

Spinons and holons for the one-dimensional three-band Hubbard models of high-temperature superconductors

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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 copper lattice. The holons are spinless noninteracting 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.

The copper sites in the CuO_2 sheets of high-temperature superconductors may be described by a single spin $\frac{1}{2}$ 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 $\frac{1}{2}$ hole in a p orbital (p_σ) pointing toward 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

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

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 oxygen 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 and 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 Fig. 1 leads to positive values for the parameters in Eq. 1. Typical values for

the parameters (3, 4) in units of J_{dd} are $J_{pd} = 7.0$, $t_{ex} = 6.6$, $t_{pdp} = 3.3$, $t_{pp}^{\text{diag}} = 4.9$. For La_2CuO_4 , $J_{dd} = 0.13$ eV (5).

In the t - J (6, 7) model of the CuO_2 sheets, the oxygen sites are eliminated by assuming that the low-energy excitations are well described by a single hybridized Cu–O band. The t - J model has been solved exactly in one dimension 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.

Here we consider a one-dimensional three-band model for the Cu–O lattice (–Cu–O–Cu–O–). By retaining the oxygen 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 one-dimensional 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 copper spins neighboring an oxygen hole couple to the hole to form the spin $\frac{1}{2}$ Emery polaron (the ground state of H_{pd} for the Cu–O–Cu triple) (1, 2). This polaron has the two copper spins in a triplet coupled to the spin $\frac{1}{2}$ oxygen hole to form an overall doublet.

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

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

Exact computations (3, 4, 11) on finite lattices find that the ground state and lowest excitations of Eq. 1 in one and two dimensions 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} , and t_{ex} (12).

Spinon and Holon Hamiltonians

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

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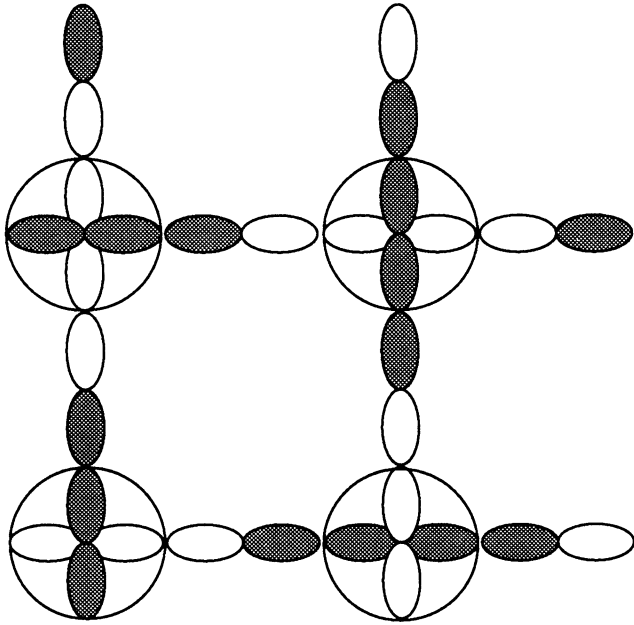


FIG. 1. The bonding phase convention on the copper $d_{x^2-y^2}$ and oxygen p_{σ} orbitals. For Hamiltonian 1, the d orbital on the copper is enclosed in a circle for clarity.

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

where

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

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 one-dimensional Heisenberg antiferromagnet on $N - M$ sites, where N is the number of copper sites and M is the number of oxygen holes (the number of sites is $N - M$ because each hole leads to an Emery polaron that couples two adjacent copper 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 noninteracting spinless fermions in the cosine band,

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

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 $\{\uparrow_{\text{E}}\}$ adjacent to a down-spin Cu $(-)$. We represent this by $\{\{\uparrow_{\text{E}}\}(-)\}$. Expanding in terms of spin functions leads to

$$\begin{aligned} \{\{\uparrow_{\text{E}}\}(-)\} &= \sqrt{\frac{2}{3}} (+ \downarrow + -) - \frac{1}{\sqrt{6}} (+ \uparrow - -) \\ &\quad - \frac{1}{\sqrt{6}} (- \uparrow + -). \end{aligned} \quad [4]$$

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

$$H[\{\uparrow_{\text{E}}\}(-)] \rightarrow T_{\text{ex}}[(+)\{\downarrow_{\text{E}}\}] + T[(-)\{\uparrow_{\text{E}}\}],$$

$$H[\{\uparrow_{\text{E}}\}(+)] \rightarrow T_{\text{ex}}[(+)\{\uparrow_{\text{E}}\}] + T[(+)\{\uparrow_{\text{E}}\}], \quad [5]$$

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

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

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

$$H_{\text{eff}}^{\text{hop}}[(\sigma'')\{\sigma_{\text{E}}\}(\sigma')] = -|T_{\text{ex}}|[(\sigma'')(\sigma)\{\sigma'_{\text{E}}\}] + [(\sigma'_{\text{E}})(\sigma)(\sigma')]. \quad [7]$$

In two dimensions, inclusion of t_{pp} , the oxygen–oxygen hybridization, leads to $T_{\text{ex}} = -10.97J_{\text{dd}}$, $T = -0.27J_{\text{dd}}$, and $|T_{\text{ex}}/T| = 41.1$.

Eq. 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 exclusion is due to hole–hole Coulomb repulsion, since such states would have two oxygen 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 copper spins is determined by the value of the operator \hat{C} that interchanges a copper spin of the polaron with an adjacent copper spin, $\langle\{\uparrow_{\text{E}}\}(-)\hat{C}|\{\downarrow_{\text{E}}\}(+)\rangle = 2/3$, leading to an effective coupling $(2/3)J_{\text{dd}}$. [This is because the z projection of the spin on a copper site in the polaron has the same sign as the total z projection of the polaron, $S_{\text{Cu}}^z = (2/3)S_{\text{E}}^z$.] 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 copper sites. They found that the holes were free Emery polarons with a slight repulsion between them.

The antiferromagnetic effective Hamiltonian $H_{\text{eff}}^{\text{dd}}$ acting on $\{(\sigma'')\{\sigma_{\text{E}}\}(\sigma')\}$ is

$$\begin{aligned} H_{\text{eff}}^{\text{dd}}[(\sigma'')\{\sigma_{\text{E}}\}(\sigma')] &= \frac{1}{2} J_{\text{dd}}[(\sigma)\{\sigma'_{\text{E}}\}(\sigma')] + [(\sigma'')\{\sigma'_{\text{E}}\}(\sigma)] \\ &\quad - \frac{1}{2} J_{\text{dd}}[(\sigma'')\{\sigma_{\text{E}}\}(\sigma')]. \end{aligned} \quad [8]$$

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 oxygen holes in one dimension as

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

where the operator P projects out states that have two oxygen holes on the same site or adjacent oxygen 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 Eq. 7, $H_{\text{holon}} = PH_{\text{eff}}^{\text{hop}}P$ shifts the locations of the polarons but *does not alter the order of the spins*. Similarly, $H_{\text{spinon}} = PH_{\text{eff}}^{\text{dd}}P$ in Eq. 8 acts on the spins but *does not change the location of the polarons*.

Exact Solution of $H_{\text{eff}} = H_{\text{spinon}} + H_{\text{holon}}$

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

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

and

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

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 $E_{\text{spinon}}(-p)$ 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,

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

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

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

with the boundary condition

$$a(0, n_2, \dots, n_{M-1}, N - M) = 0. \quad [14]$$

The solution of Eq. 13 is $E_{\text{holon}} = -2|T_{\text{ex}}|\sum_{i=1}^M \cos k_i$ and

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

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 $H_{\text{eff}}^{\text{hopp}}$. The boundary condition 14 is satisfied if the last column is a multiple of the first for $n_M = N - M$. This

leads to

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

and

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

Eqs. 16–18 constitute the complete solution to H_{eff} . The spinon spectrum is the one-dimensional Heisenberg antiferromagnet for the $N - M$ spins and hence is incommensurate with the copper 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 one-dimensional 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 $E_F = -2|T_{\text{ex}}|\cos k_F$.

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 one-dimensional three-band Hubbard model.

If similar spinons and holons are the correct quasiparticle description in two dimensions (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 two-dimensional 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.

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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