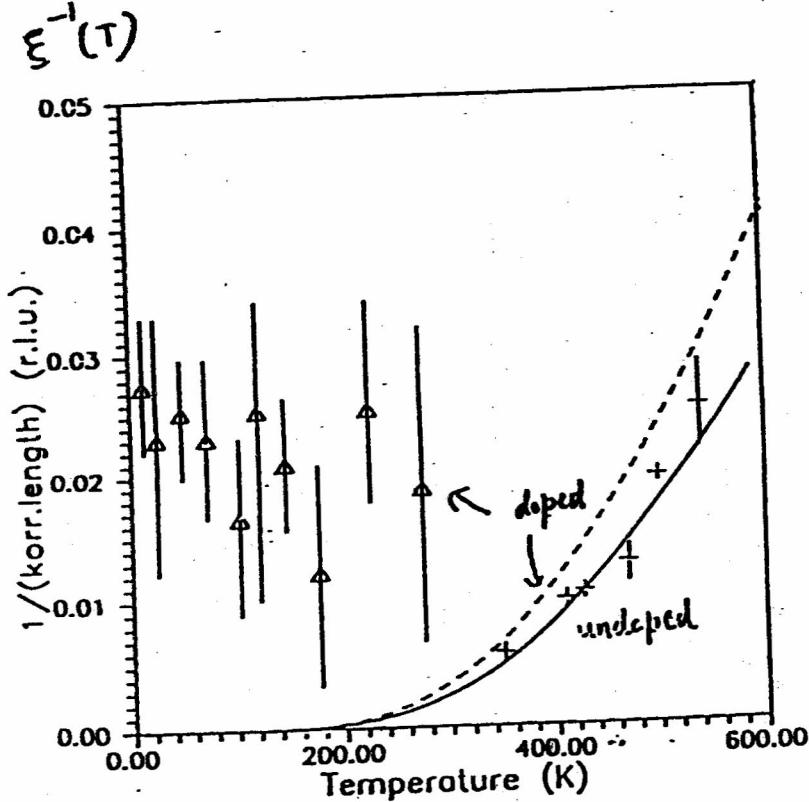
spin wave velocity  $c = z_c \cdot \sqrt{8JS}/\hbar a$

susceptibility  $\chi(F=0) = (g\mu_B)^2 \cdot z_p / 8J$

correlation length:  $\xi \sim \exp \left[ \frac{2\pi S(S+1)}{k_B T} J \cdot z_\xi \right]$

| Theory | Coefficient                                      | $S = 1/2$ | $S = 1$ |
|--------|--|-----------|---------|
| SB-HFT | $z_c$  | 1.159     | 1.079   |
| SWT    | $z_c = 1 + 158/25$                               | 1.158     | 1.078   |
| SB-HFT | $z_p$  | .53       | .73     |
| SWT    | $z_p = 1 + 582/25$                               | 4.48      | 7.24    |
| SB-HFT | $J S(S+1) d^2 z_p / dT$                          | .22       | .27     |
| SB-HFT | $z_S$  | .246      | .442    |
| CHN    | $z_\xi = \frac{k_B z_c z_p}{\alpha_B S_B (S+1)}$ | .200      | .421    |
| SB-HFT | $\delta = C_V / [T / S(S+1)J]^2$                 | 1.3       | 1.2     |

AROVAS X AUERBACH PRL



From P. Hedegård & H. Brix Pedersen (Preprint)

Dynamical str factor  
Easy to compute Bolon propagators:

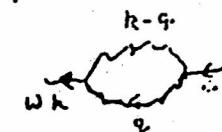
$$\langle\langle b_{k\tau}^{\dagger} \quad b_{-k\tau}^{\dagger} \quad b_{k\tau}^{\dagger} \quad b_{-k\tau}^{\dagger} \rangle\rangle$$

$$= \frac{1}{(i\nu_m - \omega_k^2)} \begin{pmatrix} i\nu_m + (\lambda + d\gamma_k) & a\phi_k \\ a\phi_k & (\lambda + d\gamma_k) - i\nu_m \end{pmatrix}$$

$$= \frac{1}{i\nu_m - \omega_k^2} \begin{pmatrix} c_k^2 & c_k s_k \\ c_k s_k & s_k^2 \end{pmatrix}$$

$$- \frac{1}{i\nu_m + \omega_k^2} \begin{pmatrix} s_k^2 & c_k s_k \\ c_k s_k & c_k^2 \end{pmatrix}$$

Hence Compute  $S(k, \omega) \Rightarrow$



$$\sum_q [1 + n(\omega_q)] [1 + n(\omega_{k+q})] s_q^2 c_{k+q}^2 \delta(\omega - \omega_q - \omega_{k+q})$$

$$+ n(\omega_q) [1 + n(\omega_{k+q})] s_q^2 c_{k+q}^2 \delta(\omega + \omega_q - \omega_{k+q})$$

$$+ - - - s_q^2 s_{k+q}^2 \delta(\omega + \omega_q - \omega_{k+q})$$

$$+ n(\omega_q) n(\omega_{k+q}) c_q^2 s_{k+q}^2 \delta(\omega + \omega_q + \omega_{k+q})$$

2 term emission

1 term

scattering

2dm abs.

Dominant contribution at low temperatures

from

$$\vec{q} = \pm \vec{k}_0 + \vec{G} \quad \left\{ \omega \vec{k} = \pm 2\vec{k}_0 + \vec{G}, \vec{G} \right.$$

$$\kappa \vec{k} \cdot \vec{q} = \pm \vec{k}_0 + \vec{G} \quad \left. \right\}$$

Each "peak" split into two at  $T \rightarrow 0$

$$\vec{k} = 2\vec{k}_0 \pm \frac{\omega}{2\Delta_0} \quad \omega_k = \sqrt{\omega_y^2 + \Delta_0^2 (k - k_s)^2}$$

Resolvable for  $\omega \gtrsim 50$  mev [ $\omega/2\Delta_0 \gtrsim .1 \text{ s}^{-1}$ ]

but not for  $\omega = 12$  mev [ $\omega/2\Delta_0 \sim .03 \text{ s}^{-1}$ ]

Separation between incommensurate peaks:

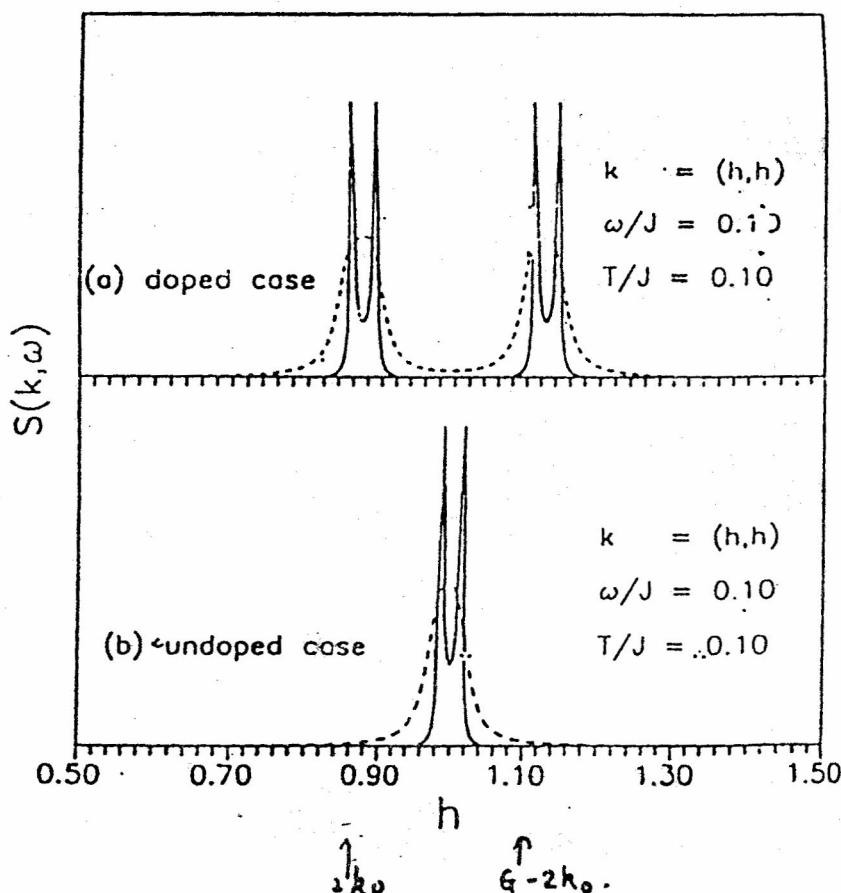
$$.13 \pm .03 \text{ s}^{-1} \quad \text{for } \delta = .11$$

$$.25 \pm \quad \quad \quad \text{for } \delta \approx .15$$

Integrated intensity:

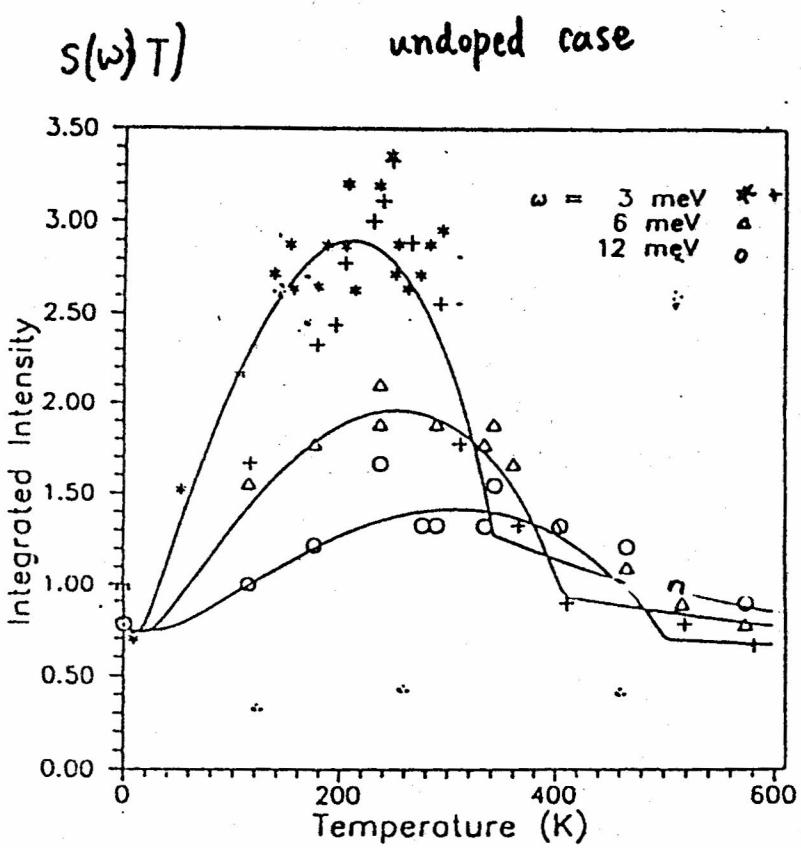
$$S(\omega) \sim \frac{\omega_0}{\omega_g} \int_{\omega_g}^{\omega_0} d\omega' [1 + n_B(\omega')] [1 + n_g(\omega - \omega')] \\ + 2 \int_{\omega_g}^{\omega_0} d\omega' n_0(\omega') \left[ 1 + n_g(\omega + \omega') \right] \frac{1}{(k - k_s)^2}$$

Fig. 1.



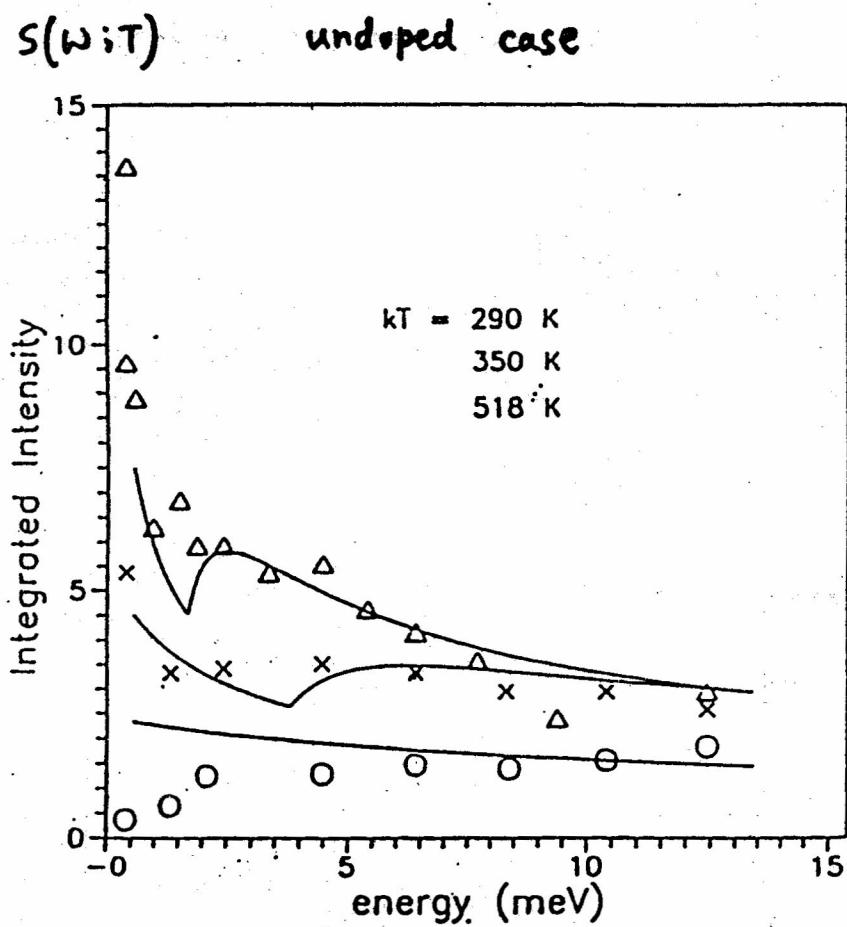
From P. Hedegard & M. Brix Pedersen (Preprint)

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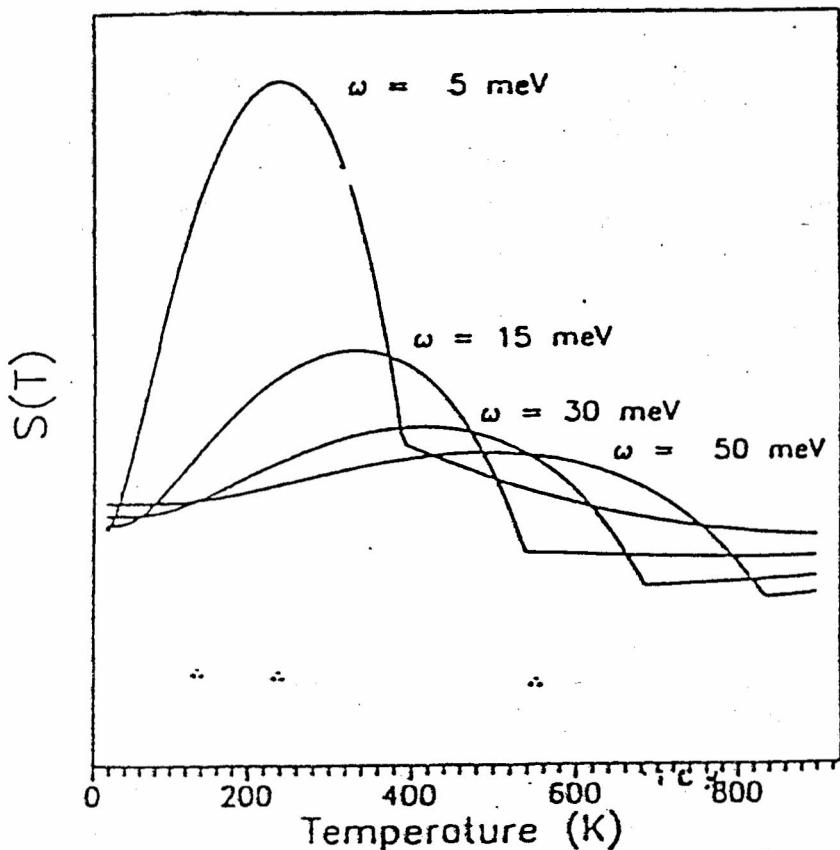
96.



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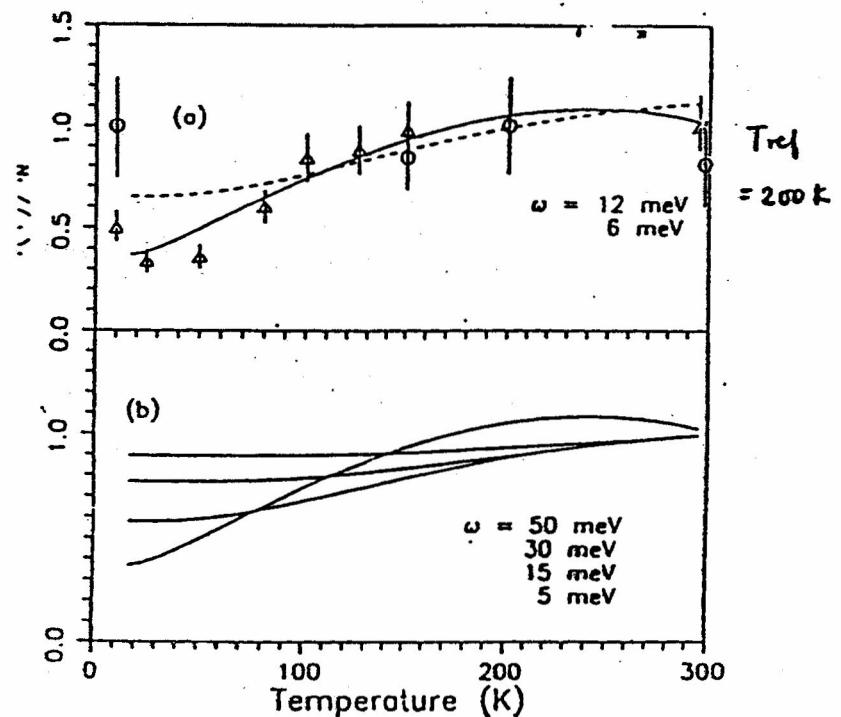
$S(\omega, T)$  doped case.  $\bar{J} = 0.1 \text{ eV}$



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$S(\omega; T) / S(\omega; T_{ref})$  doped case:



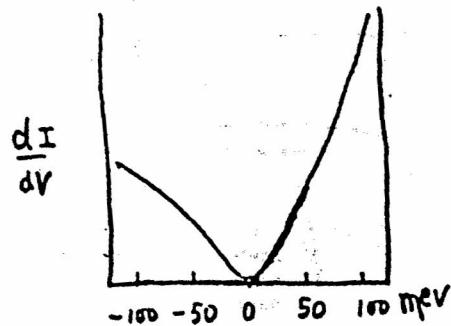
From P. Hedegård & M. Brix Pedersen (preprint)

99

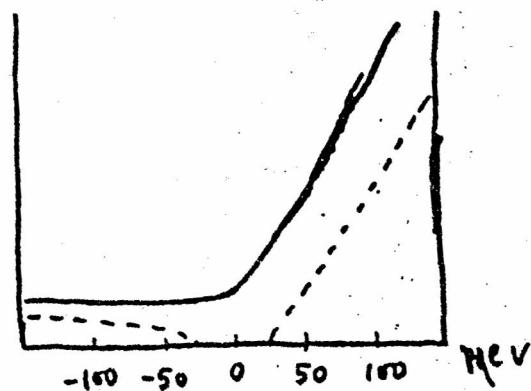
(2) Tunnelling : [Flensborg, Haldane & Pedersen]

$$I(v) \equiv \frac{e}{k} |T_0|^2 g_1 \int_0^{\text{ev}} d\omega A_2(\omega)$$

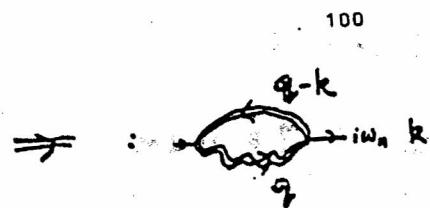
$$\frac{dI}{dv} = \frac{e}{k} |T_{12}|^2 g_1 A_2(\text{ev}).$$



holon Fermion  
x  
Spinon boson  
mft.



holon boson  
x  
Spinon fermion  
mft.



$$G(k, i\omega_n) = \sum_q \left[ C_q^2 \frac{f_{q-k} + n_g}{i\omega_n - \omega_q + \epsilon_{q-k}} - S_q^2 \frac{f_{q+k} - 1 - n_g}{i\omega_n + \omega_q + \epsilon_{q+k}} \right]$$

$$\Rightarrow A(k, \omega) = \sum_q \left[ C_q^2 (f_{q-k} + n_g) \delta(\omega - \omega_q + \epsilon_{q-k}) - S_q^2 (f_{q+k} - 1 - n_g) \delta(\omega + \omega_q + \epsilon_{q+k}) \right]$$

From summing over  $k$ ,

$$A(\omega) = P_h \sum_q [C_q^2 \delta(\omega - \omega_q) + \delta(-\omega - \omega_q) S_q^2]$$

gives result shown.

$T=0$  Spectral function  $\propto$  mom distribution function has structure corresponding to holon (non-Luttinger) Fermi Surface due to Bose condensate.

## Concluding Comments

① Bose condensation giving ferromagnetism can be fixed by considering Luttinger

Fermi-surface restoring excitations

as discussed in

Shastry, Krishnamurthy & Anderson

PRB 40 (90) p 2375

② Other order parameters (short range) have been looked at. e.g. B. Chakraborty et al (preprint).

③ Key problem is to understand what suppresses bose condensation away from half filling  $\Rightarrow$  gauge fluctuations?

### Instability of the Nagaoka ferromagnetic state of the $U = \infty$ Hubbard model

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(Received 24 April 1989)

We identify a "k<sub>f</sub> instability" of the Nagaoka ferromagnetic state of the  $U = \infty$  Hubbard model. We show rigorously that for a large enough hole concentration the ferromagnet possesses an instability with respect to overturning an up-spin electron at the Fermi surface and placing it at the bottom of a down-spin band made very narrow by correlation effects. We find a low-energy scale for spin-waves in this strong-coupling limit, in the form of a spin-wave stiffness that is much smaller than its random-phase-approximation value.

In this paper we present some variational and exact results concerning the Hubbard model in the limit of large  $U$ —pertaining mainly to the stability or otherwise of the Nagaoka ferromagnet. The result of Nagaoka<sup>1</sup> (see also Thouless<sup>2</sup>) is of considerable importance since it is a non-perturbative and exact statement about the Hubbard model for strong coupling, i.e.,  $U = \infty$ . The recent revival of interest in the Hubbard model for large (but not infinite)  $U$ , following Anderson's suggestion<sup>3</sup> of its relevance in high- $T_c$  superconductivity, has focused mainly on the so-called Heisenberg-Hubbard model, which in fact contains the  $U = \infty$  Hubbard model kinetic energy as one of its pieces. In addition, the theory of itinerant electron ferromagnetism has traditionally relied upon the Nagaoka ferromagnet as a clearly demonstrable case of the existence of ferromagnetism in a one-band Hubbard model.<sup>4</sup>

Given the importance of the Nagaoka ferromagnet, the "thermodynamic frailty" of the methods used to prove it have been a source of concern to several workers over the years. Nagaoka shows that the fully saturated ferromagnet is a ground state in the case of one hole (measured from half-filling) for  $U = \infty$  and on appropriate lattices. This method fails to prove ferromagnetism for a few as two holes. In fact in the case of two holes we can readily show, by essentially a Peierls construction, that a singlet state must exist with an energy only  $O(1/L^2)$  above that of the ferromagnet (we could cut the lattice into two equal domains and confine one hole into each, and further form the largest spin state for each domain and couple these two domain ferromagnets into a singlet—the energy cost is only a boundary effect). For a thermodynamic concentration of holes, such considerations really do not serve as proper guides. However, the one-dimensional Hubbard model, with  $U = \infty$ , has a separation of charge and spin, and so it is impossible to find a state with lower energy than the Nagaoka state at any concentration of holes. This leads to a possible scenario in which the ferromagnet could survive (at  $U = \infty$ ) in two and three dimensions for any hole concentration.

It is the purpose of this paper to show that the preceding scenario is false—we present a variational wave function with one spin down with a finite wave vector,  $k_f$ , which has a lower energy than the Nagaoka state in two and three dimensions for a sufficiently large concentration of holes. Our "excitation energy" is a strict upper bound to the true excitation energy, and becomes negative for large enough  $\delta$  (density of holes) but it remains non-negative in one dimension. In fact, our criterion for the instability of the ferromagnet (namely the "excitation energy" going negative) captures the subtleties of the Nagaoka theorem (related to the sign of the hopping matrix element on non bipartite lattices). We also present variational estimates on how large the Coulomb interaction  $U$  must be in order to stabilize the ferromagnet. These are, however, not optimal for all  $\delta$ . We believe that this is the first published demonstration of the instability of the Nagaoka state for any hole concentration (at  $U = \infty$ ) which has a variational (and hence rigorous) basis, and which is thermodynamically relevant.

In order to motivate our wave functions, we would like to review, briefly, the work of Richmond and Rickayzen,<sup>5</sup> who performed an interesting calculation with a similar objective to ours. These authors also consider the problem of  $N_1 = N_1(1 - \delta)$  up 1-spin electrons and one down 1-spin electron ( $N_1$  being the number of lattice sites) and construct a variational wave function obtained by freezing the motion of the down electron and solving exactly for the up electron gas which now sees a simple potential scatterer (strength  $U$ ) at one site. The up-electron energies are shifted by  $O(1/N_1)$  each, and the net cost is  $O(1)$ , whereas the possibility of virtually admixing the doubly occupied site gains an exchange energy. The final conclusion of this study is that the Nagaoka ferromagnet is unstable with respect to reducing  $U$  from infinity—however, they find that at  $U = \infty$  the Nagaoka ferromagnet is always stable for any  $\delta$ .

It appears that the preceding stability of the Nagaoka ferromagnet arises in their calculation by the inability of the wave function to allow the down-spin electron to hop

around. The overturned electron would prefer to be in a highly delocalized state. For, if we imagine the fully spin-polarized Stoner state (which is just the Nagaoka state at  $U = \infty$ ) and switch off  $U$ , then the leading instability would correspond to destroying an up electron at the (Stoner-Nagaoka) Fermi surface and creating a down electron at the band bottom. This picture immediately suggests that an appropriate strategy for the large- $U$  problem would be to take such a "Fermi surface restoration" excitation and to correct for strong Coulomb repulsion by a variational projection.

Explicitly we write the Hamiltonian

$$H = -\sum_{ij} t_{ij} C_{i\downarrow}^{\dagger} C_{j\downarrow} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

In the  $U = \infty$  limit, the above considerations lead us to the variational wave function<sup>8</sup>

$$|\chi_r\rangle = (N_r)^{-1/2} \sum_i e^{i k_r \cdot r} C_{i\downarrow}^{\dagger} (1 - n_{i\uparrow}) C_{i\downarrow} |F\rangle, \quad (2)$$

where  $|F\rangle$  is the ferromagnetic Nagaoka-Stoner state  $|\prod_{i\downarrow} \psi_{i\downarrow}, C_{i\downarrow}^{\dagger} |vac\rangle$ , and  $k_r$  refers to one of the Fermi-surface vectors. A straightforward calculation gives the excitation energy

$$\langle \chi_r | (H - E_0) | \chi_r \rangle / \langle \chi_r | \chi_r \rangle, \quad (3)$$

where  $E_0$  is the energy of the Nagaoka-Stoner state, as

$$\lambda_r(q) = (\mu - \epsilon_q) + \epsilon_q \delta(1 - \beta^2/z^2 r^2). \quad (4)$$

Here  $\rho = 1 - \delta$ ,  $\beta = -E_0/(Nb)$ , and  $\epsilon_q = \epsilon_{k_r}$ , with

$$\epsilon_q = -(1/N_r) \sum_j t_{qj} e^{-i k_r \cdot r_j},$$

$z$  = coordination number and further we assume that  $t_{qj} = 1$  for  $j$ , nearest neighbor and zero otherwise. In terms of the density of states  $p(\epsilon)$  per site and per spin we have

$$\beta \delta = \int_{\epsilon_F}^{\epsilon_{top}} \epsilon p(\epsilon) d\epsilon \quad \text{and} \quad \delta = \int_{\epsilon_F}^{\epsilon_{top}} p(\epsilon) d\epsilon, \quad (5)$$

where  $\epsilon_{top}$  is the band top energy, whence  $\epsilon_F \leq \mu \leq \epsilon_{top}$ . In Eq. (3), the two terms are, respectively, the energy loss of the up spins brought about by the up electrons having to avoid the inserted down spin (it is a net loss since  $\beta \geq \epsilon_q$ ) and the energy gain of the down electron that can move around on the vacant sites left behind in the ferromagnet. The coefficient of  $\epsilon_q$  in (3) represents the effective "band width" reduction factor of the down electron—which is, in fact, the hole-density-hole-density correlation function at nearest-neighbor separation in the Nagaoka ferromagnet divided by  $\delta$ . The physics of this term is simply that given a hole at a site, a down spin is inserted there, and its hopping requires a hole at a neighboring site—thus we need the conditional probability of finding a second hole at a nearest-neighbor site given one hole at a site.

Clearly the lowest value of  $\lambda_r(q)$  is obtained by setting  $\epsilon_q$  as the band bottom energy  $-|W_{top}|$ . We distinguish two cases here depending on whether (a)  $W_{top} = z|r|$  or (b)

$W_{top} < z|r|$ . Case (a) applies to the square lattice, the triangular lattice with  $r < 0$ , the simple cubic, the bcc lattice, and the fcc lattice with  $r < 0$ . Case (b) corresponds to the triangular and fcc lattices with  $r > 0$ . We assert for all the lattices in case (b) that the ferromagnet is unstable for arbitrarily small  $\delta$ ; the instability is of course exactly what Nagaoka's theorem would predict for a single hole—it arises in (3) because the first term is a positive number of  $O(\delta)$  and the second is also of  $O(\delta)$  but negative, with a larger coefficient. Case (a) is, however, more subtle. The fact that  $W_{top} = z|r|$  and Eq. (4) imply that  $(1/zr^2)$  tends to 1 as  $\delta \rightarrow 0$ , whence the second term in (3) is of  $O(\delta^2)$ . This guarantees that there must exist a nonzero region around  $\delta = 0$  where  $\lambda_r$  is non-negative—this robustness of the Nagaoka ferromagnet in this case stems from the rather curious fact that the hole-density-hole-density correlation function of the ferromagnet, at nearest-neighbor separation, is of  $O(\delta^2)$  rather than  $O(\delta^3)$  as one might naively expect. In effect holes repel very strongly in this case thereby enhancing the stability of the Nagaoka state. Table I lists the critical values of  $\delta$  above which  $\lambda_r$  goes negative in various cases. It is seen that there are surprisingly stable cases—the case (a) triangular lattice and fcc lattice, which appear to be good candidates for itinerant ferromagnetism.

Having found an excitation with possibly vanishing energy, we observe that the preceding instability has a wave vector corresponding to the Stoner-Nagaoka Fermi momentum relative to the band bottom state's momentum. This is a generalized spin wave with a (fixed) nonzero wave vector  $q = k_F$ ; and brings us to the question of the (Goldstone) long-wavelength spin waves, which must on symmetry grounds possess a vanishing energy.<sup>9</sup> We therefore construct a variational wave function which contains long-wavelength spin waves and also interpolates to contain the leading instability already discussed as

$$|\phi\rangle = \frac{1}{\sqrt{B(N_r - N)}} \sum_{i\downarrow} e^{i k_F \cdot r_i} \psi_i C_{i\downarrow}^{\dagger} (1 - n_{i\uparrow}) C_{i\downarrow} |F\rangle, \quad (6)$$

where  $\psi_i$  is an unspecified amplitude for the wave vector  $k$ . The wave function<sup>10</sup>  $|\phi\rangle$  is characterized by the wave vector  $q$ , and is motivated by the RPA (Ref. 9) which can be recovered by neglecting the (projection) factor  $(1 - n_{i\uparrow})$ . If we choose  $\psi_i$  to be a Kronecker  $\delta$  function at  $k = k_F$ , this reduces to our wave function  $|\chi_r\rangle$  in Eq. (2). If we set  $q = 0$  and let  $\psi_i$  be independent of  $k$ , then  $|\phi\rangle$  is simply the state obtained by acting on  $|F\rangle$  with the total spin lowering operator, and hence is degenerate with  $|F\rangle$ .

The constant  $\beta$  in (6) is determined by normalization as

$$\beta = \sum_i |\psi_i|^2 f_i + \frac{1}{N_r \delta} \sum_{p,k} \psi_p^* \psi_k f_p / f_k. \quad (7)$$

where  $f_k = \Theta(\epsilon_F - \epsilon_k)$  restricts the sum to the Stoner-Nagaoka Fermi sea. We calculate the "spin-wave" excitation energy [i.e.,  $\langle \phi | (H - E_0) | \phi \rangle$ ] to be

TABLE I. The spin-wave stiffness in our scheme and in the RPA, in units of  $zr$  where  $z$  is the coordination number for different lattices, and the critical hole concentration  $\delta_c$  where Eq. (3) is zero.

|              |            | Square | Triangle | sc    | bcc   | fcc   |
|--------------|------------|--------|----------|-------|-------|-------|
| $\delta=0.1$ | $D_{RPA}$  | 0.023  | 0.01     | 0.012 | 0.01  | 0.006 |
|              | $D$        | 0.009  | 0.016    | 0.006 | 0.005 | 0.004 |
| $\delta=0.2$ | $D_{RPA}$  | 0.044  | 0.036    | 0.024 | 0.015 | 0.01  |
|              | $D$        | 0.014  | 0.026    | 0.007 | 0.006 | 0.006 |
|              | $\delta_c$ | 0.49   | 1        | 0.32  | 0.32  | 0.62  |

$$\begin{aligned} \epsilon(q) = & \frac{1}{\beta} \sum_k \lambda_k(q) \psi_k^* \psi_k f_k \\ & + \frac{1}{BN_r} \sum_{kp} f_k f_p \psi_p^* \psi_k K(k, p; q), \end{aligned} \quad (8)$$

where

$$\lambda_k(q) = \mu - \epsilon_k + \delta(1 - \beta^2/z^2 r^2) \epsilon_{k+q}, \quad (9)$$

and

$$K(k, p; q) \approx (\epsilon_{k+q} + \epsilon_{p+q}) + (\beta/z) \epsilon_q + \epsilon_{k+p+q}. \quad (10)$$

Varying with respect to  $\psi_k^*$ , with the preceding normalization constraint, we find the eigenvalue equation

$$[\epsilon(q) - \lambda_k(q)] \psi_k = \frac{1}{N_r} \sum_p f_p \left[ K(k, p; q) - \frac{1}{\beta} \epsilon(q) \right] \psi_p. \quad (11)$$

This integral equation has two classes of solutions, the continuum of scattering states obtained by omitting the right-hand side [which shifts the energies only by  $O(1/N_r)$ ] and a bound state, the (Goldstone) spin wave, starting at zero energy at  $q = 0$ . The scattering continuum is analogous to the Stoner particle-hole continuum in the weak-coupling ferromagnet, and is bounded from below by the minimum of  $\lambda_k(q)$  for a given  $q$ . Its value at  $q = 0$  is the effective exchange splitting in this strong-coupling theory. The instability discussed in the previous sections is precisely contained in this scheme, since  $\lambda_k(q)$  at  $q = k_F$  has a minimum at  $k = -k_F$ , thus our previous discussion is tantamount to the statement that the lower edge of the scattering continuum has a minimum at  $q = k_F$ , and that this minimum comes down with increasing  $\delta$ , until at some critical value, it hits the abscissa, signifying the instability of the ferromagnet.<sup>10</sup> This scheme also contains the Goldstone mode, since a calculation shows that Eq. (7), in the limit of  $q = 0$ , has a zero eigenvalue with the eigenfunction  $\psi_k$  independent of  $k$ . (This phenomenon is a statement of the rotational invariance of our scheme.)

The small- $q$  spin-wave spectrum can be extracted from the (separable kernel) integral equation (10). We find the eigenfunction

$$\psi_k = 1 + g_k \phi_k + O(q^2). \quad (12)$$

and  $\phi_k$  is obtained as

$$\phi_k = \frac{\psi_{k_0}}{\lambda_k(0) + z\beta\epsilon/(2\theta)}, \quad (13)$$

where

$$\psi_{k_0} = (\partial/\partial k_x) \epsilon_{k_0},$$

and

$$I = (1/N_r) \sum_k f_k \psi_k^2 / \lambda_k(0).$$

These are appropriate in all the lattices of case (a), with energy measured in units of  $W_{top}$ . In the remainder of the paper, we use the same units. The constant  $\Theta = 1$  in all cases except the triangular lattice where  $\Theta = 2$ , and we treat this lattice as a square lattice (with lattice constant  $a$ ) and all diagonal bonds running, say, northeast. The spin-wave energy goes as

$$\epsilon_{sw}(q) = Dq^2/a^2 + O(q^4),$$

with the stiffness given (in units of  $zr$ ) by

$$D = D_{RPA} \left[ 1 - \frac{Iz}{\theta\Theta(1 + \beta Iz/2\Theta)} \right], \quad (14)$$

where  $D_{RPA} = \Theta\beta\delta/z$ . Note that  $I$  is always positive, and hence the spin waves are always softer than what RPA suggests. In Table I we list the stiffness for two typical values of  $\delta$  (0.1 and 0.2) and also the RPA values for comparison.

It is remarkable that the stiffness is much smaller than  $D_{RPA}$  and 2 orders of magnitude less than  $zr$  is almost all the cases considered. This low-energy scale of the long-wavelength excitations would lead to a transition temperature that is considerably lower than the Stoner-Hartree-Fock estimates, and has a bearing on the question of why the  $T_c$  of itinerant ferromagnets is so low.<sup>11</sup> Spin-wave theory<sup>12</sup> for the simple cubic lattice for  $\delta = 0.2$  would give a  $T_c = 0.029 zr$ . In any case our calculation gives an upper bound on the spin-wave stiffness. A finite exchange energy ( $I^2/U$ ) would reduce this further.

For general nonzero  $q$ , the integral equation (10) reduces to a set of algebraic equations by using the separability of the kernel, and was solved numerically. In Fig. 1 we sketch the bound-state spectrum and the scattering continuum for the square lattice in two cases; one case

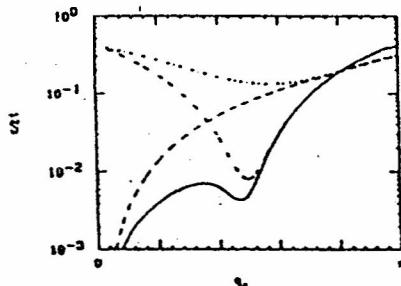


FIG. 1. The spin-wave energy (solid and dashed curves) and the bottom of the scattering continuum (dot-dashed and dotted curves) for  $\delta \leq \delta_{cr}$  and  $\delta = 0.34$ , respectively, on a logarithmic scale, against  $q$  [along (1,1) direction].

corresponds to a small enough  $\delta$  for which we only have positive-definite excitations, and the second corresponds to  $\delta = 0.49$  at which the Nagaoka ferromagnet is close to being unstable.

From Fig. 1, it is seen that the spin-wave bound state is at a much lower scale than the single-particle continuum, and unlike in the usual weak-coupling case, does not enter the continuum for any  $q$ . The effect of increasing the hole density is to bring down the entire continuum rapidly, and the dip at  $q = k_F$  precipitously. This situation is somewhat reminiscent of soft modes in ferroelectrics, but is a more severe instability since essentially an infinite number of states are going soft. The spin waves respond by going soft slightly before  $q = k_F$ , and hug the bottom of the continuum for larger  $q$ .

We have also used a simple generalization of the wave function of Eq. (2) to determine the critical value of  $U$  below which the Nagaoka state is definitely unstable. The variational function is chosen as a Gutzwiller incomplete projected version of Eq. (2) and written as

$$\langle \Phi_g \rangle = \prod_m [1 + (g-1)n_m]^{-1} C_{k_F} |F\rangle, \quad (13)$$

where  $g$  is the usual Gutzwiller parameter. The variational energy now reads

$$\lambda_g(g, q, U) = C^{-1} [(g-1)\rho\delta - C_{k_F} + g^{-1}\mu] + \epsilon_q[(\delta + \rho g)^2 - \delta^2(g-1)^2/\mu^2], \quad (14)$$

where  $C = \delta + \rho g^2$ ,  $\rho = 1 - \delta$ , and the various terms are recognizable in analogy with Eq. (3) obtained by  $g = 0$ , except the third which is the Coulomb interaction energy. For a fixed  $\delta$  and  $U$ , we can minimize Eq. (14) with respect to  $g$ ; and  $U_{cr}$  is defined by  $\lambda_g = 0$ . We believe that this estimate of  $U_{cr}$  is a reasonably good guide for  $\delta \rightarrow \delta_{cr}$ , where  $U_{cr}$  diverges [like  $(\delta_{cr} - \delta)^{-1}$ ], but is far from optimal for  $\delta = 0$ . In the limit of small  $\delta$  and large  $U$ , the main contribution to the excitation energy comes from the first, second, and last term [i.e., by ignoring the kinetic

energy of the down spin which is of  $O(\delta^3)$ ], and we find the leading behavior goes as  $(\rho - C_{k_F}) - \delta^2/U$ . Thus, both terms are of order  $\delta$  and hence we find that in order to stabilize the ferromagnet we must have  $U > U_1$  with  $U_1$  an  $O(1)$  energy [ $= \lim_{\delta \rightarrow 0} [\delta^2/(\rho - C_{k_F})]$ ]. This is not as good as the result of Richmond and Rickayzen, who find the exchange contribution [i.e., term of  $O(1/U)$ ] to be independent of  $\delta$ , whereby  $U_{cr} \rightarrow \infty$  as  $\delta \rightarrow 0$ . Their result is of course more reliable in this limit since their calculation is exact whenever the down-electron kinetic energy is neglected. In Fig. 2, we juxtapose for the square lattice our result for the stability regime with that of Ref. 4 for the case of the square lattice, to get a rigorous limit on the regime of stability of the Nagaoka ferromagnet.

In summary, we have shown in this paper that the Nagaoka ferromagnet is unstable for a sufficiently large concentration of holes at  $U = \infty$  by identifying a soft Fermi-surface restoring excitation. The Nagaoka-Stoner Fermi surface forces the kinetic energy of the up electron to be much greater than that in the Luttinger, or normal (Fermi liquid) Fermi surface, and the instability corresponds to the rectification of this state of affairs—for large enough  $\delta$ , the down-electron band width becomes large enough to benefit from this collapse. Our estimate of the down-electron band width as  $O(\delta^2)$ , rather than  $O(\delta)$  is specific to the use of our variational wave function—if this is true in general then we have a generic argument for the stability of the Nagaoka ferromagnet for small enough  $\delta$ . If a state can be found that has a band width for down electrons of  $O(\delta)$  while costing only an energy of  $O(\delta)$  for the up spins, there would be possible to destabilize the ferromagnet for any  $\delta > 0$ . Although we cannot rule out this possibility categorically, we feel it is unlikely since our wave function can only be improved upon by an admixture of particle-hole excitations in the up-electron Fermi surface, which should be quite small [to keep the up-electron energy cost low, of  $O(\delta)$ ].

The instability, with respect to reducing  $U$  from

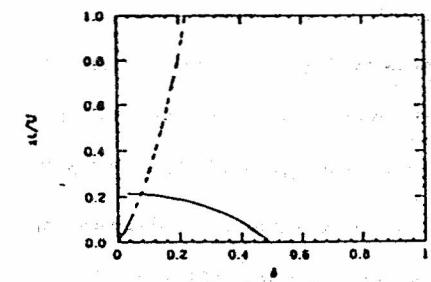


FIG. 2.  $\Delta M / M(0)$  vs  $\delta$  for the square lattice as found from our Eq. (14) (solid line) and from Ref. 4 (dashed line). The Nagaoka ferromagnetic is then definitely unstable outside the area bounded by the two curves and the abscissa.

#### ACKNOWLEDGMENTS

We would like to thank T. V. Ramakrishnan for several interesting discussions about the Nagaoka ferromagnet. We thank D. M. Edwards for bringing to our attention the work of Roth (see Refs. 6 and 10) and of the unpublished thesis of Tan, (see Ref. 10), of which we were unaware.

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†On leave from Indian Institute of Science, Bangalore, India.

‡Y. Nagaoka, Phys. Rev. 147, 392 (1966); Solid State Commun. 3, 409 (1965).

§D. J. Thouless, Proc. Phys. Soc. London B6, 893 (1965).

¶P. W. Anderson, Science 235, 1196 (1987).

•Ferromagnetism in the Hubbard model has been studied using a variety of approximate methods over the years. Some early references, apart from Hubbard's own paper, J. Hubbard, Proc. R. Soc. London A 276, 238 (1963), are J. Kanamori, Prog. Theor. Phys. 30, 276 (1963); A. B. Harris and R. V. Lange, Phys. Rev. 157, 295 (1967). For some recent reviews see *Metallic Magnetism*, edited by H. Capemann (Springer-Verlag, Berlin, 1987). In what follows, we do not attempt to review the vast literature, and cite only a few papers that are directly related to our work.

•P. Richmond and G. Rickayzen, J. Phys. C2, 528 (1969).

•This wave function turns out to have a long history, and was first written down by Laura M. Roth, J. Phys. Chem. Solids 28, 1549 (1967), who, however, seems to have missed the instability contained in it, which we discuss in what follows. The same wave function has also been rediscovered by S. Schmitt-Rink and A. Ruckenstein (unpublished).

•In the case of the electron gas the ferromagnetic state, found within the Hartree-Fock approximation by Bloch, was shown to be unstable with respect to long-wavelength spin-wave excitations in a small range of  $k$ , by Herring [C. Herring, *Magnetism*, edited by G. T. Rado and H. Suhl (Academic, New York, 1966), Vol. IV, p. 104]. It is therefore necessary to examine the long-wavelength spin waves to make sure of the stability of the ferromagnet.

•This wave function has also been discussed by L. M. Roth (Ref. 5) who used it only to study the long-wavelength spin waves.

•Reviewed by C. Herring in Ref. 2, Chap. XIV. (By RPA we refer to the limit  $U = \infty$  of the RPA results noted in this review.)

•A similar instability of the Nagaoka-Stoner state has also been discussed by Laura M. Roth, Phys. Rev. 186, 428 (1969), using a Green's-function decoupling scheme. Even though her considerations did not have a variational significance, H. W. Tan, in his unpublished thesis (Imperial College, London, 1974) has shown that Roth's decoupling scheme results can be obtained using a variational wave function for one-spin-down excitations. See also D. M. Edwards and J. A. Hertz, J. Phys. F 3, 2191 (1973); S. R. Allan and D. M. Edwards, J. Phys. F 12, 1203 (1982).

•D. M. Edwards, Magn. Magn. Mater. 15-18, 262 (1980).

•We are using a crude estimate taken from a simple minded spin-wave calculation, which gives  $\Delta M / M(0) = (0.0587 / \pi K_B T / D)^{1/2}$ , (see, e.g., C. Kittel, in *Introduction to Solid State Physics*, Sixth Ed. (Wiley, New York, 1986), p. 415), and use  $S = \frac{1}{2}$  with  $\Delta M / M(0) = 1$  in order to find the estimate quoted in the text.

### Gauge Theory Of The Hubbard Model

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An exciting result of the renewal of interest in the large U Hubbard model has been the gauge theory formalism of the model. For the first time, there is a theory of quasiparticles in a condensed matter system with interactions mediated by long ranged gauge quasiparticles. This description of the system has met with preliminary success in explaining some of the normal state transport properties of the cuprate superconductors. There are however still a host of questions, both basic theoretical ones as well as phenomenological ones that remain to be answered. Essentially, the theoretical framework has been laid out and some physics has been extracted from it. A large amount remains to be pulled out. In these three lectures, I will be reviewing the basic theoretical formalism and some recent attempts to extract phenomenological consequences.

The first two transparencies illustrate, in two simple examples, the fact that the presence of a gauge symmetry implies that the system is constrained. Namely that there are some redundant degrees of freedom. In quantum theory, there are then some unphysical states. The reason for the emergence of gauge symmetries in strongly correlated electronic systems is then clear. Because of the strong correlations, certain states ( those having double occupancies ) become high energy states. They get separated from the low energy ones by a gap ( the Mott-Hubbard gap). These states then contribute to the low energy physics only through virtual processes. So they can be "integrated out" and the effective

low energy model which includes these effects can be obtained. But now in this model the high energy states are not physically relevant. The effective model thus has a gauge symmetry which expresses this fact.

Thus the Heisenberg model, which is the low energy effective theory of the large U Hubbard model at half filling, has a local  $U(1)$  gauge symmetry which was discovered by Baskaran and Anderson<sup>(1)</sup>. This was later found to be a part of a larger  $SU(2)$  gauge symmetry by Affleck et al<sup>(2)</sup>.

The  $SU(2)$  gauge theory formalism is described in the next few transparencies. The gauge fields arise as link variables when a Hubbard-Stratanovich transformation is performed to make the theory quadratic in the fermion fields.

The physical meaning of the gauge fields in terms of the original spin variables is then sketched. The association of the magnetic field with spin chirality is discussed in more detail in references (3) and (4).

Next the question of the relevance of this formalism is discussed. It is clear that the formalism will have relevance if the fermion operators create physical quasiparticles. In the context of the gauge theory, this implies that the system is in the deconfined phase. Thus if the model is realised in the deconfined phase, then this formalism can be expected to be useful. The RVB picture of the ground state and excitations gives a physical picture of such a phase. The unpaired spins being the deconfined fermions, the dynamics of the singlet pairs being described by the gauge fields.

One point to note here is that even if the model were not realised in the deconfined phase in the strict sense of the word, but if the confinement length were large, this could

still be a useful formalism. The fermions would then not be free but would form loosely bound particle hole pairs.

To tackle the model away from half filling, i.e. the physics of the t-J model, the formalism has to be extended. This is the slave boson formalism. This formalism is described in the next few transparencies. The Hubbard model is rewritten in terms of the slave bosons. When this is done there is a U(1) gauge symmetry which comes as a consequence of the extra fields introduced and the resulting constraint. We then integrate out the doubly occupied sites in the path integral and obtain the t-J model as the low energy theory.

Some popular mean field solutions<sup>(5),(6),(3)</sup> of the Heisenberg model are then described. The electron propagator at the mean field level is simply a convolution of the boson and fermion propagator. It can then be seen that below the Bose-Einstein crossover temperature, the propagator is Fermi liquid type with a sharp quasiparticle peak in  $A(k,\omega)$ . Above  $T_{BG}$  the peak broadens and the system is no longer a Fermi liquid. At the mean field level  $T_{BG} \sim 1/t \simeq 1000$  deg K. The normal state properties like resistivity seem to be correctly reproduced only above  $T_{BG}$  i.e. in the non-Fermi liquid region. Thus the high value of  $T_{BG}$  poses a major problem for the gauge theory approach. It is speculated that the gauge field fluctuations should bring down the value of  $T_{BG}$ . How exactly this happens is an outstanding problem in the field.

Finally the method to include the effects of gauge field fluctuations in correlation functions is sketched out. The features of the calculation of the normal state resistivity are then stated. The readers are referred to references (7-9) for the thorough treatment.

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## GAUGE THEORY OF THE HUBBARD MODEL.

1. CONSTRAINTS AND GAUGE SYMMETRY
2. THE HESSENBERG MODEL
3. DOPING: THE SLAVE-BOSON FORMALISM
4. HUBBARD  $\rightarrow$  T-J
5. MEAN FIELD SOLUTIONS
6. GAUGE FIELD FLUCTUATION EFFECTS

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## GAUGE SYMMETRY

$$S = \int dt \left( \frac{1}{2} \dot{\vec{x}}^2 + \frac{1}{2} \dot{\vec{y}}^2 + \vec{x} \cdot \vec{y} \right)$$

$$\begin{aligned}\vec{x}(t) &\rightarrow \vec{x}(t) + \vec{\xi}(t) \\ \vec{y}(t) &\rightarrow \vec{y}(t) - \vec{\xi}(t)\end{aligned}$$

$S[\vec{x}(t), \vec{y}(t)]$  is invariant

$$\therefore S[\vec{x}(t), \vec{y}(t)] = \int dt \frac{1}{2} (\dot{\vec{x}}(t) + \dot{\vec{y}}(t))^2$$

## SPIN $\frac{1}{2}$ IN A MAGNETIC FIELD

$$H = \vec{B} \cdot \vec{S} \quad [S^a, S^b] = i \epsilon^{abc} S^c$$

$$\vec{S} \cdot \vec{S} = \frac{1}{2} (t+1)$$

$$\vec{S} = \frac{1}{2} S_r \vec{\sigma}_{\alpha\beta} S_{\alpha\beta} \quad (\alpha = r, \perp)$$

$$\sum S_\alpha S_\alpha = 1$$

STATES

- 113  
 114
- 1a)
  - 1b) } PHYSICAL
  - 1b)
  - 1d) } UNPHYSICAL

$$\int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{i(\sum S_a^z S_b - 1)\theta} |\Psi\rangle = |\Psi_{phys}\rangle$$

$$Z = \int_{S_a^z S_b^z}^A e^{-\int dz (\sum S_a^z (Q_a - i A_a) S_b - i A_b + \frac{1}{2} \vec{B}(z) \cdot \vec{S}(z))}$$

ACTION IS INVARIANT UNDER

$$S_a(z) \rightarrow e^{i Q_a(z)} S_a(z)$$

$$S_a^z(z) \rightarrow e^{-i Q_a(z)} S_a^z(z)$$

$$A_a \rightarrow A_a(z) + \partial_z Q_a$$

AVERAGING OVER THE GAUGE GROUP PROJECTS OUT THE "PHYSICAL" STATES DEFINED BY  $\hat{Q} |\Psi_{phys}\rangle = 0$  (GAUSS LAW).

### THE SU(2) SYMMETRY

$$Q^3 \equiv \frac{1}{2} (\sum S_a^z S_b - 1)$$

$$Q^+ \equiv S_+^z S_+^z$$

$$Q^- \equiv S_-^z S_-^z$$

$$AGAIN \quad Q^\alpha |\Psi_{phys}\rangle = 0$$

$$\int d\theta e^{i(Q^\alpha \theta^\alpha)} |\Psi\rangle = |\Psi_{phys}\rangle$$

$$\begin{pmatrix} S_+ \\ -S_-^z \end{pmatrix} \rightarrow \begin{pmatrix} \omega & \beta \\ -\beta & \omega \end{pmatrix} \begin{pmatrix} S_+ \\ -S_-^z \end{pmatrix}$$

THE HEISENBERG MODEL

$$H = \sum_{ij} J_{ij} \vec{s}_i \cdot \vec{s}_j$$

$$\vec{s}_i = \frac{1}{2} s_{i\alpha} \vec{\epsilon}_{\alpha\beta\gamma} s_{i\beta} s_{i\gamma}$$

$$H = \int d\zeta \left( \sum_i (s_{i\alpha}^r - s_{i\alpha}^a) (\partial_\zeta - i A_{i\alpha}^r \zeta^*) \begin{pmatrix} s_{i\alpha} \\ -s_{i\alpha} \end{pmatrix} + H_a \right)$$

$$Z = \int e^{-S[s_{i\alpha}^r, s_{i\alpha}^a, A_{i\alpha}^r]}$$

$s_{i\alpha}^r, s_{i\alpha}^a$   
 $A_{i\alpha}^r$

$$\begin{pmatrix} s_{i\alpha}^r \\ -s_{i\alpha}^a \end{pmatrix} \rightarrow U_i(\zeta) \begin{pmatrix} s_{i\alpha} \\ -s_{i\alpha} \end{pmatrix}$$

(Bardeen + Anderson  
Affleck, Zee + Anderson)

$$A_{i\alpha}^r \zeta^* \rightarrow U_i(\zeta) A_{i\alpha}^r U_i^*(\zeta) + i U_i \partial_\zeta U_i^*$$

GAUGE FIELDS

$$\vec{s}_i \cdot \vec{s}_j = \frac{1}{2} (\hat{x}_{ij}^+ \hat{x}_{ij}^- + \hat{d}_{ij}^+ \hat{d}_{ij}^-)$$

$$\hat{x}_{ij}^\pm \equiv \frac{1}{\sqrt{2}} \sum_\alpha s_{i\alpha}^\pm s_{j\alpha}^\pm$$

$$\hat{d}_{ij}^\pm \equiv \frac{1}{\sqrt{2}} (s_{i\alpha} s_{j\beta}^\pm - s_{i\beta} s_{j\alpha}^\pm)$$

HUBBARD - STRATANOVICH

$$\begin{aligned} H &= - \sum_{ij} J_{ij} (\hat{x}_{ij}^+ \hat{x}_{ij}^- + h.c.) + \sum_{ij} (\hat{d}_{ij}^+ \hat{d}_{ij}^- + h.c.) \\ &\quad + \sum_{ij} J_{ij} (|\hat{x}_{ij}|^2 + |\hat{d}_{ij}|^2) \\ &= - \sum_{ij} J_{ij} \Psi_i^+ \begin{pmatrix} \hat{x}_{ij}^+ & \hat{d}_{ij}^+ \\ -\hat{d}_{ij}^- & \hat{x}_{ij}^- \end{pmatrix} \Psi_j^- \quad (\Psi_i = \begin{pmatrix} s_{i\alpha} \\ -s_{i\alpha} \end{pmatrix}) \\ &\quad + \sum_{ij} J_{ij} (|\hat{x}_{ij}|^2 + |\hat{d}_{ij}|^2) \end{aligned}$$

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$$\text{Im } \hat{\chi}_{ij} \hat{\chi}_{jk} \hat{\chi}_{ki} = \vec{s}_i \cdot (\vec{s}_j \times \vec{s}_k)$$

$\hat{\chi}_{ij} \hat{\chi}_{jk} \hat{\chi}_{ki}$  ~~and~~  $e^{i\theta \vec{A} \cdot \vec{d}}$

$$\langle \hat{n}_i \hat{n}_j \hat{n}_k | \vec{s}_i \cdot (\vec{s}_j \times \vec{s}_k) | \hat{n}_i \hat{n}_j \hat{n}_k \rangle$$

$$= \hat{n}_i \cdot \hat{n}_j \times \hat{n}_k$$

IF  $\hat{n}_i$  SLOWLY VARYING,



MAGNETIC FLUX  $\sim$  SPIN CHIRALITY

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### RELEVENCE

IF THEORY IN DECONFINED PHASE

THEN  $s_{ir}^+, s_{ir}^-$  UNBOUND (LOOSELY BOUND)

SPECTRUM WILL CONTAIN SPIN  $1/2$  EXCITATIONS. MFT WITH

$\frac{1}{2}(s_{ir}^+ s_{ir}^-) = \chi_{ij}$  WILL BE GOOD

SPIN LIQUID PHASE (NO HOMOGENEITY)

IF THEORY IN CONFINED PHASE, ie  $s_{ir}^+ s_{ir}^-$  TIGHTLY BOUND MAGNETIC MOMENTS WILL EXIST

PHYSICAL PICTURE

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$$\Sigma | \begin{array}{c} \diagup \\ \diagdown \end{array} \begin{array}{c} \diagdown \\ \diagup \end{array} \rangle = \text{SPIN LIQUID GROUND STATE}$$

$$\Sigma | \begin{array}{c} \diagup \\ - \\ \diagdown \end{array} \begin{array}{c} \diagdown \\ \diagup \end{array} \rangle = \text{SPIN } \frac{1}{2} \text{ EXCITATION "SPINON"}$$

$$\Sigma | \begin{array}{c} \diagup \\ - \\ \diagdown \end{array} \begin{array}{c} \diagdown \\ \diagup \end{array} \rangle = \text{HOLON}$$

$$-\cdots \chi_{ii} \chi_{ii} \hat{x}_{ii} s_i^+ = \text{SPINON CREATION OPERATOR}$$

$$\sim e^{i \int A \cdot d\ell} s_i^+$$

$$\text{GAUGE INVARIANT OPERATOR.}$$

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MEANING OF STRING.

$$\hat{x}_{ij} = \frac{1}{2} \sum s_i^+ s_{j+}^-$$

$$\hat{x}_{ij} | 00 \rangle = | 00 \rangle$$

$$\hat{x}_{ij} | 01 \rangle = | 10 \rangle$$

$$\therefore \prod_i \hat{x}_{i,i+1} | \begin{array}{cccccc} \diagup & \diagup & \diagup & \diagup & \diagup & \dots \\ \diagdown & \diagdown & \diagdown & \diagdown & \diagdown & \dots \\ \diagup & \diagup & \diagup & \diagup & \diagup & \dots \\ \diagdown & \diagdown & \diagdown & \diagdown & \diagdown & \dots \\ \diagup & \diagup & \diagup & \diagup & \diagup & \dots \\ \diagdown & \diagdown & \diagdown & \diagdown & \diagdown & \dots \end{array} \rangle = | \begin{array}{cccccc} \diagup & \diagup & \diagup & \diagup & \diagup & \dots \\ \diagdown & \diagdown & \diagdown & \diagdown & \diagdown & \dots \\ \diagup & \diagup & \diagup & \diagup & \diagup & \dots \\ \diagdown & \diagdown & \diagdown & \diagdown & \diagdown & \dots \\ \diagup & \diagup & \diagup & \diagup & \diagup & \dots \\ \diagdown & \diagdown & \diagdown & \diagdown & \diagdown & \dots \end{array} \rangle$$

( $\therefore$  NEEC STATE SHOULD CONFIRM)

$$\prod_i \hat{x}_{i,i+1} | \begin{array}{ccc} \diagup & \diagup & \diagup \\ \diagdown & \diagdown & \diagdown \\ \diagup & \diagup & \diagup \\ \diagdown & \diagdown & \diagdown \\ \diagup & \diagup & \diagup \\ \diagdown & \diagdown & \diagdown \end{array} \rangle = | \begin{array}{ccc} \diagup & \diagup & \diagup \\ \diagdown & \diagdown & \diagdown \\ \diagup & \diagup & \diagup \\ \diagdown & \diagdown & \diagdown \\ \diagup & \diagup & \diagup \\ \diagdown & \diagdown & \diagdown \end{array} \rangle$$

## SLAVE BOSONS

$e_i, d_i, \delta_{i\sigma}, \delta_{i\sigma}^+$

$$[e_i, e_j^\dagger] = \delta_{ij}, \quad [d_i, d_j^\dagger] = \delta_{ij}$$

$$\{\delta_{i\sigma}, \delta_{j\sigma'}\} = \delta_{ij} \delta_{\sigma\sigma'}, \quad [e_i, d_i] = [\delta_{i\sigma}, e_i] = 0$$

$$[d_i, \delta_{i\sigma}] = 0$$

$$c_{i\sigma} = e_i^\dagger \delta_{i\sigma} + \sigma d_i \delta_{i\sigma}^T$$

$$c_{i\sigma}^\dagger = e_i \delta_{i\sigma}^\dagger + \sigma d_i^\dagger \delta_{i\sigma}$$

$$e_i^\dagger e_i + d_i^\dagger d_i + \delta_{i\sigma}^\dagger \delta_{i\sigma} + \delta_{i\sigma}^\dagger \delta_{i\sigma} = 1$$

$$\Rightarrow \{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}$$

$$e_i^\dagger |0\rangle \leftrightarrow |0\rangle$$

$$d_i^\dagger |0\rangle \leftrightarrow |1\rangle$$

$$\delta_{i\sigma}^\dagger |0\rangle \leftrightarrow |1\rangle$$

$$\delta_{i\sigma}^\dagger |0\rangle \leftrightarrow |1\rangle$$

$$|0\rangle, e_i^\dagger |0\rangle, e_i^\dagger d_i^\dagger |0\rangle, \delta_{i\sigma}^\dagger \delta_{i\sigma} |0\rangle$$

$e_i^\dagger \delta_{i\sigma}^\dagger |0\rangle, \dots \text{UNPHYSICAL.}$

## HUBBARD MODEL

$$H = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i$$

$$n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}, \quad n_i \equiv \sum_{\sigma} n_{i\sigma}$$

$$n_i \leftrightarrow \sum_{\sigma} \delta_{i\sigma}^\dagger \delta_{i\sigma}$$

$$n_{i\uparrow} n_{i\downarrow} \leftrightarrow d_i^\dagger d_i$$

$$\sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) = \sum_{\sigma} e_i^\dagger \delta_{i\sigma} \delta_{j\sigma} c_j^\dagger + h.c.$$

$$- \sum_{\sigma} d_i^\dagger \delta_{i\sigma} \delta_{j\sigma} c_j^\dagger + h.c.$$

$$+ \sum_{\sigma} d_i^\dagger \delta_{i\sigma} \delta_{j\sigma}^T d_j$$

DEFINE

$$J_i = t \delta_{ij} e_j^\dagger, \quad J_i^T = t e_j \delta_{ij}^\dagger$$

$$H = \sum_{\langle i,j \rangle} (e_i^\dagger e_j^\dagger \delta_{i\sigma} \delta_{j\sigma} + h.c.) - \mu \sum_{i\sigma} \delta_{i\sigma}^\dagger \delta_{i\sigma}$$

$$+ \sum_{\langle i,j \rangle} d_i^\dagger - c_j^\dagger \delta_{ij} d_j + U \sum_i d_i^\dagger d_i - \sum_i d_i^\dagger J_i +$$

$$e_i^\dagger e_i + d_i^\dagger d_i + \sum_{\sigma} \delta_{i\sigma}^\dagger \delta_{i\sigma} = 1$$

$$Z = \int e^{-\int dz \left[ \sum_i c_i^T (z_i - iA_i) c_i + d_i^T (z_i - iA_i) d_i + \sum_r S_{ir}^T (z_r - iA_{ir}) S_{ir} - iA_{ir} \right] + H\omega} \quad (1)$$

 $e^* e_i$  $d_i d_i^*$  $S_{ir}^* S_{ir}$  $A_i$ 

$\therefore U(1)$  GAUGE SYMMETRY PRESENT  
AT ALL VALUES OF  $U$ .

DECONFINED PHASE:  $e$ ,  $S_r$  ARE INDEPENDENT QUASI PARTICLES  $\Leftrightarrow$  "SPIN-CHARGE DECOUPLING."

CONFINED PHASE:  $e_0$ ,  $e_s$ ,  $s_s$  BIND  
TO FORM  $c_o$

$\therefore U=0$  IS IN THIS LANGUAGE  
A CONFINED PHASE.

### T-J MODEL

FOR LARGE  $U$ ,  $d^T$  WILL CREATE HIGH ENERGY EXCITATIONS AND WE CAN INTEGRATE IT OUT TO OBTAIN THE EFFECTIVE LOW ENERGY THEORY.

$$e^{\int dz \left[ \sum_{ij} d_i^T (z_i - iA_0 + US_{ij} - \chi_{ij}) - \sum_i g_i^T J_i + h.c. \right]} \\ = e^{-\text{Tr} \ln (D_0 + \chi) + J^T (D_0 + \chi)^{-1} J}$$

$$(D_0)_{ij}(z_1, z_2) \equiv (z_1 - iA_0 + U) S_{ij} S(z_1 - z_2)$$

$$(D_0')_{ij}(z_1, z_2) = e^{iA_0(z_1 - z_2)} e^{-U(z_1 - z_2)} \theta(z_1 - z_2) \quad (\text{AC } \beta = \infty)$$

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$\text{Tr } \ln(D_0 + t\hat{x})$  DOES NOT CONTRIBUTE  
TO ORDER  $\frac{t^2}{U}$ , CORRESPONDS TO  
PROCESSES  $\pi, \pi_b \rightarrow \pi_b, \pi$

$$J^T (D_0 + t\hat{x}) J = J^T D_0^{-1} J + \dots$$

$$= \frac{2t^2}{U} \sum_{ijk} \hat{A}_{ij}^T \hat{A}_{ik} e_j e_k^T$$

CONSIDER THE  $j=k$  TERMS

$$= \frac{2t^2}{U} \sum_{ij} (\vec{s}_i \cdot \vec{s}_j - \frac{1}{4} n_i n_j)$$

THIS MOTIVATES THE STUDY OF  
THE FOLLOWING T-J MODEL

$$H_T = -t \sum_{ij} (e_i s_{ir}^T s_{jr} e_j^T + h.c.) - \mu \sum_i s_{ir}^T s_{ir}$$

$$+ J \sum_{ij} (\vec{s}_i \cdot \vec{s}_j - \frac{1}{4} n_i n_j)$$

$$J = \frac{2t^2}{U}, \quad e_i^T e_i + \sum_r s_{ir}^T s_{ir} = 1$$

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### M.F.T. OF T-J MODEL

HUBBARD - STRATANOVICH IT TILL  
QUADRATIC COME.

$$H = \sum_{ij} -t (\hat{\Phi}_{ij}^+ \hat{x}_{ij} + h.c.)$$

$$- \frac{J}{4} (\hat{x}_{ij}^T \hat{x}_{ij} + \hat{d}_{ij}^T \hat{d}_{ij} + \hat{\Phi}_{ij}^+ \hat{\Phi}_{ij})$$

$$+ \sum_i (i A_{0i} - \mu^0) e_i^T e_i + \sum_i (i A_{0i} - \mu_i) \hat{d}_{ir}^T \hat{d}_{ir}$$

$$H = - \sum_{ij} e_i^T (t 2\hat{x}_{ij}^T + \frac{J}{4} \hat{\Phi}_{ij}^+) e_j + h.c.$$

$$- \sum_{ij} (g_{ir}^T g_{jr}) \left( \frac{1}{2} \hat{x}_{ij}^T + \frac{1}{2} \hat{\Phi}_{ij}^+ - \frac{\hat{d}_{ij}^T}{2} \right) \frac{g_{ir}}{D_{ij} - \frac{J}{4} \hat{x}_{ij}^T + \hat{\Phi}_{ij}^+}$$

$$+ \sum_i (i A_{0i} + \mu^0) e_i^T e_i + \sum_{ir} (i A_{0i} - \mu_i) \hat{d}_{ir}^T \hat{d}_{ir}$$

$$+ \sum_{ij} \frac{J}{4} (|\hat{x}_{ij}|^2 + |\hat{d}_{ij}|^2 + |\hat{\Phi}_{ij}|^2) + t(\hat{x}_{ij}^T \hat{d}_{ij} + h.c.)$$

SADDLE POINT / MEAN FIELD EQUATIONS  
ARE THEN

$$\chi_{ij} = \sum_{\sigma} \langle \delta_{ir}^{\dagger} \delta_{j\sigma} \rangle$$

$$\Delta_{ij} = \sum_{\sigma} \langle \delta_{ir} \delta_{j\sigma} - \delta_{is} \delta_{jr} \rangle$$

$$\phi_{ij} = \langle e_i^{\dagger} e_j \rangle$$

IF  $A_{oi}$  IS TAKEN TO BE SITE INDEPENDENT & IMAGINARY CONST

$$i A_{oi} + \mu_B \equiv \mu_B$$

$$i A_{oi} - \mu_F \equiv \mu_F$$

$$\langle \delta_{ir}^{\dagger} \delta_{i\sigma} \rangle = \frac{1-\delta}{2}$$

$$\langle e_i^{\dagger} e_i \rangle = \delta$$

$$\therefore \langle e_i^{\dagger} e_i + \sum_{\sigma} \delta_{ir}^{\dagger} \delta_{i\sigma} \rangle = 1$$

$\therefore$  CONSTRAINT IS IMPOSED ON THE AVERAGE.

### LARGE N $\approx$ FORMALISM

$$\delta_{ir} \sigma = i \dots N$$

$$t \rightarrow \frac{t}{N}, J \rightarrow \frac{J}{N},$$

$$e_i^{\dagger} e_i + \sum_{\sigma} \delta_{ir}^{\dagger} \delta_{i\sigma} = \frac{N}{2}$$

$$\langle e_i^{\dagger} e_i \rangle = \frac{\delta N}{2}$$

$\delta_{ij}$  NOW IS NOT A SU(N) SINGLET & HENCE CANNOT CONDENSE IN THE  $N = \infty$  LIMIT.

MEAN FIELD SOLUTIONS

$$A. \delta = 0 \Rightarrow \Phi_{ij} = 0$$

$$\sum_i \delta_{i\sigma}^{\dagger} \delta_{i\sigma} = 1$$

1.  $B \geq A$  / EXTENDED-S / UNIFORM

$$\chi_{ij} = \chi \quad \Delta_{ij} = \Delta$$

SU(2) ROTATED TO  $\Delta = 0$

M.F HAMILTONIAN

$$H_{MF} = -J \sum_{\langle ij \rangle} \chi (\delta_{i\sigma}^{\dagger} \delta_{j\sigma} + \text{H.c.})$$

QP SPECTRUM

$$E_k = -J\chi (2\cos k_x + 2\cos k_y)$$

NOTE: STANDARD MFT  
ASSUMPTION THAT

MF DOES NOT DEFORM IN PRESENCE  
OF Q.P. MAY NOT BE TRUE AT  $N=2$ .



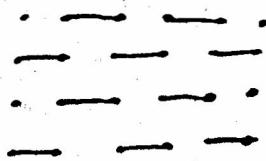
2. FLUX PHASE (5+1d)  $\alpha$  wave pairing

$$+ \boxed{1/2} \operatorname{tr} U_1 U_2 U_3^T U_4^T = -e^{i\pi} = -1$$

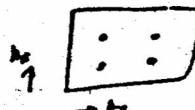
ONE WAY  $\Delta = 0$

$$\cdots \Rightarrow x = 0$$

$$\cdots \Rightarrow x = -1$$



$$E_k = J\chi \sqrt{\cos^2 k_x + \cos^2 k_y}$$

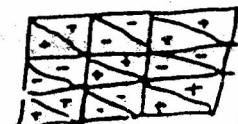


NEAR ZEROS

$$E_k \propto ck$$

$\therefore 4$  MASSLESS DIRAC FERMIONS.

3. CHIRAL PHASE



$$E_k = c \sqrt{k^2 + m^2}$$

TIME REV BROKEN.

SPINON FERMI SURFACE IS  
REFLECTED IN ELECTRON  
GREENS FUNCTION.

UNIFORM PHASE SEEM MORE  
IN LINE WITH EXPERIMENT AS  
COMPARED TO FLUX OR CHIRAL  
PHASES.

THIS DOES NOT PRECLUDE OTHER  
MF SOLNS WHICH HAVE A  
SPINON FERMI SURFACE. THERE  
MAY BE SUCH SOLNS IN PRE-  
SENCE OF DOPING.

<sup>131</sup>  
B.M.F. ELECTRON PROPAGATOR

$$\begin{aligned} G_{ij}^{el}(z) &= \langle T(C_i^{\dagger}(z) C_j(z)) \rangle \\ &= \langle T(e_i^r(z) e_j(z) S_i(z) S_j^r(z)) \rangle \\ &= G_{ij}^B(z) G_{ij}^F(z) \end{aligned}$$

$$G_{ij}^F(k, \omega) = \int \frac{d^3q}{(2\pi)^3} \frac{n_B(\vec{k}-\vec{q}) + n_F(\vec{q})}{\omega + i\varepsilon - (E_F(\vec{q}) - E_B(\vec{k}-\vec{q}))}$$

$$A(k, \omega) = \int \frac{d^3q}{(2\pi)^3} (n_B(k-q) + n_F(q)) \delta(\omega - (E_F(q) - E_B(k-q)))$$

$$n_k = \frac{(-s)^2}{2} + \int \frac{d^3q}{(2\pi)^3} n_B(\vec{q}) n_F(\vec{k}-\vec{q})$$

1.  $n_F$  PART GIVES INCOHERENT  
BACKGROUND,  $n_B$  PART GIVES "Q.P." PEAK

2.  $\int d\omega A(k, \omega) = \frac{1+s}{2} \because \{C_i^{\dagger}, C_i\} = 1 - s_i^2 s_i$   
 $\therefore$  SOME SPECTRAL WEIGHT PUSHED TO  $\infty$ .

ONE IMPORTANT TEMPERATURE

HERE IS THE BOSE-EINSTEIN  
Crossover TEMPERATURE

$$kT_{BE} \approx \frac{2\pi^2 \hbar}{m_B}$$

THE<sup>A</sup><sub>L</sub> WAVELENGTH = INTER PARTICLE  
DISTANCE.

Below  $T_{BE} \sim$  FERMI LIQUID

Above  $T_{BE} \sim$  NON FERMI LIQUID.

If  $m_B \sim \frac{1}{t}$  THEN  ~~$T_{BE}$~~  IS VERY HIGH. SOME MECHANISM

ARISING FROM THE FACT THAT

HOLONS ARE NOT INTERACTING

SHOULD REDUCE  $T_{BE}$

## GAUGED FIELD FLUCTUATIONS IN THE UNIFORM PHASE

(N. NAGOSA  
& P. LEE)

PR L 54, 2450 (1970)

IOFFE + LARKIN

PR 32, 3928 (1974)

APPROXIMATE COEFF  $\sim 1 - \frac{\alpha^2}{2}$  AND  
CONSIDER THE HAMILTONIAN.

$$H = \int d^2x \frac{1}{2m_B} e^\dagger (\vec{p} - i\vec{a})^2 c(\omega) + \frac{1}{2m_F} \sum \vec{p}^2 c^2(\omega)$$

$$Z = \int e^{-\int dz (e^\dagger(x)(\omega_z - i\omega_0)c^\dagger(z) + s_z^\dagger(\omega_z - i\omega_0)s_z + \dots)}$$

$e^\dagger e$

$s_z^\dagger s_z$

$\vec{a}, \omega$

DIRECTLY IMPLIES.

$$\left[ \begin{array}{l} \frac{1}{2m_B} \sim \chi_L \\ \frac{1}{2m_F} \sim \chi_J \end{array} \right]$$

$$\partial_\mu^B(x) + J_\mu^F(x) = 0$$

$$\partial_\mu^B = \frac{1}{m_B} e^\dagger(\omega) (\vec{p} - \vec{a}) c(\omega) \rightarrow \partial_\mu^F = \frac{1}{m_F} \sum s_z^\dagger(\vec{p} - \vec{a}) s_z$$

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IN PRESENCE OF EXTERNAL  
E.M. FIELD

$$e^+(\alpha) (\vec{p} - \vec{\alpha})^2 e(\alpha) \rightarrow e^+(\alpha) (\vec{p} - \vec{\alpha} - \frac{e}{c} \vec{A}) e(\alpha)$$

$$\vec{J}_B = \sigma_B (\vec{E} + \vec{\epsilon})$$

$$\vec{J}_F = \sigma_F (\vec{E})$$

$$\vec{J}_F + \vec{J}_B = 0$$

$$\vec{J}_B = \sigma_B (\vec{E} - \frac{\vec{J}_B}{\sigma_F})$$

$$\vec{J}_B = \frac{\sigma_F \sigma_B}{\sigma_F + \sigma_B} \vec{E}$$

$$\therefore \vec{J}_B = \frac{1}{\sigma} = \frac{1}{\sigma_F} + \frac{1}{\sigma_B}$$

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TO COMPUTE CORRELATION  
FUNCTIONS.

$$\langle \hat{O} \rangle = \frac{1}{Z} \int_{ee^*}^{ss^*} \hat{O} e^{-S[ee^*, ss^*; a^*]}$$

INTEGRATE OUT THE FERMIONS &  
HOLONS

$$= \frac{1}{Z} \int_a \langle \hat{O} \rangle_a e^{-S_{eff}[a]}$$

TO SECOND ORDER IN  $a$

$$S_{eff}[a] = \int a_\mu \circlearrowleft a_\nu + a_\mu \cdots a_\nu$$

$\circlearrowleft$  — BOSON LINE  
----- FERMION LINE

$\circlearrowright$  — CURRENT CURRENT CORR.

GAUGE FIELD  
PROPAGATOR  
(TRANSVERSE  
PART)

$$= \frac{(k^2 \delta_{\mu\nu} - k_\mu k_\nu)}{k(\omega_n + \chi \frac{k^2}{R^2})}$$

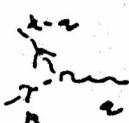
$$\chi_d = \chi_F + \chi_B$$

$$\chi_F = \frac{1-\delta}{m_F} \quad \chi_B = \frac{2\pi g \beta}{m_B^2}$$

$$\frac{1}{\sigma_B} \sim T \quad (T > T_{cB})$$



$$\frac{1}{\sigma_F} \sim T^{4/3}$$



$$2 \quad \sigma_B \ll \sigma_F$$

$$\therefore \frac{1}{\sigma} \sim T$$

NOTE  $T \ll T_{cB}$   $\sigma_B \rightarrow \infty$

$$\frac{1}{\sigma} \sim \frac{1}{\sigma_F} \sim T^{4/3}$$

## Numerical Techniques for solving Hubbard models

S. RAMASESHIA

Indian Institute of Science, Bangalore

In this set of transparencies, a valence bond (VB) method for evaluating the eigen states of finite Hubbard and extended Hubbard models is presented. The VB approach exploits both the total spin invariance and the invariance of the z-component of the total spin of these model Hamiltonians. The VB functions are spin adapted functions that can be represented as integers on a computer and hence can be easily manipulated. The Hamiltonian matrix in the VB basis is nonsymmetric but sparse. Efficient algorithms exist for obtaining eigen values and eigen functions of a few low-lying states of the matrix. The ground state energy per site, excitation gaps, etc. can be reliably extrapolated to the infinite system value since the finite systems are exactly solved and hence the solutions are size consistent. This method has been applied to polyenes for studying effect of correlations on dimerization and optical gaps. The exact dynamic properties of the model systems, such as dynamic polarizabilities, second harmonic and third harmonic generation coefficients etc can also be obtained exactly using a recent formulation. The resonant situations can be handled through a life-time parameter since pole strengths at resonances can be exactly evaluated. Finally, the feasibility of a Quantum Monte Carlo procedure using the VB basis is discussed. This has the advantage of reducing the sample variance by working in the desired spin sub space.

## Numerical Techniques for Solving Hubbard Models

### Importance of Numerical Techniques

- (a) Obtain Reliable Solutions if Exact Analytic Methods do not work.
- (b) Check on Approximate Analytical Methods

### Types of Numerical Techniques

- (a) Configuration Interaction Technique
- (b) Quantum Monte Carlo Technique
- (c) Quantum Renormalization Group Technique

Mostly (a) and a little of (b)

(c) has inherent difficulties and will not be discussed.

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### Configuration Interaction Techniques

- (i) Variational
- (ii) Perturbative
- (iii) Exact.

(i) is O.K. for a single finite system.

Not good for extrapolations as the procedure is not size consistent

(ii) good if the series converge. Size consistent in every order

(iii) Possible for finite model Hamiltonians since they span finite-dimensional Hilbert space. Size consistent and hence possible to obtain reliable extrapolations to infinite systems.

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## Exact Techniques for Finite Hubbard and Related Models

# of degrees of freedom at a site

$$4 \rightarrow 0, \uparrow, \downarrow, \uparrow\downarrow$$

# of possible configurations for  $N$  sites

$$P(N) \sim 4^N$$

To solve large systems, Exploit all possible symmetries:

Hubbard model derived from a general nonrelativistic Hamiltonian

$$H_{\text{tot}} = \sum_{ij\sigma} f_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{1}{2} \sum_{ijkl} \sum_{\sigma\tau} \langle ij|g|kl \rangle a_{i\sigma}^\dagger a_{j\sigma} a_{k\tau}^\dagger a_{l\tau}$$

$$H_{\text{Hub.}} \text{ for } t_{i,j\pm 1} = f_{ij} \delta_{i,j\pm 1}$$

$$\epsilon_i = f_{ii} \delta_{ii}$$

$$U = \langle ij|g|kl \rangle \delta_{ij} \delta_{kl} \delta_{jk}$$

Extended Hubbard Model if  $\delta_{jk}$  is relaxed.  
Conserves  $S_z$  and  $S_{\text{tot}}^2$ .

To exploit the invariance

$$[H, S_{\text{tot}}^2] = [H, S_{\text{tot}}^2] = 0,$$

use as basis functions, simultaneous eigenstates of  $S_{\text{tot}}^2$  &  $S_{\text{tot}}^z$ .

Slater Determinantal basis ( $|SD\rangle$ ) trivially exploits  $S_{\text{tot}}^2$  invariance

i.e.

$$S_{\text{tot}}^2 |SD\rangle = M_{\text{tot.}} |SD\rangle$$

But total spin invariance is not exploited in general, i.e.

$$S_{\text{tot.}}^2 |SD\rangle \neq S_{\text{tot.}}(S_{\text{tot.}}+1) |SD\rangle$$

Advantages in exploiting total spin invariance

- Smaller basis sets
- Straight forward spin labelling of states

This has been a major preoccupation of quantum chemists for several decades.

<sup>144</sup>  
Dimension of Complete subspaces with  $S=0(\gamma_2)$  for even (odd) number  $N_e$  of electrons on  $N$  sites

| <u><math>N_e/N</math></u> | <u>Dimension (<math>S</math>)</u> | <u>Dimension (<math>S_z</math>)</u> |
|---------------------------|-----------------------------------|-------------------------------------|
| 6/6                       | 175 ( $S=0$ )                     | 400 ( $S_z=0$ )                     |
| 8/8                       | 1,764 ("")                        | 4,900 ("")                          |
| 10/10                     | 19,404 ("")                       | 63,504 ("")                         |
| 12/12                     | 226,512 ("")                      | 853,776 ("")                        |
| 14/14                     | 2,760,615 ("")                    | 11,778,624 ("")                     |
| 7/7                       | 784 ( $S=\gamma_2$ )              | 1,225 ( $S_z=\gamma_2$ )            |
| 9/9                       | 8,820 ("")                        | 15,786 ("")                         |
| 11/11                     | 104,544 ("")                      | 213,444 ("")                        |

Dimension of  $S=0$  and  $S_z=0$  separate subspaces

| <u><math>N</math></u> | <u>Dimension (<math>S=0</math>)</u> | <u>Dimension (<math>S_z=0</math>)</u> |
|-----------------------|-------------------------------------|---------------------------------------|
| 14                    | 429                                 | 3,432                                 |
| 16                    | 1,430                               | 12,870                                |
| 18                    | 4,862                               | 48,620                                |
| 20                    | 16,796                              | 184,756                               |
| 22                    | 58,786                              | 705,432                               |
| 24                    | 208,012                             | 2,704,156                             |

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Methods for constructing spin adapted functions:

- (i) Direct diagonalization of  $S^2$  in Slater Determinantal basis
- (ii) Use of Projection Operators  $[S^2 - S(S+1)]$
- (iii) Branching diagram technique of van Vleck & Sherman (based on symmetric groups and Young Tableau)
- (iv) Unitary Group Approach - Gelfand patterns and Paldus arrays.
- (v) Pauling's explicit spin pairing technique and VB diagrams.

The VB approach is simplest and most physical.

In this approach a VB diagram of a given spin  $S$ , with  $N_e$  electrons on  $N$  orbitals will consist of an arrow passing through 25 vertices, crosses at  $m$  vertices, and  $p$  lines, with each line connecting 2 vertices, such that

$$N_e = 2S + 2m + p$$

The number of vertices are equal to the No. of Orbitals  $N$ . For odd  $N_e$  a "phantom" orbital is introduced that always participates in a line. This orbital is reckoned only in the diagrams but does not appear in the Hamiltonian.

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A line between vertices  $q$  and  $q'$  represents

$$\overbrace{q \quad q'} = \frac{1}{\sqrt{2}} (a_{q\alpha}^\dagger a_{q'\beta}^\dagger - a_{q\beta}^\dagger a_{q'\alpha}^\dagger) |0\rangle$$

A cross at a vertex  $q$  represents

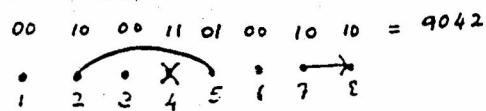
$$\times_q \equiv a_{q\alpha}^\dagger a_{q\beta}^\dagger |0\rangle$$

(Phase convention  $\alpha$  to the left has +ve coefficient).

An arrow through sites  $q_1 q_2 \dots q_{25}$  represents

$$\overrightarrow{q_1 \quad q_2 \dots \quad q_{25}} \equiv a_{q_1\alpha}^\dagger a_{q_2\alpha}^\dagger \dots a_{q_{25}\alpha}^\dagger |0\rangle, q_1 < q_2 < \dots < q_{25}$$

A typical VB diagram for  $S=1$ ,  $N_e=6$ ,  $N=8$  would look like



and will represent

$$a_{7\alpha}^\dagger a_{8\alpha}^\dagger \frac{(a_{2\alpha}^\dagger a_{5\beta}^\dagger - a_{2\beta}^\dagger a_{5\alpha}^\dagger)}{\sqrt{2}} a_{4\alpha}^\dagger a_{4\beta}^\dagger |0\rangle$$

The total Number of linearly independent diagrams is given by the Weyl formula

$$P_S = \frac{2S+1}{N+1} \left( \frac{N+1}{2} - S \right) \left( N - \frac{N_e}{2} - S \right)$$

For  $S=0$ , Rumer rule states that the set of diagrams with noncrossing lines (when the orbitals are arranged on the vertices of a polygon) forms a complete and linearly independent set. This is because

$$\begin{array}{c} 4 \\ \diagup \quad \diagdown \\ 1 \quad 2 \end{array} = - \begin{array}{c} 4 \quad 3 \\ \diagup \quad \diagdown \\ 1 \quad 2 \end{array} - \begin{array}{c} 4 \quad 3 \\ | \quad | \\ 1 \quad 2 \end{array}$$

For  $S \neq 0$ , a second condition, that an arrow should not be enclosed by a line, is also necessary, because

$$\overbrace{\begin{array}{c} \rightarrow \rightarrow \\ 1 \quad 2 \quad 3 \quad 4 \end{array}} = \begin{array}{c} \rightarrow \rightarrow \\ 1 \quad 2 \quad 3 \quad 4 \end{array} + \begin{array}{c} \rightarrow \rightarrow \\ 1 \quad 2 \quad 2 \quad 4 \end{array} + \overbrace{\begin{array}{c} \rightarrow \rightarrow \\ 1 \quad 2 \quad 3 \quad 4 \end{array}}$$

Using these rules, it is possible to write down the complete set of linearly independent VB diagrams for any  $N$ ,  $N_e$  and  $S$ .

This is done very simply on a computer by assigning 2 bits to each orbital. The state '00'  $\rightarrow$  empty orbital; '11'  $\rightarrow$  doubly occ. (x) '10'  $\rightarrow$  beginning of a line or part of an arrow & '01'  $\rightarrow$  end of a line. With extended Rumer rules, each VB diagram is represented by a  $2N$  bit integer, uniquely and generated as an increasing sequence of integers, by simple bit manipulations.

Method of generating VB diagrams on a computer.

Start with the lowest integer that represents the VB diagram of the given system.  
e.g. 6e/10 sites,  $S=1$

Needs 20 bits

Start with

00 00 00 00 00 00 10 10 11 11

6 - '1' bits for 6 electrons

20 bits in the integer. (All higher bits set to '0' for convenience)

Next higher integer with same # of '1' bits is

00 00 00 00 00 00 10110111

A singlet not a triplet so reject

Next higher integer

00 00 00 00 00 00 10 11 10 11

'Legal' Triplet VB diagram.

Continue process until no higher integer can be created.

### Adaption of Spatial Symmetries

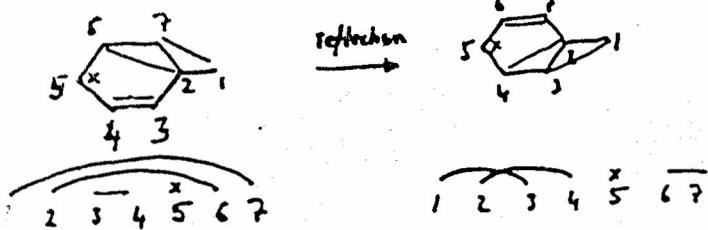
Spatial symmetries whose operations do not lead to crossing diagrams can be easily adopted

$$\hat{R}|i\rangle = |j\rangle$$

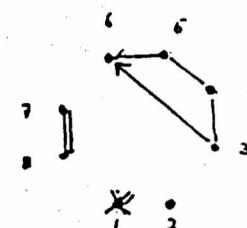
$$\Psi_T = \sum_R \chi_p(\hat{R}) \hat{R}|i\rangle$$

In the event of crossing diagrams Abelian groups do not in general present difficulties

Symmetry adaption for nonabelian groups underway. Involves uncrossing crossed or "illegal" VB diagrams to obtain a combination of uncrossed or "legal" diagrams.



The VB basis, although linearly independent is nonorthogonal. The overlap integral  $S_{ij}$  between two VB states of the same spin is nonzero, if (i) The distribution of electrons in the orbitals in both  $|i\rangle$  and  $|j\rangle$  are identical and (ii) the arrows in  $|i\rangle$  and  $|j\rangle$  fall in the same 'island'. The 'island' counting rule of Pauling is easily generalized to obtain the



sign and magnitude of the overlap integral.

To set up the H matrix, we define the operator

$$(i,j) \equiv [a_{id}^+ a_{jd} + a_{ip}^+ a_{jp}]$$

The operators  $(i,j)$  satisfy the commutation relation

$$(i,j) = [(i,k), (k,j)]_-$$

so that we need know the action of  $(i,i+1)$  on a VB diagram to be able to set up the Hamiltonian matrix.

Action of  $(i, i+1)$  on a VB state

$$\begin{array}{ll}
 \text{b} & \begin{array}{c} i \\ \downarrow \\ i+1 \\ \times \end{array} \\
 \cdot & \begin{array}{c} \text{coeff. } \frac{1}{\sqrt{2}} \\ \rightarrow \\ +\sqrt{2} \end{array} \\
 \hline
 \text{---} & \begin{array}{c} i \\ \downarrow \\ i+1 \\ \times \end{array} \\
 \cdot & \begin{array}{c} \text{---} \\ \rightarrow \\ +1 \end{array} \\
 \hline
 \text{---} & \begin{array}{c} i \\ \downarrow \\ i+1 \\ \times \end{array} \\
 \text{---} & \begin{array}{c} -1 \\ \rightarrow \\ -\frac{1}{\sqrt{2}} \end{array} \\
 \hline
 \rightarrow & \begin{array}{c} \text{---} \\ \rightarrow \\ 0 \end{array}
 \end{array}$$

[Arrows and lines behave identically but for the last exception].

With the help of the commutation relations and the above rules, we can compute the result of a general nonrelativistic many electron Hamiltonian

$$H = \sum_{ij} \langle i | f | j \rangle \langle i, j \rangle + \frac{1}{2} \sum_{ijkl} \left\langle \langle ij | \frac{e^2}{r_{ij}} | kl \rangle \right\rangle [ \langle i, k \rangle \langle j, l \rangle - \delta_{jk} \langle i, l \rangle ]$$

The matrix representation  $h$  of the Hamiltonian  $H$  is obtained as

$$H |k\rangle = \sum_j h_{kj} |j\rangle$$

where  $|k\rangle$  and  $|j\rangle$  are VB states. Ordered integer sequence of diagrams speeds up generation of  $h_{kj}$ .

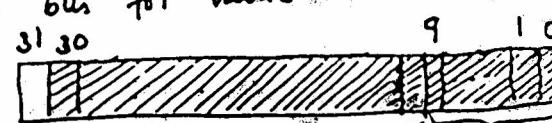
Sparse matrix storage:

- No. of Unique nonzero elements usually small.
- Waste of storage & CPU in doing arithmetic with zeroes.
- Efficient packing as follows:

In a given row store the column index of the nonzero element in increasing order.

No. of columns  $\sim 10^6$ . So 21 bits for column address.

No. of Unique nonzero elements  $\leq 10^3$   
10 bits for value



column address      matrix element.

- Store the element # with which the first element in a row appears

Total storage required

$$\sim (N + R) \times 4 \text{ Bytes}$$

N-dimensionality of matrix  
R - No. of nonzero matrix elements.

In model systems of finite size the matrix  $h$  is an exact representation of the model Hamiltonian since the VB basis is complete & finite.

$h$  is a real non-symmetric matrix since the VB basis is non-orthogonal.

$h$  is a sparse matrix as with any CI methods Symmetric representation of  $H$  can be obtained as

$$h_{\text{symm.}} = hS \quad \text{with}$$

$$h_{\text{symm.}} \in = E S \in$$

as the eigen value equation. We avoid this step and work directly with  $h$ . Eigen values & Eigen functions are obtained by Rettig's algorithm, for the low-lying states.

Start with  $m$  orthonormal vectors  $\vec{Q}_i$

Set up matrix  $A^{(m)}$ :  $a_{ij} = (\vec{Q}_i, h \vec{Q}_j)$

Obtain  $e_j^{(m)}$  and  $\vec{C}_j^{(m)}$  ( $j=1$  is g.s.) where

$$A^{(m)} \vec{C}_j^{(m)} = e_j^{(m)} \vec{C}_j^{(m)}$$

Get the difference vector

$$\vec{R}_j^{(m)} = (h - e_j^{(m)} I) \vec{C}_j^{(m)}$$

and the correction vector  $W_j^{(m)}$

$$W_j^{(m)}(i) = R_j^{(m)}(i) / (e_j^{(m)} - h_{ii})$$

Augment the orthonormal set  $\{\vec{Q}_i\}$  by adding

$$\vec{Q}_{m+1} = \vec{Q}'_{m+1} / \| \vec{Q}'_{m+1} \| \quad \text{where}$$

$$\vec{Q}'_{m+1} = \vec{w}_q^{(m)} - \sum_{k=1}^m (W_q^{(m)}, \vec{Q}_k) \vec{Q}_k$$

This process is iterated until a stable  $\vec{Q}_q$  is obtained. The process converges rapidly, usually about 30 iterations may be required, for satisfactory convergence.

### Matrix elements between VB Eigen States

Besides energy, there are many other quantities of interest Eg., Transition dipoles, spin densities, bond orders, charge densities, spin-spin correlations, charge correlations, polarizabilities etc.

VB basis is non-orthogonal. Appears cumbersome to even normalize eigen states of say  $N=14$ ,  $N_e=14$ ,  $S=0$  case.

However 2 VB diagrams with same  $N, N_e, S \& S_z$  are orthogonal if the charge distribution among the orbitals in the two diagrams are not identical

$$\text{i.e., } \langle - | \cdot \times \rangle = 0$$

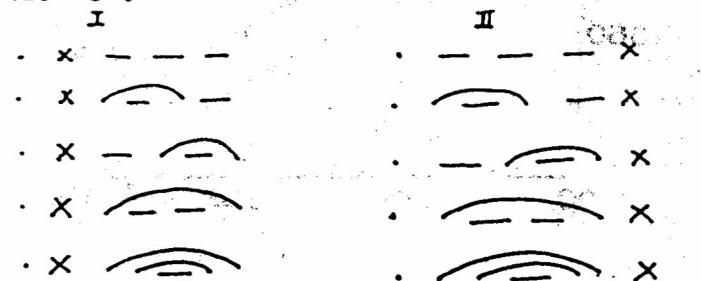
$\Rightarrow$  VB basis can be rearranged to have a block-diagonal structure of the overlap matrix. Rule - start with a given charge distribution, exhaust all possible pairings before moving to next charge distribution.

Eg.  $N = N_e = 6$ ;  $S=0$

- (i) Exhaust all covalent diagrams
- (ii) Consider a specific singly ionic case, exhaust the 2 diagrams
- (iii) move the charges and in each case exhaust the 2 diagrams in the same order of connectivity
- (iv) repeat (ii) & (iii) for doubly ionic and triply ionic diagrams.

For a given ionicity, repeating diagrams in the same order of connectivity for two different charge distributions ensures overlap blocks of same size are identical. Consider the

two sets



For this arrangement

$$S_{ij}^I = S_{ij}^{II} \quad \text{for all } i, j$$

By virtue of (iii) overlap matrix need be calculated only once for a block of a given size.

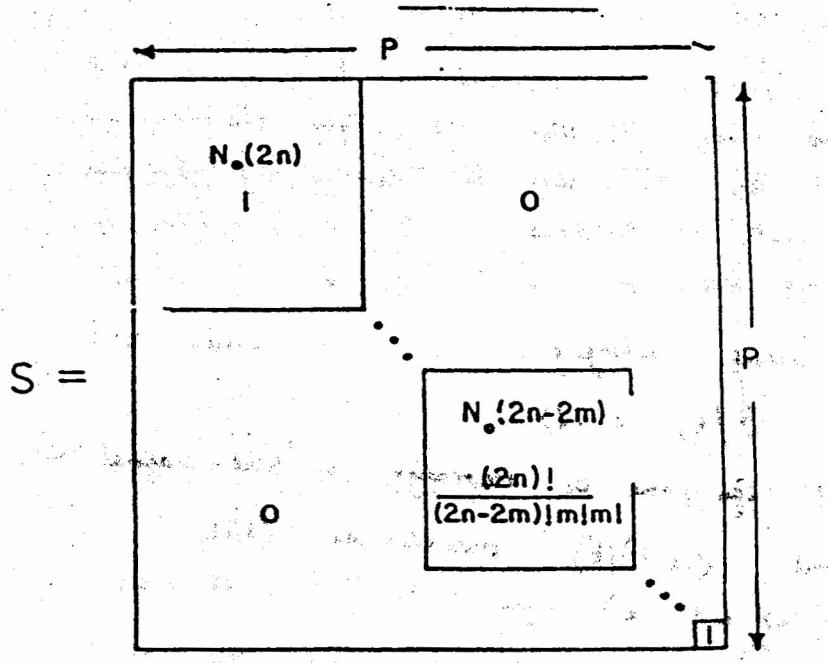


FIG.3. Block diagonal structure of overlap matrix arising from the charge orthogonality of VB diagrams.

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The eigen state can be easily transformed from 'discreet integer' basis to 'block-diagonal' basis, via a 'correspondence' vector.

Calculation of matrix elements of operators that are diagonal in VB basis is now straight forward. Eg. transition dipoles,  $P_{ij}$ ,  $P_i P_j$  etc.

Operators not diagonal in VB basis can be of two kinds (i) those that scramble charges and (ii) those that alter the spin pairing say from singlets to triplets. Eg. of (i) operators for bond orders and of (ii) site spin operator  $s_i^z$ .

Operators belonging to (i) can be handled easily

$$\hat{O}|k\rangle = |l\rangle$$

$|l\rangle$  can now be rearranged in 'block-diagonal' basis and  $\langle k'| \hat{O} | k \rangle$  evaluated as  $\langle k' | l \rangle$ .

[ $|k\rangle$  and  $|l\rangle$  eigen states of  $\hat{H}$  in VB basis]

Operators of class (ii) need developing new techniques for instance ..

$\langle k' | s_i^z s_j^z | k \rangle$  between singlet eigenstates can be evaluated as triplet overlap integrals since

$$s_i^z |i\rangle = -|i\rangle$$

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### Test of finite size calculations

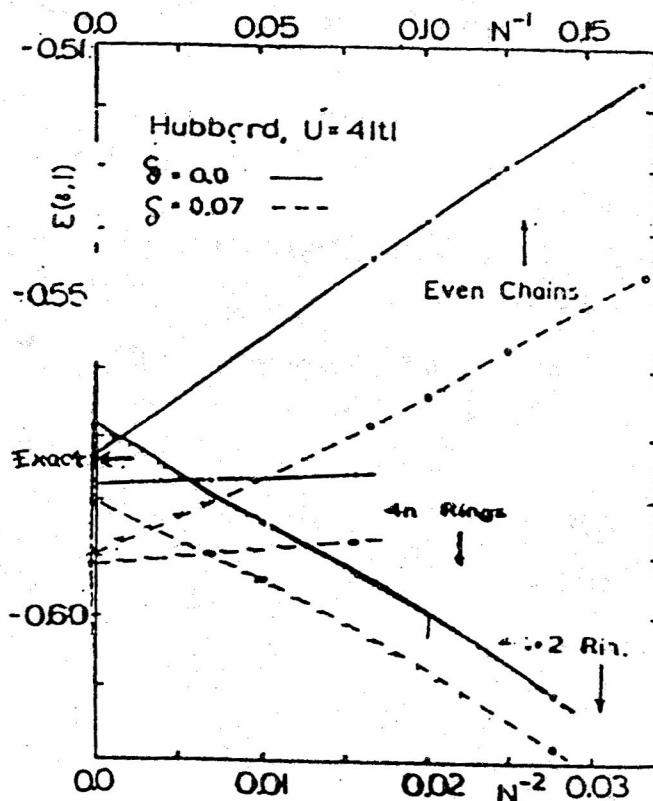


FIG. 2. Ground-state energy per site  $\epsilon$  in units of  $|t|$  vs  $N^{-1}$  for chains and  $N^{-2}$  for rings in regular ( $\delta=0.0$ ) and alternating ( $\delta=0.07$ ) Hubbard models with  $U=4|t|$ ; the exact  $\delta=0.0$  result is from Ref. 7.

Exact =  $-0.57373$       Extrapolated =  $-0.573 \pm 0.005$

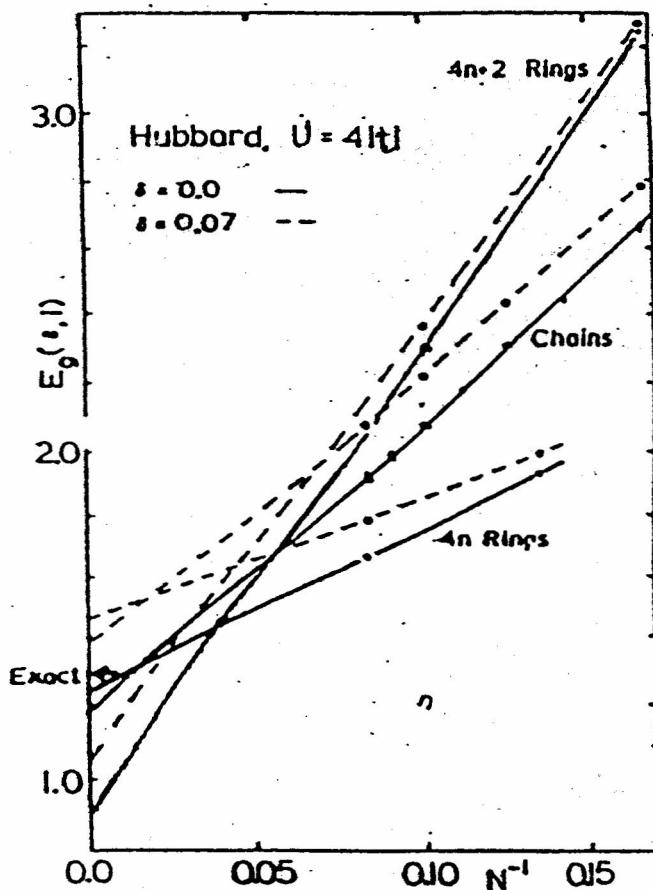


FIG. 3. Optical gap  $E_g$  in units of  $|t|$  vs  $N^{-1}$  for regular and alternating Hubbard models with  $U=4|t|$ ; the exact  $\delta=0.0$  result is from Ref. 17.

Note : Increase in  $E_g$  due to bond alternation is very little. The gap is predominantly due to correlations.

$$\delta=0 \quad \text{exact } 1.2867 \quad E_g \text{ extrapolated } 1.20 \pm 0.10$$

### Effect of Correlations on Periodic Dimerization

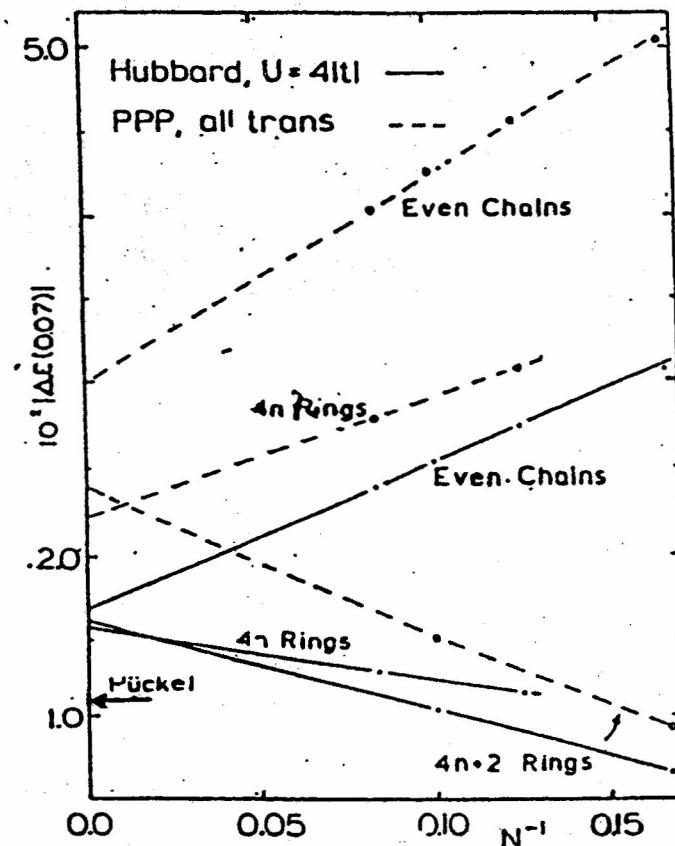


FIG. 4. Electronic energy gain per site,  $|\Delta E|/|t|$  vs  $N^{-1}$  for alternating  $\delta=0.07$  in  $U=4|t|$  Hubbard models and in PPP models with standard molecular parameters; the exact Hückel result is given by Eqs. (18) and (14).

### Optical gap in polyenes

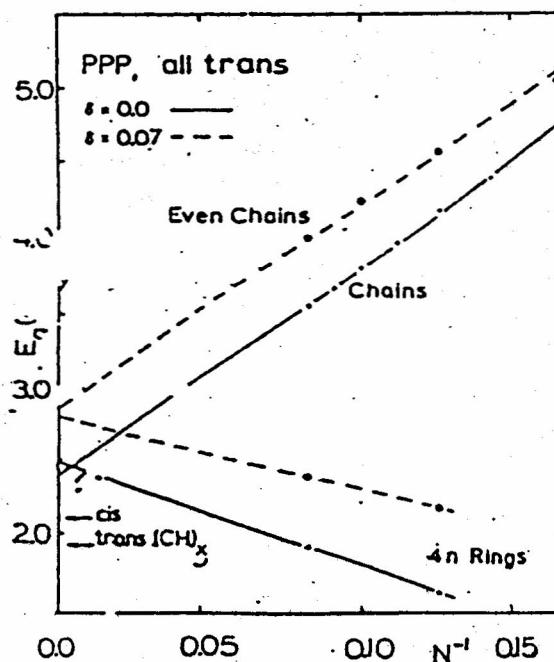


FIG. 7. Optical gap  $E_g$  vs  $N^{-1}$  of regular and alternating PPP model with molecular correlations.

$\delta=0.0$  Extrapolated gap  $2.4 \pm 0.2$

$\delta=0.07$  Extrapolated gap  $2.8 \pm 0.2$

Exptl: all trans  $(CH)_x \sim 1.8$

### Optical gaps in charged and neutral solitons and cyanine Dyes

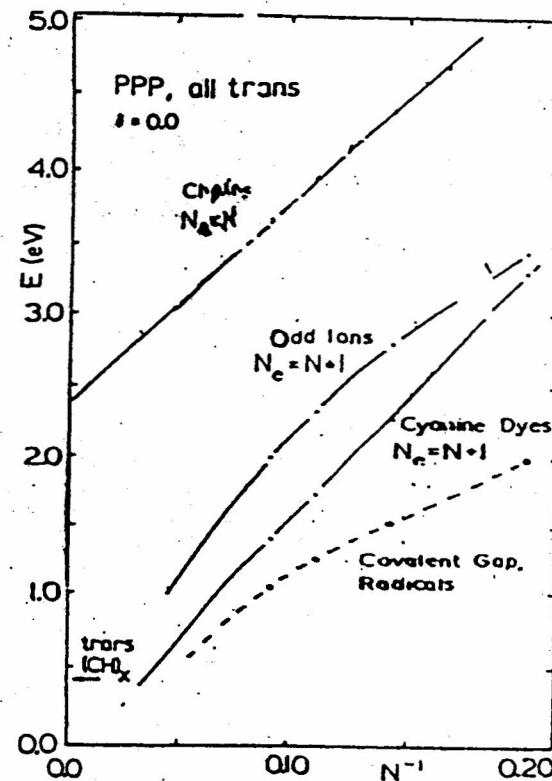


FIG. 8. Optical gaps vs  $N^{-1}$  of regular PPP chains with molecular correlations, ions of odd segments representing charged solitons and linear cyanine dyes; the covalent gap of radicals is dipole forbidden.

Singlet-Triplet and Singlet-Singlet gaps in a system with two sectors, are function of distance of separation between sectors.

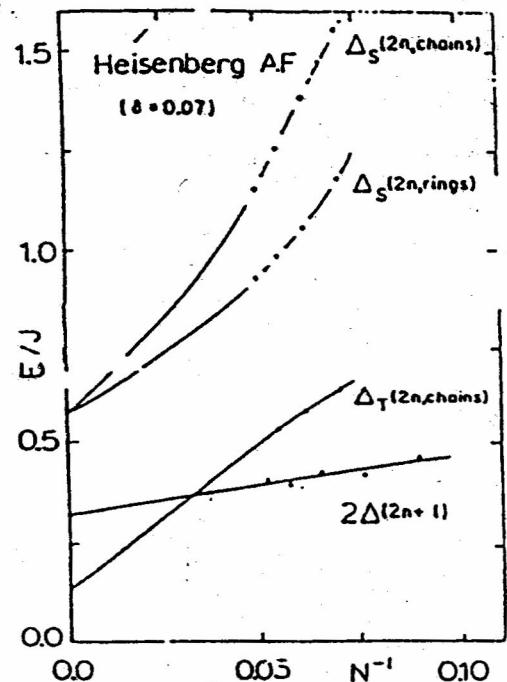
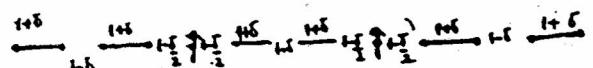


FIG. 3. Excitations of alternating Heisenberg anti-ferromagnets:  $\Delta_T(2n)$  and  $\Delta_S(2n)$  are triplet and singlet excitations with two domain walls indicated in Fig. 1(b); least-square extrapolations of  $\Delta_S$  are constrained to coincide at  $N = \infty$ . The "midgap" excitation energy  $\Delta(2n+1, \delta)$  of odd chains is given by (5).



$$\Delta(2n+1) = {}^2E_0(2n+1, \delta) - [{}^1E_0(2n, \delta) + {}^1E_0(2n+2, \delta)]/2$$

### Dynamic Response of Extended Hubbard Systems

Perturbation expressions for  $\alpha_{ij}$ ,  $\beta_{ijk}$  &  $\gamma_{ijkl}$

Simplest cases  $i=j=k=l$ . These expressions have been known for a very long time

$$\alpha_{xx}(\omega) = \sum_Q \frac{\langle G/\mu_x | Q \rangle \langle Q | \mu_x | G \rangle E_Q}{2(E_Q^2 - \hbar^2 \omega^2)} \quad (6)$$

$$\beta_{xxx}(\omega_r, \omega_s) = \frac{1}{8\hbar^2} \sum_{SR} \langle G/\mu_x | R \rangle \langle R | \mu_x | S \rangle \langle S | \mu_x | G \rangle$$

$$x \left[ \frac{1}{(\omega_R - \omega_1 - \omega_2)(\omega_S - \omega_2)} + \frac{1}{(\omega_R + \omega_1)(\omega_S - \omega_2)} \right. \\ \left. + \frac{1}{(\omega_R - \omega_2)(\omega_S - \omega_1)} + \text{3 more terms} \right] \quad (7)$$

$$\gamma_{xxx}(\omega_r, \omega_s, \omega_t) = \frac{1}{8\hbar^3} \sum_{RST} \langle G/\mu_x | R \rangle \langle R | \mu_x | S \rangle \langle S | \mu_x | T \rangle \langle T | \mu_x | G \rangle$$

$$x \left[ \frac{1}{(E_R - 3\omega)(E_S - 2\omega)(E_T - \omega)} + \frac{1}{(E_R + 3\omega)(E_S + 2\omega)(E_T + \omega)} \right. \\ \left. + \frac{1}{(E_R - \omega)(E_S - 2\omega)(E_T - \omega)} + \frac{1}{(E_R - \omega)(E_S + 2\omega)(E_T + \omega)} \right]$$

Evaluation of  $\alpha_{xx} \rightarrow$  One sum

$\beta_{xxx} \rightarrow$  Two sums

$\gamma_{xxx} \rightarrow$  Three sums

(25)

### Approaches to evaluating polarizabilities

- (i) Truncation of infinite or large sums to finite sums.
- (ii) finite level - systems, such as T.L.S. etc.
- (iii) Obtaining these as derivatives of corrections to  $E$  in the presence of applied fields (static) - (a) finite field method  
(b) density functional method
- (iv) via calculation of perturbed wave fn. using a variational approximation to it.

Mostly dealing with non-interacting systems or interacting systems in a mean field approx.

### Correlated Model Systems : Relevance to Organics

- (i) Observation of  $2^1\text{Ag}$  state in pheno below  $E_g$
- (ii) Qualitatively different extrapolations of  $E_g$  in finite polymers and cyanine dyes
- (iii) Observation of negative spin densities in Radicals of polymers
- (iv) Lower than expected oscillator strength for dipole transitions  
PPF or Extended Hubbard Model

Approximate closed form solutions only for non-interacting models.

For interacting models, usually sum over states approach. For  $\beta$  there exist a few variational approach calculations.

Our approach - calculate functions such as  $\phi_i^{(k)}(\omega_i)$ ,  $\phi_{ij}^{(k)}(\omega_2, \omega_1)$  exactly where  $\phi_i^{(V)}(\omega_i)$  is defined as

$$(H - E_G + i\omega_1) \phi_i^{(V)}(\omega_1) = - \tilde{\mu}_i \phi_G \quad (9)$$

$$\text{and } (H - E_G + i\omega_2) \phi_{ij}^{(V)}(\omega_2, \omega_1) = - \tilde{\mu}_j \phi_i^{(V)}(\omega_1) \quad (10)$$

$$\tilde{\mu} = \vec{\mu} - \vec{\mu}_G.$$

$$\phi_i^{(V)}(\omega_1) = - \sum_R \frac{\langle R | \tilde{\mu}_i | G \rangle}{E_R + i\omega_1} |R\rangle \quad (11)$$

and

$$\phi_{ij}^{(R)}(\omega_2, \omega_1) = \sum_R \sum_S \frac{\langle G | \tilde{\mu}_i | R \rangle \langle R | \tilde{\mu}_j | S \rangle}{(E_R + i\omega_1)(E_S + i\omega_2)} |S\rangle \quad (12)$$

If we can solve for  $\phi_i^{(V)}(\omega_i)$ , we can write

$$\alpha_{ij}(\omega) = [\langle G | \tilde{\mu}_i | \phi_j^{(V)}(\omega) \rangle + \langle G | \tilde{\mu}_i | \phi_j^{(R)}(\omega) \rangle] / 4 \quad (13)$$

Eqn. (13) is exact, i.e. it includes sum over all excited states.

Static polarizability is given by

$$\alpha_{ij}(0) = \langle G | \tilde{\mu}_i | \phi_j^{(0)}(0) \rangle / 2$$

Similarly

$$\begin{aligned} \beta_{XXX}(0,0,0) &= [\langle \tilde{\phi}_x^{(1)}(-\omega_1, -\omega_2) | \tilde{\mu}_x | \phi_x^{(1)}(-\omega_3) \rangle \\ &\quad + \langle \phi_x^{(1)}(\omega_1, \omega_2) | \tilde{\mu}_x | \phi_x^{(1)}(\omega_3) \rangle] / 8 \quad (15) \end{aligned}$$

and

$$\begin{aligned} \gamma_{XXXX}(0,0,0,0) &= \frac{1}{8} [\langle \tilde{\phi}_x^{(1)}(-3\omega) | \tilde{\mu}_x | \phi_x^{(1)}(-2\omega, -\omega) \rangle \\ &\quad + \langle \phi_{xx}^{(4)}(2\omega, \omega) | \tilde{\mu}_x | \phi_x^{(1)}(-\omega) \rangle + \omega \rightarrow -\omega] \quad (16) \end{aligned}$$

Similar expressions can be derived for any general coefficient.

Formal expressions such as (14) to (16) have existed in literature for quite some time. These expressions are for nonresonant hyper polarizability.

Static hyper polarizabilities can also be expressed in a form similar to (4) e.g.

$$\begin{aligned} \gamma_{XXXX}(0,0,0) &= \frac{1}{6} \left[ + \langle \tilde{\phi}_{xx}^{(2)}(\omega, 0) | \tilde{\mu}_x | \phi_x^{(0)}(0) \rangle - \langle \tilde{\phi}_{xx}^{(1)}(2\omega, 0) | \tilde{\mu}_x | \phi_x^{(0)}(0) \rangle \right. \\ &\quad \left. - \langle \phi_x^{(0)}(0) | \tilde{\mu}_x | \zeta \rangle \langle \phi_x^{(1)}(0) | \phi_x^{(0)}(0) \rangle + \omega \rightarrow -\omega \right] \quad (17) \end{aligned}$$

Evaluation of  $\phi_i^{(1)}(\omega)$  and  $\phi_{ij}^{(1)}(\omega_2, \omega_1)$ .

- Expand  $\phi_i^{(1)}(\omega)$  as a linear combination of symmetry adopted valence bond (VB) functions.

$$\phi_x^{(1)}(\omega_1) = \sum_j c_{xj} | j \rangle \quad (18)$$

$$\text{We know } H | j \rangle = \sum_k h_{jk} | k \rangle \quad (19)$$

Therefore

$$(H - E_G + \hbar\omega_1) \phi_x^{(1)}(\omega_1)$$

$$= \sum_j c_{xj} \left( \sum_k h_{jk} - E_G + \hbar\omega_1 \right) | k \rangle$$

$$= - \sum_k d_{Gk} \tilde{\mu}_x | k \rangle = - \sum_k d_{Gk} \mu_{Xk} | k \rangle \quad (20)$$

Since the VB basis is complete & linearly indep., we can equate coefficients of  $| k \rangle$  on either side to obtain

$$\sum_j h_{jk} c_{xj} + (\hbar\omega_1 - E_G) c_{Xk} = - \mu_{Xk} d_{Gk}, \quad (21)$$

for every  $k$ .

We can derive a similar equation for  $\phi_{ij}^{(1)}(\omega_1, \omega_2)$ .

Numerical solution of  $\phi_i^{(1)}(\omega_1)$  &  $\phi_{ij}^{(2)}(\omega_2, \bar{\omega}_1)$

for  $\hbar\omega > 0$ , eqn. (21) can be solved by Gauss-Seidel iteration scheme.

However, for  $\hbar\omega_2 < 0$ , in the solution of  $\phi_{ij}^{(2)}(\omega_2, \omega_1)$  Gauss-Seidel iteration scheme bombs. We use a conjugate-gradient technique [ $|Ax - b|^2$  is minimized w.r.t.  $x$ ]

This is a very slow process and currently the most time consuming step.

#### Checks on the procedures:

The coefficients  $a_{il}$  in  $\phi_i^{(1)}$  can be directly evaluated as

$$\langle \phi_i^{(1)} | \phi_l^{(0)} \rangle \text{ as well as } \quad (22)$$

$$\langle \phi_G | \tilde{\mu}_l | \phi_l^{(0)} \rangle / (E_G - E_l)$$

for small values of  $l$   $\phi_l^{(0)}$  can be obtained using Rethrop Algorithm with 'dial-back' feature.

Small matrix algorithm for Large linear systems

$$Ax = b, \quad A \text{ is a } N \times N \text{ matrix}$$

Gauss-Seidel fails if  $A$  is nondefinite.

But Gauss-Seidel of

$$A^T A x = A^T b$$

converges, although very slowly, since  $A^T A$  is ~~nondef.~~

Gauss-Seidel on  $A^T A x = A^T b$  is equivalent to minimization of  $|Ax - b|^2$  by successively relaxing components of ~~the~~  $x$ .

In small matrix algorithm, start with an-space {Q<sub>i</sub>},  $n \ll N$ . Assume

$$x^{(0)} = \sum_{i=1}^n c_i^{(0)} Q_i, \quad Q_i \text{'s are } N \text{-vectors.}$$

Determine  $c_i$ 's by inverting  $\tilde{A}$  in the eqn.  $\tilde{A} c^{(0)} = \tilde{b}$ ,  $\tilde{A}_{ij} = (Q_i, A Q_j)$ ,  $\tilde{b}_i = (Q_i, b)$

From  $c^{(0)}$ , we have  $x^{(0)}$ , use  $x^{(0)}$  and obtain the correction vector  $\alpha$  from Jacobi relaxation on  $A^T A x = A^T b$

$$\alpha_i = \left( \sum_{k=1}^N r_k^{(0)} a_{ki} \right) / \left( \sum_{k=1}^N a_{ki} \alpha_{ki} \right)$$

$$\text{where } r^{(0)} = Ax^{(0)} - b$$

$$\text{Obtain } Q_{n+1} = [x - \sum_{i=1}^n (\alpha, Q_i) Q_i] / \| \dots \|$$

Construct  $\tilde{A}^{(0)} [(a_{n+1}) x(n+1)]$  obtain  $x^{(0)}$  & so on until  $|r_k^{(k)}| < \epsilon$  for all  $k=1, 2, \dots, N$

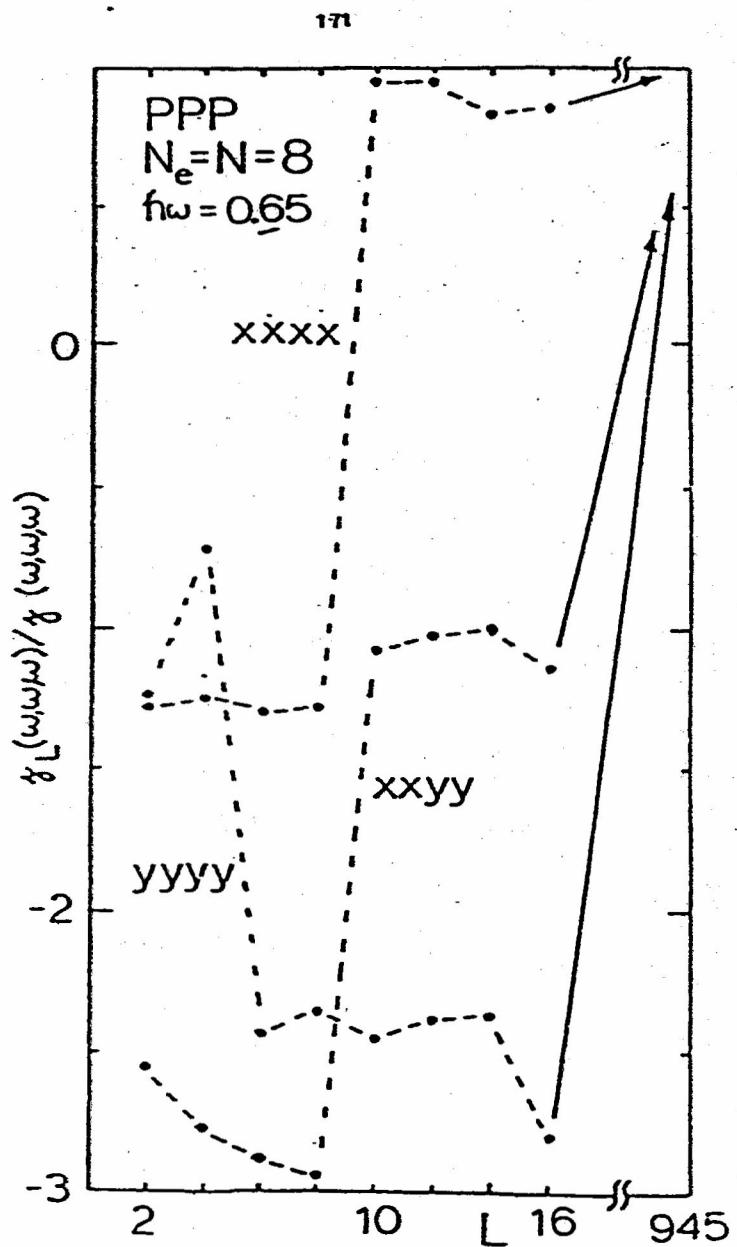


Fig. 1. Self-consistent variational basis approach to ground state energies

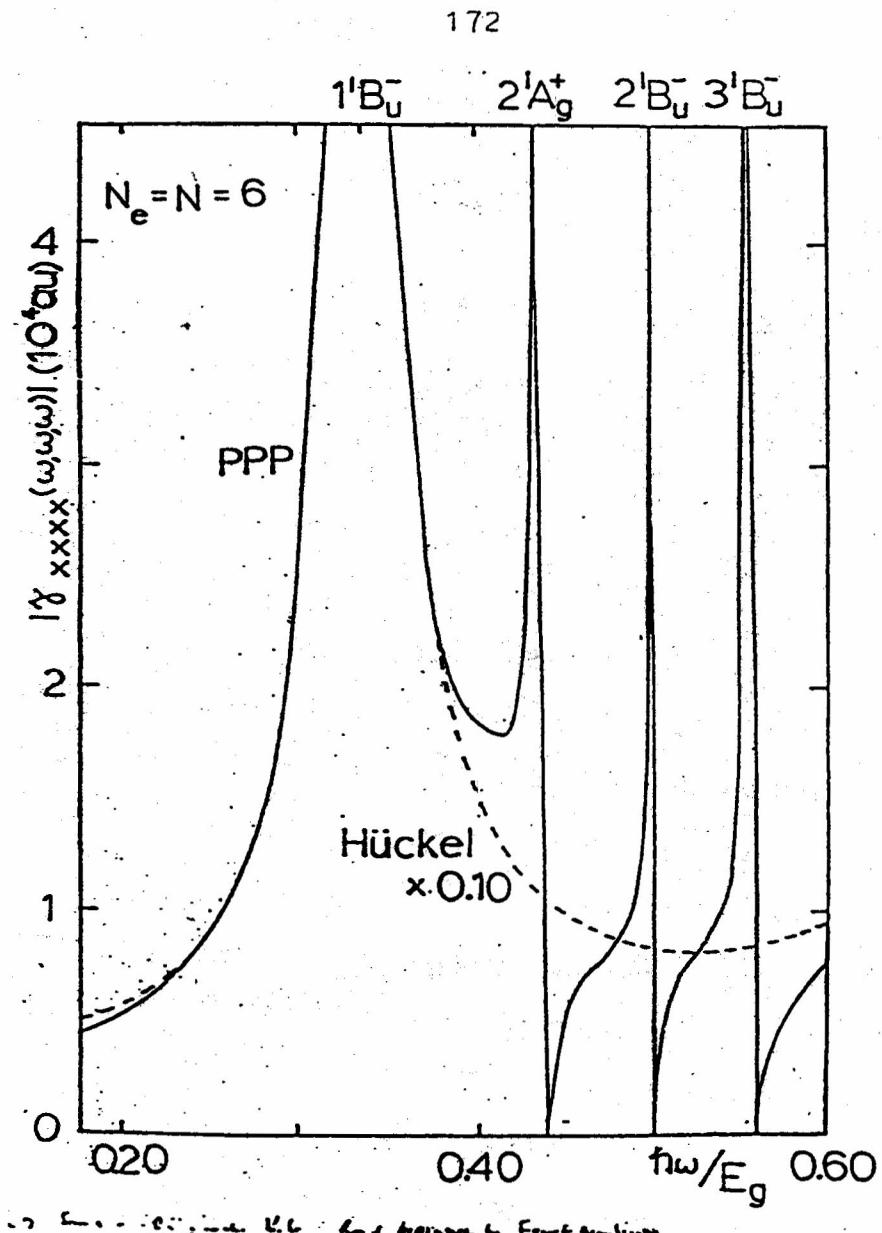


Fig. 2. Self-consistent variational basis approach to excited states

For small problems  $\phi_i^{(0)}(\omega_i)$  and  $\phi_{i;j}^{(2)}(\omega_i, \omega_j)$  can be calculated as sums over transition matrix elements by energy denominator.

These can be checked against  $\phi_i^{(0)}(\omega_i)$  and  $\phi_{i;j}^{(2)}(\omega_2, \omega_1)$  calculated from 'direct' procedure.

### Resonant contributions

Whenever an energy denominator in the S.O.S. expression for  $\alpha$ ,  $\beta$  or  $\gamma$  goes to zero at a specified frequency, we have a resonance. It is unphysical for such quantities as  $\alpha$ ,  $\beta$  or  $\gamma$  to become infinite. If we do perturbation to all orders, this unphysicalness will disappear.

Another practical way of handling resonance is to introduce a broadening parameter  $\Gamma$  which bypasses the singularity.

In  $\gamma$  we have two types of singularities

- (i) A-type corresponding to  $2\omega$  resonance
- (ii) B-type corresponding to  $\omega$  or  $3\omega$  resonance

Pole strength of  $2\omega$  resonances can be expressed as

$$\begin{aligned}\zeta_{2A}^{xxxx} = & [\langle \phi_x^{(0)}(-3\omega) | \mu_x | 2A \rangle \langle 2A | \mu_x | \phi_x^{(0)}(-\omega) \rangle \\ & + \langle \phi_x^{(0)}(-\omega_2) | \mu_x | 2A \rangle \langle 2A | \mu_x | \phi_x^{(0)}(\omega_2) \rangle] / 8\end{aligned}\quad (23)$$

$$\zeta_{1B}^{xxxx} = \langle G | \mu_x | 1B \rangle \langle 1B | \mu_x | \phi_{xx}^{(2)}(-2\omega_1, -\omega_1) \rangle / 8 \quad (24)$$

where

$$\gamma_{xxxx}(\omega, \omega_1, \omega_2) = \frac{C_p}{\omega - \omega_p + i\Gamma_p} + \text{Nonresonant terms} \quad (25)$$

$\Gamma_p$  for an A-type resonance is very small since the transition dipole between  $\langle G \rangle$  and  $|1B\rangle$  states is zero.

For B-type resonance  $\Gamma$  is very large because life-times of B-type states is small since  $\langle G | \mu_x | 1B \rangle$  is not zero by symmetry.

Table 4: Amplitude  $|c_p|/E_g$ , in atomic units, and energies, in ev, of  $\gamma_{xxx}(\nu,\nu,\nu)$ , for three-photon resonances to  $1^1B_u^-$  states and two-photon resonances to  $1^1A_g^+$  states (for PPP models of trans hexatriene and octatetraene;  $E_g$  is the excitation energy to  $1^1B_u$ ).

| N | State(p)   | $\Delta\nu_p$ (ev) | $ c_p /E_g$ ( $10^3$ au) |
|---|------------|--------------------|--------------------------|
| 6 | $1^1B_u$   | 1.6821             | 2.669 (26.03)*           |
|   | $2^1A_g$   | 2.1907             | 0.171 (179.4)            |
|   | $2^1B_u$   | 2.5241             | 0.069                    |
|   | $3^1B_u$   | 2.7999             | 0.144                    |
|   | $3^1A_g^+$ | 3.4971             | 0.640                    |
| 8 | $1^1B_u$   | 1.5203             | 6.652 (150.7)            |
|   | $2^1A_g^+$ | 1.8826             | 0.736 (693.6)            |
|   | $2^1B_u$   | 2.3605             | 0.235                    |
|   | $3^1B_u$   | 2.4965             | 0.465                    |
|   | $3^1A_g^+$ | 2.6687             | 0.039                    |

\* Hückel value

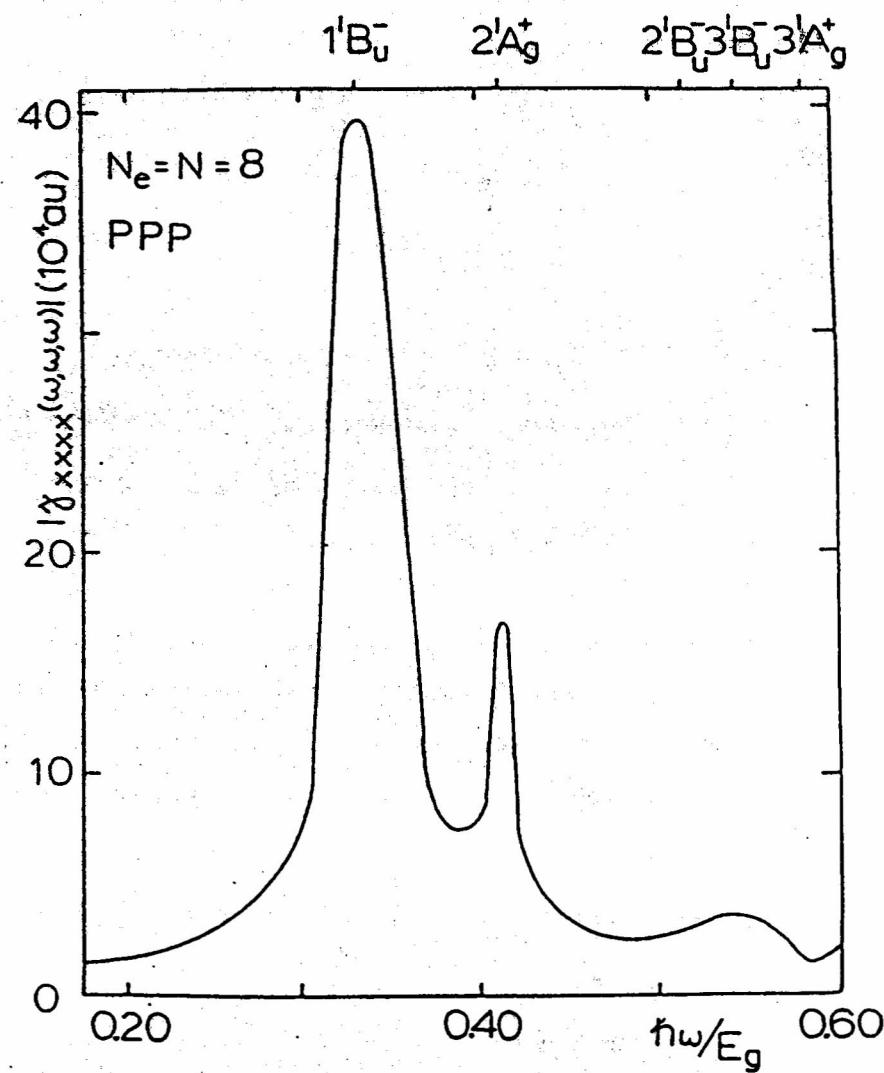


Fig. 5. Three-photon resonance signals from resonance to excited A<sub>1</sub> states.

### Quantum Monte Carlo with Valence Bond Basis

#### 1. Monte Carlo Simulations - Classical Systems

$$Z = \int \exp\{-\beta H(I, P)\} dI dp$$

$$\propto \int \exp\{-\beta V(z)\} dz$$

$$\langle A \rangle = \int A(I, P) e^{-\beta H(I, P)} dI dp \times Z^{-1}$$

Estimated by Importance Sampling Technique

Direct importance sampling requires knowledge of  $Z$ .

We resort to MC estimates since  $Z$  can not be evaluated directly.

Way out of the vicious circle - Devise a Markov chain with limiting probability same as thermodynamic probability. And estimate thermodynamic properties by averaging over states of Markov chain after the chain has attained limiting behaviour.

#### 2. Monte Carlo simulations - Quantum systems.

$$Z = \text{Tr}_n e^{-\beta \hat{H}}$$

$$\hat{H} = \hat{T} + \hat{V}$$

Energy of the system is no longer the sum of individual kinetic and potential energies since  $\hat{t}$  and  $\hat{p}$  do not commute.

$Z$  can be calculated after solving the Schrödinger eqn. as

$$Z = \sum_i e^{-\beta E_i}$$

Often this is not simple and we need to obtain estimates of physical properties without explicitly solving the S.E.

First successful Monte Carlo route to this end was due to Handcomb.

If  $\hat{H}$  can be divided into

$$\hat{H} = \hat{H}_0 + \sum_i \hat{H}_i ; [\hat{H}_0, \hat{H}_i] = 0 \text{ for all } i, \quad -(1)$$

$$\text{then } \langle \hat{F} \rangle = \frac{\text{Tr} \hat{F} e^{-\beta \hat{H}}}{\text{Tr} e^{-\beta \hat{H}}} = \frac{\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{Y_n} f(Y_n) e^{-\beta \hat{H}_0} [\hat{H}_1, \hat{H}_2, \dots, \hat{H}_n]}{\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{Y_n} e^{-\beta \hat{H}_0} [\hat{H}_1, \hat{H}_2, \dots, \hat{H}_n]}$$

$$\equiv \sum_n \sum_{Y_n} f(Y_n) \pi(Y_n)$$

$$f(Y_n) = \frac{\text{Tr}_n \{ \hat{F} e^{-\beta \hat{H}_0} \hat{H}_1, \hat{H}_2, \dots, \hat{H}_n \}}{\text{Tr}_n \{ e^{-\beta \hat{H}_0} \hat{H}_1, \hat{H}_2, \dots, \hat{H}_n \}}$$

$$\pi(Y_n) = A (-\beta)^n \text{Tr} \{ e^{-\beta \hat{H}_0} \hat{H}_1, \hat{H}_2, \dots, \hat{H}_n \}$$

Devise a Markov chain with limiting probability proportional to  $\pi(Y_n)$ . If the traces can be easily evaluated then we have a way of estimating  $\langle \hat{F} \rangle$ . Applied to Heisenberg spin system.

Draw backs with Handscomb's method :-  
Specific to certain types of Hamiltonians  
Laborious to compute traces.

## 3. Trotter Formula

$$\hat{H} = \sum_{i=1}^n \hat{H}_i$$

$$\exp(-\beta \hat{H}) = \lim_{n \rightarrow \infty} \left[ \exp\left(-\frac{\beta \hat{H}_1}{n}\right) \exp\left(-\frac{\beta \hat{H}_2}{n}\right) \cdots \exp\left(-\frac{\beta \hat{H}_n}{n}\right) \right]^n$$

Introducing complete sets of states, we have

$$\begin{aligned} Z &= \text{Tr}[\exp(-\beta \hat{H})] \\ &= \sum_{\alpha} \langle \alpha | \exp(-\beta \hat{H}) | \alpha \rangle \\ &= \lim_{n \rightarrow \infty} \sum_{\alpha} \sum_{i_1, i_2, \dots, i_n} \langle \alpha | \exp\left(-\frac{\beta \hat{H}_1}{n}\right) | \alpha_{i_1} \rangle \langle \alpha_{i_1} | \exp\left(-\frac{\beta \hat{H}_2}{n}\right) | \alpha_{i_2} \rangle \cdots \\ &\quad \langle \alpha_{i_{n-1}} | \exp\left(-\frac{\beta \hat{H}_n}{n}\right) | \alpha_{i_n} \rangle \langle \alpha_{i_n} | \exp\left(-\frac{\beta \hat{H}_1}{n}\right) | \alpha_{i_1} \rangle \cdots \\ &\quad \langle \alpha_{i_{n-1}} | \exp\left(-\frac{\beta \hat{H}_n}{n}\right) | \alpha_{i_n} \rangle \langle \alpha_{i_n} | \exp\left(-\frac{\beta \hat{H}_1}{n}\right) | \alpha_{i_1} \rangle \cdots \\ &\quad \times \langle \alpha_{i_n} | \exp\left(-\frac{\beta \hat{H}_n}{n}\right) | \alpha \rangle \end{aligned}$$

Suzuki used this approach to show the equivalence between d-dimensional quantum spins and (d+1)-dimensional Ising spin systems. Suzuki and coworkers carried out MC simulations on the (d+1)-dimensional Ising spin system to study the d-dimensional quantum spin system.

Burna and Sastri extended Suzuki's approach to Fermion systems, in one-dimension. Consider the 1-d spinless fermion model (non interacting)

$$H = -t \sum_i [c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i]$$

Using B-S break up we can write

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

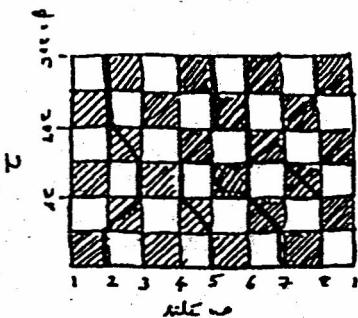
$$\hat{H}_1 = -t \sum_{i \text{ odd}} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)$$

$$\hat{H}_2 = -t \sum_{i \text{ even}} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)$$

All the terms in  $\hat{H}_1$  commute with each other, similarly in  $\hat{H}_2$ . Therefore, matrix elements of  $\exp(-\beta \hat{H}_1)$  as well as those of  $\exp(-\beta \hat{H}_2)$  can be evaluated exactly with ease. Applying Trotter Formula we have

$$Z = \sum_{i_1, i_2, \dots, i_n} \langle i_1 | e^{-\beta \epsilon \hat{H}_1} | i_2 \rangle \langle i_2 | e^{-\beta \epsilon \hat{H}_2} | i_3 \rangle \langle i_3 | e^{-\beta \epsilon \hat{H}_1} | i_4 \rangle \cdots \langle i_{2L} | e^{-\beta \epsilon \hat{H}_2} | i_1 \rangle \quad (2)$$

where  $\beta \epsilon = \beta/L$  and since in Trotter formula we have used  $e^{-\beta \epsilon (\hat{H}_1 + \hat{H}_2)} \approx e^{-\beta \epsilon \hat{H}_1} e^{-\beta \epsilon \hat{H}_2}$ , the error introduced is of order  $(\beta \epsilon)^2$ . In the occupation number representation, every term in the expansion can be represented by a configuration of Fermion world lines or a checker board pattern. In each time slice (imaginary time  $\tau$  representing temperature) there is one action by  $e^{-\beta \epsilon \hat{H}_1}$  and  $e^{-\beta \epsilon \hat{H}_2}$  each. Because the summation in (2) can be regarded as summation over all possible fermion world line configurations, this approach is equivalent to the path integral approach.



In the Monte Carlo procedure, states of the Markov chain correspond to a single term in eqn. ② or equivalently to a specific checker board configuration. To generate different states of the Markov chain we need to alter the configuration of world lines, based on a few simple rules. To evaluate the new term  $\alpha$  in ② arising from this we need to know the result of operation by  $\exp(-\beta t H_{i,i+1})$  on the state of the system at sites  $i$  and  $i+1$ . This can be simply evaluated and the results are

$$\exp(-\beta t H_{i,i+1}) |0,0\rangle = |0,0\rangle$$

$$\exp(-\beta t H_{i,i+1}) |1,1\rangle = |1,1\rangle$$

$$\exp(-\beta t H_{i,i+1}) |1,0\rangle = \cosh(\beta t) |1,0\rangle + \sinh(\beta t) |0,1\rangle$$

$$\exp(-\beta t H_{i,i+1}) |0,1\rangle = \cosh(\beta t) |0,1\rangle + \sinh(\beta t) |1,0\rangle$$

To thermalise, the ratio of the two terms is computed and the new configuration accepted with a probability given by the ratio.

This MC algorithm has been used by Hirsch and others in studying Hubbard models and Kondo necklace models.

#### 4. Quantum Monte Carlo with VB basis

Even in the case of Fermions with spin, and in the models that conserve total spin, the basis set used to get matrix representation of Trotter formula conserve only total  $S_z$ , i.e., the basis sets are simple Slater determinants. Complete

VB basis which comprise eigen states of  $S^2$ , are usually much smaller than the complete Slater det. basis

[for a Hubbard chain with  $2n$  electrons on  $2n$  sites,  $S=0$  VB basis is smaller than  $S_z=0$  Slater det. basis by a factor  $\frac{n}{2}+1$  for large  $n$ .]

If the VB basis is employed in Trotter representation, the population from which we sample reduces [in the above example, by a factor  $(\frac{n}{2}+1)^L$  where  $L$  is the No. of lattice points along the Trotter axis], thereby increasing enormously the efficiency of the method.

VB basis is nonorthogonal, hence

$$I = \sum_k \sum_l |k\rangle S^{-1}_{kl} \langle l|$$

This at first glance appears to wipe away the advantage

However, the Trotter representation for  $Z$  reduces to [for the noninteracting fermion Hamiltonian]

$$Z = \sum_{i_1, i_2, \dots, i_L} \langle i_1 | e^{-\alpha t H_1} | i_2 \rangle \langle i_2 | e^{-\alpha t H_2} | i_3 \rangle \dots \langle i_L | e^{-\alpha t H_L} | i_1 \rangle S_{i_1, i_2, \dots, i_L}$$

where  $S_{i_1, i_2, \dots, i_L}$  is an overlap integral which can be easily computed. We also need to know the effect of  $e^{-\alpha t H_{c,c+1}}$  on a VB diagram. The result is

$$\begin{aligned} e^{-\alpha t H_{c,c+1}} |x \ x\rangle &= |x \ x\rangle \\ " | \cdot \cdot \rangle &= | \cdot \cdot \rangle \\ " | \cdot x\rangle &= \frac{1}{2} \left[ [\cosh(2\alpha t) + 1] | \cdot x\rangle \right. \\ &\quad \left. + [\cosh(2\alpha t) - 1] | x \cdot \rangle - \frac{1}{\sqrt{2}} \sinh(2\alpha t) | \cdot \cdot \rangle \right] \\ " | \rightarrow \rangle &= \cosh(2\alpha t) | \rightarrow \rangle - \frac{1}{\sqrt{2}} \sinh(2\alpha t) [ | \cdot x\rangle + | x \cdot \rangle] \end{aligned}$$

$$\begin{aligned} " | \overbrace{\downarrow}^i \overbrace{\uparrow}^j \rangle &= | \overbrace{\downarrow}^i \overbrace{\uparrow}^j \rangle + \frac{1}{2} (1 - \cosh(\alpha t)) | \overbrace{\cdots}^{i-1} \overbrace{\cdots}^{j+1} \rangle \\ &\quad + \frac{1}{2\sqrt{2}} \sinh(\alpha t) \left[ | \overbrace{\cdots}^{i-1} \overbrace{\cdots}^{j+1} \rangle + | \overbrace{\cdots}^{j+1} \overbrace{\cdots}^{i-1} \rangle \right] \end{aligned}$$

$$" | x \curvearrowleft \rangle = \cosh(\alpha t) | x \curvearrowleft \rangle + \sinh(\alpha t) | \curvearrowleft x \rangle$$

$$" | \cdot \curvearrowleft \rangle = \cosh(\alpha t) | \cdot \curvearrowleft \rangle - \sinh(\alpha t) | \curvearrowleft \cdot \rangle$$

Introduction of the interaction part is quite straightforward. Even in this rep the checker board pattern is useful. However, the checker board corr. to  $\uparrow \downarrow$  spins evolve in a generalized manner.

## Numerical Approach to Strongly Correlated Systems

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## Numerical Approach to strongly Correlated systems

### (1) Technique(s)

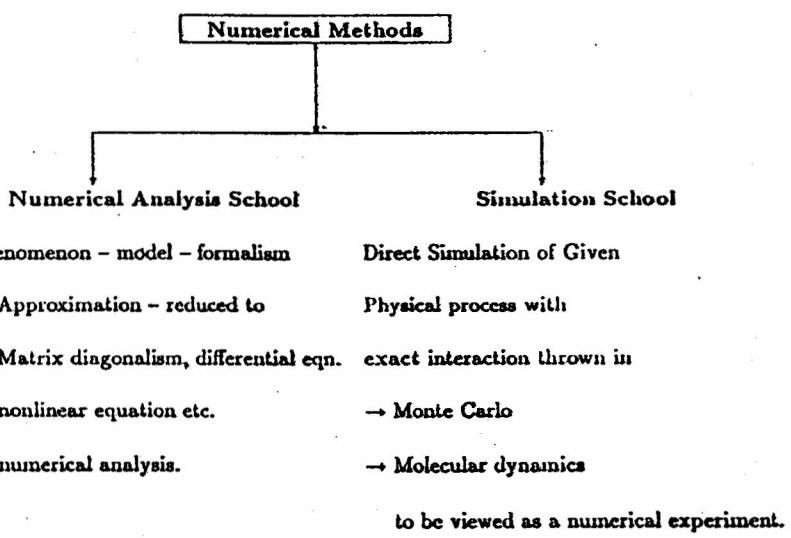
### (2) What can be studied?

- Binding Energies - Ground state, 1h, 2h
- Phase Diagram  $U-V$  model {extended Hubbard}
- Optical Conductivity
- one hole: dynamical properties
- Phases — non Fermi liquid
  - ↓ wave chiral
  - ...

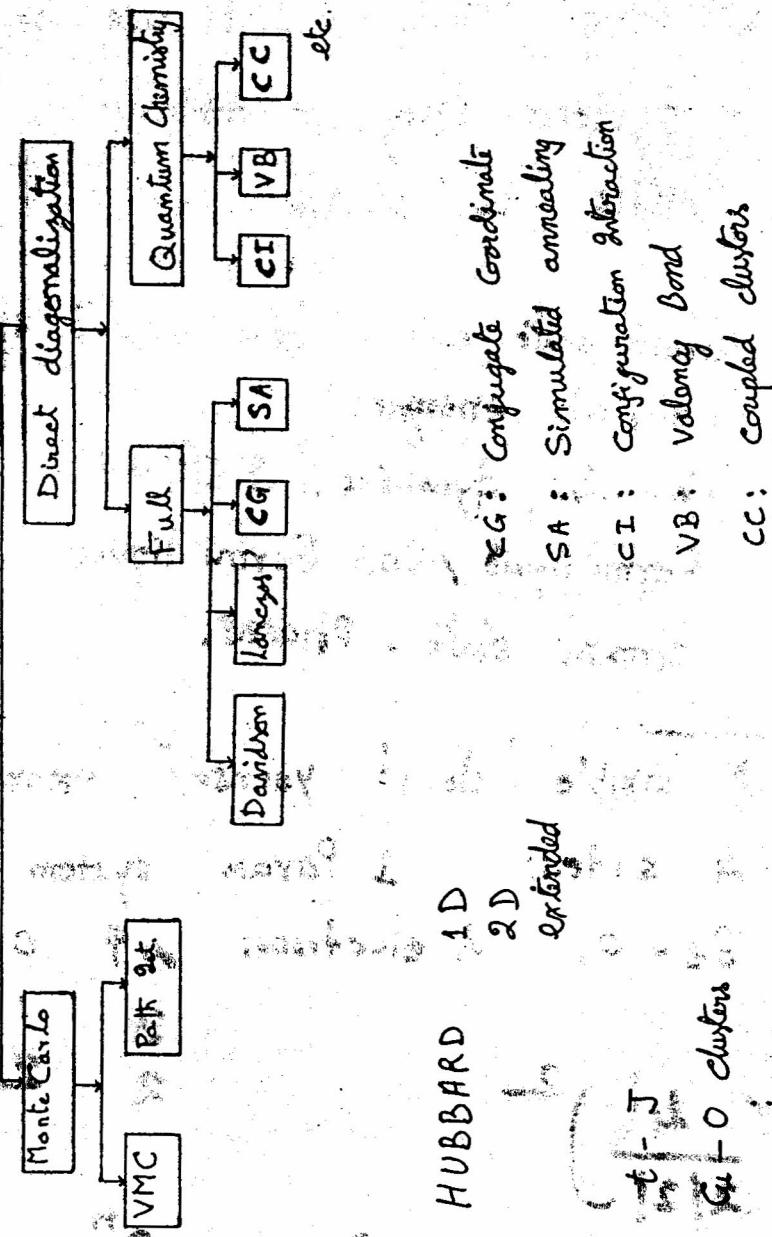
### (3) CI Techniques

### (4) Simulated annealing - large sparse matrices

Numerical Calculations gives you numbers ask questions to get physics.

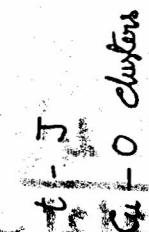


## NUMERICS



187

HUBBARD  
1 D      2 D  
extented



Cu - O clusters

188

The States :  $S_z = 0$  Total  $6 \times 6 = 36$

$|0011\rangle$

$|0101\rangle$

$|1001\rangle$

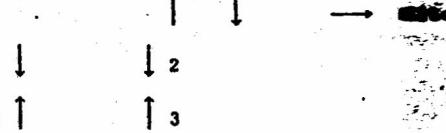
$|0110\rangle$

$|1010\rangle$

$|1100\rangle$

Same for up and down electrons

Typical State  $|0011/1100\rangle$



Diagonalization of  $36 \times 36$  matrix gives all eigenstates for 6 sites.

Note : States can be classified as with 0 sites double occupied

1 site doubly occupied

N/2 site doubly occupied

(N = Number of Electrons)

i.e.

(A)  $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$  Neel type (2)

$\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$ ,  $\uparrow\uparrow\downarrow\downarrow$ ,  $\downarrow\uparrow\uparrow\downarrow$ ,  $\downarrow\downarrow\uparrow\uparrow$

(4) : RVB type

[total of 6 singly occupied]

+ 1 site D and 2 site D.

### Configuration Interaction Technique

Solid state communication : 77 (613) 91.

As we have seen, large clusters means very large number of basis functions :  
 $N = 16, NB \approx 1.6 \times 10^6$ . Hence Try CI : ie. try to pickup only significant configurations.

(A) Conventional CI : i diagonal or single particle basis

$$\Psi_C = C_{HF} \psi_{HF} + \sum_a C_a^r \psi_a^r + \sum_{ab} C_{ab}^r \psi_{ab}^r + \dots$$

a,b,c run over occupied orbitals, in HF state

r,s run over unoccupied orbitals in HF state.

(B) Useful for large U : Site basis most dominant states : No double occupancy

then all states with 1 site double occupancy etc

$$\Psi_C = \sum_a C_a^0 \psi_a^0 + \sum_b C_b^1 \psi_b^1 + \dots - \sum_c C_c^2 \psi_c^2 + \dots$$

$\psi_x^n \equiv x^{th}$  multiparticle state with n doubly-occupied sites for large U : B much better than U.

Warning! These results are on finite systems. Any resemblance to infinite lattice is purely .....

Ground state and a few excited states

1h, 2h energies

1h, 2h, dynamics:  $S(\vec{k}, \omega)$

Fermi liquid / Non Fermi liquid

Ground state : Phases:

A simple 'do it yourself' example

4 sites: 1 Param system

$S_z = 0$ , 4 electrons:  $\frac{1}{2} \uparrow \frac{1}{2} \downarrow \frac{1}{2} \uparrow \frac{1}{2} \downarrow$

$$\left( \frac{4!}{2!2!} \right)^2$$

$$\begin{matrix} 3 & 1 \\ 2 & 2 \end{matrix}$$

Analysis of Wave f<sup>n</sup>

(a) Reference state: half filled

add hole: and then another

$$\Delta_N(n) = [E_0(n+2) - E_0(n+1)] - [E(n+1) - E_0(n)]$$

$$= E(2h) - 2E(1h)$$

measure of Pairing interaction between 2h

$\Delta_n < 0$  two holes bind,  $-\Delta$  binding energy  
in infinite limit

stability 3rd hole should not bind.

$$\frac{\partial^2 G}{\partial n^2} > 0$$

$$\Delta'_N(n) = E_0(n+3) - E_0(n+2) - [E_0(n+1) - E_0(n)]$$

look for region

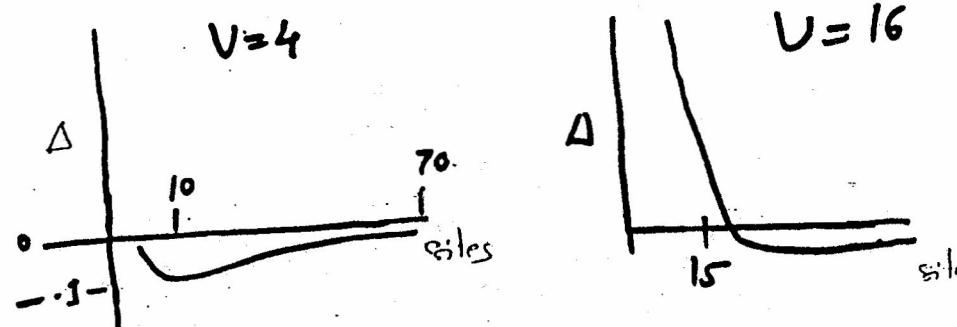
$\Delta(n) < 0$  attractive

$\Delta'(n) > 0 \rightarrow$  stability.

Binding energy of

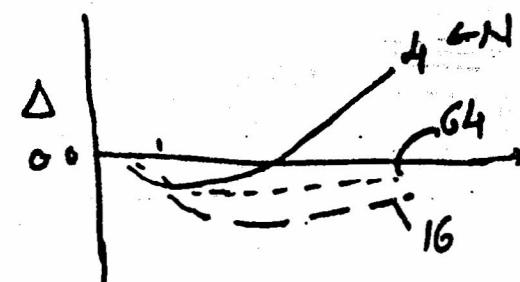
$2h$

binding energy: example 1 U:



(1) For  $U \leq 4.5$  initial increase in B.E.  
slow decay

(2)  $U > 4.5$  There is  $N_c$  critical size  
for B.E.,  
For large  $U$ ,  $N_c \rightarrow$  increases



$U \rightarrow$

note decrease in B.E. in going from 16 to 64

great care must be exercised: in interpreting finite cluster results.  
Role of boundary Cond:

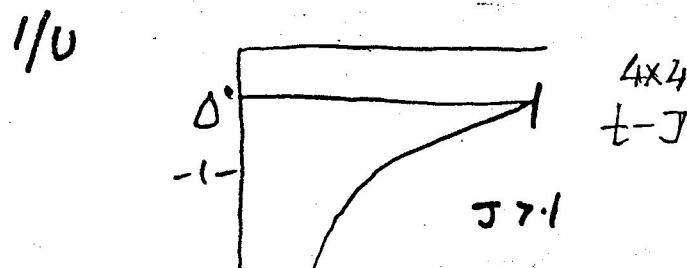
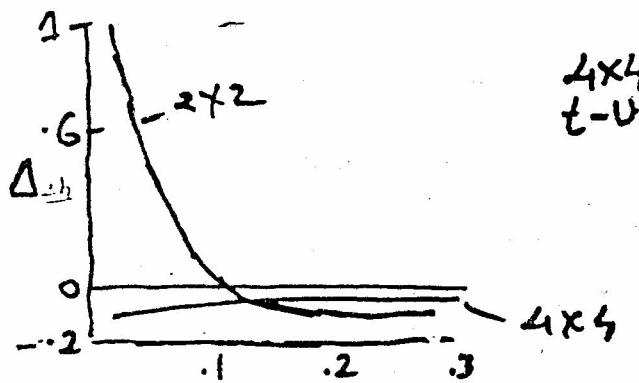
1D  $E_B^{th} \rightarrow 0$  in thermodynamic limit

No binding for any size with Antiperiodic BC

[Fye: Martin-  
Scatterer

P.R. B at 90

2D:



Clusters:

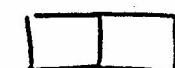
Investigated  
(36)

dep. of the  
matrix

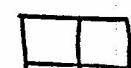
+ 6 and 8 sites hexagon and  
octagon



4



6



9

(15876)

Correlation functions:

SPIN

$$L_{ij} = \frac{1}{4} \langle G((n_{iq} - n_{if})(n_{jt} - n_{jf})) \rangle_G$$

charge:

$$D_{ij} = \langle n_i n_j \rangle$$

Pairing:

$$P_{ij} = \langle o_i o_j^\dagger \rangle$$

Local Singlet:  $o_i = C_{ip} C_{if}$

Extended Singlet:

$$o_i = \frac{1}{\sqrt{2}} (C_{ip} C_{i+x_f} - C_{if} C_{i+x_p})$$

Triplet:  $o_i = C_{ip} C_{i+x_p}$

Structure factors:

$$S_S(\bar{q}) = \frac{1}{N} \sum_{ij} e^{i\bar{q} \cdot (\bar{R}_i - \bar{R}_j)} L_{ij} \quad (2)$$

$$\bar{q} = \pi \quad \therefore (\pi, \pi)$$

In addition: def:  $C = \sum_{j=-M}^M [D_{ij} s_i s_j - \left(\frac{n_e}{N}\right)^2]$

$$M = \frac{1}{2} \left( \frac{n_e}{2} - 1 \right)$$

for integer values

If  $C > 0$ : condensation

Describe the system: CDW  
SDW  
Condensation  
Pairing

= 2D clusters

half filled +

one and two holes over half filled band

195

AF spin structure factor  $S_S(\pi)$ : Half filled case note

a) Increase in S with size  
b) Increases with  $U \frac{t}{t} \approx 20 \rightarrow$  large U limit

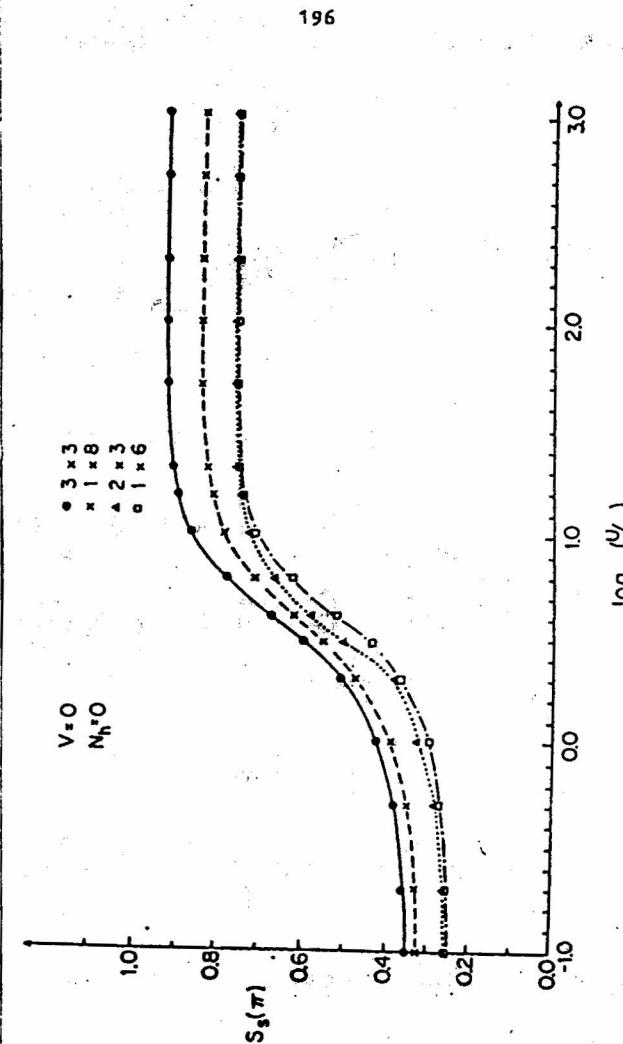


Figure 2.

Simple Hubbard model:  $V=0$

Features: (1) Formation of local moment

$$\bar{m} = 4 \langle S_{iz}^2 \rangle N/n_e \quad \text{for large } U$$

→ 1 independent of

But:  
coupling between the moments on different  
sites depends on Geometry / occupancy

⇒ Investigate  $S_s(\pi)$  (AF)

Fig 4 square system:

Fig 5 Significant reduction in  $S_s(\pi)$  for holes  
reduction in magnetic order

Fig 6 first and second nn spin corr. functions

④ Indicates: magnetic correlations are  
greatly reduced in strength beyond 1<sup>st</sup> n.

⇒ Binding of 2 holes:

$$E_B = E(0) - 2E(1) + E(2)$$

Z

Effect of holes  
on AF order

lower curves are  
for unpaired, i.e. U,  
above which ground  
state is not of the  
spin

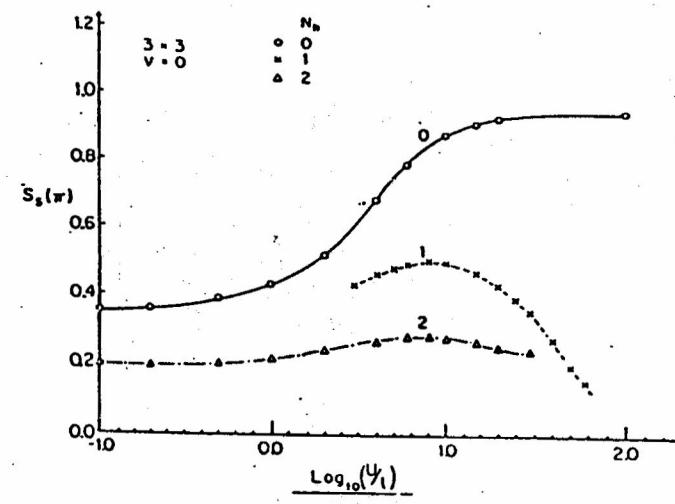


Figure 5.

— Single Pairing  
--- charge  
(Two squares, symm.)

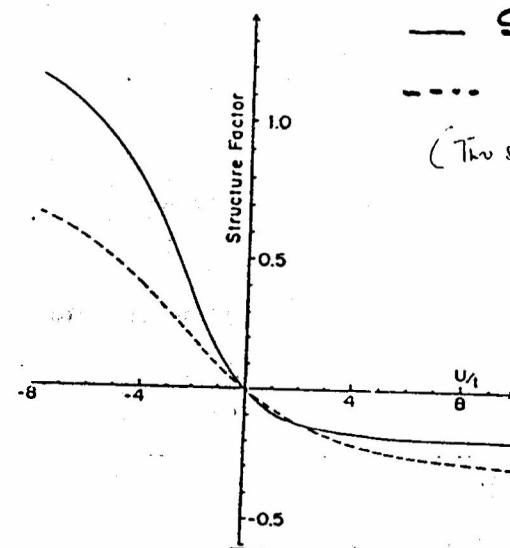
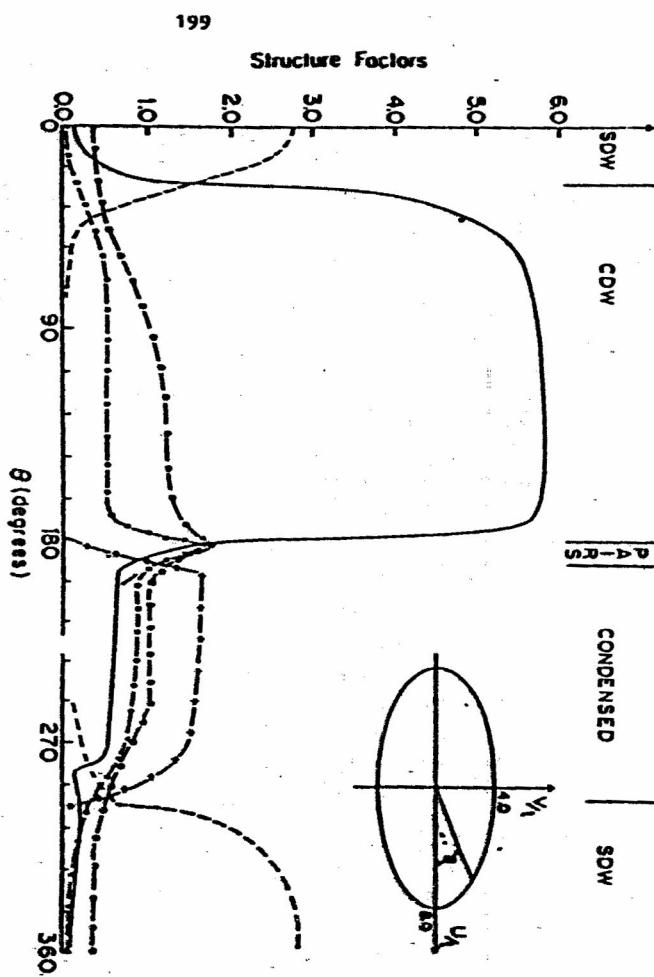


Figure 6.

co-existence of Pairing (single) and charge CDW in-U region.

Figure 9:  
 - - - charge structure factor  $S_c(\pi)$   
 - - - local singlet pairing  
 - - - charge structure factor  $S_c(\pi)$   
 - - - local singlet pairing parameter



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Property dependent on Geometry

- (1) No binding for 2 square or 4 squares
- (2) Weak binding for octagon

Stability: | binding influenced by  
 $V$

$\Rightarrow$  Co-existence of pairing and CDW  
 for  $-ve \underline{V}$

Fig. 8

charge st. factor —  
 local singlet Pairing -----

Extended Hubbard model:

Phase diagram  $U - V$ ;  $\theta = \tan^{-1}(U/V)$

Fig. 9

around ellipse  

$$U^2 + 4V^2 = a^2$$

$$\frac{U}{4V} t^2$$

$S_c(\pi)$  —

$S_s(\pi)$  -----

$S_p(\alpha)$  (Local singlet) +--o | ---  $\propto (4\pi)$

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The 2D clusters show:

Fig 8

Transition  $\rightarrow$  from AF - SD  $\rightarrow$  CSW

for values of  $V$  significantly smaller than  
 $V/2$  (for large system  $V = U/t$ )

Fig 10:  $S_S$  and  $S_C$  for  $V=2$

$$V \approx 0.555$$

Interesting Result: 2 holes in half filled band:

$V$  can favour either spin alignment or

Fig 1 Pairing for certain range of Params

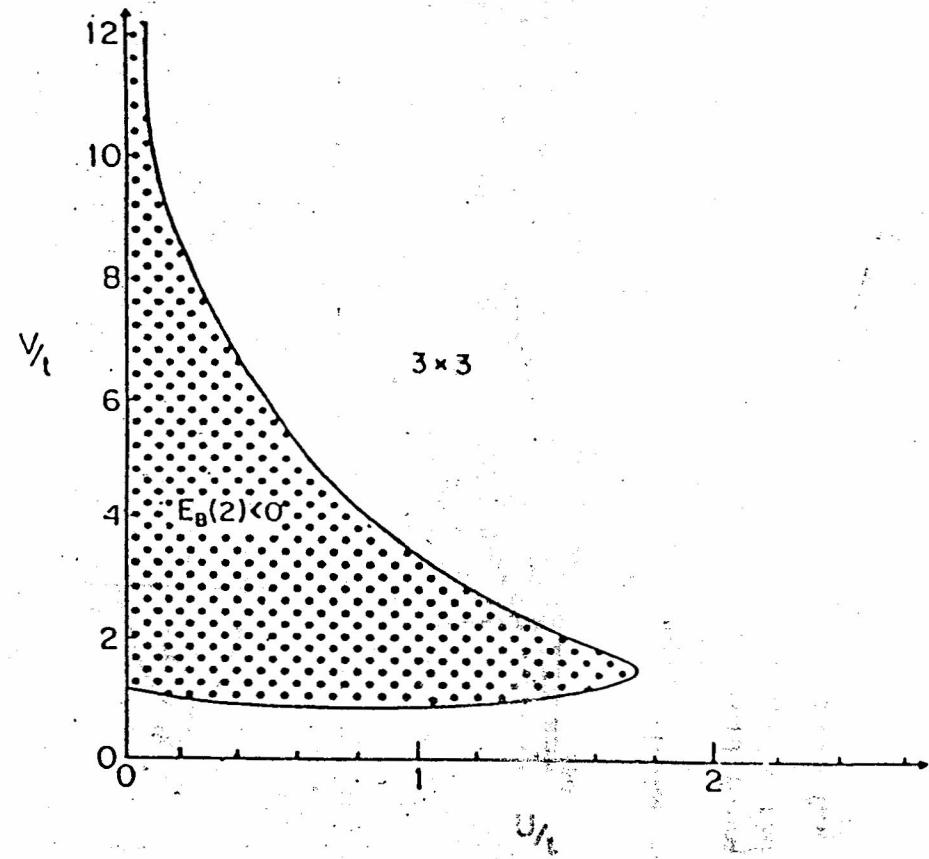
2.895 and 4.895: 2 Regions of  $V_1 V_2$  plane alignment

for  $V=c_1$  large  $V$ ,  $S=3$ , 4cb2sg syst.

Binding of 2 holes [effect of  $V$ ]

202

2 holes 3x3  
7el.



Region of hole binding for 7 electron in 9 sites

Figure 12

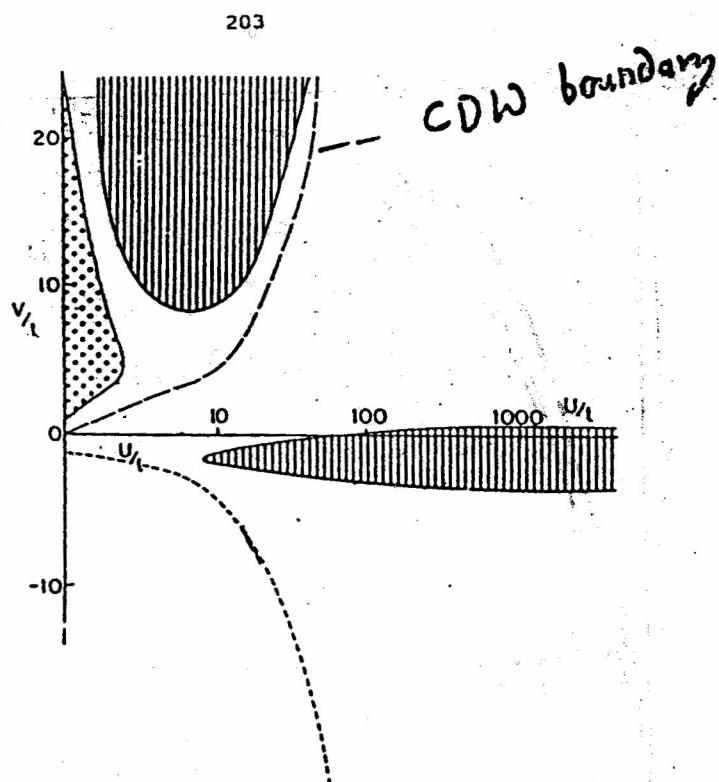


Figure 11:

2 holes :

Regions with II spin

Two hole binding  $E_B < 0$

## Results

Fig.12 : % ground state (exact) energies as a function of  $U$  : (conventional CI Scheme)

Curve A: HF

Curve B: HF + upto 2 Fold excitations.

Curve C: HF + upto 4 Fold excitations.

Fig.13: Same as above, full for "site basis" CI

A : 6 site cluster

B : 7 site cluster

C : 8 "

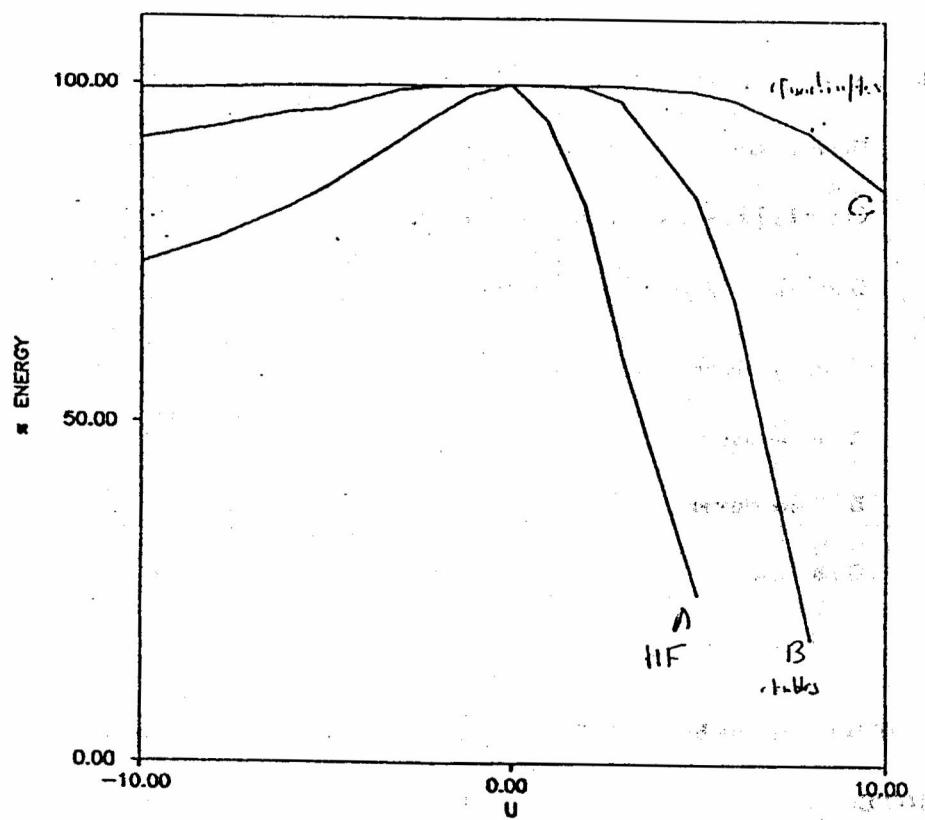
D : 9 "

All the cases with basis including all 0 occupancy + all 1 site double occupancy.

## NOTE:

1. HF is Ok for low  $U$  and -ive  $U$  but even 2 fold excitation is not enough for moderate  $U$ .
2. 2nd scheme is much better for large approximate size consistency seen.

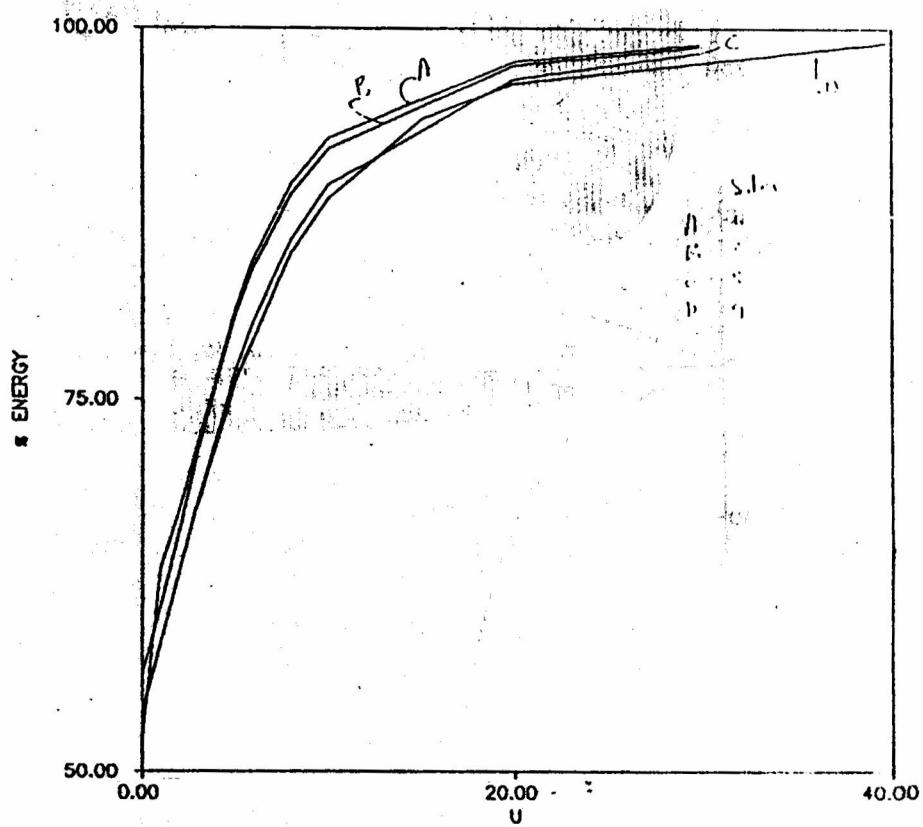
205



% ground state energies U 6 sites

[Fig. 12]

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x ground state energies (exact) as a function of U second CI scheme  
[one site doubly occupied]

[Fig. 13]

### I: Generic Results:

- (a) Formation of local spin moment - large  $U$
- (b) existence of SDW or AF correlations for half filled bands
- (c) Reduction of the range of spin correlations by hole doping except when a Ferromagnetic ground state is formed
- (d) Occurrence of local singlet Pairing for  $-ve U$
- (e) A transition to CDW order for some  $V$
- (f) enhancement of magnetic corr. ( $U > 0$  case) and pairing for  $-ve V$  due to small  $-ve U$

Geometrically Sensitive result:  $\rightarrow$  values of parameters

- (1) Occurrence of ground state with  $S=0, \frac{1}{2}$  for 2 hole system in large  $U$  limit
- (2) Binding of two holes

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