Exact solution to a strongly coupled Hubbard model in one dimension for high-T_c superconductors

Jamil Tahir-Kheli and William A. Goddard III
Materials and Molecular Simulation Center, Beckman Institute 139-74, California Institute of Technology, Pasadena, California 91125
(Received 3 September 1992)

A Hamiltonian for the motion of oxygen holes strongly coupled to the Cu spins in a one-dimensional (1D) 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 1D antiferromagnet incommensurate with the Cu lattice and the holons are spinless noninteracting 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 $x=1$.

In the three-band Hubbard models for the CuO_2 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, $t_{pdp}\sum p^\dagger_\sigma p_\sigma$, and (ii) hopping *with* spin exchange of the intervening Cu spin, $t_{ex}\sum p^\dagger_{\sigma'} p_\sigma d^\dagger_\sigma d_{\sigma'}$, where the sum is taken over all σ, σ'. $p^\dagger_{m\sigma}$ creates an O hole at m with z projection of spin σ and $d^\dagger_{i\sigma}$ 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 1D 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,

$$H=H_{\text{spinon}}+H_{\text{holon}}\ . \tag{1}$$

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 1D antiferromagnet on a lattice incommensurate with the Cu lattice and the holon Hamiltonian H_{holon} is simply the motion of spinless fermions on a 1D 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 1D: spinons and holons. It is from this strong-coupling solution ($t_{pdp}=0, J_{pd}=J_{dd}$, and $t_{ex}\neq 0$) that perturbation theory should be applied, rather than from $t_{ex}=0$.

Consider a 1D Cu-O lattice as shown in Fig. 1. In this report, we solve the following spin-exchange hopping Hamiltonian for $J_{pd}=J_{dd}$:

$$\begin{aligned} H&=P\left[J_{dd}\sum_{\langle ij\rangle}{}'\,\mathbf{S}_i\cdot\mathbf{S}_j+J_{dd}\sum_{\langle im\rangle}\mathbf{S}_i\cdot\mathbf{S}_m\right.\\ &\qquad\left.+t_{ex}\sum_{\substack{\langle \lim\rangle\\ \sigma\sigma'}} p^\dagger_{l\sigma'}p_{m\sigma}d^\dagger_{i\sigma}d_{i\sigma'}\right]P\ ,\\ &=H'_{dd}+H_{pd}+H_{ex}\ , \end{aligned} \tag{2}$$

where the first term $H'_{dd}=J_{dd}\sum'\mathbf{S}_i\cdot\mathbf{S}_j$ 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 $H_{pd}=J_{pd}\sum\mathbf{S}_i\cdot\mathbf{S}_m$ is the antiferromagnetic coupling of the oxygen holes S_m to neighboring copper spins S_i. The final term $H_{ex}=t_{ex}\sum p^\dagger pd^\dagger d$ 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 Eq. (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 Eq. (2), the sum over nearest-neighbor pairs and O-Cu-O triples is taken once. The effect of the first two terms of Eq. (2), $H'_{dd}+H_{pd}$, is shown in Fig. 2.

Two other terms in three-band Hubbard models are *not* included in Eq. (2). 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 Fig. 3, which leads to positive values for the parameters

— Cu — O — Cu — O —

FIG. 1. The 1D Cu-O infinite lattice.

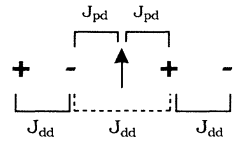

FIG. 2. The coupling of copper and oxygen spins due to $H'_{dd}+H_{pd}$. The oxygen spin is represented by the arrow and the dotted line indicates the copper coupling *not* included in H'_{dd}.

in Eq. (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, $J_{dd}=0.13$ eV.[4]

Define a new representation for the general description of eigenstates of Eq. (2) as linear combinations of product wave functions $\Theta_{spinon}\Gamma_{holon}$: (i) $\Theta_{spinon}=(\sigma_1,\ldots,\sigma_{N+M})$ where σ_i is the z projection (in spin space) of the ith spin (copper or oxygen hole) on the N+M periodic lattice, and (ii) $\Gamma_{holon}=\psi_{n_1,\ldots,n_M}$ where $n_1,\ldots,n_M$ are the locations of the oxygen holes with $n_1<\cdots<n_M$. This is shown clearly in Fig. 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 Eq. (2), 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 define the eigenstates of Eq. (2) unambiguously. P in Eq. (2) is *necessary* in order to use the CR.

The effect of H_{ex} is particularly simple in the CR of the state. H_{ex} acts only on the holon piece of the wave function (Fig. 5),

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

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,

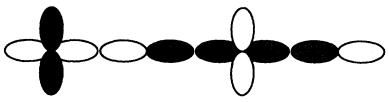

FIG. 3. The Bonding Phase Convention on the Cu $d_{x^2-y^2}$ and O p_σ orbitals.

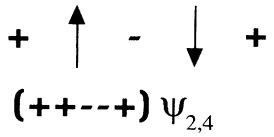

FIG. 4. The Coupled Representation (CR). The first line shows a particular Cu and O-hole state in the standard representation. The second line is the same state in the CR. The arrows are O-hole spins.

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

$$H_{spinon}=P(H'_{dd}+H_{pd})P ,$$
$$H_{holon}=PH_{ex}P . \tag{4}$$

H_{spinon} acts *only on the spinon wave function* Θ and is the 1D Heisenberg antiferromagnet on an $N+M$ site lattice. H_{holon} acts *only on the holon wave function* 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 $\Gamma=\sum a_p(n_1,\ldots,n_M)\psi_{n_1,\ldots,n_M}$ 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 $a_p(n_1,\ldots,n_M)$ (including n_1 for notational simplicity) is

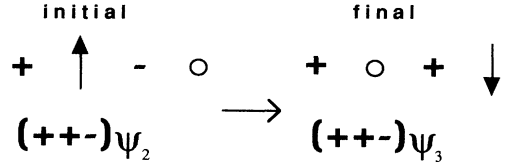

FIG. 5. The effect of a right spin-exchange hop in the standard and coupled representations (CR). As before, the arrow is an O-hole spin and the circle is an O site without a hole. In the CR, the spinon part is unchanged due to the hole hop.

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

with the boundary condition

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

The solution is

$$a_p(n_1,\ldots,n_M)=\det\begin{vmatrix} e^{ik_1n_1} & e^{ik_1(n_2-1)} & \cdots & e^{ik_1(n_M-M+1)} \\ e^{ik_2n_1} & e^{ik_2(n_2-1)} & \cdots & e^{ik_2(n_M-M+1)} \\ \vdots & \vdots & \ddots & \vdots \\ e^{ik_Mn_1} & e^{ik_M(n_2-1)} & \cdots & e^{ik_M(n_M-M+1)} \end{vmatrix}\ , \quad (7)$$

with $E_{\text{holon}}=2t_{\text{ex}}\sum_{i=1}^{M}\cos k_i$ 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 momentum 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 1D 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 $\langle \mathbf{S}_1\cdot\mathbf{S}_2\rangle_{AF}$ of the Heisenberg antiferromagnet in 1D (-0.443) (Ref. 6) to the value of the *next*-nearest-neighbor correlation $\langle \mathbf{S}_1\cdot\mathbf{S}_3\rangle_{AF}$ of the antiferromagnet in 1D [≈ 0.19 (Ref. 9)].

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

$$\frac{(N-M)}{N}\langle \mathbf{S}_1\cdot\mathbf{S}_2\rangle_{AF}+\frac{M}{N}\langle S_1\cdot S_3\rangle_{AF}$$

or

$$(1-x)\langle \mathbf{S}_1\cdot\mathbf{S}_2\rangle_{AF}+x\langle \mathbf{S}_1\cdot\mathbf{S}_3\rangle_{AF}\ . \quad (10)$$

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

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

[1] V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).

[2] V. J. Emery and G. Reiter, Phys. Rev. B **38**, 4547 (1988).

[3] M. S. Hybertsen, M. Schlüter, and N. E. Christensen, Phys. Rev. B **39**, 9028 (1989).

[4] P. E. Sulewski, P. A. Fleury, K. B. Lyons, S. W. Cheong, and Z. Fisk, Phys. Rev. B **41**, 225 (1990).

[5] H. A. Bethe, Z. Phys. **71**, 205 (1931); A. Sommerfeld and H. A. Bethe, *Handbuch der Physik* (Springer-Verlag, Berlin, 1933), Vol. 24, Part 2, pp. 604–618.

[6] L. Hulthén, Ark. Mat. Astron. Fys. (Sweden) **26A**, No. 1 (1938).

[7] R. Orbach, Phys. Rev. **112**, 309 (1958).

[8] R. B. Griffiths, Phys. Rev. **133**, A768 (1963).

[9] J. C. Bonner and M. E. Fisher, Phys. Rev. **135**, A640 (1964). Bonner and Fisher calculate all spin correlations for periodic lattices with up to 11 sites and extrapolate to infinity. The expected error for the value of the next nearest correlation is a few percent.