

**SPINONS AND HOLONS FOR THE
ONE-DIMENSIONAL THREE-BAND HUBBARD
MODELS OF HIGH T_c SUPERCONDUCTORS**

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Abbreviations: 1D, one-dimension; 2D, two dimensions.

ABSTRACT

The one-dimensional three-band Hubbard Hamiltonian is shown to be equivalent to an effective Hamiltonian that has independent spinon and holon quasiparticle excitations plus a weak coupling of the two. The spinon description includes both copper sites and oxygen hole sites leading to a one-dimensional antiferromagnet incommensurate with the Cu lattice. The holons are spinless non-interacting fermions in a simple cosine band. Because the oxygen sites are in the Hamiltonian, the quasiparticles are much simpler than in the exact solution of the t-J model for $2t = \pm J$. If a similar description is correct for two dimensions, then the holons will attract in a p-wave potential.

INTRODUCTION

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 $d_{x^2-y^2}$ with adjacent copper spins coupled antiferromagnetically. Doping of the system (removing electrons) 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. The mixing of the copper and oxygen orbitals leads to the three-band Hubbard models of superconductivity (1,2), with Hamiltonian,

$$\begin{aligned}
 H = & J_{dd} \sum_{\langle ij \rangle} S_i \cdot S_j + J_{pd} \sum_{\langle im \rangle} S_i \cdot S_m + \left(-t_{pp} \sum_{\text{diag} \langle mn \rangle} p_{n\sigma}^\dagger p_{m\sigma} - t_{pdp} \sum_{\langle mn \rangle} p_{n\sigma}^\dagger p_{m\sigma} \right) \\
 & + t_{ex} \sum_{\langle \substack{im \\ \sigma\sigma'} \rangle} p_{l\sigma'}^\dagger p_{m\sigma} d_{i\sigma}^\dagger d_{i\sigma'} \\
 = & H_{dd} + H_{pd} + H_{band} + H_{ex}. \tag{1}
 \end{aligned}$$

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 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 . H_{band} is the oxygen hopping *without* spin exchange of the intervening copper. The t_{pp} term in H_{band} describes direct O-O coupling between diagonally adjacent O sites (say the x-axis to the y-axis) whereas, t_{pdp} describes the hopping due to the copper-mediated non-spin exchange hopping for both diagonal and same axis hops. 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 sum in H_{ex} is over all spins σ, σ' and the pairs in H_{dd} and H_{pd} are summed over once. $p_{m\sigma}^\dagger$ creates an oxygen hole of spin σ at m and $d_{i\sigma}^\dagger$ creates a copper hole of spin σ at i . Using the Bonding Phase Convention illustrated in figure 1 leads to positive values for the parameters in [1]. Typical values for the parameters (3,4) are $J_{pd} = 7.0$, $t_{ex} = 6.6$, $t_{pdp} = 3.3$, $t_{pp}^{diag} = 4.9$ in units of J_{dd} . For La_2CuO_4 , $J_{dd} = 0.13\text{eV}$ (5).

In the t-J (6,7) model of the CuO₂ sheets, the oxygen sites are eliminated by assuming the low-energy excitations are well described by a single hybridized Cu-O band. The t-J model has been solved exactly in 1D with a Bethe Ansatz for the supersymmetric case, $2t = \pm J$ (8,9). The low lying excitations are found to consist of two parts: one for the spin degrees of freedom (spinons) and the other for the charge degrees of freedom (holons). The spinon spectrum is a pure spin excitation only for the case of exactly the half-filled band (no holes). With doping charge mixes into the spinon states, destroying a simple picture of two uncoupled quasiparticle excitations.

In this letter, we consider a 1D three-band model for the Cu-O lattice in figure 2. By retaining the O sites, the Hamiltonian [1] can be reduced to an effective Hamiltonian that can be solved exactly. We find simple independent spinon and holon quasiparticle excitations where the spinon spectrum is a 1D Heisenberg antiferromagnet incommensurate with the Cu lattice and the holons are spinless fermions in a cosine band. This solution is a generalization to the full three-band Hamiltonian [1] of our exact solution (10) on a Cu-O chain assuming $J_{pd}=J_{dd}$ and only spin-exchange hopping ($t_{ex} \neq 0, t_{pdp} = t_{pp} = 0$).

In the three-band model, the two Cu spins neighboring an oxygen hole couple to the hole to form the spin 1/2 Emery polaron (the ground state of H_{pd} for the Cu-O-Cu triple)(1,2). This polaron has the two Cu spins in a triplet coupled to the spin 1/2 O hole to form an overall doublet.

$$\begin{aligned} \{\uparrow_E\} &= \sqrt{\frac{2}{3}}(+\downarrow+) - \frac{1}{\sqrt{6}}(+\uparrow-) - \frac{1}{\sqrt{6}}(-\uparrow+), \\ \{\downarrow_E\} &= -\sqrt{\frac{2}{3}}(-\uparrow-) + \frac{1}{\sqrt{6}}(+\downarrow-) + \frac{1}{\sqrt{6}}(-\downarrow+), \end{aligned} \quad [2]$$

where $\{\uparrow_E\}$ has $M_z = +1/2$ and $\{\downarrow_E\}$ has $M_z = -1/2$. The +, - are Cu spins and \uparrow, \downarrow represent the O hole spin.

Exact computations (3,4,11) on finite lattices find that the ground state and lowest excitations of [1] in 1D and 2D have large (> 90%) projections onto the Emery polaron.

This is due not only to the J_{pd} hole-Cu coupling, but also to the nature of the hopping terms t_{pp} , t_{pdp} , t_{ex} (12).

SPINON AND HOLON HAMILTONIANS

Assuming the Emery polaron is the correct description of the low-energy physics, we will show that the Hamiltonian [1] can be written as,

$$H = H_{eff} + H', \quad [1']$$

where

$$H_{eff} = H_{spinon} + H_{holon}.$$

Here H_{eff} dominates and can be exactly solved while H' is a perturbation. The two pieces of H_{eff} are: (i) H_{spinon} , the 1D Heisenberg antiferromagnet on $N - M$ sites where N is the number of Cu sites and M is the number of O holes. The number of sites is $N - M$ because each hole leads to an Emery polaron that couples two adjacent Cu sites and, (ii) H_{holon} the Hamiltonian for the motion of M spinless fermions on an $N - M$ site lattice. H_{spinon} is soluble by the Bethe Ansatz (13-16). The solutions of H_{holon} describe the motion of M non-interacting spinless fermions in the cosine band,

$$\epsilon(k) = -(1/3)(4t_{pdp} + 5t_{ex}) \cos k. \quad [3]$$

H_{eff} is an effective “spin-exchange” hole hopping Hamiltonian on a reduced set of spins that are coupled antiferromagnetically. The remainder, H' leads to coupling of the exact quasiparticles (spinons and the holons).

To evaluate the effective hopping of an Emery polaron, consider an up spin polaron $\{\uparrow_E\}$ adjacent to a down spin Cu $(-)$. We represent this by $[\{\uparrow_E\}(-)]$. Expanding in terms of spin functions leads to,

$$[\{\uparrow_E\}(-)] = \sqrt{\frac{2}{3}}(+\downarrow+-) - \frac{1}{\sqrt{6}}(+\uparrow--)- \frac{1}{\sqrt{6}}(-\uparrow+-). \quad [4]$$

On the right-hand side of the equation, \uparrow and \downarrow is the spin of the O hole. Neglecting non-Emery states and using conservation of total spin, a hop to the *right* must be of the form,

$$\begin{aligned} H[\{\uparrow_E\}(-)] &\rightarrow T_{ex}[(+)\{\downarrow_E\}] + T[(-)\{\uparrow_E\}], \\ H[\{\uparrow_E\}(+)] &\rightarrow T_{ex}[(+)\{\uparrow_E\}] + T[(+)\{\uparrow_E\}], \end{aligned} \quad [5]$$

where T_{ex} is the matrix element for “spin-exchange” hopping and T is hopping “without spin-exchange.” The matrix elements are,

$$T_{ex} = -\frac{1}{6}(4t_{pdp} + 5t_{ex}), \quad T = \frac{1}{6}(t_{ex} - t_{pdp}). \quad [6]$$

For the values of the parameters given above, $T_{ex} = -7.7J_{dd}$, $T = 0.55J_{dd}$ and $|T_{ex}/T| = 14$. Since the Emery polaron [2] is symmetric under interchange of its Cu spins, a hop to the left will have the same T_{ex} and T . Thus, neglecting the T term in [5], we define H_{eff}^{hop} as,

$$H_{eff}^{hop}[(\sigma'')\{\sigma_E\}(\sigma')] = -|T_{ex}|([\sigma''](\sigma)\{\sigma'_E\}] + [\{\sigma''_E\}(\sigma)(\sigma')]). \quad [7]$$

In 2D, including t_{pp} , the oxygen-oxygen hybridization, leads to $T_{ex} = -10.97J_{dd}$, $T = -0.27J_{dd}$ and $|T_{ex}/T| = 41.1$.

Equation [7] also defines the reduced spin Hilbert space of H_{eff} . We also assume that two Emery polarons cannot occupy the same site in this Hilbert space. This is due to hole-hole Coulomb repulsion since such states would have two O holes on the same site or adjacent sites. (Also the dopings of interest to superconductivity are small.)

The antiferromagnetic coupling of the total polaron spin to the neighboring Cu spins is determined by the value of the operator \hat{C} that interchanges a copper spin of the polaron with an adjacent Cu spin, $\langle \{\uparrow_E\}(-) | \hat{C} | \{\downarrow_E\}(+) \rangle = \frac{2}{3}$, leading to an effective coupling $(2/3)J_{dd}$. [This is because the z-projection of the spin on a Cu site in the polaron has the same sign as the total z-projection of the polaron, $S_{Cu}^z = (2/3)S_E^z$.] In defining H_{eff} , we

will use a net coupling of J_{dd} with the remainder included in H' . Our assumption that H' may be considered a small perturbation to H_{eff} is supported by the calculations of Ding and Goddard (4) for one and two holes on a Cu-O chain with 16 Cu sites. They find that the holes are free Emery polarons with a slight repulsion between them.

The antiferromagnetic effective Hamiltonian H_{eff}^{dd} acting on $[(\sigma'')\{\sigma_E\}(\sigma')]$ is,

$$H_{eff}^{dd}[(\sigma'')\{\sigma_E\}(\sigma')] = \frac{1}{2}J_{dd}\{[(\sigma)\{\sigma_E''\}(\sigma')] + [(\sigma'')\{\sigma_E'\}(\sigma)]\} - \frac{1}{2}J_{dd}[(\sigma'')\{\sigma_E\}(\sigma')]. \quad [8]$$

Here we have used the relation $S_1 \cdot S_2 = (1/2)\hat{C}_{1,2} - 1/4$, where $\hat{C}_{1,2}$ interchanges spins at sites 1 and 2.

Thus we define the effective Hamiltonian for the motion of O holes in 1D as,

$$H_{eff} = P[H_{eff}^{dd} + H_{eff}^{hop}]P = H_{spinon} + H_{holon}, \quad [9]$$

where the operator P projects out states that have two O holes on the same site or adjacent O sites (due to Coulomb repulsion). That is, P does not allow Emery polarons to be on the same site in the reduced spin Hilbert space.

From [7], $H_{holon} = PH_{eff}^{hop}P$ shifts the locations of the polarons but *does not alter the order of the spins*. Similarly, $H_{spinon} = PH_{eff}^{dd}P$ in [8] acts on the spins but *does not change the location of the polarons*.

EXACT SOLUTION OF $H_{eff} = H_{spinon} + H_{holon}$

We will now describe a general state of H as a linear combination of product wavefunctions $\Theta_{spinon}\Gamma_{holon}$ (N Cu sites and M O holes): (i) $\Theta_{spinon} = (\sigma_1, \dots, \sigma_{N-M})$ where σ_i is the z-projection of the i^{th} spin (Cu or polaron) on the $N - M$ site lattice, and (ii) $\Gamma_{holon} = \psi_{n_1, \dots, n_M}$ where $0 \leq n_1 < \dots < n_M \leq N - M - 1$ are the locations of the Emery polarons. Hence,

$$H_{holon}\psi_{n_1, \dots, n_M} = -|T_{ex}| \sum_{i=1}^M (\psi_{n_1, \dots, n_{i-1}, \dots, n_M} + \psi_{n_1, \dots, n_{i+1}, \dots, n_M}), \quad [10]$$

$$H_{spinon}\Theta = J_{dd}[S_1 \cdot S_2 + \dots + S_{M-1} \cdot S_M + S_M \cdot S_1]\Theta. \quad [11]$$

To uniquely specify a state $\Theta\Gamma$, we require that every Θ has as the first spin a polaron with the oxygen hole at the same particular oxygen site, $n_1 = 0$. By translational symmetry, a complete set of states can be specified by the total momentum K , the spinon state Θ , and the holon state ψ_{n_1, \dots, n_M} with $n_1 = 0$ and $n_M < N - M$. The holon state with $n_M = N - M$ is not allowed due to Coulomb repulsion with the holon at $n_1 = 0$. This is the boundary condition.

Let $\Theta(-p)$ be an eigenstate of H_{spinon} with energy $E_{spinon}(-p)$ and momentum $-p$. Let $\Gamma = \sum a(n_1, \dots, n_M)\psi_{n_1, \dots, n_M}$ be an eigenstate of H_{holon} with energy E_{holon} such that $\Theta(-p)\Gamma$ has total momentum K . Then,

$$H_{eff}[\Theta(-p)\Gamma] = [E_{spinon} + E_{holon}][\Theta(-p)\Gamma], \quad [12]$$

and the energy equation for E_{holon} (we include n_1 for notational simplicity, although $n_1 = 0$) is,

$$e^{i(K-p)}a(n_1, n_2 - 1, \dots, n_M - 1) + e^{-i(K-p)}a(n_1, n_2 + 1, \dots, n_M + 1) + \sum_{i=2}^M [a(n_1, \dots, n_i - 1, \dots, n_M) + a(n_1, \dots, n_i + 1, \dots, n_M)] = \frac{E_{holon}}{T_{ex}}a(n_1, \dots, n_M), \quad [13]$$

with the boundary condition,

$$a(0, n_2, \dots, n_{M-1}, N - M) = 0. \quad [12]$$

The solution to Eqn. [13] is $E_{holon} = -2|T_{ex}| \sum_{i=1}^M \cos k_i$ and

$$a(n_1, n_2, \dots, n_M) = Det \begin{vmatrix} e^{ik_1 n_1} & e^{ik_1 n_2} & \dots & e^{ik_1 n_M} \\ e^{ik_2 n_1} & e^{ik_2 n_2} & \dots & e^{ik_2 n_M} \\ \vdots & \vdots & \ddots & \vdots \\ e^{ik_M n_1} & e^{ik_M n_2} & \dots & e^{ik_M n_M} \end{vmatrix}, \quad [15]$$

where

$$K = p + \sum_{i=1}^M k_i. \quad [16]$$

Note that a is zero if two holons are on the same site or if any two holon momenta are equal.

It is the operator P that induces the fermionic statistics on the holons or the excitations of H_{eff}^{hop} . The boundary condition [14] is satisfied if the last column is a multiple of the first for $n_M = N - M$. This leads to,

$$k_i - k_j = \frac{2\pi}{(N - M)} \lambda_{i,j}, \quad \lambda_{i,j} = integer \neq 0, \quad [17]$$

and

$$E_{eff}(K) = E_{spinon}(-p) - 2|T_{ex}| \sum_{i=1}^M \cos k_i. \quad [18]$$

Equations [16-18] constitute the complete solution to H_{eff} . The spinon spectrum is the 1D Heisenberg antiferromagnet for the $N-M$ spins and hence is incommensurate with the Cu lattice. It is linear in momentum for small p . The holons are spinless fermions in a cosine band with a Fermi surface and Fermi energy. In the thermodynamic limit, the ground state of H_{eff} has total momentum $K = 0$ with a spinon wavefunction corresponding to the ground state of the 1D Heisenberg antiferromagnet ($p = 0$) and the holon state with Fermi momentum $k_F = \pi x / (1 - x)$ ($x = M/N$ is the doping) and Fermi energy $E_F = -2|T_{ex}| \cos k_F$.

The energies from the exact solution of H_{eff} are in excellent agreement with numerical studies using the full Hamiltonian (4). This shows that the coupling H' of the spinons and holons is small so that spinons and holons may be regarded as the correct zeroth order quasiparticle of the 1D three-band Hubbard model.

If similar spinons and holons are the correct quasiparticle description in 2D (17), then the weak coupling H' will lead to a net attraction of holons and superconductivity. The attractive coupling of holons must be p-wave because the holons are spinless fermions.

The spinon spectrum of the 2D antiferromagnet is also linear for small momentum (just as for phonons) although the coupling of the spinons to holons will be different from the coupling of phonons to electrons.

DISCUSSION AND SUMMARY

In this paper we define spinon and holon Hamiltonians that include the dominant part of the full Hamiltonian yet permit exact solutions. The resulting spinon and holon states are *decoupled independent of doping*. This separability differs drastically from the spinons and holons of the t-J Hamiltonians.

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FIGURE CAPTIONS

1. The Bonding Phase Convention on the Cu $d_{x^2-y^2}$ and O p_σ orbitals. For Hamiltonian [1], the d orbital on the Cu is enclosed in a circle for clarity.
2. The 1D Cu-O infinite lattice.

