

EXACT SOLUTION TO A STRONGLY COUPLED HUBBARD MODEL IN 1-D FOR HIGH T_c SUPERCONDUCTORS

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ABSTRACT

A Hamiltonian for the motion of oxygen holes strongly coupled to the Cu spins in a 1-D Cu-O lattice is solved exactly for all dopings. This Hamiltonian retains the dominant O hole hopping term, that is, spin-exchange hopping of the hole spin with the intervening Cu spin and neglects the weaker non-spin-exchange hopping term. The excitations naturally separate into two independent quasiparticles: spinons and holons. It is this Hamiltonian that should be taken as the correct “zeroth order” Hamiltonian from which perturbation theory should be applied. We show that the spinon spectrum is the spectrum of the 1-D antiferromagnet incommensurate with the Cu lattice and 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 antiferromagnetic (-0.443) at $x = 0$ to ferromagnetic (≈ 0.19) at $x = 1$.

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In the three-band Hubbard models for the CuO₂ sheets of high temperature superconductors [1,2], there are two kinds of O hole hopping terms: (i) hopping *without* spin-exchange with the intervening Cu, $t_{pdp} \sum p_{\sigma}^{\dagger} p_{\sigma}$, and (ii) hopping *with* spin-exchange of the intervening Cu spin, $t_{ex} \sum p_{\sigma'}^{\dagger} p_{\sigma} d_{\sigma}^{\dagger} d_{\sigma'}$ where the sum is taken over all σ, σ' . $p_{m\sigma}^{\dagger}$ creates an O hole at m with z-projection of spin σ and $d_{i\sigma}^{\dagger}$ creates a Cu hole at i with spin σ . Due to the strong overlap of the Cu $d_{x^2-y^2}$ and the O p_{σ} orbitals, the spin-exchange hopping, t_{ex} is typically 2-3 times larger than t_{pdp} , hopping without spin-exchange.

In this paper, we solve a 1-D “three-band” Hubbard model exactly for all dopings of O holes. In this model, we retain only the spin-exchange hopping term, t_{ex} , neglecting t_{pdp} . By setting the hole-Cu antiferromagnetic coupling J_{pd} , to be equal to the Cu-Cu antiferromagnetic coupling J_{dd} ($J_{pd} = J_{dd}$), the Hamiltonian separates into two exactly soluble Hamiltonians,

$$H = H_{spinon} + H_{holon}. \quad (1)$$

H_{spinon} is the Hamiltonian for the spin degrees of freedom (spinons) and H_{holon} is for the charge degrees of freedom of the O holes (holons). The spinon Hamiltonian H_{spinon} , is the 1-D antiferromagnet on a lattice incommensurate with the Cu lattice and the holon Hamiltonian H_{holon} , is simply the motion of spinless fermions on a 1-D lattice with a hard-core repulsion of one lattice spacing.

The important physical point is that the dominant O hopping term due to the strong coupling of the hole to the Cu background spins naturally separates the system into two independent quasiparticle excitations in 1-D: spinons and holons. It is from this “strong coupling” solution ($t_{band} = 0, J_{pd} = J_{dd}$, and $t_{ex} \neq 0$) that perturbation theory should be applied, rather than from $t_{ex} = 0$.

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

$$H = P \left[J_{dd} \sum_{\langle ij \rangle} S_i \cdot S_j + J_{dd} \sum_{\langle im \rangle} S_i \cdot S_m + t_{ex} \sum_{\substack{\langle lim \rangle \\ \sigma \sigma'}} p_{l\sigma'}^{\dagger} p_{m\sigma} d_{i\sigma}^{\dagger} d_{i\sigma'} \right] P, \quad (2)$$

$$= H'_{dd} + H_{pd} + H_{ex},$$

where the first term $H'_{dd} = J_{dd} \sum' S_i \cdot S_j$, is the antiferromagnetic coupling between adjacent copper spins $\langle ij \rangle$. 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 $H_{ex} = t_{ex} \sum p^\dagger p d^\dagger d$, is the copper mediated hopping of oxygen holes with spin exchange of the hole and the intervening copper. The operator $P = \prod (1 - n_{m\uparrow} n_{m\downarrow})$ in (2) 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 (2), the sum over nearest neighbor pairs and O-Cu-O triples is taken once. The effect of the first two terms of (2), $H'_{dd} + H_{pd}$, is shown in figure 2.

Two other terms in three-band Hubbard models are *not* included in (2). These are the direct O-O hopping $-t_{pp} \sum p_{l\sigma}^\dagger p_{m\sigma}$ and the copper mediated O-O hopping *without* spin exchange $H_{pdp} = -t_{pdp} \sum p_{l\sigma}^\dagger p_{m\sigma}$. 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 (2), 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 , $J_{dd} = 0.13\text{eV}$ [4].

Define a new representation for the general description of eigenstates of (2) as linear combinations of product wavefunctions $\Theta_{spinon} \Gamma_{holon}$: (i) $\Theta_{spinon} = (\sigma_1, \dots, \sigma_{N+M})$ where σ_i is the z-projection (in spin space) of the i^{th} spin (copper or oxygen hole) on the $N + M$ periodic lattice, and (ii) $\Gamma_{holon} = \psi_{n_1, \dots, n_M}$ where n_1, \dots, n_M are the locations of the oxygen holes with $n_1 < \dots < n_M$. This is shown clearly in figure 4. We call $(\sigma_1, \dots, \sigma_{N+M})$ the spinon state and ψ_{n_1, \dots, n_M} the holon state.

In this Coupled Representation (CR), the projection operator P in (2) due to Coulomb repulsion, requires that the holon states ψ_{n_1, \dots, 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 (2). P in (2) 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),

$$H_{ex}\psi_{n_1, \dots, n_M} \rightarrow t_{ex} \sum_{i=1}^M (\psi_{n_1, \dots, n_{i-1}, \dots, n_M} + \psi_{n_1, \dots, n_i+1, \dots, n_M}). \quad (3)$$

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 (2) 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 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 (2) can be written as the sum of two independent Hamiltonians (1) where,

$$\begin{aligned} H_{spinon} &= P[H'_{dd} + H_{pd}]P, \\ H_{holon} &= PH_{ex}P. \end{aligned} \quad (4)$$

H_{spinon} acts *only on the spinon wavefunction* Θ and is the 1-D Heisenberg antiferromagnet on an $N + M$ site lattice. H_{holon} acts *only on the holon wavefunction* Γ and is the nearest neighbor hopping of M holons on an $N + M$ site periodic lattice with an infinitely hard-core repulsion of one lattice spacing.

The Hamiltonian H_{spinon} , for the spin degrees of freedom of the system is soluble by the Bethe Ansatz (BA) [5-8]. The eigenstates of H_{holon} are simpler and are derived below.

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 $\Gamma = \sum a_p(n_1, \dots, n_M)\psi_{n_1, \dots, n_M}$ is an eigenstate of H_{holon} with energy E_{holon} . Assume $\Theta(-p)\Gamma$ has total translational symmetry K . The eigenvalue equation for the coefficients $a_p(n_1, \dots, n_M)$ (including n_1 for notational simplicity) is,

$$e^{i(K-p)}a_p(n_1, n_2 - 1, \dots, n_M - 1) + e^{-i(K-p)}a_p(n_1, n_2 + 1, \dots, n_M + 1) + \sum_{i=2}^M [a_p(n_1, \dots, n_i - 1, \dots, n_M) + a_p(n_1, \dots, n_i + 1, \dots, n_M)] = \frac{E_{holon}}{t_{ex}}a_p(n_1, \dots, n_M), \quad (5)$$

with the boundary condition,

$$a_p(0, n_2, \dots, n_{M-1}, N + M - 1) = 0. \quad (6)$$

The solution is,

$$a_p(n_1, \dots, n_M) = \det \begin{vmatrix} e^{ik_1 n_1} & e^{ik_1(n_2-1)} & \dots & e^{ik_1(n_M-M+1)} \\ e^{ik_2 n_1} & e^{ik_2(n_2-1)} & \dots & e^{ik_2(n_M-M+1)} \\ \vdots & \vdots & \ddots & \vdots \\ e^{ik_M n_1} & e^{ik_M(n_2-1)} & \dots & e^{ik_M(n_M-M+1)} \end{vmatrix}, \quad (7)$$

with $E_{holon} = 2t_{ex} \sum_{i=1}^M \cos k_i$ and $K = p + \sum_{i=1}^M k_i$. The boundary condition (6) requires that the first and last columns in (7) be multiples of each other for $n_M = N + M - 1$. This leads to,

$$k_i - k_j = \frac{2\pi\lambda_{i,j}}{N}, \quad \lambda_{i,j} = \text{integer} \neq 0. \quad (8)$$

Note that the number of O holes M , has dropped out of the quantization condition (8).

No two holon momenta may be equal because the determinant in (7) will be identically zero for all n_i . Therefore, *the holons may be considered to be spinless fermions*. It is the difference in the holon momenta that must be commensurate with the Cu lattice,

rather than the momenta k_i . Thus, each holon momenta can be written as the sum of two terms φ and k'_i where k'_i is commensurate with the Cu lattice.

$$k_i = \varphi + k'_i, \quad k'_i = \frac{2\pi\mu_i}{N}, \quad \mu_i = \text{integer}. \quad (9)$$

Since the spinon momentum p is incommensurate with the lattice, φ is necessary in order to make the total momentum K commensurate.

As $N \rightarrow \infty$, 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 .

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 $\langle S_1 \cdot S_2 \rangle_{AF}$ of the Heisenberg antiferromagnet in 1-D (-0.443) [6] to the value of the *next* nearest neighbor correlation $\langle S_1 \cdot S_3 \rangle_{AF}$ of the antiferromagnet in 1-D (≈ 0.19 [9]).

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

$$\frac{(N-M)}{N} \langle S_1 \cdot S_2 \rangle_{AF} + \frac{M}{N} \langle S_1 \cdot S_3 \rangle_{AF},$$

or,

$$(1-x) \langle S_1 \cdot S_2 \rangle_{AF} + x \langle S_1 \cdot S_3 \rangle_{AF}. \quad (10)$$

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

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

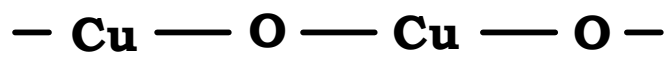


Figure 2

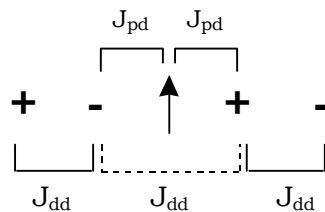


Figure 3

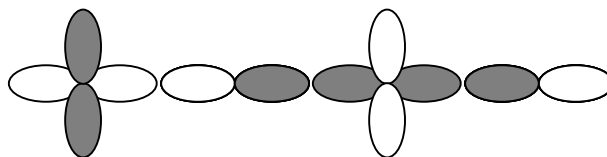


Figure 4

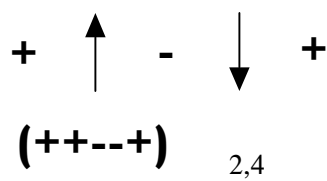


Figure 5

