The Infinite Range Heisenberg Model and High Temperature Superconductivity

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To My Parents

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Abstract

The thesis deals with the theory of high temperature superconductivity from the standpoint of three-band Hubbard models.

Chapter 1 of the thesis proposes a strongly coupled variational wavefunction that has the three-spin system of an oxygen hole and its two neighboring copper spins in a doublet and the background Cu spins in an eigenstate of the infinite range antiferromagnet. This wavefunction is expected to be a good "zeroth order" wavefunction in the superconducting regime of dopings. The three-spin polaron is stabilized by the hopping terms rather than the copper-oxygen antiferromagnetic coupling J_{pd}. Considering the effect of the copper-copper antiferromagnetic coupling J_{dd}, we show that the three-spin polaron cannot be pure Emery (D_g), but must have a non-negligible amount of doublet-u (D_u) character for hopping stabilization. Finally, an estimate is made for the magnitude of the attractive coupling of oxygen holes.

Chapter 2 presents an *exact* solution to a strongly coupled Hamiltonian for the motion of oxygen holes in a 1-D Cu-O lattice. The Hamiltonian separates into two pieces: one for the spin degrees of freedom of the copper and oxygen holes, and the other for the charge degrees of freedom of the oxygen holes. The spinon part becomes the Heisenberg antiferromagnet in 1-D that is soluble by the Bethe Ansatz. The holon piece is also soluble by a Bethe Ansatz with simple algebraic relations for the phase shifts.

Finally, we show that the nearest neighbor Cu-Cu spin correlation increases linearly with doping and becomes positive at $x \approx 0.70$.

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Chapter 1

The Infinite Range Heisenberg Model and High Temperature Superconductivity

ABSTRACT

A new strongly coupled variational wavefunction, the doublet spin projected Néel state (DSPN), is proposed for a single oxygen hole in three-band models of high temperature superconductors. This wavefunction has the three-spin system of the oxygen hole plus the two neighboring coppers coupled in a spin 1/2 doublet. The remaining copper spins of the crystal are in an eigenstate of the infinite range Heisenberg antiferromagnet (SPN state). The doublet three-spin magnetic polaron or hopping polaron (HP) is stabilized by the hopping terms t_σ, t_τ, rather than by the copper-oxygen antiferromagnetic coupling J_{pd}. Although, the HP has a large projection onto the Emery (D_g) polaron, a non-negligible amount of doublet-u (D_u) character is *required* for optimal hopping stabilization. This is due to J_{dd}, the copper-copper antiferromagnetic coupling.

The SPN state allows simple calculations of various couplings of the oxygen hole with the copper spins. For doping in the range 0.06 to 0.25 oxygen holes per in plane copper (the superconductive phase), the copper-copper antiferromagnetic coupling can be considered to be almost infinite ranged.

The general DSPN wavefunction is constructed for the motion of a single quasiparticle in an antiferromagnetic background. The energy minimum is found at symmetry $(\pi/2, \pi/2)$ and the bandwidth scales with J_{dd}. These results are in agreement with exact computations on a lattice.

The coupling of the quasiparticles leads to an attraction of holes and its magnitude is estimated.

I. INTRODUCTION

The copper-oxide high T_c superconductors generally involve unpaired spins on the Cu^{++} sites that couple with each other antiferromagnetically plus holes resulting from doping that lead to unpaired spins predominantly on the bridging oxygen atoms. The copper sites residing in the CuO_2 planes are in Cu^{++} (d^9) states and can be described by a single spin 1/2 hole with orbital symmetry $d_{x^2-y^2}$. Doping of the system leads to holes that tend to localize on the oxygen sites with an unpaired spin in the p orbital pointing towards the adjacent copper atoms. This hole is denoted as p_σ, where the axis of symmetry is to its two neighboring copper sites. The mixing of the spins in these copper $d_{x^2-y^2}$ orbitals and the oxygen p_σ orbitals lead to the three-band Hubbard models of superconductivity.[1,2]

The important interactions in this system are[1–5]

(i) Antiferromagnetic coupling between adjacent Cu spins, $H_{dd} = J_{dd} \sum S_i \cdot S_j$. The ground state spin coupling is complicated but adjacent spins tend to be opposite.

(ii) Direct hopping of the oxygen hole between oxygen sites, $H_{pp} = -t_{pp} \sum p^\dagger_{m\sigma} p_{n\sigma}$, where only the diagonally adjacent oxygen sites need be considered.

(iii) Bond pairing of the O p_σ orbital with the two adjacent Cu d orbitals, $H_{pd} = J_{pd} \sum S_i \cdot S_n$. Considering a single oxygen hole and the two adjacent copper spins leads to a doublet ground state referred to as the Emery polaron.[1,2]

(iv) Copper mediated hopping $H_{pdp} = -t_a \sum p^\dagger_{m\sigma} p_{n\sigma} + (t_a + t_b) \sum p^\dagger_{m\sigma'} p_{n\sigma} d^\dagger_{i\sigma} d_{i\sigma'}$. The Cu-O bonding interactions lead to additional O-O hopping terms that leave the O spin unaltered (the $-t_a$ term) or swap the O spin with the inter-

mediate Cu (the $t_a + t_b$ term).

The details of these Hamiltonians will be discussed more below. Because these five terms are strongly coupled, particularly at the high dopings necessary for the best superconductors, it has been difficult to obtain a simple description adequate for qualitative reasoning.

A major obstacle to a theoretical understanding of high temperature superconductivity is the lack of a "zeroth order" wavefunction that is valid in the superconducting regime of doping. In this paper, we propose the Hopping Polaron (HP) wave function that reproduces the major effects observed in accurate calculations. This HP wavefunction is factored in terms of two pieces: (a) the three-spin system of the hole and its two adjacent coppers, and (b) the effective configuration of the remaining copper spins.

Since the background copper spins are *included* in this wavefunction, the HP is optimized for the complete Hamiltonian (1) *with* the J_{dd} coupling (in contrast to the models of Emery,[1,2] and of Zhang and Rice[6]). We believe this formalism is useful for both qualitative reasoning and for semi-quantitative calculations.

Our starting point is the Spin Projected Néel (SPN) description of the Cu d spins that we use to model spins in the vicinity of a hole. In the SPN state, the background Cu sites are partitioned into two interpenetrating lattices A and B with the total spin on each sublattice taking its maximum allowed value and coupled together to form a total spin $S = S_A + S_B = 0, 1, 2, \ldots$. The SPN states are the low energy eigenstates of the Infinite Range Heisenberg Antiferromagnet (IRHA). Although the range of J_{dd} in H_{dd} is one lattice spacing, we argue that SPN coupling (which is correct for infinite ranged J_{dd}) is an accurate approximation for highly

doped systems. A justification for considering SPN as a good approximation is provided by neutron scattering experiments[7] that indicate the correlation length of the copper spins is equal to the mean separation of holes and does not change appreciably over a large temperature range. For dopings in the superconducting phase, we argue that SPN is the best simple description for the background Cu spins.

Considering the three-spin system consisting of the hole on the oxygen and its two neighboring copper spins, the optimum bonding for Hamiltonian H_{pd} leads to a particular doublet ($J = 1/2$) state known as the Emery polaron (denoted D_g). There is a second possible doublet state (denoted D_u) and a quartet ($J = 3/2$) state (denoted Q). For H_{pd}, the D_u state is J_{pd} above D_g, while Q is $3/2J_{pd}$ above D_g.

Considering only copper mediated hopping, H_{pdp}, in a sea of Cu spins, we show that the three-spin polaron is predominantly doublet. In fact, for $J_{pd} = 0$, the three-spin polaron remains an almost exact doublet. However, the three-spin polaron favored by H_{pdp} is a mixture of D_g (the Emery polaron) and D_u.

Combining the SPN background with the doublet quasiparticle leads to the Doublet Spin Projected Néel (DSPN) wavefunction. For a system with total spin 1/2, there are only two SPN states that may couple to the three-spin doublet. They are $J_{SPN} = 0, 1$. There are two independent doublets for the Cu-O-Cu set: D_g and D_u. The D_g state is symmetric under reflection about the oxygen or identically under interchange of the two coppers. D_u is antisymmetric under reflection. D_g is the three-spin state originally suggested by Emery[1,2] as the quasiparticles for high T_c systems and is known as the Emery polaron. It has the two coppers adjacent

to the hole coupled into a triplet; D_u has the coppers coupled in a singlet. Hence, there are four independent doublet SPN states for an oxygen hole at a given site. Using translational invariance leads to an 8×8 matrix for the Hamiltonian in two dimensions with symmetry vector k. This reduction of the state space and the simplicity of the SPN states permits us to analytically evaluate the necessary matrix elements of the Hamiltonian for a single hole in an arbitrarily large lattice. For total spin 1/2, the DSPN state has a minimum at $(\pi/2, \pi/2)$ in agreement with exact calculations.[3,5] We find that the three-spin polaron is stabilized by a *mixture* of the D_g (Emery) and D_u states (about 75% Emery for $J_{pd} = 0$). This mixing of D_u into D_g is primarily due to the J_{dd} coupling of the background copper spins. We believe the DSPN wavefunction provides a useful framework for describing and predicting properties of these systems.

The paper is arranged as follows. Section II. evaluates the eigenstates of the infinite range Heisenberg antiferromagnet and defines the SPN states. The spin correlation of the SPN states is also evaluated. In Section III. A, the hole hopping terms H_{pp} and H_{pdp} are written in a form that makes the total spin symmetry manifest. This leads naturally to the definitions of singlet hops, t_σ, and triplet hops, t_τ. The expressions for t_σ, t_τ are derived in terms of the t_a, t_b, t_{pp} of H_{pp} and H_{pdp}. For the parameters of interest in superconductivity, the singlet hop $t_\sigma \approx 3t_\tau$ for hops along the same axis, whereas for diagonal hops, $t_\sigma \approx 20t_\tau$. Section III. B defines the states of the three-spin Cu-O-Cu subsystem: the two doublets (D_g, D_u) and the quartet (Q). They are eigenstates of H_{pd}. The doublets are written as a sum of terms with the hole coupled to one or the other of the coppers in a pure singlet, whereas, the quartet has only triplet coupling to the

coppers. Thus we expect negligible quartet character in the lowest eigenstates of the Hamiltonian. In Section IV. A, the Hamiltonian matrix for the total spin one-half DSPN wavefunctions is calculated in one dimension. We show that even for a single oxygen hole in an infinitely large lattice, there is always finite scattering into SPN configurations from the total Hamiltonian (1). The matrix is then generalized to two dimensions in Section IV. B. Since the form of the SPN states is independent of the dimensionality of the system, this process is straightforward. Finally, Section V. discusses the qualitative effect of two holes moving in a SPN type background. We find a short range attraction between the holes.

The phases of the copper d and oxygen p hole orbitals are chosen so that each Cu-O bond has positive overlap as in figure 1. This Bonding Phase Convention results in copper hopping interactions having the same sign regardless of the direction of the hopping. This convention leads to a shift in momentum of (π, π) from the standard phase convention in which the phases of the orbitals are the same in every unit cell. The total Hamiltonian is the sum of (i)-(iv),

$$H = J_{dd} \sum_{<ij>} S_i \cdot S_j - t_{pp} \sum_{\substack{<mn>_{diag} \\ \sigma}} p^\dagger_{m\sigma} p_{n\sigma} + J_{pd} \sum_{<in>} S_i \cdot S_n$$

$$-t_a \sum_{\substack{<min> \\ \sigma}} p^\dagger_{m\sigma} p_{n\sigma} + (t_a + t_b) \sum_{\substack{<min> \\ \sigma\sigma'}} p^\dagger_{m\sigma'} p_{n\sigma} d^\dagger_{i\sigma} d_{i\sigma'}. \qquad (1)$$

In this equation, m, n are oxygen sites and i, j are copper sites. $< min >$ represents two oxygen sites neighboring the copper at i. The $< ij >$ are adjacent copper sites and $< mn >_{diag}$ represents diagonally adjacent oxygen sites, i.e., sites on different axes. $p^\dagger_{n\sigma}$ creates a hole of spin σ on the oxygen site n, and similarly $d^\dagger_{i\sigma}$ creates a hole of spin σ on copper site i. J_{dd} is the antiferromagnetic coupling of adjacent

coppers and t_{pp} is the direct oxygen-oxygen hopping between diagonally adjacent sites. J_{pd} is the antiferromagnetic coupling of an oxygen hole to neighboring coppers. The t_a and t_b are copper mediated hopping processes.[3,4] They are second order in t_{pd}, the matrix element representing mixing of copper d and oxygen p orbitals. In the Bonding Phase Convention, all parameters in (1) are positive. The summations in equation (1) are to be taken over every pair just once. Thus, the energy separation between the singlet and triplet states for two copper ions is J_{dd} similarly for J_{pd}. For typical high T_c superconductors, t_a, t_b, t_{pp}, J_{pd} are approximately equal and around 4 to 5 times as large as J_{dd}.[3,5,8-10] J_{dd} is $0.13eV$ for $La_{2-x}Sr_xCuO_4$, while J_{dd} is $0.12ev$[11-13] for $Y_1Ba_2Cu_3O_6$. There are relationships between these parameters, but for formal analysis, we may vary them independently.

With no holes on the oxygen sites, J_{dd} is the only nonzero term and the Hamiltonian reduces to the spin 1/2 Heisenberg antiferromagnet. Recent experiments[14] find the magnon spectrum for a two-dimensional antiferromagnet to be identical to the spin wave theory spectrum with a quantum scale factor $Z \approx 1.18$. This has been observed theoretically using slave boson techniques[15] and by exactly diagonalizing the 4×4 system with periodic boundary conditions.[16] The energy maxima are at symmetry vectors $k = (\pi/2, \pi/2)$, $(0, \pi)$ and symmetry equivalents. The minimum is at $k = (0, 0)$. The gap between the lowest $k = (\pi, \pi)$ and the ground state at $(0, 0)$ tends to zero as $N \to \infty$.

If, the direct oxygen-oxygen hopping t_{pp} is the only nonzero parameter, then the minimum is at $k = (0, 0)$. (This is $k = (\pi, \pi)$ in the standard phase convention.)

Calculations of a single hole in a 4×4 lattice[3,5,17] for the complete Hamiltonian (1) find the minimum to be at $(\pi/2, \pi/2)$ for a large range of parameters. Also, the

bandwidth for the lowest excited states is found to scale as J_{dd}.

II. THE INFINITE RANGE HEISENBERG MODEL AND THE SPN STATES

Consider an infinite lattice of spins $S = 1/2$ that can be partitioned into two sublattices A, B such that the nearest neighbor of every A site is a B site and vice versa. For the Hamiltonian H_{dd} in two dimensions, there is little hope at present of writing down explicit wavefunctions for the ground state and the lowest energy excitations. However, there is a sister system that can be solved exactly. This is the Infinite Ranged Heisenberg Antiferromagnet (IRHA).

If every A spin interacts with every B spin with the same coupling, then the Hamiltonian can be written as,

$$H^{IRHA} = J_{dd} \sum_{\substack{i \in A \\ j \in B}} \underline{S}_i \cdot \underline{S}_j = J_{dd} \underline{S}_A \cdot \underline{S}_B, \tag{2}$$

where $\underline{S}_A$, $\underline{S}_B$ are the total spins on the A, B lattices respectively. This is easily diagonalized,

$$H = \frac{1}{2} J_{dd} (\underline{S}^2 - \underline{S}_A{}^2 - \underline{S}_B{}^2), \tag{3}$$

where $\underline{S}$ is the total spin angular momentum $\underline{S}_A + \underline{S}_B$ of the lattice. The ground state and the lowest energy excitations have each sublattice in a state of *maximum* spin, (i.e., ferromagnetic), but coupled to form a state of small total spin, $S = 0, 1, 2, \ldots$. These states are exactly the spin projections[18] of the classical Néel state onto states of total spin $S = 0, 1, 2, \ldots$. This can be seen by observing that the two sublattices of the Néel state have maximum spin and opposite z-projections. We denote these states as the Spin Projected Néel (SPN) states and write the SPN

state of total spin S and z-projection M as $|SM>_{SPN}$. The nearest neighbor spin correlation for the SPN state is easy to evaluate by noticing that in the SPN state there is no information on the separation between spins. In the SPN state, every A site looks the same as every other A site and the correlation of two neighboring A and B sites is the same as the correlation between any two A and B sites.

$$_{SPN}<00|\underline{S}_1\cdot\underline{S}_2|00>_{SPN}=(2/N)<\underline{S}_A\cdot\underline{S}_2>=(2/N)^2<\underline{S}_A\cdot\underline{S}_B>,$$

where N is the total number of sites, half A and half B. Since, $S_A^2 = S_B^2 = (N/4)[(N/4)+1]$, we obtain,

$$<\underline{S}_1\cdot\underline{S}_2>=-\frac{1}{4}-\frac{1}{N}. \tag{4}$$

As $N\to\infty$, $<S_1\cdot S_2>\to -\frac{1}{4}$, the correlation of the classical Néel state. This is not a good approximation to the ground state of the Heisenberg Hamiltonian (where with only nearest neighbor coupling, $<S_1\cdot S_2>=-0.3346\pm 0.0001$ for a square lattice[19−23]). On the other hand, for small N the SPN states become good representations of the eigenstates of the Heisenberg Antiferromagnet.

For periodic 4×1 and 2×2 copper lattices, the system is effectively infinite ranged and the SPN states are indeed the exact eigenstates. For 1-D, the $k=\pi/2$ state is not a SPN state since the two sublattices have different spins. However, it is an eigenstate of (2), the infinite range Hamiltonian. A single oxygen hole in the 4×1 and 2×2 copper lattices has only $2^2-2=2$ remaining copper spins participating in the SPN state. In this case, the spins on the two sublattices are necessarily the same ($S_A=S_B=1/2$) and the background is exactly represented by SPN states.

From direct calculations, the 4×4 lattice with periodic boundary conditions has nearest neighbor spin correlation[16,24] -0.3509 whereas the SPN singlet gives -0.3125. When the lattice has a single hole, there are $4^2 - 2 = 14$ remaining spins to form an SPN state. This leads to a correlation of -0.3214 for this doping of $1/16 = 6.25\%$. This doping is at the lower end of the range for high T_c superconductors and hence the SPN description should be a good approximation for the superconductive phase.

The SPN states have either $k = (0, 0)$ or (π, π). Thus the SPN states cannot be used directly to model the excitation spectrum of the Heisenberg antiferromagnet. However, for small systems, the SPN singlet and triplet are good approximations to the ground state and first excited state.

The correlation length of the copper spins is found by neutron scattering[7] to be equal to the mean separation of the oxygen holes and is independent of temperature in the superconducting range of dopings. Hence, we may consider the copper spins surrounding an oxygen hole as antiferromagnetically coupled to each other but not strongly coupled to the copper spins more than one hole-hole separation apart. If the number of copper spins surrounding an oxygen hole is small, then the lowest excitations of the spins are well approximated by SPN states. As the doping is increased, fewer copper spins per hole are available to form an SPN state leading to increasingly better approximations to the antiferromagnetic ground state. In the superconducting regime, the SPN states describe the effect of the antiferromagnetic coupling of the copper spins.

For dopings in the superconducting regime, the following sections incorporate the effects of the J_{dd} term by requiring the background to be in an SPN state.

Increased doping leads to an effective lattice size of the Heisenberg Antiferromagnetic Hamiltonian that is reduced, yet the range of the J_{dd} term remains one lattice spacing. The ratio of the range of the antiferromagnetic coupling to the size of the system tends to unity so that the system behaves more and more like an Infinite Ranged Heisenberg Antiferromagnetic. Thus, above $\approx 6\%$ doping, *no knowledge of the excitations of the Heisenberg Antiferromagnet is required. The system has "no options" but to become more and more SPN-like as information about the relative separation of spins is lost.*

III. THE THREE-SPIN POLARON

A. SINGLET AND TRIPLET HOPPING TERMS

Consider an oxygen hole and a single neighboring copper spin coupled into a state of spin S and z-projection M. If the hole hops to another oxygen bound to the same copper site, then total spin symmetry implies that the hole and the copper spin in the new configuration have the same S and M. Suppressing the orbital part, this can be written as, $|SM> \rightarrow C|SM>$ where S, M are the spin and z-projection of the hole-copper pair and C is a constant that can be a function of S. The state of the remaining spins not involved in the hop remains unchanged and so is not written. The only possible pairs are singlet $J = 0$ and triplet $J = 1$. The most general singlet and triplet hops (singlet and triplet copper-oxygen bond resonances) can be written as,

$$|1M> \rightarrow t_\tau |1M>, \tag{5a}$$

$$|00> \rightarrow -t_\sigma |00> . \tag{5b}$$

The minus sign on the singlet bond resonance is chosen so that t_τ, t_σ will be positive and in defining the singlet and triplet states, the hole spin is *always* taken first. Typically, $t_\sigma \approx 3t_\tau$ when direct oxygen-oxygen hopping (t_{pp}) is not considered. In band theory, there is no coupling to the background spins so $t_\tau = -t_\sigma$.

To find expressions for t_τ, t_σ in terms of t_a, t_b, we consider separately the hopping of singlet and triplet pairs. Assume a hole hops to the right. Represent the hole spin by an arrow and the copper spin by a plus or minus sign. For singlet hopping,

$$\sqrt{2}|00>= (\uparrow -) - (\downarrow +) \rightarrow - t_a(-\uparrow) + (t_a + t_b)(+\downarrow) + t_a(+\downarrow) - (t_a + t_b)(-\uparrow),$$

$$= -(2t_a + t_b)[(-\uparrow) - (+\downarrow)].$$

Therefore,

$$t_\sigma = 2t_a + t_b, \tag{6a}$$

and similarly,

$$t_\tau = t_b. \tag{6b}$$

Next we include the H_{pp} hopping terms with H_{pdp}. t_{pp} represents the delocalization of the p_σ orbital into its neighboring diagonally adjacent hole sites. In the Bonding Phase Convention, t_{pp} as defined in (1) is always positive, $t_{pp} = |t_{pp}|$. Let $t_\tau^{pp}, t_\sigma^{pp}$ be the total matrix elements for triplet and singlet hops in the diagonal directions. Then, the combined H_{pdp} and H_{pp} leads to,

$$t_\tau^{pp} = t_\tau - |t_{pp}|, \tag{7a}$$

$$t_\sigma^{pp} = t_\sigma + |t_{pp}|. \tag{7b}$$

Typically, $t_{pp} \approx t_a, t_b$ so singlet hops dominate for diagonal hops. There is a wide range of parameters[8,9,10] that may be used in calculations. We find that there is no

qualitative difference for different choices. In this paper, we take, $t_{pp} = 3$, $t_a = 2.5$, $t_b = 3.5$, $J_{pd} = 5$, resulting in $t_\tau = 3.5$, $t_\sigma = 8.5$, $t_\tau^{pp} = 0.5$, $t_\sigma^{pp} = 11.5$ in units of J_{dd}. For oxygen hops along the same axis, the t_{pp} hopping term is much smaller (our Hamiltonian neglects it) so that t_τ *cannot* be neglected in comparison to t_σ.

B. DOUBLET AND QUARTET STATES

By lattice translational invariance, the eigenstates of the Hamiltonian are completely specified by the symmetry vector $\underline{k}$ and linear combinations of all the configurations with the hole restricted to the x-axis and y-axis site in a single unit cell. It is convenient to classify the eight possible states that can be formed with a hole at a fixed site and its two adjacent copper spin sites. We use as a basis the eigenstates of the Hamiltonian containing solely the J_{pd} antiferromagnetic coupling of the hole with the two copper sites. There are three eigenstates: two doublets $J = 1/2$ and one quartet $J = 3/2$. The ground state (denoted D_g) has energy $-J_{pd}$ and spin $J = 1/2$ with the two copper spins in a triplet; it is symmetric under reflection about the oxygen site. D_g is the Emery[1,2] state and can be written,

$$(+\frac{1}{2})_{D_g} = \sqrt{\frac{2}{3}} \downarrow |11> - \sqrt{\frac{1}{3}} \uparrow |10> . \tag{8a}$$

In this expression, the $+1/2$ is the spin projection along the z direction (in spin space), the subscript is the symmetry, the arrows are the hole spin projections, and $|JM>$ represents the state of the two copper spins. The D_u and Q states are defined as,

$$(+\frac{1}{2})_{D_u} = \uparrow |00>, \tag{8b}$$

$$(+\frac{3}{2})_{Q} = \uparrow |11>, \tag{8c}$$

with energies $E_{D_u} = 0$, $E_Q = +\frac{1}{2}J_{pd}$. The Hamiltonian is taken to be $H_{pd} = J_{pd}[\underline{\sigma} \cdot \underline{S}_L + \underline{\sigma} \cdot \underline{S}_R]$; L, R are the copper spins to the left and right of the hole. For two dimensions, the hole may also be on the y-axis site and a convention is necessary for the ordering of the adjacent copper sites. For a hole on the x-axis, the adjacent spins can be considered as the East and West spins and for a hole on the y-axis, the South and North spins. We take the West and South copper spins to be first when constructing the coupled copper spin states adjacent to the hole.

The D_g and D_u states both involve a resonance between the two states with the hole singlet coupled to one or the other of the adjacent copper spins. The Q state, having total spin 3/2 cannot have the hole singlet coupled to either copper spin. The D_g and Q states have the two coppers triplet coupled whereas, in D_u, they are singlet coupled. Letting (00) represent the hole and adjacent copper in a spin singlet state, these relations are,

$$(\sigma)_{D_g} = -\frac{1}{\sqrt{3}}\Big[\big(\sigma(00)\big) + \big((00)\sigma\big)\Big], \tag{9a}$$

$$(\sigma)_{D_u} = \big(\sigma(00)\big) - \big((00)\sigma\big). \tag{9b}$$

σ can take values + or −. Once again, the hole spin is always taken first when coupled to an adjacent copper. When the hole hops to a new site around the right copper, the first term on the right hand side of (9) leads to a singlet hop with matrix element $-t_\sigma$. The second term represents the hole bonded to the left copper spin. This term needs to be rewritten in terms of configurations where the hole is coupled to the copper on the right. The relations for the transformation of a singlet bond to bonds on the opposite copper are,

$$\big((00)+\big) = \frac{1}{\sqrt{2}}\big(-(11)\big) - \frac{1}{2}\big(+(10)\big) + \frac{1}{2}\big(+(00)\big), \tag{10a}$$

$$\big((00)-\big) = -\frac{1}{\sqrt{2}}\big(+(1-1)\big) + \frac{1}{2}\big((-(10)\big) + \frac{1}{2}\big(-(00)\big), \tag{10b}$$

$$\big(+(00)\big) = \frac{1}{\sqrt{2}}\big((11)-\big) - \frac{1}{2}\big((10)+\big) + \frac{1}{2}\big((00)+\big), \tag{10c}$$

$$\big(-(00)\big) = -\frac{1}{\sqrt{2}}\big((1-1)+\big) + \frac{1}{2}\big((10)-\big) + \frac{1}{2}\big((00)-\big). \tag{10d}$$

It is most convenient for further development to write the expressions for the D_g and D_u states as linear combinations of terms with the hole coupled to a particular copper site. Both states have total spin 1/2 and since the singlet bonding configuration (e.g., $(\sigma(00))$ has $J = 1/2$, the terms with triplet coupling must also have $J = 1/2$. There is only one way to make a total $J = 1/2$ from a triplet and a $j = 1/2$ spinor. Let $(\sigma)^R_{\frac{1}{2}}$ be the right side triplet coupled $J = 1/2$ state with z-projection σ. The superscript is the copper site to which the hole is coupled; the subscript is the total spin (in this case 1/2). The spin 1/2 triplet states can be written,

$$(+)^R_{\frac{1}{2}} = \sqrt{\frac{2}{3}}\big(-(11)\big) - \frac{1}{\sqrt{3}}\big(+(10)\big), \tag{11a}$$

$$(-)^R_{\frac{1}{2}} = -\sqrt{\frac{2}{3}}\big(+(1-1)\big) + \frac{1}{\sqrt{3}}\big(-(10)\big). \tag{11b}$$

The relations for left triplet coupling are obtained by interchanging the left and right spins,

$$(+)^L_{\frac{1}{2}} = \sqrt{\frac{2}{3}}\big((11)-\big) - \frac{1}{\sqrt{3}}\big((10)+\big), \tag{11c}$$

$$(-)^L_{\frac{1}{2}} = -\sqrt{\frac{2}{3}}\big((1-1)+\big) + \frac{1}{\sqrt{3}}\big((10)-\big). \tag{11d}$$

Combining (9),(10),(11),

$$(\sigma)_{D_g} = -\frac{\sqrt{3}}{2}\big(\sigma(00)\big) - \frac{1}{2}(\sigma)^R_{\frac{1}{2}} = -\frac{\sqrt{3}}{2}\big((00)\sigma\big) - \frac{1}{2}(\sigma)^L_{\frac{1}{2}}, \tag{12a}$$

$$(\sigma)_{D_u} = \frac{1}{2}\big(\sigma(00)\big) - \frac{\sqrt{3}}{2}(\sigma)^R_{\frac{1}{2}} = -\frac{1}{2}\big((00)\sigma\big) + \frac{\sqrt{3}}{2}(\sigma)^L_{\frac{1}{2}}, \tag{12b}$$

with corresponding inverse relations,

$$\big(\sigma(00)\big) = -\frac{\sqrt{3}}{2}(\sigma)_{D_g} + \frac{1}{2}(\sigma)_{D_u}, \tag{13a}$$

$$\big((00)\sigma\big) = -\frac{\sqrt{3}}{2}(\sigma)_{D_g} - \frac{1}{2}(\sigma)_{D_u}, \tag{13b}$$

$$(\sigma)^R_{\frac{1}{2}} = -\frac{1}{2}(\sigma)_{D_g} - \frac{\sqrt{3}}{2}(\sigma)_{D_u}, \tag{13c}$$

$$(\sigma)^L_{\frac{1}{2}} = -\frac{1}{2}(\sigma)_{D_g} + \frac{\sqrt{3}}{2}(\sigma)_{D_u}. \tag{13d}$$

For completeness, the transformations between Q states and triplet coupled states is included.

$$(+\frac{3}{2})_Q = \big(+(11)\big), \tag{14a}$$

$$(+\frac{1}{2})_Q = \frac{1}{\sqrt{3}}\big(-(11)\big) + \sqrt{\frac{2}{3}}\big(+(10)\big), \tag{14b}$$

$$(-\frac{1}{2})_Q = \frac{1}{\sqrt{3}}\big(-(1-1)\big) + \sqrt{\frac{2}{3}}\big(+(10)\big), \tag{14c}$$

$$(-\frac{3}{2})_Q = \big(-(1-1)\big). \tag{14d}$$

The inverse relations for triplet coupling in terms of the $j = 1/2,\, 3/2$ states are,

$$\big(+(11)\big) = (+\frac{3}{2})_Q, \tag{15a}$$

$$\big(-(11)\big) = \sqrt{\frac{2}{3}}(+\frac{1}{2})^R_{\frac{1}{2}} + \frac{1}{\sqrt{3}}(+\frac{1}{2})_Q, \tag{15b}$$

$$\big(+(10)\big) = -\frac{1}{\sqrt{3}}(+\frac{1}{2})^R_{\frac{1}{2}} + \sqrt{\frac{2}{3}}(+\frac{1}{2})_Q, \tag{15c}$$

$$\big(+(1-1)\big) = -\sqrt{\frac{2}{3}}(-\frac{1}{2})^{R}_{\frac{1}{2}} + \frac{1}{\sqrt{3}}(-\frac{1}{2})_{Q}\,, \tag{15d}$$

$$\big(-(10)\big) = \frac{1}{\sqrt{3}}(-\frac{1}{2})^{R}_{\frac{1}{2}} + \sqrt{\frac{2}{3}}(-\frac{1}{2})_{Q}\,, \tag{15e}$$

$$\big(-(1-1)\big) = (-\frac{3}{2})_{Q}\,. \tag{15f}$$

Again, interchanging the left and right spins gives the equivalent relations for left coupling.

If t_σ, t^{pp}_σ, and J_{pd} are the only non-zero interactions, then because the Q state has no singlet bond character, the D states cannot mix at all with Q. Therefore, one expects to see very little Q character when the $t_\tau, t^{pp}_\tau, J_{dd}$ interactions are turned on. This can be inferred from the calculations of Lang et al.[5] who calculated the ground state energy and wavefunction at each symmetry $\underline{k}$ for a single mobile hole in a 4×4 lattice with periodic boundary conditions. The spin-spin correlation was evaluated for the hole with its two adjacent Cu spins and also the correlation of the left and right Cu with each other is calculated.

To extract the amount of Q character from the results of Ref. 5, we use the following observation. Using the notation from above, we define $\underline{\sigma}$ to be the hole spin and $\underline{S}_L$, $\underline{S}_R$ the spins of the adjacent copper sites. Form the total angular momentum operator of the three spins $J = \sigma + S_R + S_L$. J can take the values 1/2, 3/2. Now the sum of the correlations of the hole to the Cu plus the Cu-Cu correlation is,

$$< \sigma \cdot S_R > + < \sigma \cdot S_L > + < S_R \cdot S_L >= \frac{1}{2}J^2 - \frac{9}{8}. \tag{16}$$

For the D state, $J = 1/2$ and the sum is $-3/4$; for pure Q, $J = 3/2$ and the sum becomes $+3/4$. For parameters typical of high T_c systems, Lang et al.[5] find the

sum is at most 2% larger than -0.75 leading to less than 2% Quartet character. Therefore, we can neglect all scattering into Q states.

IV. SINGLE HOLE INTERACTING WITH Cu SPIN BACKGROUND

A. ONE DIMENSION

Allowing those states in which the three spins copper-hole-copper form a doublet and the remaining spins form an SPN configuration, we find the minimum energy at $\pi/2$.

Here we calculate the energies of the states with total spin of 1/2. The formalism is most easily developed in 1-D. The generalization to 2-D is carried out in the following section.

Assume that the effect of J_{dd} is to drive the background spin into an SPN configuration. This is only valid for sufficiently large doping, but we assume SPN regardless of doping. We first construct a general DSPN (doublet SPN) state. To make a total spin of one half, the background SPN spins must be either singlet or triplet. There are only two possibilities for each of the three-spin systems, D_g or D_u. This leads to a total of four possible spin one half states. (In 2-D, there will be exactly eight possible states, four on the x-axis and four on the y-axis.) Due to total spin conservation, we need to consider only the $+1/2$ z-projection.

In general, the Hamiltonian can be written in terms of six hopping coefficients containing all the information about the lattice size. Three of the coefficients arise from singlet hops and the other three from triplet hops.

We define four singlet bond states:

$$|0>^{R}_{SPN} = [+(00)]|00>_{SPN}, \tag{17a}$$

$$|1>^{R}_{SPN}= \sqrt{\frac{2}{3}}[-(00)]|11>_{SPN} -\frac{1}{\sqrt{3}}[+(00)]|10>_{SPN}, \tag{17b}$$

$$|0>^{L}_{SPN}= [(00)+]|00>_{SPN}, \tag{17c}$$

$$|1>^{L}_{SPN}= \sqrt{\frac{2}{3}}[(00)-]|11>_{SPN} -\frac{1}{\sqrt{3}}[(00)+]|10>_{SPN} . \tag{17d}$$

The convention on the ordering of the spin sublattices is the site to the left of the three-spin system is *always* on the A sublattice and the site to the right is *always* on the B sublattice. In the SPN state, the A lattice spins are taken first.

Taking $t_\sigma = -1$ in equation $(5b)$, define the constants $A_\sigma, B_\sigma, C_\sigma, D_\sigma$ by the mixing of a right hop,

$$|0>^{R}_{SPN} \rightarrow A_\sigma |0>^{L}_{SPN} + B_\sigma |1>^{L}_{SPN}, \tag{18a}$$

$$|1>^{R}_{SPN} \rightarrow C_\sigma |0>^{L}_{SPN} + D_\sigma |1>^{L}_{SPN} . \tag{18b}$$

If there are N sites in the SPN state, there are $N/2$ on each sublattice making the total spin of each sublattice $J = N/4$. Under inversion about the hole site, the two sublattices are swapped. Therefore, $|00>_{SPN} \rightarrow s|00>_{SPN}, |1M>_{SPN} \rightarrow (-s)|1M>_{SPN}$ where $s = (-)^{2J}$. Applying the inversion operator to equations (17) gives the corresponding relations for left hops of left coupled states. Since the Hamiltonian is Hermitian, $C_\sigma = -B_\sigma$. The general formulas for the coefficients are,

$$A_\sigma = (-)^{2J+1}(-\frac{1}{2}), \tag{19a}$$

$$B_\sigma = (-)^{2J+1}(\frac{1}{2}\sqrt{\frac{J+1}{J}}), \tag{19b}$$

$$D_\sigma = (-)^{2J+1}[\frac{1}{2}(\frac{J-1}{J})]. \tag{19c}$$

These equations are derived in the appendix. As $J \to \infty$, $-A_\sigma = B_\sigma = D_\sigma \to 1/2(-)^{2J+1}$. *No matter how large the lattice becomes, there is always finite scattering into SPN states.* Also, note that A_σ, B_σ are never zero while $D_\sigma = 0$ at $J = 1$.

We now define the four states,

$$|1>=(+)_{D_g}|00>_{SPN}, \tag{20a}$$

$$|2>=\sqrt{\frac{2}{3}}(-)_{D_u}|11>_{SPN}-\frac{1}{\sqrt{3}}(+)_{D_u}|10>_{SPN}, \tag{20b}$$

$$|3>=\sqrt{\frac{2}{3}}(-)_{D_g}|11>_{SPN}-\frac{1}{\sqrt{3}}(+)_{D_g}|10>_{SPN}, \tag{20c}$$

$$|4>=(+)_{D_u}|00>_{SPN}\ . \tag{20d}$$

$|1>$ and $|2>$ transform with parity $+s$ under inversion while $|3>$ and $|4>$ have parity $-s$.

Using equations (9) and (18), the Hamiltonian matrix for the t_σ hops is,

$$H = P(-t_\sigma)\begin{pmatrix} \frac{3}{2}A_\sigma\cos k & \frac{\sqrt{3}}{2}B_\sigma\cos k & -i\frac{3}{2}B_\sigma\sin k & -i\frac{\sqrt{3}}{2}A_\sigma\sin k \\ \frac{\sqrt{3}}{2}B_\sigma\cos k & -\frac{1}{2}D_\sigma\cos k & i\frac{\sqrt{3}}{2}D_\sigma\sin k & -i\frac{1}{2}B_\sigma\sin k \\ i\frac{3}{2}B_\sigma\sin k & -i\frac{\sqrt{3}}{2}D_\sigma\sin k & \frac{3}{2}D_\sigma\cos k & -\frac{\sqrt{3}}{2}B_\sigma\cos k \\ i\frac{\sqrt{3}}{2}A_\sigma\sin k & i\frac{1}{2}B_\sigma\sin k & -\frac{\sqrt{3}}{2}B_\sigma\cos k & -\frac{1}{2}A_\sigma\cos k \end{pmatrix}, \tag{21}$$

where k is the symmetry vector or momentum. P is the parity of the translation operator used after a hole hop to translate the system so that the hole returns to its starting position. It arises from the total antisymmetry of the wave function. This is most easily seen by the following simple example. Consider a hole in a 2×1 lattice that is originally in the state $(\uparrow ++) = p^\dagger_\uparrow d^\dagger_{1+} d^\dagger_{2+}|vacuum>$. A hop to the right and then a translation to the left gives the state $t_\tau p^\dagger_\uparrow d^\dagger_{2+} d^\dagger_{1+}|vac>=$

$-t_\tau p^\dagger_\uparrow d^\dagger_{1+} d^\dagger_{2+}|vac>$. Therefore $P=-1$. In one dimension, P is just the parity of the cycle $(1,2,\ldots,L)$ where L is the number of copper spins. For L even, this cycle is always odd. In two dimensions, $P=1$ for $L\times L$ lattices with L even. Physically, the parity is not important; it can be absorbed into the momentum $k\to k+\pi$ for $P=-1$.

If t_σ is the only non-zero parameter (J_{dd}, J_{pd}, t_τ all zero), then the ground state of the Hamiltonian has $k=\pi$ and the three-spin polaron is pure Emery (D_g). The background copper spins are completely ferromagnetic and the total spin of the ground state is $J_{max}-1$, where J_{max} is the maximum possible spin of the complete copper and oxygen hole system. This is true *regardless* of the dimensionality of the lattice for pure singlet hops *only*. The proof uses the method of Lieb, Schultz, and Mattis[25] for the spin symmetry of the ground state of the Heisenberg Antiferromagnet. Thus the ground state is DSPN with maximum J_{SPN}. For the state with total spin J_{max}, only triplet (t_τ) hops are possible and so $E(J_{max})=0$.

When J_{dd} is non-zero, the pure D_g ground state is unfavorable due to the ferromagnetic background. H_{dd} prefers a small total spin whereas, t_σ prefers a large spin. This suggests that the background becomes ferromagnetic when the doping is increased sufficiently (since the number of background copper spins per oxygen hole is reduced). Figures 2*a* and 2*b* show the energies for a single hole in a 4×1 lattice assuming the three-spin polaron can only be a doublet. Figures 3*a* and 3*b* show the projection onto the D_g state. Figures 2*a* and 3*a* have $J_{dd}=0$, while figures 2*b* and 3*b* have $J_{dd}=0.1t_\sigma$. For nonzero J_{dd}, the ground state has spin 1/2 and there is strong mixing of D_g and D_u for all k [see (21)]. *It is the coupling of the background copper spins that strongly mixes D_g (Emery) with D_u.* The effect

of H_{dd} has been directly incorporated into the SPN background.

For triplet hops, equations analogous to (17) may be defined with the three spin states from equations $(13a), (13b)$ replaced by the corresponding $J = 1/2$ triplet coupled states in equations $(13c), (13d)$. In the same way, coefficients A_τ, B_τ, D_τ are defined that contain all the lattice size information in the Hamiltonian for triplet hops. The triplet hop coefficients are derived in the appendix; their values are,

$$A_\tau = (-)^{2J+1}(-\frac{1}{2}), \tag{22a}$$

$$B_\tau = (-)^{2J+1}(-\frac{1}{6})\sqrt{\frac{J+1}{J}}, \tag{22b}$$

$$D_\tau = (-)^{2J+1}(\frac{3J+1}{6J}). \tag{22c}$$

As $J \to \infty$, $-A_\tau = D_\tau \to (-)^{2J+1}(1/2)$, $B_\tau \to (-)^{2J+1}(-\frac{1}{6})$. There is always finite triplet scattering into SPN states regardless of the lattice size.

From (9), the Hamiltonian for triplet hops is,

$$H = P(t_\tau) \begin{pmatrix} \frac{1}{2}A_\tau \cos k & -\frac{\sqrt{3}}{2}B_\tau \cos k & -i\frac{1}{2}B_\tau \sin k & i\frac{\sqrt{3}}{2}A_\tau \sin k \\ -\frac{\sqrt{3}}{2}B_\tau \cos k & -\frac{3}{2}D_\tau \cos k & -i\frac{\sqrt{3}}{2}D_\tau \sin k & -i\frac{3}{2}B_\tau \sin k \\ i\frac{1}{2}B_\tau \sin k & i\frac{\sqrt{3}}{2}D_\tau \sin k & \frac{1}{2}D_\tau \cos k & \frac{\sqrt{3}}{2}B_\tau \cos k \\ -i\frac{\sqrt{3}}{2}A_\tau \sin k & i\frac{3}{2}B_\tau \sin k & \frac{\sqrt{3}}{2}B_\tau \cos k & -\frac{3}{2}A_\tau \cos k \end{pmatrix}. \tag{23}$$

In this basis, the J_{pd} contribution to the Hamiltonian is diagonal, equations $(8), (20)$. The matrix is,

$$H = (J_{pd}) \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{24}$$

The contribution to the Hamiltonian due to the J_{dd} coupling can be broken into two pieces: the first matrix $(25a)$ containing the coupling of the three-spin

polaron to the two neighboring copper spins and the second matrix $(25b)$ containing the energies of the SPN spin background states plus the energy of the two copper spins neighboring the hole.

Since $S_1 \cdot S_2 = \frac{1}{2}C_{1,2} - \frac{1}{4}$, where $C_{1,2}$ is the transposition swapping the $1, 2$ spins, it is the C term that mixes various hole states. The action of the C operator leads to exchange coefficients in correspondence to $(19), (22)$. The first matrix becomes,

$H/(\frac{1}{2}J_{dd}) =$

$$\begin{pmatrix} \frac{3}{2}A_\sigma^C + \frac{1}{2}A_\tau^C - 1 & \frac{\sqrt{3}}{2}B_\sigma^C - \frac{\sqrt{3}}{2}B_\tau^C & 0 & 0 \\ \frac{\sqrt{3}}{2}B_\sigma^C - \frac{\sqrt{3}}{2}B_\tau^C & \frac{1}{2}D_\sigma^C + \frac{3}{2}D_\tau^C - 1 & 0 & 0 \\ 0 & 0 & \frac{3}{2}D_\sigma^C + \frac{1}{2}D_\tau^C - 1 & \frac{\sqrt{3}}{2}B_\sigma^C - \frac{\sqrt{3}}{2}B_\tau^C \\ 0 & 0 & \frac{\sqrt{3}}{2}B_\sigma^C - \frac{\sqrt{3}}{2}B_\tau^C & \frac{1}{2}A_\sigma^C + \frac{3}{2}A_\tau^C - 1 \end{pmatrix}. \tag{25a}$$

There is a factor of $1/2$ in front of the matrix because for 1-D, there is only one copper spin adjacent to one of the coppers in the polaron. In 2-D, there are three copper spins adjacent to either copper spin in the polaron leading to a factor of $3/2$. The coefficients A_σ^C, B_σ^C, etc. can be written in terms of the A_σ, B_σ, etc. as shown in the appendix. The relations are: $A_\sigma^C = sA_\sigma$, $B_\sigma^C = (-s)B_\sigma$, $D_\sigma^C = (-s)D_\sigma$ and similarly for A_τ^C, etc.

The second matrix is very simple. The nearest neighbor spin correlation for the SPN state with total spin σ is $(\frac{1}{2}\sigma^2)(2/N)^2 - \frac{1}{4} - \frac{1}{N}$. This correlation is multiplied by the number of possible nearest neighbor spin pairs that can be formed; in one dimension, this is $(N+2)-3 = N-1$ or $4J-1$ where J is total spin on a sublattice. For the two-dimensional lattice, this is $2(N+2) - 7 = 8J - 3$. Define G to be this number. There is a total energy shift of $E_{shift} = G(-1/4 - 1/N)J_{dd}$. For states

with the SPN total spin of one, there is an additional term $+(2/N)^2 G J_{dd}$. Finally, for D_g states, there is a $+(1/4)J_{dd}$ and for D_u, $-(3/4)J_{dd}$ due to the two copper spins adjacent to the hole. Thus the second matrix is,

$$H = (J_{dd}) \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & (\frac{1}{2J})^2 G - \frac{3}{4} & 0 & 0 \\ 0 & 0 & (\frac{1}{2J})^2 G + \frac{1}{4} & 0 \\ 0 & 0 & 0 & -\frac{3}{4} \end{pmatrix} + E_{shift}. \qquad (25b)$$

The sum of equations $(21), (23) - (25)$ is the full one-dimensional Hamiltonian for a total spin 1/2. The effect of J_{dd} is incorporated by the choice of spin one-half DSPN wavefunctions.

For the final Hamiltonian, the minimum energy is found at $\pi/2$ for all lattice sizes (see figure 4). The projection of these eigenstates onto the Emery polaron is typically from 65% to 80% *even when the hole-copper antiferromagnetic coupling J_{pd} is zero. The singlet and triplet hopping terms are sufficient to select a large projection onto the Emery state.* The hopping terms have no knowledge of the Emery and D_u states; they select between singlet coupling and triplet coupling configurations. Since singlet hops are the dominant effect, the Hamiltonian for the singlet hopping term (21) is most important.The diagonal elements for the Emery states $(20a)$, $(20c)$ are about three times as large as the D_u diagonal terms. For all k values, the off diagonal terms in (21) for the mixing of the two Emery states are three times larger than the mixing of the two D_u states. This leads to an Emery projection that is three times larger than the D_u projection, or Emery is $\approx 75\%$. Hence, the hopping polaron (HP) must always have some D_u character.

B. SINGLE HOLE IN TWO DIMENSIONS

The power of using the SPN state becomes obvious in higher dimensions. Since for the SPN state, (i) *every* spin on a particular sublattice looks exactly the

same as any other spin on the same sublattice and (ii) spin-spin correlations between sublattices are independent of the particular spins chosen, then the background spins do not know from which direction the hole hopped. This enormous simplification allows the same six hopping coefficients, equations (19), (22), and spin interchange coefficients, to be used in constructing the total Hamiltonian.

The first step in writing the 8×8 matrix for the Hamiltonian in two dimensions, is defining a convention on the ordering of spins in the D_u and the SPN parts of the wavefunction. In two dimensions it is not correct to label the adjacent copper spins to a hole by whether they are left or right of the hole. In Section III. B., the spin positions were defined by the directions East, West, South, and North. When constructing the coupled copper spins for a hole on the x-axis, the West spin is taken first and for the y-axis, the South spin is taken first. The first copper spin to the West (South) of the hole and its adjacent copper is always on the A sublattice and the spin to the East (North) is always on the B sublattice. This is illustrated in Figure 5.

We define the corresponding states to equation (20) for the hole on the y-axis as,

$$|5>=(+)_{D_g}|00>_{SPN}, \tag{26a}$$

$$|6>=\sqrt{\frac{2}{3}}(-)_{D_u}|11>_{SPN}-\frac{1}{\sqrt{3}}(+)_{D_u}|10>_{SPN}, \tag{26b}$$

$$|7>=\sqrt{\frac{2}{3}}(-)_{D_g}|11>_{SPN}-\frac{1}{\sqrt{3}}(+)_{D_g}|10>_{SPN}, \tag{26c}$$

$$|8>=(+)_{D_u}|00>_{SPN}\ . \tag{26d}$$

There are two kinds of hops in the Hamiltonian; hops to the same axis or diagonal hops to the other axis. For hops to the same axis, the Hamiltonian for the 1-D

system is correct, the only change being $k \rightarrow k_x, k_y$ and $P = 1$. For diagonal hops, the matrix is,

$H/(-t_\sigma^{pp}) =$

$$\begin{pmatrix} \frac{3}{4}A_\sigma s f_+(k_x)f_+^*(k_y) & \frac{\sqrt{3}}{4}B_\sigma s f_+(k_x)f_+^*(k_y) & \frac{3}{4}B_\sigma s f_-(k_x)f_+^*(k_y) & \frac{\sqrt{3}}{4}A_\sigma s f_-(k_x)f_+^*(k_y) \\ \frac{\sqrt{3}}{4}B_\sigma s f_+(k_x)f_+^*(k_y) & -\frac{1}{4}D_\sigma s f_+(k_x)f_+^*(k_y) & -\frac{\sqrt{3}}{4}D_\sigma s f_-(k_x)f_+^*(k_y) & \frac{1}{4}B_\sigma s f_-(k_x)f_+^*(k_y) \\ \frac{3}{4}B_\sigma s f_+(k_x)f_-^*(k_y) & -\frac{\sqrt{3}}{4}D_\sigma s f_+(k_x)f_-^*(k_y) & -\frac{3}{4}D_\sigma s f_-(k_x)f_-^*(k_y) & \frac{\sqrt{3}}{4}B_\sigma s f_-(k_x)f_-^*(k_y) \\ \frac{\sqrt{3}}{4}A_\sigma s f_+(k_x)f_-^*(k_y) & \frac{1}{4}B_\sigma s f_+(k_x)f_-^*(k_y) & \frac{\sqrt{3}}{4}B_\sigma s f_-(k_x)f_-^*(k_y) & \frac{1}{4}A_\sigma s f_-(k_x)f_-^*(k_y) \end{pmatrix} \quad (27)$$

where $f_\pm(k) = 1 \pm se^{ik}$ and $s = (-)^{2J}$ is the parity of $|00>_{SPN}$ under reflection, as before. Equation (27) represents the singlet hopping of x-axis states to y-axis states. There is a similar contribution due to hops from the y-axis to the x-axis. This is obtained from (27) by interchanging k_x, k_y and taking the transpose.

The triplet hop matrix can be obtained easily from the singlet hop matrix (27) by the following transformations:

$$A_\sigma \rightarrow A_\tau, \quad B_\sigma \rightarrow B_\tau, \quad D_\sigma \rightarrow D_\tau, \quad (28a)$$

$$< D_g|H|D_g > \rightarrow \frac{1}{3} < D_g|H|D_g >, \quad < D_u|H|D_u > \rightarrow 3 < D_u|H|D_u >,$$

$$< D_g|H|D_u > \rightarrow - < D_g|H|D_u >, \quad (28b)$$

$$-t_\sigma^{pp} \rightarrow t_\tau^{pp}. \quad (28c)$$

The D_g and D_u in equation (28b) just represent those states that have doublet g or u character respectively. For example, $< 1|H_{t_\sigma}|8 >$ is a matrix element of type $< D_g|H|D_u >$, so under the transformation it acquires a minus sign.

We find that $(\pi/2, \pi/2)$ is the minimum for all reasonable values of the parameters regardless of the lattice size. Figures 6a and 6b show the energy and Emery

projections for $t_\sigma = 8.5$, $t_\tau = 3.5$, $t_{pp} = 3$, and $J_{pd} = 0$ and 5 in units of J_{dd} for a 4×4 lattice. Lang et al.[5] find that the minimum energy states for $(\pi/2, \pi/2)$ and $(\pi, \pi/2)$ have total spin of one half. They find the separation of these states to be $\approx J_{dd}$ for a large range of parameters. Similar results are observed by Frenkel et al.[3] This is in agreement with the results obtained from the above 8×8 matrix. The projection onto the Emery polaron is in the range $65 - 80\%$ (figure 6*b*) compared to 90% for the exact calculations.[3,5]

C. ATTRACTION OF HOLES

A simple qualitative argument makes it clear that there is a net short range attraction between holes. The argument is based upon the number of nearest neighbor background spin pairs G (see IV. A.). The attractive coupling arises from the changes in antiferromagnetic energy of the background spins that comprise the SPN states. When the holes are sufficiently close, there are more nearest neighbor background spin pairs as compared to when the spins are sufficiently far apart. For example, consider two holes on a 4×4 lattice, figures 7a and 7b. The doping is 12.5% and there are $16 - 4 = 12$ background spins in the SPN configuration. When the holes are far apart (figure 7a), two extra pairs become available and there are a total of 18 nearest neighbor bonds for the background spins. This change gives a lowering of the antiferromagnetic energy of $2(+1/4 + 1/12)J_{dd}$ or $(2/3)J_{dd}$. Due to Coulomb repulsion of the two holes, we only allow hole configurations in which the two three-spin polarons do not overlap. This leads to 12 configurations with an extra bond for the background spins and 3 configurations with two extra bonds. There are 10 configurations with no extra background bonds. Averaging over these

configurations leads to a binding energy for the pair

$$\Delta E_{pair} = \frac{12 \cdot 1 + 3 \cdot 2}{12 + 3 + 10} \cdot (+\frac{1}{4} + \frac{1}{12}) J_{dd}$$

$$\Delta E_{pair} = \frac{6}{25} J_{dd}. \tag{29}$$

For $J_{dd} = 1450K$, $\Delta E_{pair} = 348K$.

This calculation leads to only a qualitative estimate of the attractive coupling. No account has been taken of the possible momenta of the holes and with it the probabilities of the holes being on the different axes. Also, in the above discussion the background spins are assumed to be predominantly in a singlet configuration. There is also the issue of whether the 12 background spins form a single SPN state as above, or two SPN states with 6 spins in each. For scaling arguments to make sense, the latter should be the case. Breaking the 12 spins into two 6 spin SPN states corresponds to keeping the correlation length of the copper spins the same as the mean separation of the holes.

A second estimate of the pairing energy is as follows. The energy is $-81.00 J_{dd}$ for two holes in a 4×4 periodic lattice with the 12 remaining background copper spins in a single SPN state. The total spin is taken to be singlet. The three-spin polarons are not allowed to overlap as above. The ground state is at $k = (0,0), (\pi,0), (0,\pi)$ with $(0,0)$ doubly degenerate (figure 8). Adding this to the energy of a 4×4 Heisenberg Antiferromagnet ($E_{AF} = -11.23 J_{dd}$) leads to an energy $-92.23 J_{dd}$, more than twice the energy of a single DSPN hole in a 4×4 periodic lattice by $0.60 J_{dd} = 870K$ using the parameters in figure 8. We believe this method of calculating the binding energy of two holes is not reliable, since energies are compared at *different* dopings (in this case 6.25% and 12.5%).

V. CONCLUSIONS

By writing the Hamiltonian in a form that makes spin conservation most apparent, we see that the matrix elements for singlet hops are about three times greater than triplet hops for hops along the same axis. For diagonal hops, the direct oxygen-oxygen delocalization t_{pp}, reduces the triplet hopping further while enhancing singlet hops, leading to $t_{\sigma}^{pp} \approx 20 t_{\tau}^{pp}$.

The hole-copper antiferromagnetic coupling J_{pd}, gives a natural basis of states for representing the three-spin system of a hole and its two neighbors. The two doublet states, D_g and D_u, can be written solely as linear combinations of configurations with singlet coupling of the hole to one of the coppers. The state Q has no singlet coupling; it is unfavorable not only because of the J_{pd} term but also because singlet hops are dominant. These observations allow the Quartet polaron configuration to be neglected in calculating the ground state and low energy excitations of the system. The Hopping Polaron (HP) is a linear combination of the D_g (Emery) state and D_u with a projection onto D_g that for $J_{pd} = 0$ is about three times larger than D_u. Mixing of D_u into the HP is a result of the hopping terms and the J_{dd} Cu-Cu antiferromagnetic coupling. The D_u term cannot be neglected even for nonzero J_{pd}.

The antiferromagnetic coupling is included by the observation that the Heisenberg Antiferromagnet becomes effectively infinite ranged for small lattice sizes. The effects of doping the system destroy the long range order of the antiferromagnet and allow eigenstates of the IRHA to be used locally to model the copper-copper spin coupling. The low energy excitations of the infinite range Hamiltonian are spin projections of the classical Néel state and are denoted SPN states. In an SPN state, every spin on one sublattice is equally correlated to every spin on the other

sublattice and the sublattices take the maximum spin allowed.

A variational wavefunction is constructed that contains only doublet three-spin polaron character with the remaining spins in an SPN state. These are the DSPN states. Only states with total spin 1/2 are considered. In evaluating the mean energy of the trial state, one sees that there is always finite scattering into SPN states by singlet or triplet hops regardless of the lattice size.

The minimum at $(\pi/2, \pi/2)$ observed in accurate calculations (of a single hole in a 4×4 lattice) is obtained by minimizing this simpler DSPN wavefunction. The bandwidth scales as J_{dd}, in agreement with calculations. With an SPN background, the minimum at this symmetry persists as the lattice size becomes infinite.

Finally, a qualitative argument is given for a net attraction between holes at 12.5% doping, leading to $\Delta E_{pair} \approx 6/25 J_{dd}$. This is based on the geometry of the SPN state. The energy of a SPN state can be reduced solely by increasing the connectivity of the spins in this state. A short range attraction is expected due to this effect.

VI. APPENDIX

To evaluate the coefficients in (19), (22), explicit representations of the singlet and triplet SPN states are needed. In the SPN state, each sublattice has maximum spin, say j. The SPN singlet and triplet states with each sublattice of spin j can be written,[26]

$$|00>_{SPN} = \sum_m |j; -m>_A \, |j; m>_B \, \frac{(-)^{j-m}}{\sqrt{2j+1}}, \tag{30a}$$

$$|11>_{SPN} = \sum_m |j; -m>_A \, |j; m+1>_B \, (-)^{j-m+1}(-)^{2j+1} \sqrt{\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}, \tag{30b}$$

$$|10>_{SPN}=\sum_m |j;m>_A\ |j;-m>_B\ (-)^{j-m}m\sqrt{\frac{3}{(2j+1)(j+1)j}}, \qquad (30c)$$

$$|1-1>_{SPN}=\sum_m |j;m>_A\ |j;-m-1>_B\ (-)^{j-m-1}\sqrt{\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}, \quad (30d)$$

where the subscript A, B refers to the sublattice. Note that under interchange of sublattices, $A \leftrightarrow B$, the SPN singlet transforms as, $|00>_{SPN} \rightarrow s|00>_{SPN}$ where $s=(-)^{2j}$. The triplet states transform with parity $-s$. Equations (30) are useful with A and B interchanged. For example, in (30b), this requires $-m \rightarrow m+1$. One final relation is necessary. That is the Clebsch-Gordon coefficients for the coupling of a $j-\frac{1}{2}$ spin with a spin $\frac{1}{2}$ to form a total spin j. This is derived by applying the spin lowering operator to $|jj>=|j-\frac{1}{2};j-\frac{1}{2}>\uparrow$, and gives,

$$|jm>=\sqrt{\frac{j+m}{2j}}|j-\frac{1}{2};m-\frac{1}{2}>\uparrow+\sqrt{\frac{j-m}{2j}}|j-\frac{1}{2};m+\frac{1}{2}>\downarrow . \qquad (31)$$

Consider equation (18a) and $t_\sigma=-1$. The site to the left of the three spin polaron is on the A sublattice, therefore the site to the right of the polaron is on the B sublattice. For a hop to the right, the B sublattice spin becomes part of the polaron and the + spin that was part of the polaron becomes the spin to the left. But then the A and B sublattices must be interchanged in order that the spin to the left is again on the A sublattice. Equation (32) shows this process explicitly.

$$(\bullet^B\ \bullet^A\ [+(00)]\ \bullet^B\ \bullet^A) \rightarrow_{Right} (\bullet^B\ \bullet^A\ +[(00)\bullet]\ \bullet^A)$$

$$\rightarrow_{A\leftrightarrow B} (\bullet^A\ \bullet^B\ +^A[(00)\bullet]\ \bullet^B). \qquad (32)$$

Applying (31) to the B sublattice in (30a),

$$[+(00)]|00>_{SPN}=\frac{1}{\sqrt{2j+1}}\sum_m(-)^{j-m}\left\{\sqrt{\frac{j-m}{2j}}|j-\frac{1}{2};-m-\frac{1}{2}>_B\uparrow\right.$$

$$+\sqrt{\frac{j+m}{2j}}|j-\frac{1}{2};-m+\frac{1}{2}>_B\downarrow\Bigg\}[+(00)]|j;m>_A, \tag{33}$$

where $\uparrow$, $\downarrow$ represent the spin on the B sublattice site to the right of the polaron. Hopping to the right and letting $A \leftrightarrow B$ gives,

$$\frac{1}{\sqrt{2j+1}}\sum_m(-)^{j-m}\Bigg\{\sqrt{\frac{j-m}{2j}}|j-\frac{1}{2};-m-\frac{1}{2}>_A\uparrow[(00)+]$$

$$+\sqrt{\frac{j+m}{2j}}|j-\frac{1}{2};-m+\frac{1}{2}>_A\uparrow\Bigg\}[(00)-]|j;m>_B, \tag{34}$$

The overlap of (34) with $[(00)+]|00>_{SPN}$ is A_σ.

$$A_\sigma=\sum_m\frac{1}{2j+1}\left[\sqrt{\frac{j-m}{2j}}\right]^2(-)^{j+m}(-)^{j-m}$$

$$=(-)^{2j}\{\frac{1}{2}\sum\frac{1}{2j+1}-\frac{1}{2j(2j+1)}\sum m\},$$

$$A_\sigma=(-)^{2j+1}\left(-\frac{1}{2}\right). \tag{35}$$

Taking the overlap of (34) with $[(00)+]|10>_{SPN}$ will give $-1/\sqrt{3}B_\sigma$,

$$-\frac{1}{\sqrt{3}}B_\sigma=\frac{1}{\sqrt{2j+1}}\sum(-)^{j-m}(-)^{j+m+1}m\sqrt{\frac{3}{j(2j+1)(j+1)}}\left[\sqrt{\frac{j-m}{2j}}\right]^2$$

$$=(-)^{2j}\frac{1}{2j(2j+1)}\sqrt{\frac{3}{j(j+1)}}\sum m^2.$$

Using the relation,

$$\sum_{m=-(2j+1)}^{2j+1}m^2=\frac{1}{3}j(2j+1)(j+1), \tag{36}$$

leads to,

$$B_\sigma=(-)^{2j+1}\left[\frac{1}{2}\sqrt{\frac{j+1}{j}}\right]. \tag{37}$$

For $-1/\sqrt{3}D_\sigma$, the overlap of $[(00)+]|10>_{SPN}$ with a right hop of $\sqrt{2/3}[-(00)]|11>_{SPN}$ $-1/\sqrt{3}|10>_{SPN}$ is required.

$$[-(00)]|11>_{SPN}=[-(00)]\sum(-)^{j-m+1}(-)^{2j+1}\sqrt{\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}$$

$$\left\{\sqrt{\frac{j+m+1}{2j}}|j-\frac{1}{2};m+\frac{1}{2}>_B\uparrow+\sqrt{\frac{j-m-1}{2j}}|j-\frac{1}{2};m+\frac{3}{2}>_B\downarrow\right\}|j;-m>_A .$$

Hopping to the right with sublattice interchange leads to,

$$[(00)+]\sum(-)^{j-m+1}(-)^{2j+1}\sqrt{\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}\sqrt{\frac{j+m+1}{2j}}|j-\frac{1}{2};m+\frac{1}{2}>_A\downarrow\ |j;-m>_B$$

$$+(term\ with\ [(00)-]).$$

Overlap with $[(00)+]|10>_{SPN}$ is,

$$\sum(-)^{j-m+1}(-)^{j-m}m\sqrt{\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}}\times$$

$$\sqrt{\frac{3}{(2j+1)(j+1)j}}\sqrt{\frac{j+m+1}{2j}}\sqrt{\frac{j-m}{2j}}$$

$$=(-)^{2j+1}\sum(-)\frac{1}{2\sqrt{2}}\cdot\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)j^2}\cdot m. \tag{38}$$

Similarly the contribution from $\sqrt{2/3}[-(00)]|11>_{SPN}$ is,

$$\sum(-)^{2j+1}\left(\frac{3}{2}\right)\frac{m^2(j-m)}{(j+1)(2j+1)j^2}. \tag{39}$$

Adding (38), (39) and multiplying by $-\sqrt{3}$,

$$D_\sigma=(-)^{2j+1}\cdot\frac{3}{2}\left[\frac{(j-1)}{(j+1)(2j+1)j^2}\right]\sum m^2.$$

Therefore,

$$D_\sigma = (-)^{2j+1}\left[\frac{1}{2}\left(\frac{j-1}{j}\right)\right]. \tag{40}$$

The triplet coefficients (22) may be derived by the same methods as in the singlet case. The algebra is a little more involved due to the the triplet bonded DSPN states having more terms. The A_τ coefficient is the overlap of $[(11)-]|00>_{SPN}$ with a right triplet hop ($t_\tau = 1$) of $[-(11)]|00>_{SPN}$. This is formally identical to the derivation of A_σ with the singlet bond (00) in (34) replaced everywhere with the triplet bond (11). Hence,

$$A_\tau = (-)^{2j+1}\left(-\frac{1}{2}\right). \tag{41}$$

The B_τ coefficient may be determined by calculating the scattering into the states $[(11)-]|10>_{SPN}$, $[(10)+]|10>_{SPN}$ and subtracting the quartet three-spin polaron piece. The $[-(11)]|00>_{SPN} \rightarrow [(11)-]|10>_{SPN}$ overlap is,

$$\sum (-)^{j-m}(-)^{j+m+1}\frac{m}{\sqrt{2j+1}}\sqrt{\frac{3}{(2j+1)(j+1)j}}\left[\sqrt{\frac{j+m}{2j}}\right]^2$$

$$= (-)^{2j+1}\cdot\frac{1}{2}\sqrt{\frac{j+1}{3j}}. \tag{42}$$

The overlap $[+(10)]|00>_{SPN} \rightarrow [(10)+]|10>_{SPN}$ is equal to,

$$\sum (-)^{j-m}(-)^{j+m+1}\frac{m}{\sqrt{2j+1}}\sqrt{\frac{3}{(2j+1)(j+1)j}}\left(\frac{j-m}{2j}\right)$$

$$= (-)^{2j+1}\left(-\frac{1}{2}\right)\sqrt{\frac{j+1}{3j}}. \tag{43}$$

This is exactly the negative of (42). Hence,

$$\sqrt{\frac{2}{3}}[-(11)]|00>_{SPN} -\frac{1}{\sqrt{3}}[+(10)]|00>_{SPN} \rightarrow K\left\{\sqrt{\frac{2}{3}}[(11)-]+\frac{1}{\sqrt{3}}[(10)+]\right\}|10>_{SPN},$$

where K is the right hand side of (42) and only those terms with a projection onto $(+)^L_{\frac{1}{2}}|10>_{SPN}$ are shown. Using equations (11) for the left bonded triplets, leads to the expression for B_τ,

$$-\frac{1}{\sqrt{3}}B_\tau = K\left(\left[\sqrt{\frac{2}{3}}\right]^2 + \frac{1}{\sqrt{3}}\cdot\frac{-1}{\sqrt{3}}\right),$$

$$B_\tau = (-)^{2j+1}\left(-\frac{1}{6}\right)\sqrt{\frac{j+1}{j}}. \tag{44}$$

Once again, the quartet scattering has to be subtracted in order to determine D_τ. This is most easily done by finding the coefficient of $[(11)+]|1-1>_{SPN}$. Only $-1/\sqrt{3}(+)^R_{\frac{1}{2}}|10>_{SPN}$ can scatter into this state and then only the term, $(-1/\sqrt{3})(\sqrt{2/3})[-(11)]|10>_{SPN}$. The overlap $\sqrt{2/3}(-)^R_{\frac{1}{2}}|11>_{SPN}$ $-1/\sqrt{3}(+)^R_{\frac{1}{2}}|10>_{SPN} \rightarrow [(11)+]|1-1>_{SPN}$ has coefficient, $(-)^{2j+1}[-1/(6j)]$. Therefore,

$$\sqrt{\frac{2}{3}}(-)^R_{\frac{1}{2}}|11>_{SPN} -\frac{1}{\sqrt{3}}(+)^R_{\frac{1}{2}}|10>_{SPN} \rightarrow D_\tau\left[\sqrt{\frac{2}{3}}(-)^L_{\frac{1}{2}}|11>_{SPN} -\frac{1}{\sqrt{3}}(+)^L_{\frac{1}{2}}|10>_{SPN}\right]$$

$$+Q\left[\frac{1}{\sqrt{2}}(+\frac{3}{2})_Q|1-1>_{SPN} -\frac{1}{\sqrt{3}}(+\frac{1}{2})_Q|10>_{SPN} +\frac{1}{\sqrt{6}}(-\frac{1}{2})_Q|11>_{SPN}\right], \tag{45}$$

and

$$Q = (-)^{2j+1}\left(-\frac{1}{3\sqrt{2}j}\right). \tag{46}$$

In (45), the scattering into SPN singlet states is not shown. Once the coefficient for scattering of the left hand side of (45) into $[(1-1)+]|11>_{SPN}$ is known, then from

the right hand side of (45) and (46), D_τ can be determined. The only term in (45) that can scatter into $[(1-1)+]|11>_{SPN}$ is $-2/3[+(1-1)]|11>_{SPN}$. The overlap $[+(1-1)]|11>_{SPN} \rightarrow [(1-1)+]|11>_{SPN}$ is,

$$\sum (-)^{j+m}(-)^{2j+1}(-)^{j-m+1}(-)^{2j+1}\left[\frac{3(j-m)(j+m+1)}{(j+1)(2j+1)(2j)}\right]\left(\frac{j+m+1}{2j}\right)$$

$$= (-)^{2j+1}\left[\frac{(2j+1)}{4j}\right].$$

Equating the two sides of (45) for the coefficient of $[(1-1)+]|11>_{SPN}$,

$$-\frac{2}{3}D_\tau + \frac{1}{3\sqrt{2}}Q, = \left(-\frac{2}{3}\right)(-)^{2j+1}\left[\frac{2j+1}{4j}\right]$$

and solving for D_τ,

$$D_\tau = (-)^{2j+1}\left(\frac{3j+1}{6j}\right). \tag{47}$$

A^C_σ, B^C_σ, D^C_σ are defined in complete analogy to the singlet hopping coefficients in equations (18) where instead of a right singlet hop, the right copper spin in the polaron is swapped with the adjacent spin in the SPN state. Denote this operation by C_R with an analogous definition for C_L.

$$|0>^R_{SPN} \rightarrow A^C_\sigma|0>^L_{SPN} + B^C_\sigma|1>^L_{SPN}, \tag{48a}$$

$$|1>^R_{SPN} \rightarrow -B^C_\sigma|0>^L_{SPN} + D^C_\sigma|1>^L_{SPN}\ . \tag{48b}$$

These coefficients are related in a simple way to the singlet hopping coefficients already derived in this appendix. Consider equation (32). The intermediate step before the sublattice exchange $A \leftrightarrow B$, just represents the interchanging of a B sublattice spin with the + spin in the polaron. Note that by definition of the SPN

state, it is irrelevant which B sublattice spin is involved in the swap with the polaron. Thus, the effect of a singlet right hop ($t_\sigma = -1$) *without sublattice interchange on* $[+(00)]|00>_{SPN}$ *gives the same result as* C_R *acting on* $[(00)+]$. Therefore, by applying sublattice interchange $A \leftrightarrow B$ to the right hand side of equations (18) gives equations (48). The parity of a singlet SPN state under interchange is $s = (-)^{2j}$ and $-s$ for SPN triplets. Therefore,

$$A^C_\sigma = sA_\sigma, \quad B^C_\sigma = (-s)B_\sigma, \quad D^C_\sigma = (-s)D_\sigma. \tag{49}$$

Similarly,

$$A^C_\tau = sA_\tau, \quad B^C_\tau = (-s)B_\tau, \quad D^C_\tau = (-s)D_\tau. \tag{50}$$

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FIGURE CAPTIONS

1. The Bonding Phase Convention. With this choice of phases, the first three terms in (1) have the same sign regardless of the direction of the hole hop.
2. Energy of a single hole in a 4×1 periodic Cu-O lattice. The three-spin polaron is assumed to be a doublet. The total spin is $S = 1/2$ ($\bullet$) and $S = 3/2$ ($\circ$) where, (a) $J_{dd} = 0$, and (b) $J_{dd} = 0.1t_\sigma$. J_{pd} and t_τ are zero.
3. D_g (Emery) projection of a single hole in a 4×1 periodic lattice. As in figure 2, the three-spin polaron is assumed to be a doublet. The total spin is $S = 1/2$ ($\bullet$) and $S = 3/2$ ($\circ$), where $J_{dd} = 0$ in (a) and $J_{dd} = 0.1t_\sigma$ in (b). All remaining parameters are zero.
4. (a) Energy and (b) Emery projection for a single Doublet hole in an infinite SPN 1-D Cu-O lattice. The values of the parameters are, $t_\sigma = 8.5$, $t_\tau = 3.5$, $J_{dd} = 1.0$, with $J_{pd} = 0$ ($\bullet$) and $J_{pd} = 5.0$ ($\circ$).
5. Definition of the A and B sublattices of the copper spins ($\bullet$), for a hole ($\circ$) on the x and y axes. For an oxygen hole on the x-axis, the West copper site is on the A sublattice and for a hole on the y-axis, the South copper is on the A sublattice. For the D_u state on the x(y) axis, the Western(Southern) copper spin is taken first.
6. (a) Energy and (b) Emery projection for a single hole in a 4×4 periodic lattice. We take $t_\sigma = 8.5$, $t_\tau = 3.5$, $t_{pp} = 3.0$, $J_{dd} = 1.0$, with $J_{pd} = 0.0$ ($\bullet$) and $J_{pd} = 5.0$ ($\circ$).
7. Two holes in a 4×4 lattice with periodic boundary conditions. The dotted lines connect copper adjacent pairs that are not counted in calculating the energy of the SPN state of the remaining background copper spins of the

lattice. In (a), there are 14 such pairs leading to $G = 32 - 14 = 18$ pairs in the SPN background. In (b), the holes are closer together increasing the number of available pairs for the SPN state by 2. So $G = 20$.

8. Energies of the lowest and first excited states of two Doublet holes in a single SPN background on a 4×4 periodic lattice. We assume that the two three-spin polarons do not overlap. The parameters are, $t_\sigma = 8.5$, $t_\tau = 3.5$, $t_{pp} = 3.0$, $J_{dd} = 1.0$, $J_{pd} = 5.0$. $k = (0, 0)$ is doubly degenerate and has the same energy as $(\pi, 0)$ and $(0, \pi)$.

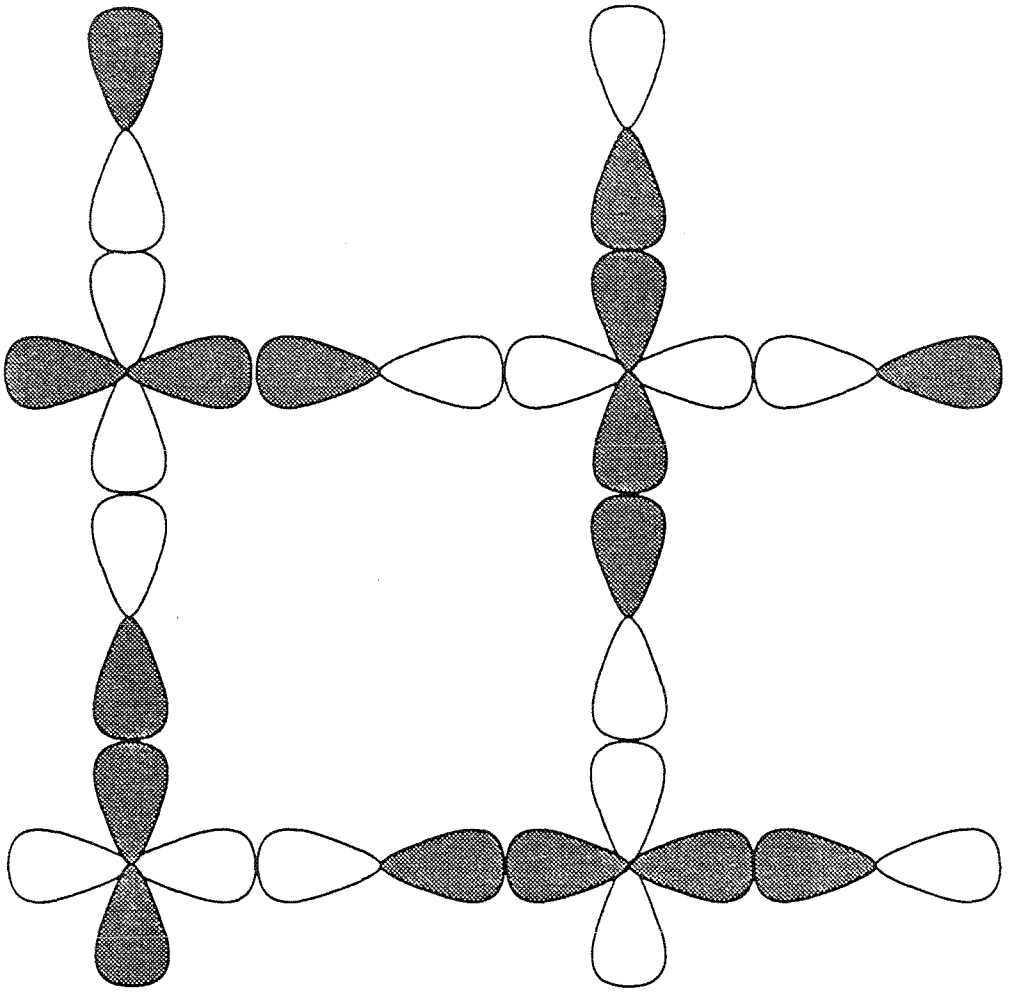

Figure 1

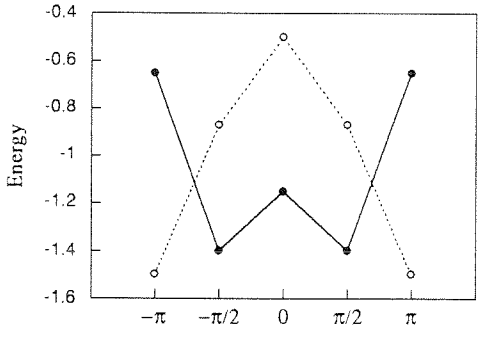

Figure 2a

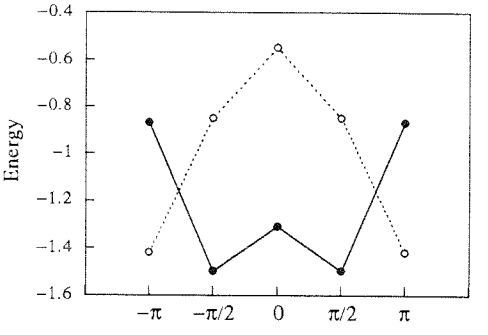

Figure 2b

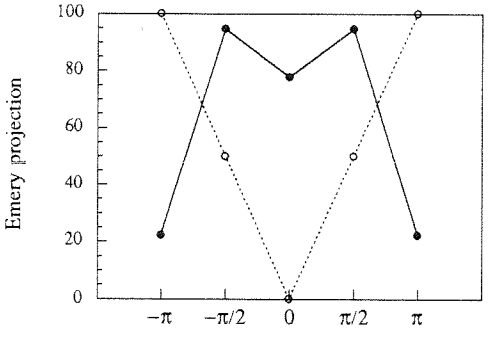

Figure 3a

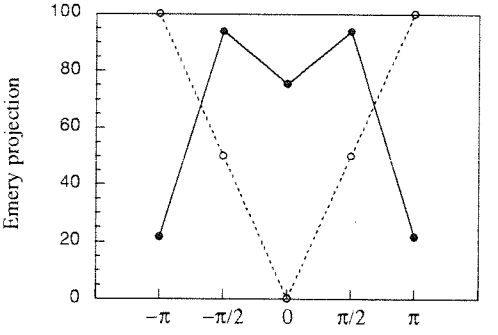

Figure 3b

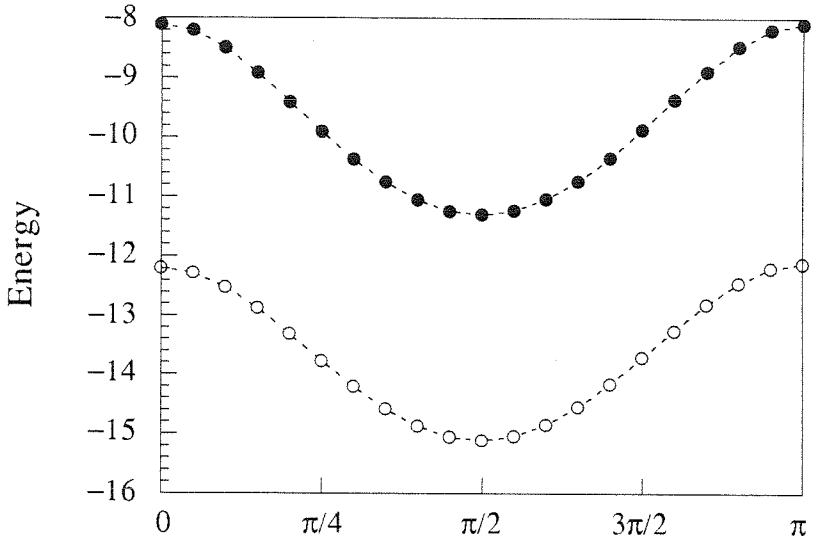

Figure 4a

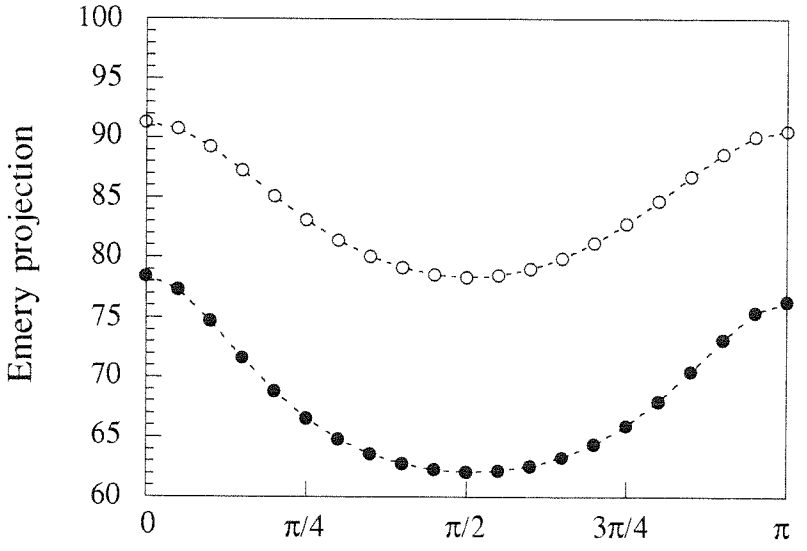

Figure 4b

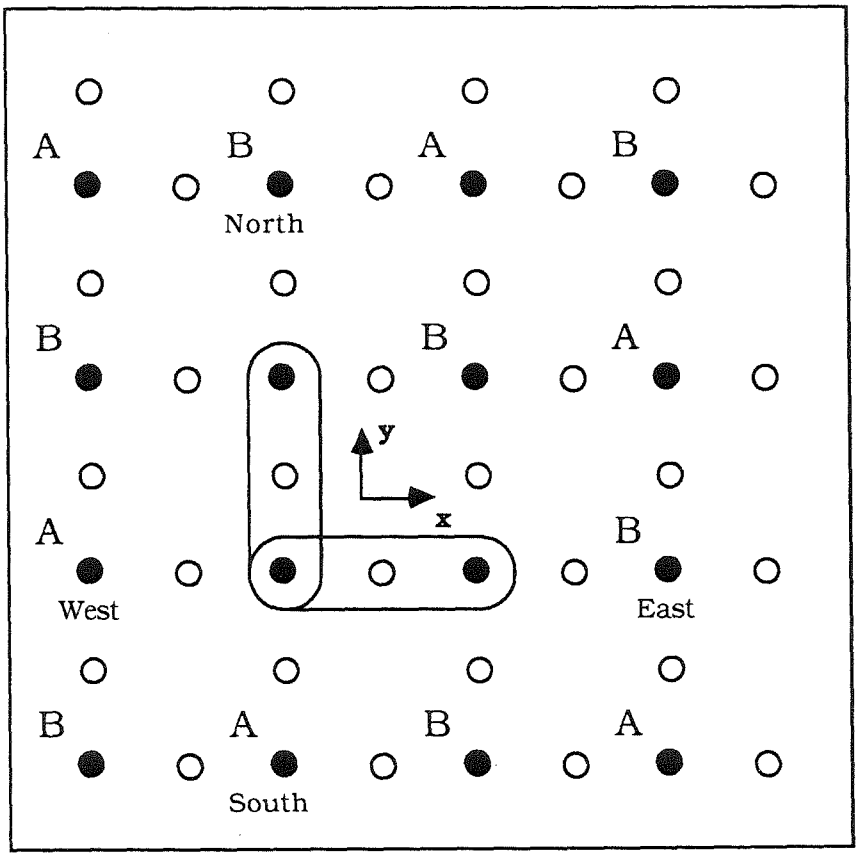

Figure 5

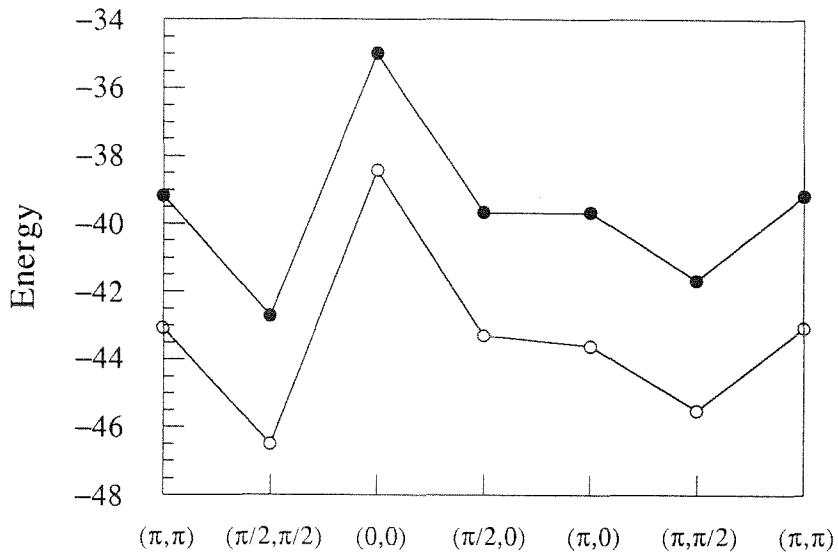

Figure 6a

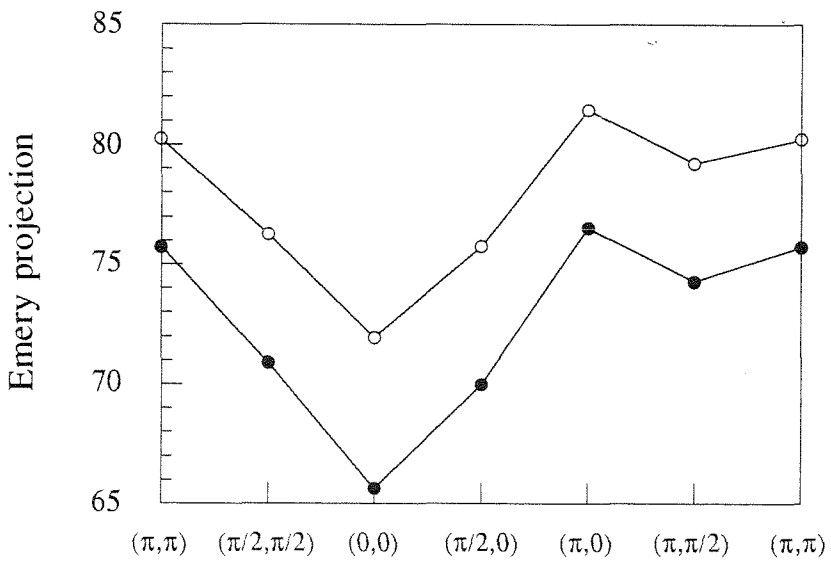

Figure 6b

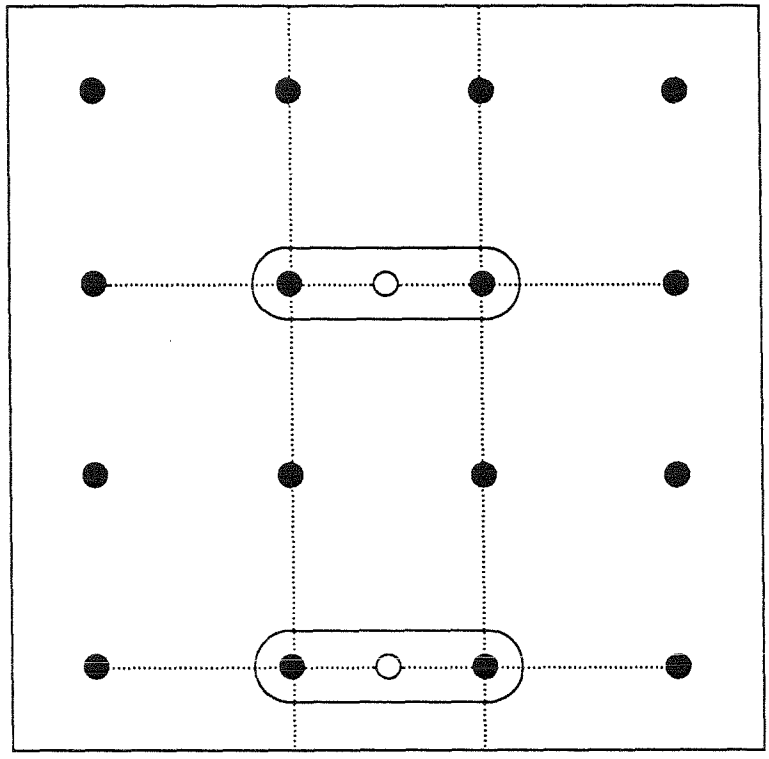

Figure 7a

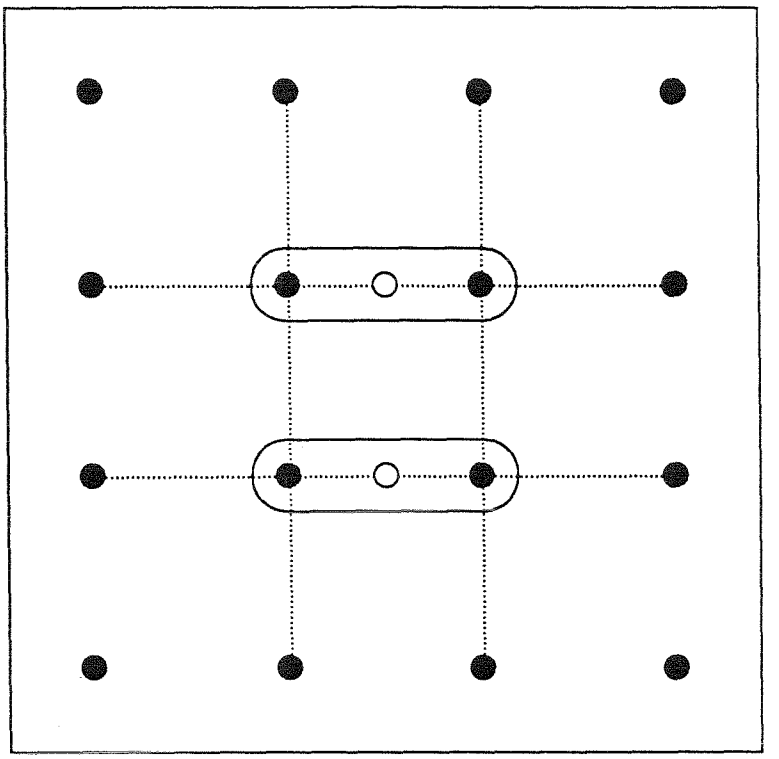

Figure 7b

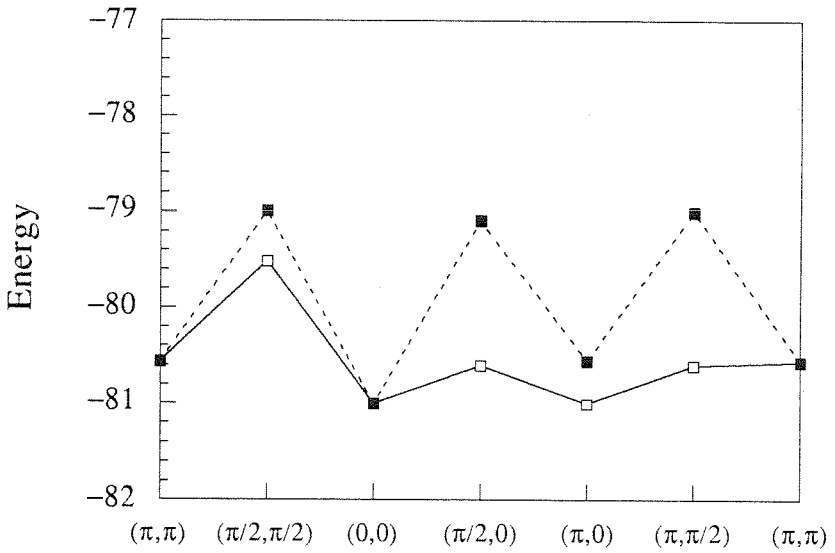

Figure 8

Chapter 2

An Exact Solution to a Strongly Coupled Hubbard Model in 1-D for High T_c Superconductors: Cu Ferromagnetism in 1-D

ABSTRACT

A stongly coupled Hamiltonian for the motion of oxygen holes in a 1-D Cu-O lattice is solved exactly for all dopings. The Hamiltonian is based upon the three-band Hubbard models for high T_c superconductors with the restrictions that oxygen holes may only hop to neighboring oxygen sites, exchanging spin with the intervening copper in the process, and that oxygen holes may not reside on the same site.

The spin and charge degrees of freedom (spinons and holons) of the system decouple. The spinon spectrum is the spectrum of the 1-D Heisenberg Antiferromagnet. The holons are spinless non-interacting fermions in a cosine band.

The Cu-Cu spin correlation in the ground state increases linearly with doping from the value for an infinite antiferromagnet (-0.443) to the value of the *next* nearest spin correlation (≈ 0.19) for an antiferromagnet. At doping, $x \approx 0.70$, the correlation becomes positive.

THE MODEL

The copper sites in the CuO_2 sheets of high temperature superconductors may be described by a single spin 1/2 hole with orbital symmetry $d_{x^2-y^2}$. Doping of the system leads to unpaired spins on the oxygen sites that can be described by a spin 1/2 hole in a p orbital (p_σ) pointing towards the two adjacent copper sites. Adjacent copper spins are coupled antiferromagnetically and the mixing of the copper and oxygen orbitals leads to the three-band Hubbard models of superconductivity [1,2].

Consider a one-dimensional Cu-O lattice as shown in figure 1. In this letter, we solve the following "spin-exchange hopping" Hamiltonian for $J_{pd} = J_{dd}$,

$$H = P\left[J_{dd}\sum_{<ij>}{}' S_i \cdot S_j + J_{pd}\sum_{<im>} S_i \cdot S_m + \frac{1}{2}t_{ex}\sum_{\substack{<lim> \\ \sigma\sigma'}} p^\dagger_{l\sigma'}p_{m\sigma}d^\dagger_{i\sigma}d_{i\sigma'}\right]P, \quad (1)$$

where the first term $H'_{dd} = J_{dd}\sum' S_i \cdot S_j$, is the antiferromagnetic coupling between adjacent copper spins $< ij >$. The prime on the summation indicates that the terms coupling two copper spins surrounding an oxygen hole to each other are not included in this sum. The second term $H_{pd} = J_{pd}\sum S_i \cdot S_m$, is the antiferromagnetic coupling of the oxygen holes S_m to neighboring copper spins S_i. The final term $H_{ex} = \frac{1}{2}t_{ex}\sum p^\dagger p d^\dagger d$, is the copper mediated hopping of oxygen holes with spin exchange of the hole and the intervening copper. $p^\dagger_{m\sigma}$ creates an oxygen hole of spin σ at m and $d^\dagger_{i\sigma}$ creates a copper hole of spin σ at i. The operator $P = \prod(1-n_{m\uparrow}n_{m_\downarrow})$ in (1) projects out states that have two oxygen holes on the same site. This is due to the large on-site coulomb repulsion of holes. In (1), the sum over nearest neighbor pairs and O-Cu-O triples is taken once. The effect of the first two terms of (1), $H'_{dd} + H_{pd}$, is shown in figure 2.

Two other terms in three-band Hubbard models are *not* included in (1). These are the direct O-O hopping $-t_{pp}\sum p^{\dagger}_{l\sigma}p_{m\sigma}$ and the copper mediated O-O hopping *without* spin exchange $H_{pdp} = -t_{pdp}\sum p^{\dagger}_{l\sigma}p_{m\sigma}$. The direct O-O hopping (t_{pp} term) is usually neglected for hops along the same axis in three-band Hubbard models. In two dimensions, the t_{pp} term for diagonal hops (from say the x-axis to the y-axis) cannot be neglected.

We use the Bonding Phase Convention illustrated in figure 3, that leads to positive values for the parameters in (1), and also for t_{pp} and t_{pdp}. Typical values for the parameters [3] are $J_{pd} = 5.1$, $t_{ex} = 10.3$, $t_{pdp} = 2.6$, $t_{pp}^{diag} = 5.2$ in units of J_{dd}. For La_2CuO_4, $J_{dd} = 0.13$eV [4].

When $J_{pd} = J_{dd}$, the first two terms in (1) reduce to the 1-D antiferromagnetic Hamiltonian on $N + M$ sites, where N is the number of copper spins and M is the number of oxygen holes.

We define a new representation for the general description of eigenstates of (1) as the product of two states: (i) $(\sigma_1, \ldots, \sigma_{N+M})$ where σ_i is the z-projection (in spin space) of the i$^{\text{th}}$ spin (copper or oxygen hole) on the $N + M$ periodic lattice, and (ii) $\psi_{n_1,\ldots,n_M}$ where $n_1, \ldots, n_M$ are the locations of the oxygen holes with $n_1 < \ldots < n_M$. This is shown clearly in figure 4. We call $(\sigma_1, \ldots, \sigma_{N+M})$ the spinon state and $\psi_{n_1,\ldots,n_M}$ the holon state.

In this Coupled Representation (CR), the projection operator P in (1) due to Coulomb repulsion, requires that the holon states $\psi_{n_1,\ldots,n_M}$, are *not* allowed, if $n_{i+1} = n_i + 1$ for some i. The Coulomb repulsion becomes a hard-core repulsion of one lattice spacing in the CR. If oxygen holes were permitted to reside on the same site, then the CR would not unambiguously define the eigenstates of (1). P in (1)

is *necessary* in order to use the CR.

The effect of H_{ex} is particularly simple in the CR of the states. H_{ex} acts only on the holon piece of the wavefunction (figure 5),

$$H_{ex}\psi_{n_1,\ldots,n_M} \rightarrow \frac{1}{2}t_{ex}\sum_{i=1}^{M}\left(\psi_{n_1,\ldots,n_i-1,\ldots,n_M} + \psi_{n_1,\ldots,n_i+1,\ldots,n_M}\right). \qquad (2)$$

In the CR, spin-exchange hopping (H_{ex}) is completely analogous to direct hopping (H_{pdp}) in the standard representation. In fact, direct hopping in the CR is analogous to spin-exchange hopping in the standard representation. By transforming to the CR, the *strong coupling* Hamiltonian (1) has been mapped into a band theory problem for the motion of spinless holes with a hard-core Coulomb repulsion that we exactly solve below. Since the spin-exchange term $(1/2)t_{ex}$ is typically two times larger than t_{pdp}, it is not reliable to apply perturbation theory assuming small t_{ex}. The above approach takes us directly into the strong coupling regime and from there perturbation theory may be applied.

The Hamiltonian (1) separates into two independent pieces: (i) the spin 1/2 Heisenberg Antiferromagnet in 1-D on a periodic $N+M$ site lattice, $H_{spinon} = H'_{dd} + H_{pd}$, that acts on the spinon part of the wavefunction, and (ii) nearest neighbor hopping of M holons on an $N+M$ site periodic lattice with an infinitely hard-core repulsion of one lattice spacing, $H_{holon} = H_{ex}$. H_{ex} acts only on ψ, the holon wavefunction.

The Hamiltonian H_{spinon}, for the spin degrees of freedom of the system is soluble by the Bethe Ansatz (BA) [5-8]. We show that the second Hamiltonian for the charge degrees of freedom of the system, H_{holon}, is also soluble by a BA. The BA for the antiferromagnet results in non-trivial transcendental equations for the

momentum (phase) shifts of the magnons, whereas, the phase shifts for H_{holon} are simple.

To uniquely specify a state in the CR, we require that the first spin is always an oxygen hole at a fixed oxygen site. By translational symmetry, a complete set of states can be specified by the total symmetry K, the spinon state, and the holon state with $n_1 = 0$ and $n_M < N+M$. If $n_M = N+M-1$, then the holon state is not allowed due to Coulomb repulsion with the hole at $n_1 = 0$. This is the boundary condition.

Let $\Theta(p)\Gamma$ be an eigenstate of the total Hamiltonian (1) where the spinon state $\Theta(p)$, is an eigenstate of the $N+M$ site antiferromagnet (H_{spinon}) with momentum p and $\Gamma = \sum a_p(n_1, \ldots, n_M)\psi_{n_1,\ldots,n_M}$. Assume $\Theta(p)\Gamma$ has total translational symmetry K. The eigenvalue equation for the coefficients $a_p(n_1, \ldots, n_M)$ (we write n_1 for notational simplicity) is,

$$e^{i(K+p)}a_p(n_1, n_2-1, \ldots, n_M-1) + e^{-i(K+p)}a_p(n_1, n_2+1, \ldots, n_M+1) +$$

$$\sum_{i=2}^{M}\left[a_p(n_1, \ldots, n_i-1, \ldots, n_M) + a_p(n_1, \ldots, n_i+1, \ldots, n_M)\right] = \frac{2E_{holon}}{t_{ex}}a_p(n_1, \ldots, n_M), \tag{3}$$

with the boundary condition,

$$a_p(0, n_2, \ldots, n_{M-1}, N+M-1) = 0. \tag{4}$$

To solve (3), consider a single hole ($M = 1$) in an N site copper lattice. There is only one value of $a(n_1)$, $a(0) = 1$, leading to $E_{holon} = t_{ex}\cos(K+p)$.

For two holes, $M = 2$, and we try the BA with $n_1 < n_2$,

$$a_p(n_1, n_2) = e^{i(k_1 n_1 + k_2 n_2 + \frac{1}{2}\varphi)} + e^{i(k_2 n_1 + k_1 n_2 - \frac{1}{2}\varphi)}. \tag{5}$$

For this choice of $a(n_1, n_2)$ to be an eigenstate of H_{holon}, E_{holon} must equal $t_{ex}(\cos k_1 + \cos k_2)$ and $k_1 + k_2 = K + p$. Due to the hard-core repulsion, we require $a(n_1, n_1 + 1) = 0$. The solution is

$$\varphi = k_1 - k_2 \pm \pi. \tag{6}$$

Substituting the above BA into the boundary condition (4) leads to

$$(N+1)k_2 + \frac{1}{2}\varphi = (N+1)k_1 - \frac{1}{2}\varphi - 2\pi\lambda + \pi,$$

where λ is an integer. From (6), we see that the boundary condition is satisfied if

$$k_1 - k_2 = \frac{2\pi\lambda}{N}, \tag{7}$$

where $k_1 = k_2$ is not allowed because (5) becomes identically zero.

The general case $M > 2$ can be solved by the BA,

$$a_p(n_1, \ldots, n_M) = \sum_P \exp\ i\left[\sum_{i=1}^{M} k_{P(i)} n_i + \frac{1}{2}\sum_{i<j} \varphi(k_{P(i)}, k_{P(j)})\right], \tag{8}$$

where the first sum is over all permutations P on the integers $(1, \ldots, M)$ and

$$\varphi(k, k') = \begin{cases} k - k' + \pi, & k < k'; \\ k - k' - \pi, & k > k'. \end{cases} \tag{9}$$

The spin-exchange momenta, $k_1, \ldots, k_M$ satisfy $\sum k_i = K + p$ and $E_{holon} = t_{ex} \sum \cos k_i$.

To show that the phase shifts in (9) satisfy the hard-core repulsion condition, let $n_{i+1} = n_i + 1$ for some i. For every even permutation P in (8), with $P(i) = q$ and $P(i+1) = q'$, there is an associated odd permutation P' such that $P'(i) = q'$

and $P'(i+1) = q$. The contribution to $a_p(n_1, \ldots, n_i, n_i+1, \ldots, n_M)$ due to the permutations P and P' is proportional to,

$$e^{i(qn_i + q'n_{i+1} + \frac{1}{2}\varphi(q,q'))} + e^{i(q'n_i + qn_{i+1} - \frac{1}{2}\varphi(q,q'))} = 0,$$

as in the two hole case.

The only condition that remains is the boundary condition (4). Consider the even permutation P such that $k_{P(1)} = q$ and $k_{P(M)} = q'$. Let P' be the corresponding odd permutation with $P'(1) = P(M)$ and $P'(M) = P(1)$. If the contribution to the left hand side of (4) from P and P' is zero for all P, then the boundary condition is satisfied. This leads to the condition,

$$(N+M-1)q' + \frac{1}{2}\sum_{1<i<M-1}\left[\varphi(q, k_{P(i)}) + \varphi(k_{P(i)}, q')\right] + \frac{1}{2}\varphi(q, q')$$

$$= (N+M-1)q + \frac{1}{2}\sum_{1<i<M-1}\left[\varphi(q', k_{P(i)}) + \varphi(k_{P(i)}, q)\right] + \frac{1}{2}\varphi(q', q) + 2\pi\mu + \pi. \quad (10)$$

From (9), we see that $\varphi(k, k') = -\varphi(k', k)$ and that $\varphi(q, k) + \varphi(k, q') = q - q' + 2\pi\nu$, where ν is an integer. Hence, (10) becomes, $q - q' = 2\pi\lambda/N$, where λ is an integer. Therefore, the boundary conditions lead to,

$$k_i - k_j = \frac{2\pi\lambda_{ij}}{N}, \quad (11)$$

with integer λ_{ij}. As in the two hole case, a_p is identically zero unless all the k_i are different. Thus, *the allowed shifted momenta for M holons in an $N+M$ site lattice are the allowed momenta for a non-interacting holon in an N site lattice.* The dispersion relation for the holon band is $\epsilon(k) = t_{ex}\cos k$. As $N \to \infty$, the ground state of (1) has total momentum $K = 0$, the spinon piece is the ground

state of the 1-D antiferromagnet (singlet with $p = 0$), and the holons fill all the k states from $\pi(1-x)$ to $\pi(1+x)$, where x is the doping M/N.

Lieb and Mattis [9] proved that there is no ferromagnetism in one dimension at $T = 0$. We show that, in the ground state, the nearest neighbor copper spin correlation increases linearly with doping from the value of the nearest neighbor spin correlation $< S_1 \cdot S_2 >_{AF}$ of the Heisenberg antiferromagnet in 1-D (-0.443) [6] to the value of the *next* nearest neighbor correlation $< S_1 \cdot S_3 >_{AF}$ of the antiferromagnet in 1-D (≈ 0.19 [10]).

In the ground state of (1), the spinon state is the ground state of the antiferromagnet and the holon state has Fermi energy $\epsilon_F = -t_{ex} \cos \pi x$. Evaluating the mean value of the Cu-Cu spin correlation, leads to the result,

$$\frac{(N-M)}{N} < S_1 \cdot S_2 >_{AF} + \frac{M}{N} < S_1 \cdot S_3 >_{AF},$$

or,

$$(1-x) < S_1 \cdot S_2 >_{AF} + x < S_1 \cdot S_3 >_{AF} . \tag{12}$$

Thus the Cu-Cu correlation becomes ferromagnetic when $x \approx 0.70$.

This is not in contradiction to the result of Lieb and Mattis. Although the total copper spin has significant high spin character (ferromagnetic), the *combined* spin symmetry of the copper and oxygen spins is singlet for the ground state.

For both 1-D and 2-D, the preference for antiferromagnetic pairing decreases with doping. It is interesting to consider whether higher doping in the 2-D systems will lead to the ferromagnetic pairing we find in 1-D for high doping.

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FIGURE CAPTIONS

1. The 1-D Cu-O infinite lattice.
2. The coupling of copper and oxygen spins due to $H'_{dd} + H_{pd}$. The oxygen spin is represented by the arrow and the dotted line indicates the copper coupling *not* included in H'_{dd}.
3. The Bonding Phase Convention on the Cu $d_{x^2-y^2}$ and O p_σ orbitals.
4. The Coupled Representation (CR). The first line shows a particular Cu and O hole state in the standard representation. The second line is the same state in the CR. The arrows are O hole spins.
5. The effect of a right spin-exchange hop in the standard and coupled representations (CR). As before, the arrow is an O hole spin and the circle is an O site without a hole. In the CR, the spinon part is unchanged due to the hole hop.

Figure 1

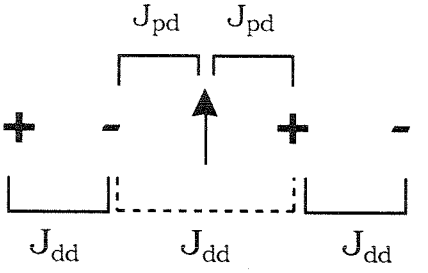

Figure 2

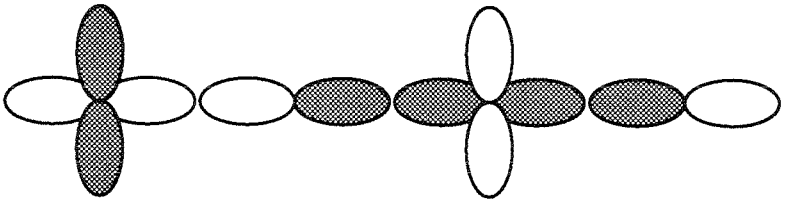

Figure 3

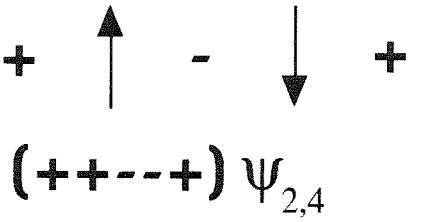

Figure 4

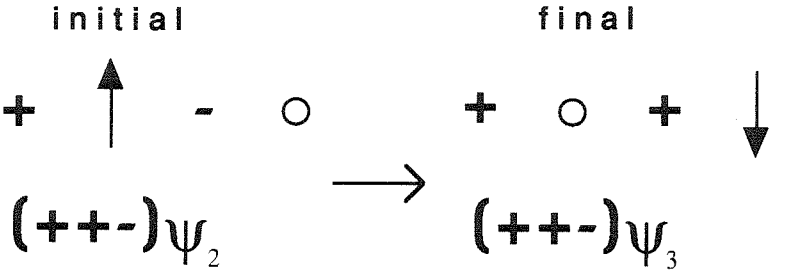

Figure 5