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# Two-electron bound state formation in the $t$ - $J$ - $U$ model for exchange-coupled planes

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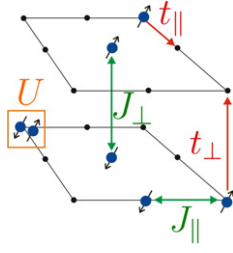
## Abstract

An anisotropic  $t$ - $J$ - $U$  model Hamiltonian is used to model electron behaviour in quasi-two-dimensional materials in the dilute limit, and as a highly simplified representation of the weakly coupled  $\text{CuO}_2$  planes of the high- $T_c$  cuprates we model the very poor out-of-plane conductivity via the complete suppression of interplanar hopping. However, we do include the very weak interplanar superexchange, and are thus considering a model of exchange-coupled planes. For an isotropic three-dimensional system in the dilute limit, we find that the formation of two-particle bound states requires  $J_c/t \gtrsim 5.9$ . Also, it is known that  $J_c/t = 2$  for a two-dimensional square lattice. However, for our model of exchange-coupled planes any infinitesimal interplanar exchange ( $J_c = 0$ ) is adequate for forming bound states.

## 1. Motivation and introduction

The discovery of high-temperature superconductivity in copper-based transition metal oxides was made by Alex Müller and Georg Bednorz in 1986 (see [1] for more information). They found that the copper oxide compound  $(\text{La, Ba})_2\text{CuO}_4$  became a superconductor at  $T_c \approx 30$  K, which was substantially higher than for other any other compounds known at that time. At present one can find transition temperatures at ambient pressure close to 138 K for other cuprate-based systems. The mechanism for this novel behaviour is still a subject of spirited debate, but one idea that has been put forward repeatedly is the Heisenberg superexchange between neighbouring Cu sites, a by-product of the strong repulsive electronic (Hubbard-type) correlations that are present on the transition metal sites.

The structure of all of the cuprate materials is similar, in that  $\text{CuO}_2$  planes are stacked one on top of another to produce a quasi-two-dimensional crystallographic arrangement. This characterization of these materials is supported by their very poor interplanar conducting behaviour [2], at least in the weakly doped regime [3, 4]. The so-called  $c$ -axis puzzle has been studied extensively [5], and its relation to the superconductivity has been discussed [6]. Further, given the dependence of  $T_c$  on the number of  $\text{CuO}_2$  planes per unit cell [7], the possibility of an



**Figure 1.** A schematic representation of the various terms that appear in the  $t$ - $J$ - $U$  model Hamiltonian. The electron hopping  $t$ , both in-plane ( $t_{\parallel}$ ) and inter-plane ( $t_{\perp}$ ), spin exchange  $J$ , again for both in-plane ( $J_{\parallel}$ ) and inter-plane ( $J_{\perp}$ ), and the on-site Coulomb repulsion  $U$ .

(This figure is in colour only in the electronic version)

interplanar pairing mechanism cannot be ignored, and indeed previous work has shown [8, 9], within various approximations, that any interplanar interaction increases  $T_c$ .

In this paper we examine the two-electron problem (namely the dilute limit) in the highly simplified situation of zero interplanar hopping. That is, our model is meant to be a very rough approximation to the extremely low out-of-plane conductivity, but leaving the residual interplanar superexchange found in the cuprates, the latter produced by strong electronic correlations. We refer to this situation as *exchange-coupled planes*. We solve for the conditions under which a two-particle bound state is formed, and in particular determine the minimum value of superexchange ( $J_c/t$ ) for which bound states appear. Our results make evident the potential benefit of having electrons confined to individual planes that can only move between planes via the spin-exchange ( $\frac{J}{2}S_i^+S_j^-$ ) process. To be specific, we find that while for a two-dimensional plane ( $J_c/t = 2$ ) or an isotropic three-dimensional system ( $J_c/t \approx 5.9$ ) one requires a superexchange much larger than that found experimentally ( $J/t \sim 0.3$ ), for exchange-coupled planes one requires only an infinitesimal ( $J_c = 0$ ) interaction. Therefore, even the very small out-of-plane exchange coupling (estimated to be roughly  $10^{-4}$  of the in-plane exchange) would suffice to form bound states. We note that similar results were found previously for exchange-coupled chains [10], emphasizing the potential importance of such *electronic confinement*.

## 2. Formalism

### 2.1. Model Hamiltonian

We consider the so-called  $t$ - $J$ - $U$  or Heisenberg-Hubbard model Hamiltonian, given by

$$\mathcal{H} = - \sum_{\langle i,j \rangle, \sigma} (t_{i,j} c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + \sum_{\langle i,j \rangle} J_{i,j} (\mathbf{S}^{(i)} \cdot \mathbf{S}^{(j)} - \frac{1}{4} n_i n_j) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

In this Hamiltonian  $i, j$  label the sites of the lattice, the notation  $\langle i, j \rangle$  denotes neighbouring lattice sites in *any* of the  $x, y$  or  $z$  directions, each near-neighbour pair is counted once only, and  $c_{i,\sigma}/c_{i,\sigma}^\dagger/n_{i,\sigma}$  denotes the annihilation/creation/number operator for an electron at site  $i$  with spin  $\sigma$ . We will consider the dilute limit, and in particular only two electrons, and therefore the frustrating geometry of some the high- $T_c$  cuprates (such as occurs for a body-centred tetragonal structure) can be ignored. Therefore, we consider a simple tetragonal lattice structure, which reduces to a simple cubic structure for isotropic hopping and exchange (see below).

For the energy parameters in the Hamiltonian we consider the following situations: a schematic of these parameters is shown in figure 1. First, the hopping frequency is restricted to

be near neighbour only, and in-plane and out-of-plane hopping frequencies are allowed to be different:

$$\begin{aligned} t_{i,j} &= t_{\parallel} && \text{when } i, j \text{ are near neighbours in either the } x \text{ or } y \text{ directions} \\ &= t_{\perp} && \text{when } i, j \text{ are near neighbours in the } z \text{ direction.} \end{aligned} \quad (2)$$

Similarly for the superexchange integral:

$$\begin{aligned} J_{i,j} &= J_{\parallel} && \text{when } i, j \text{ are near neighbours in either the } x \text{ or } y \text{ directions} \\ &= J_{\perp} && \text{when } i, j \text{ are near neighbours in the } z \text{ direction.} \end{aligned} \quad (3)$$

The Hubbard on-site repulsion energy is parametrized by  $U$ .

Strong coupling expansions of the Hubbard model show that to lowest order in  $t/U$  one has  $J = 4t^2/U$ , and in the  $t$ - $J$ - $U$  model this exchange interaction is included explicitly. Note, however, that this model Hamiltonian does *not* involve projection operators that project from doubly occupied sites, as one considers in  $t$ - $J$  model studies [11]. Instead, we take the limit  $U \rightarrow \infty$  to represent the high cost of doubly occupied sites, similar to what has been done in previous studies [10, 12]. That is,  $J$  is the effective interaction that is created by some finite value of  $U$  [13], and we then reduce the Hilbert space by taking the  $U \rightarrow \infty$  limit leaving  $J$  nonzero.

As we have discussed in section 1, in this paper we compare the bound states for a two-electron system, described by the Hamiltonian of (1), when interplanar hopping does not occur (that is  $t_{\perp} = 0$ ), with the situation in which each of the hopping and superexchange energies in (2) and (3) are the same in all three directions.

Consider the two-electron,  $S_{\text{total}}^z = 0$  state

$$|\psi\rangle = \sum_{m,n} \phi(m,n) c_{m,\uparrow}^{\dagger} c_{n,\downarrow}^{\dagger} |0\rangle \quad (4)$$

created from the empty lattice,  $|0\rangle$ . With the added symmetry  $\phi(m,n) = \phi(n,m)$ ,  $|\psi\rangle$  will be a singlet state. We use the following for the Fourier coefficients for  $\phi(i,j)$ :

$$\phi(\mathbf{k}_1, \mathbf{k}_2) \equiv \frac{1}{N} \sum_{i,j} e^{-i(\mathbf{k}_1 \cdot \mathbf{r}_i + \mathbf{k}_2 \cdot \mathbf{r}_j)} \phi(i,j). \quad (5)$$

Introducing  $\mathbf{k}_1 = \frac{\mathbf{Q}}{2} + \mathbf{q}$  and  $\mathbf{k}_2 = \frac{\mathbf{Q}}{2} - \mathbf{q}$ , we restrict our attention to zero centre-of-mass momentum states, and therefore solve for solutions in terms of

$$\phi(\mathbf{k}_1, \mathbf{k}_2) = \phi(\mathbf{q}, -\mathbf{q}) \equiv \phi(\mathbf{q}). \quad (6)$$

We make the following definitions:

$$\epsilon(\mathbf{k}) \equiv -2\{t_{\parallel}[\cos(\mathbf{k} \cdot \mathbf{x}) + \cos(\mathbf{k} \cdot \mathbf{y})] + t_{\perp} \cos(\mathbf{k} \cdot \mathbf{z})\} \quad (7)$$

$$J(\mathbf{k}) \equiv 2\{J_{\parallel}[\cos(\mathbf{k} \cdot \mathbf{x}) + \cos(\mathbf{k} \cdot \mathbf{y})] + J_{\perp} \cos(\mathbf{k} \cdot \mathbf{z})\} \quad (8)$$

and find [12, 10] that  $H|\psi\rangle = E|\psi\rangle$  is equivalent to solving the following equation:

$$\phi(\mathbf{q}) = \frac{\frac{U}{N} \sum_{\mathbf{p}} \phi(\mathbf{p}) - \frac{1}{N} \sum_{\mathbf{p}} J(\mathbf{q} - \mathbf{p}) \phi(\mathbf{p})}{E - 2\epsilon(\mathbf{q})}. \quad (9)$$

To simplify (9) it is convenient to make the following definitions (with  $x_i$  and  $x_j$  being any of  $x$ ,  $y$  or  $z$ ):

$$C_0 \equiv \frac{1}{N} \sum_{\mathbf{k}} \phi(\mathbf{k}) \quad C_{x_i} \equiv \frac{1}{N} \sum_{\mathbf{k}} \cos(k_{x_i}) \phi(\mathbf{k}) \quad (10)$$

$$\begin{aligned}
I_0 &\equiv \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{E + 4(t_{\parallel}[\cos(\mathbf{q} \cdot \mathbf{x}) + \cos(\mathbf{q} \cdot \mathbf{y})] + t_{\perp} \cos(\mathbf{q} \cdot \mathbf{z}))} \\
I_{x_i} &\equiv \frac{1}{N} \sum_{\mathbf{q}} \frac{\cos(\mathbf{q} \cdot \hat{\mathbf{x}}_i)}{E + 4(t_{\parallel}[\cos(\mathbf{q} \cdot \mathbf{x}) + \cos(\mathbf{q} \cdot \mathbf{y})] + t_{\perp} \cos(\mathbf{q} \cdot \mathbf{z}))} \\
I_{x_i, x_j} &\equiv \frac{1}{N} \sum_{\mathbf{q}} \frac{\cos(\mathbf{q} \cdot \hat{\mathbf{x}}_i) \cos(\mathbf{q} \cdot \hat{\mathbf{x}}_j)}{E + 4(t_{\parallel}[\cos(\mathbf{q} \cdot \mathbf{x}) + \cos(\mathbf{q} \cdot \mathbf{y})] + t_{\perp} \cos(\mathbf{q} \cdot \mathbf{z}))}.
\end{aligned} \tag{11}$$

By substituting these definitions into (9) one straightforwardly obtains a system of equations that one can solve for the bound states of the problem:

$$\begin{aligned}
C_0 &= UI_0 C_0 - 2J_{\parallel}(I_x C_x + I_y C_y) - 2J_{\perp} I_z C_z \\
C_x &= UI_x C_0 - 2J_{\parallel}(I_{xx} C_x + I_{xy} C_y) - 2J_{\perp} I_{xz} C_z \\
C_y &= UI_y C_0 - 2J_{\parallel}(I_{xy} C_x + I_{yy} C_y) - 2J_{\perp} I_{yz} C_z \\
C_z &= UI_z C_0 - 2J_{\parallel}(I_{xz} C_x + I_{yz} C_y) - 2J_{\perp} I_{zz} C_z.
\end{aligned} \tag{12}$$

### 3. Results

We analysed the above system of equations for two geometries of lattices: infinite in all directions (referred to as the three-dimensional *case*), as well as for  $L_x = L_y = \infty$  and  $L_z = 2$  (referred to as the *two-plane problem*). For the three-dimensional case, where  $L_x, L_y, L_z \rightarrow \infty$ , the sums in (10) and (11) become

$$\frac{1}{N} \sum_{\mathbf{q}} \rightarrow \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} dq_x \int_{-\pi}^{\pi} dq_y \int_{-\pi}^{\pi} dq_z \tag{13}$$

and similarly for an isotropic two-dimensional lattice. Also, for  $L_x, L_y \rightarrow \infty$  in the two-plane problem ( $L_z = 2$ ) the sums become

$$\frac{1}{N} \sum_{\mathbf{q}} \rightarrow \frac{1}{2} \sum_{q_z=0, \pi} \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dq_x \int_{-\pi}^{\pi} dq_y. \tag{14}$$

For the  $t$ - $J$ - $U$  model with isotropic hopping ( $t$ ) and exchange ( $J$ ) in dimension  $d$ , the minimum (total) energy for two non-interacting electrons is  $-4dt$ , and therefore the energy of a bound state must be less than this energy. For convenience, we define a scaled energy  $A$  by

$$A \equiv \frac{E}{4t}. \tag{15}$$

One of our results will be related to the simpler and lower-dimensional isotropic single-plane problem, and thus here we outline a method of solving such a problem. Eliminating the  $z$  dependence and using the equivalence of the  $x$  and  $y$  directions, (12) reduces to

$$\begin{aligned}
C_0 &= UI_{0,2d} C_0 - 4JI_{x,2d} C_x \\
C_x &= UI_{x,2d} C_0 - 2JI_{xx,2d} C_x - 2JI_{xy,2d} C_x.
\end{aligned} \tag{16}$$

One can further simplify these equations using the identities [12]

$$\begin{aligned}
I_{x,2d} &= \frac{1}{8t} - \frac{AI_{0,2d}}{2} \\
I_{xx,2d} &= -I_{xy,2d} - AI_{x,2d}
\end{aligned} \tag{17}$$

and one can integrate  $I_{0,2d}$  to obtain

$$I_{0,2d} = \frac{1}{2\pi t A} K(2/A) \tag{18}$$

where  $K(x)$  is the complete elliptic integral of the first kind. Thus  $I_{0,2d}$  is a symmetric function of  $A$ , which is defined for  $|A| > 2$  and diverges as  $|A| \rightarrow 2^+$ . Now we eliminate  $C_0$  and  $C_x$  from the equation set (one can show that no solutions exist if either of these is zero—see below for three dimensions), and then take the strong Coulombic repulsion limit of  $U \rightarrow \infty$ , and then solve for  $J$ . One finds

$$J = \frac{-16I_{0,2d}t^2}{-1 + 4AI_{0,2d}t}. \quad (19)$$

Noting the dependence of  $I_{0,2d}$  on energy, this equation (and we will derive similar equations for three dimensions below) then solves for the bound state energy in terms of  $J$ . Alternatively, one can use this equation to solve for the minimum value of  $J/t$  that is required for a bound state to form. That is, by using (18) one finds that as  $A \rightarrow -2^-$   $I_{0,2d}$  diverges and the limiting value of  $J/t$  is 2. Hence a critical value of  $J_c/t = 2$  is obtained in the two-dimensional isotropic case, which is in agreement with the results obtained elsewhere [10, 12, 14].

### 3.1. Three dimensions—*isotropic hopping*

The elliptic integrals of (11) become impossible to solve analytically in higher dimensions. However, to make progress with the three-dimensional problem it is necessary to understand as much about the properties of these integrals as possible.  $I_{0,nd}$  is an odd function that is only defined for  $|A| > n$  and it is negative for  $A < -n$ . It is an important fact that the behaviour of  $I_{0,nd}$  is qualitatively different for  $n < 3$  than for  $n \geq 3$ . This is because the limit as  $A \rightarrow -n^-$  is divergent for  $n < 3$  but finite for  $n \geq 3$ , a result that can be obtained, e.g. by writing  $I_{0,nd}$  in  $n$ -dimensional polar coordinates.

To get a simple expression of  $J$  as a function of the energy  $A$  in three dimensions, analogous to (19), one can derive a set of equations analogous to (17), namely

$$\begin{aligned} I_{x,3d} &= \frac{2}{3} \left( \frac{1}{8t} - \frac{AI_{0,3d}}{2} \right) \\ I_{xx,3d} &= -AI_{x,3d} - 2I_{xy,3d}. \end{aligned} \quad (20)$$

Here we analyse the infinite three-dimensional lattice with completely isotropic hopping frequencies and spin exchanges:  $J = J_{\parallel} = J_{\perp}$  and  $t = t_{\parallel} = t_{\perp}$  with  $L_x = L_y = L_z = \infty$ . Starting from (12), and accounting for the symmetries in the elliptic integrals ( $I_x = I_y = I_z$ ,  $I_{xy} = I_{yz} = I_{xz}$ ,  $I_{xx} = I_{yy} = I_{zz}$ —note that below, for simplicity, we refrain from using the 3d label for these integrals), one can eliminate  $C_x$ ,  $C_y$  and  $C_z$  from the equation set to obtain the equation:

$$(-2I_{xx}J + 2I_{xx}JU I_0 - 6UI_x^2J - 4JI_{xy} + 4JI_{xy}UI_0 - 1 + UI_0)C_0 = 0. \quad (21)$$

First we assume that  $C_0 \neq 0$  and solve for  $U$ :

$$U = \frac{2I_{xx}J + 1 + 4JI_{xy}}{2I_{xx}JI_0 - 6I_x^2J + 4JI_{xy}I_0 + I_0}. \quad (22)$$

For finite  $A$  and  $J$ , the numerator of this expression is bounded—the  $I$  integrals are convergent for  $|A| > 3$  and finite. Thus taking the limit that  $U \rightarrow \infty$  is equivalent to setting the denominator to zero:

$$2I_{xx}JI_0 - 6I_x^2J + 4JI_{xy}I_0 + I_0 = 0 \quad (23)$$

and then solving for  $J$  gives

$$J = -\frac{1}{2} \frac{I_0}{I_{xx}I_0 - 3I_x^2 + 2I_{xy}I_0}. \quad (24)$$

Finally, (20) can be used to give the simplest form for  $J$ , similar to (19), which again only depends on the elliptic integral  $I_0$ :

$$J = \frac{24I_0t^2}{-1 + 4AI_0t}. \quad (25)$$

The right-hand side of equation (25) is a monotonically decreasing function as  $A$  approaches  $-3$  from below, and therefore the minimal value of  $J$  is found from this limit. One can evaluate the right-hand side of this equation numerically to a very high accuracy. For example, one can complete the lattice sums of equation (11) with larger and larger lattices in the limit of  $E$  approaching the bottom of the non-interacting band, that is  $-12t$ . However, a more accurate determination of this quantity can be obtained from the integral form of  $I_0$ , which, using the properties of elliptic integrals to simplify the multidimensional integral to an integration over a single variable, is given by

$$I_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{K(2/(A + \cos q))}{(2\pi)^2 t (A + \cos q)} dq \quad (26)$$

where  $K(x)$  is the complete elliptic integral of the first kind. Again, examining the limit of  $A$  approaching  $-3$  from below, and carefully accounting for the properties of the integrand near  $q = 0$ , one finds, in agreement with the lattice sum method mentioned above, that  $I_0(A \rightarrow -3) = (-0.12633 \pm 0.00009)/t$ . Therefore, for this system we find  $J_c/t = 5.877 \pm 0.008$ .

As mentioned, in the above derivation we have assumed for this solution that  $C_0 \neq 0$  in writing down (22). Putting  $C_0 = 0$  into the initial equation set, (12) gives us either the trivial solution  $C_0 = C_x = C_y = C_z = 0$  or a new equation for  $J$ . First we set  $C_0 = 0$  in (12), and eliminating  $C_x$ ,  $C_y$ ,  $C_z$  from the equations yields

$$J = \frac{12t}{-A + 4A^2I_0t - 36I_{xx}t}. \quad (27)$$

Numerical studies also indicate that this  $J$  has a similar qualitative behaviour as (25), so if the limit as  $A \rightarrow -3^-$  of (27) is less than  $5.877$  then the initial calculation of  $J_c = (5.877 \pm 0.008)t$  will be supplanted by the lower value. However, numerical calculations give a limit of  $J$  in (27) of about  $10.7$ . We note that this solution has a different symmetry from the first, a result that follows immediately from  $C_0 = 0$ ; so, this latter bound state is not an on-site or extended  $s$ -wave solution (see [14] for a discussion of analogous results in two dimensions).

Finally, the critical spin exchange in the isotropic three-dimensional case is determined to be  $J_c = (5.877 \pm 0.008)t \neq 2t$ . In part, we have provided this detailed analysis here because our results contradict a statement in [12] that the value of  $J_c/t = 2$  (in the isotropic case) is independent of the lattice size and dimensionality.

### 3.2. Two planes with no $z$ hopping

We now consider the anisotropic case of no  $z$  hopping in the lattice, for the reasons already reviewed in the introduction to this paper. Physically, one can see that to study an electron pair with no  $z$  hopping then one need only study the two-plane problem since if the electrons are to see each other at all, they must be either on the same plane or on adjacent  $z$  planes where they may interact via the spin exchange interaction  $J_{\parallel}$  or  $J_{\perp}$ . We only consider a single electron pair, and they are restricted to be in two neighbouring planes, so the problem collapses entirely to the two-plane problem. Further, due to this restricted hopping the bottom of the two-electron scattering continuum will correspond to  $E = -8t$ .

We start with the two-plane problem,  $L_x = L_y = \infty$  and  $L_z = 2$ , that is isotropic in  $x$  and  $y$  and has zero  $z$ -hopping frequency. Here, as in (10)–(12), set  $J_{\parallel} = J$ . (The fact that for

a spatial extent of  $L_z = 2$  it is necessary to specify open or periodic boundary conditions does not affect our results—see below.) Also, for the hopping we take  $t_{\parallel} = t$  and  $t_{\perp} = 0$ . A great deal of simplification may be made with the  $I$  integrals of (11) because the denominator of the integrand is independent of  $q_z$  (and  $z$  is the only coordinate exhibiting anisotropy), and we can relate these integrals (which we denote by  $\tilde{I}$ ) to their counterparts in the two-dimensional fully isotropic case. For example:

$$\begin{aligned}\tilde{I}_{zz} &= \frac{1}{2L_x L_y} \sum_{m_z=0,1} \sum_{q_x, q_y} \frac{\cos^2(2\pi m_z/2)}{E + 4t(\cos(q_x) + \cos(q_y))} \\ &= \frac{1}{L_x L_y} \sum_{q_x, q_y} \frac{1}{E + 4t(\cos(q_x) + \cos(q_y))} \\ &= I_{0,2d}.\end{aligned}\quad (28)$$

Similarly

$$\begin{aligned}\tilde{I}_0 &= I_{0,2d} \\ \tilde{I}_{\alpha} &= I_{\alpha,2d} \quad \text{where } \alpha = x, y \\ \tilde{I}_{\alpha,\beta} &= I_{\alpha,\beta,2d} \quad \text{where } \alpha, \beta = x, y \\ \tilde{I}_z &= 0 \\ \tilde{I}_{\alpha z} &= 0 \quad \text{where } \alpha = x, y \\ \tilde{I}_{zz} &= I_{0,2d}.\end{aligned}\quad (29)$$

With these simplifications, (12) simplifies significantly:

$$\begin{aligned}C_0 &= U I_{0,2d} C_0 - 2J I_{x,2d} C_x - 2J I_{y,2d} C_y \\ C_x &= U I_{x,2d} C_0 - 2J I_{xx,2d} C_x - 2J I_{xy,2d} C_y \\ C_y &= U I_{y,2d} C_0 - 2J I_{xy,2d} C_x - 2J I_{yy,2d} C_y \\ C_z &= -2J_{\perp} I_{0,2d} C_z.\end{aligned}\quad (30)$$

What is interesting about this set of equations is that the first three equations are identical to the two-dimensional isotropic case, so for  $C_0 \neq 0$  we find that (19) holds here as well. We can satisfy the third equation simply by setting  $C_z = 0$ . Since the  $z$  spin exchange is completely irrelevant to the equation, this physically means that this solution puts both electrons on the *same* plane, and thus the problem reduces completely to the two-dimensional isotropic case.

However, in our two-plane problem we can also obtain an equation for (in this case)  $J_{\perp}$  by allowing  $C_x = C_y = C_0 = 0$ , and not get a trivial zero solution to the eigenvector of the Hamiltonian by having  $C_z \neq 0$ . Hence from (30) we immediately obtain

$$J_{\perp} = -\frac{1}{2} \frac{1}{I_{0,2d}}.\quad (31)$$

In this case  $J_{\parallel}$  has dropped completely out of the equations, and this case corresponds to putting the two electrons on different planes, so they can only interact through  $J_{\perp}$ . Recalling that  $I_{0,2d}$  diverges this gives us a critical spin coupling constant of  $J_c = J_{\perp,c} = 0$ . That is, we may obtain bound state solutions for arbitrarily small values  $J_{\perp}$  (for any  $J$ ).

#### 4. Discussion

We have considered a model Hamiltonian motivated in part by the cuprate superconductors, and have examined the formation of two-electron bound states in the dilute limit. Work on related Hamiltonians [12, 10, 14] and on other model Hamiltonians motivated by the cuprates [15]



also followed this approach in the hope of better understanding the complicated many-electron states of these highly correlated systems.

This paper analysed the formation of electron pair bound states in a three-dimensional lattice by comparing the minimum spin–exchange interaction that is necessary to allow for the formation of bound states for isotropic hopping and exchange, and for the complete suppression of interplanar hopping. We found that the minimum attractive interaction required is infinitesimal for the case where  $t_{\perp}$  is zero, and hence the critical spin coupling for exchange-coupled planes is

$$J_c = 0. \quad (32)$$

The problem remains of trying to extrapolate with this very simple model to the physics of two-electron bound state formation of the cuprate superconductors (albeit in the dilute limit for each plane). A three-dimensional  $t$ – $J$ – $U$  model that takes into account the correct anisotropies of the hopping and superexchange, and for which  $t_{\perp}$  is very small, could indeed yield a two-electron bound state solution for very small values of  $J_{\perp}$  if the limit of  $J_c$  is continuous as  $t_{\perp} \rightarrow 0$ . However, in general  $J_{\perp,c}$  will depend on both  $t_{\perp}$  and  $J_{\parallel}$ , and the present study has not examined the parameter space associated with this much more difficult (numerically, that is) problem. (Note from equation (31) that there is no dependence on  $J_{\parallel}$  when  $t_{\perp} = 0$ , and for isotropic hopping and superexchange there is only dimensionless ratio,  $J/t$ .)

Our results could be of interest for the study of ultra-cold atoms (see [16] and references therein for the connection of such systems to the kind of model Hamiltonians studied in connection with the cuprate superconductors). That is, in such systems one can tune the interactions (and with optical lattices, the geometries) for such model Hamiltonians, so perhaps the limit that was examined in this paper can be created in such systems.

The above result necessarily leads to the question of the superconducting properties for such a model Hamiltonian in the dilute limit. As shown in [9], and as found for the case of exchange-coupled chains [17], weak (or in our case zero) interplanar electronic hopping leads to a large density of states at half filling (the density of states for a two-dimensional square lattice diverges logarithmically at the middle of band), necessarily leading to large increases in  $T_c$  when compared to the situation found when the hopping frequency is isotropic. Therefore, using a weak-coupling BCS approach one indeed expects this model to show a large increase in  $T_c$  relative to the three-dimensional lattice. What happens in the strong coupling limit remains a topic for conjecture. In contrast to this result, note that for exchange-coupled chains [17] the electronic density of states is in fact divergent at the band edges, and thus not surprisingly one finds the greatest enhancement of  $T_c$  at very low fillings.

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