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A pure Hubbard model with demonstrable pairing adjacent to the Mott-insulating phase

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Abstract

We introduce a Hubbard model on a particular class of geometries, and consider the effect of doping the highly spin-degenerate Mott-insulating state with a microscopic number of holes in the extreme strong-coupling limit. The geometry is quite general, with pairs of atomic sites at each superlattice vertex, and a highly frustrated inter-atomic connectivity: the one-dimensional realization is a chain of edge-sharing tetrahedra. The sole model parameter is the ratio of intra-pair to inter-pair hopping matrix elements. If the intra-pair hopping is negligible then introducing a microscopic number of holes results in a ferromagnetic Nagaoka groundstate. Conversely, if the intra-pair hopping is comparable with the inter-pair hopping then the groundstate is low spin with short-ranged spin correlations. We exactly solve the correlated motion of a pair of holes in such a state and find that, in 1d and 2d, they form a bound pair on a length scale that increases with diminishing binding energy. This result is pertinent to the long-standing problem of hole motion in the CuO_2 planes of the high-temperature superconductors: we have rigorously shown that, on our frustrated geometry, the holes pair up and a short-ranged low-spin state is generated by hole motion alone.

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1. Introduction

In the years since the discovery of high-temperature superconductors, a wide spectrum of ideas about the fundamental cause of superconductivity in CuO_2 planes has been proposed, but as yet none have been accepted as correct. In this paper we revisit Anderson's early suggestion of a resonating-valence-bond (RVB) state, with 'pre-formed' pairs [1], which at the time lacked rigorous support.

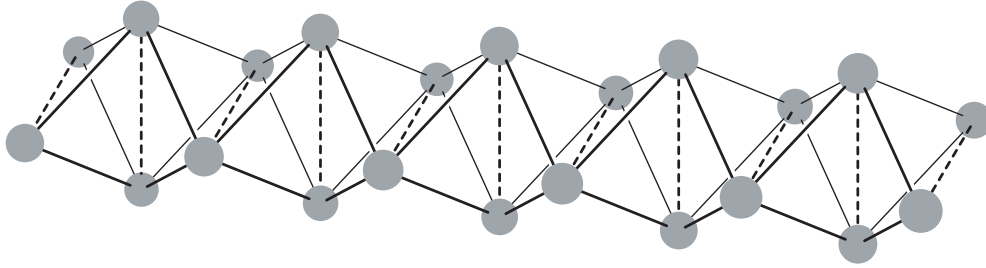


Figure 1. A chain of edge-sharing tetrahedra, a one-dimensional example of the class of geometry considered in this paper. The inter-pair hopping (—) is, in general, not the same strength as the intra-pair hopping (- - -).

A suggestion currently popular in the literature is that the three-band Hubbard model in the strong-coupling regime can be mapped onto the t - J model via the idea of Zhang–Rice singlets [2]. We believe that this reduction eliminates important physics: for example, the t -term alone can only generate Nagaoka ferromagnetism [3]—in order to account for the observed low-spin state one has to rely on the higher-order J term. In the accompanying paper by IBS and MWL [4], evidence is provided to support the hypothesis that the three-band model allows an RVB state to be generated solely by the hole motion.

The three-band model for CuO_2 planes is highly frustrated in a subtle way [5], and it is this frustration that is lost in the reduction to the t - J model. In this paper we provide rigorous evidence for energetically favourable hole-pairing in a not dissimilar highly-frustrated Hubbard model in the strong-coupling limit. The frustration is crucial, as it is this that stabilizes the short-range correlated low-spin state, which is generated by hole motion alone.

2. The model and geometry

In this study we consider a repulsive Hubbard model on a particular class of highly-connected lattice. The geometry is that of a superlattice of vertex pairs. In one dimension we will consider a linear-chain superlattice, in two a square superlattice and in three a cubic superlattice. The linear-chain situation, where each superlattice site has a co-ordination number $Z = 2$, can be realized physically as a chain of edge-sharing tetrahedra, as illustrated in figure 1.

The single-particle part of the model Hamiltonian can be specified by the options open to a charged spin-half fermion on any particular vertex. The fermion can hop to any of the vertices in the Z neighbouring pairs with a matrix element $-t$. It can also hop to the other vertex in the pair with a matrix element which, for convenience, we define to be $-Z\lambda t$. The parameter λ expresses the difference in energy scales between inter- and intra-pair hopping. The electrostatic correlations between the charged fermions are included via an on-site Hubbard term: two particles occupying the same vertex incur a Coulomb penalty U . The second-quantized Hamiltonian is

$$H = -t \sum_{\langle i, i' \rangle} \sum_{\tau, \tau', \sigma} p_{i\tau\sigma}^\dagger p_{i'\tau'\sigma} - Z\lambda t \sum_{i, \tau, \sigma} p_{i\tau\sigma}^\dagger p_{i\bar{\tau}\sigma} + \frac{U}{2} \sum_{i, \tau, \sigma} p_{i\tau\sigma}^\dagger p_{i\tau\sigma} p_{i\tau\bar{\sigma}}^\dagger p_{i\tau\bar{\sigma}} \quad (1)$$

where $p_{i\tau\sigma}^\dagger$ creates a fermion of spin σ on vertex τ of the pair on superlattice site i . The complementary spin, or vertex, is denoted by a bar, and $\langle i, i' \rangle$ indicates summation over nearest neighbours i and i' .

We are concerned with behaviour adjacent to the Mott insulator, and so it is appropriate to rewrite the Hamiltonian in terms of fermionic hole operators, via the mapping $p_{i\tau\sigma}^\dagger \mapsto h_{i\tau\sigma}$. Then, up to an ignorable constant, the hole Hamiltonian is

$$H = t \sum_{(i,i')} \sum_{\tau,\tau',\sigma} h_{i\tau\sigma}^\dagger h_{i'\tau'\sigma} + Z\lambda t \sum_{i,\tau,\sigma} h_{i\tau\sigma}^\dagger h_{i\bar{\tau}\sigma} + \frac{U}{2} \sum_{i,\tau,\sigma} h_{i\tau\sigma}^\dagger h_{i\tau\sigma} h_{i\bar{\tau}\sigma}^\dagger h_{i\bar{\tau}\sigma}. \tag{2}$$

In this paper we restrict our attention to the extreme strong-coupling limit of $U = \infty$ with a finite positive t . At maximal filling in the finite energy subspace the system is a Mott insulator with one particle (or, equivalently, one hole) per vertex: this state is hugely spin-degenerate because the super-exchange energy scale, J , is rigorously equal to zero. We address the problem of how this degeneracy is lifted by the inclusion of a microscopic number of holes. This particular geometry is useful because we can treat the doping of one and two holes analytically. Before the more interesting issue of a two-hole bound state we will introduce the two competing styles of groundstate via the more straightforward single-hole situation.

3. Local symmetries and one-hole behaviour

Eigenstates respect the symmetries of the Hamiltonian, and this is useful when categorizing the possible styles of solution. For example, the model that we consider in this paper preserves the spin of a hole when it hops: as a result of this global symmetry, the total spin of a state is conserved. There also exists a collection of N local symmetries, where N is the number of superlattice sites: these arise from the fact that the Hamiltonian is unchanged when the two vertices of any pair are swapped. In looking for the groundstate of our Hamiltonian we categorize the eigenstates by their symmetry with respect to these N Hamiltonian-preserving operations. We consider states that are either symmetric or antisymmetric with respect to all N of the local symmetries: we do not deal with the mixed-symmetry states.

3.1. The high-spin state

Setting the parameter λ to zero effectively removes all the intra-pair bonds; if the superlattice is bi-partite then the connectivity is no longer frustrated, and hence the one-hole groundstate will exhibit Nagaoka ferromagnetism.

In the real-space representation that we choose to work with, every site is occupied with either a spinless fermionic hole or a hard-core bosonic spin. To illustrate this, consider a small part of the geometry comprising two nearest-neighbour vertex pairs in the ferromagnetic one-hole state: if the hole is on one of the vertices then the other three vertices accommodate parallel spins. In pictorial form, the action of the Hamiltonian on this unit is simply

$$H \begin{array}{|c|c|} \hline \text{h} & \sigma \\ \hline \sigma & \sigma \\ \hline \end{array} = Z\lambda t \begin{array}{|c|c|} \hline \sigma & \sigma \\ \hline \text{h} & \sigma \\ \hline \end{array} + t \left[\begin{array}{|c|c|} \hline \sigma & \text{h} \\ \hline \sigma & \sigma \\ \hline \end{array} + \begin{array}{|c|c|} \hline \sigma & \sigma \\ \hline \sigma & \text{h} \\ \hline \end{array} \right]. \tag{3}$$

We can use this representation to write the Bloch state for one hole with momentum k in a ferromagnetic background:

$$|F_{k\sigma}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} \frac{1}{\sqrt{2}} \left[\begin{array}{|c|c|c|c|} \hline \sigma & \sigma & \text{h} & \sigma \\ \hline \sigma & \sigma & \sigma & \sigma \\ \hline \end{array} \begin{array}{|c|c|c|c|} \hline \sigma & \sigma & \sigma & \sigma \\ \hline \sigma & \sigma & \sigma & \sigma \\ \hline \end{array} + \begin{array}{|c|c|c|c|} \hline \sigma & \sigma & \sigma & \sigma \\ \hline \sigma & \sigma & \text{h} & \sigma \\ \hline \end{array} \begin{array}{|c|c|c|c|} \hline \sigma & \sigma & \sigma & \sigma \\ \hline \sigma & \sigma & \sigma & \sigma \\ \hline \end{array} \right]. \tag{4}$$

The one-dimensional lattice is used for illustration here because it is simple to depict; it is obvious how this representation extends to the two- and three-dimensional lattices. This state is ‘fully symmetric’ since it maps onto itself when the vertices of any particular pair are interchanged.

With the aid of equation (3) it is straightforward to show that $|F_{k\sigma}\rangle$ is an eigenstate of the Hamiltonian with an energy eigenvalue

$$\epsilon_{k\sigma}^{(\text{high},1)} = \lambda + 2\gamma_k. \tag{5}$$

Throughout this paper, energy eigenvalues, denoted by ϵ , are ‘per hole’ and in units of Zt . The one-hole groundstate has the wavevector \mathbf{k} that minimizes the superlattice structure factor γ_k : for the cubic family of superlattices that we are considering here this means that $\mathbf{k} = \mathbf{Q} \equiv (\pi, \pi, \dots)$ and therefore

$$\epsilon_{Q\sigma}^{(\text{high},1)} = \lambda - 2. \tag{6}$$

3.2. The low-spin state

The other class of state that we consider is the complement of the high-spin state, in that it has low-spin and is ‘fully anti-symmetric’ with respect to the vertex-pair-swapping symmetry.

In our chosen representation any real-space pair that is free from holes must accommodate two bosonic spins: in order to make this pair of bosons antisymmetric, the spins must be correlated in a total-spin singlet. We depict the singlet in the following way:

$$\begin{array}{|c} \uparrow \\ \circ \\ \downarrow \end{array} \equiv \frac{1}{\sqrt{2}} \left[\begin{array}{|c} \uparrow \\ \circ \\ \downarrow \end{array} - \begin{array}{|c} \downarrow \\ \circ \\ \uparrow \end{array} \right] = (-1) \begin{array}{|c} \downarrow \\ \circ \\ \uparrow \end{array} \tag{7}$$

The antisymmetric property of the bosonic singlet is evident from the fact that swapping the ‘head’ and ‘tail’ generates a factor of -1 .

The one-hole antisymmetric low-spin state is

$$|L_{k\sigma}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} \frac{1}{\sqrt{2}} \left[\begin{array}{cccc} & & \text{h} & \\ \circ & \circ & \circ & \circ \\ & & \text{h} & \end{array} - \begin{array}{cccc} & & \sigma & \\ \circ & \circ & \circ & \circ \\ & & \text{h} & \end{array} \right] \tag{8}$$

where the anti-phase combination guarantees antisymmetry with respect to vertex exchange on the hole’s pair.

The action of the Hamiltonian on a two-pair unit that contains the hole is

$$H \begin{array}{|c} \text{h} \\ \diagdown \\ \circ \\ \diagup \\ \sigma \end{array} = Z\lambda t \begin{array}{|c} \sigma \\ \diagdown \\ \text{h} \\ \diagup \\ \circ \end{array} + t \left[\begin{array}{|c} \text{h} \\ \diagdown \\ \sigma \\ \diagup \\ \circ \end{array} + \begin{array}{|c} \circ \\ \diagdown \\ \sigma \\ \diagup \\ \text{h} \end{array} \right]. \tag{9}$$

Acting the Hamiltonian on the state $|L_{k\sigma}\rangle$ creates states where singlets extend from one superlattice site to another. Such states have a non-zero overlap with the original state, and we can use the spin identity

$$\begin{array}{|c} \text{h} \\ \diagdown \\ \sigma \\ \diagup \\ \circ \end{array} - \begin{array}{|c} \sigma \\ \diagdown \\ \text{h} \\ \diagup \\ \circ \end{array} = \begin{array}{|c} \text{h} \\ \diagdown \\ \circ \\ \diagup \\ \sigma \end{array} \tag{10}$$

to show that $|L_{k\sigma}\rangle$ is in fact an eigenstate of the Hamiltonian with energy eigenvalue

$$\epsilon_{k\sigma}^{(\text{low},1)} = -\lambda + \gamma_k. \tag{11}$$

As was the case for the ferromagnetic one-hole state, the lowest energy state has $k = Q$. By comparing equations (6) and (11) it is obvious that the groundstate is ferromagnetic when $\lambda < 1/2$ and low-spin with short-range correlations when $\lambda > 1/2$.

4. Two-hole behaviour

In the previous section we saw that the one-hole solutions were trivial to find once a suitable representation had been established. With this framework in place, we are now ready to tackle the two-hole problem. The high-spin state is simple to describe because the interaction is irrelevant and we simply occupy a single non-interacting band; the low-spin problem is not so straightforward, and we make use of the Greens function impurity technique to deal with the interaction.

4.1. The high-spin state

The single-hole problem in the symmetric subspace was solved by including a symmetric hole with wavevector Q ; all other sites feature a spin σ hence the state was described as ‘high spin’. If we include another symmetric hole from the corner of the Brillouin zone, with the same spin as the first, then Pauli exclusion prevents double-occupancy of any vertex. On a macroscopic lattice these two holes, which are in orthogonal single-hole states, can have an arbitrarily close energy. Hence the lowest energy *per hole* of the two-hole high-spin state is the same as the single-hole minimum, namely

$$\epsilon_{Q\sigma}^{(\text{high},2)} = \lambda - 2. \tag{12}$$

4.2. The low-spin state

Here we restrict attention to states where the pair of fermionic holes, h_1 and h_2 , have zero total momentum. The other degree of freedom is the separation between the two holes on the superlattice, $R = r_2 - r_1$, and we use this quantity to label the low-spin state basis.

Consider the $R = 0$ state which, in its properly normalized form, is

$$|R = 0\rangle = \frac{1}{\sqrt{N}} \sum_i \text{Diagram} \tag{13}$$

This state has total-spin zero, short-range spin correlations and is overall antisymmetric since swapping a singlet’s head and tail, or exchanging h_1 and h_2 , results in a minus sign.

As before, consider a unit of this state comprising the vertex pair containing h_1 and h_2 , and one of its nearest neighbour pairs that must feature a singlet. The action of the Hamiltonian on this unit can be written as

$$H \text{Diagram} = t \left[\text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \right]. \tag{14}$$

Note that no use is made of the intra-pair hopping, as this is prohibited by the $U = \infty$ Coulomb penalty.

Now, any particular superlattice site has Z nearest neighbours; let us denote the Z vectors that translate to the nearest neighbours as $\mathbf{n}_1, \mathbf{n}_2, \dots, \mathbf{n}_Z$. We then choose to define the overall antisymmetric two-hole state where the holes are separated by one lattice spacing as

$$|\mathbf{R} \neq 0\rangle = \frac{1}{\sqrt{N}} \sum_i \frac{1}{2} \left[\begin{array}{c} \uparrow \quad \text{h}_2 \\ \diagdown \quad \diagup \\ \text{h}_1 \quad \downarrow \end{array} + \begin{array}{c} \text{h}_1 \quad \downarrow \\ \diagdown \quad \diagup \\ \uparrow \quad \text{h}_2 \end{array} - \begin{array}{c} \uparrow \quad \downarrow \\ \diagdown \quad \diagup \\ \text{h}_1 \quad \text{h}_2 \end{array} - \begin{array}{c} \text{h}_1 \quad \text{h}_2 \\ \diagdown \quad \diagup \\ \uparrow \quad \downarrow \end{array} \right] \quad (15)$$

where it is implied that all other vertex-pairs feature a spin singlet. The convention is to put an \uparrow spin on the same pair as the hole h_1 , and a \downarrow with h_2 ; the factor of $1/2$ ensures correct normalization. It is then possible to express the outcome of applying the Hamiltonian to $|\mathbf{R} = 0\rangle$ as

$$H|\mathbf{R} = 0\rangle = 2\sqrt{2}t \sum_{j=1}^Z |\mathbf{R} = \mathbf{n}_j\rangle. \quad (16)$$

The states for all other \mathbf{R} , i.e. $\mathbf{R} \neq 0, \mathbf{n}_1, \mathbf{n}_2, \dots, \mathbf{n}_Z$, are defined in a similar way to $|\mathbf{R} = \mathbf{n}_j\rangle$. The fact that these states have the holes more than one hop apart means that they move as ‘independent holes’. The reasoning from section 3.2 applies, and thus

$$H|\mathbf{R} \neq 0, \mathbf{n}_1, \mathbf{n}_2, \dots, \mathbf{n}_Z\rangle = -2Z\lambda t|\mathbf{R}\rangle + 2t \sum_{j=1}^Z |\mathbf{R} + \mathbf{n}_j\rangle \quad (17)$$

where the factor of two arises because there are *two* independent holes.

The action of the Hamiltonian on the nearest-neighbour states is a combination of the two above styles of behaviour. The holes are on different vertex pairs, so they can gain the intra-pair hopping energy. Hopping in one particular direction will bring both holes onto the same site, and hopping in all the other directions is ‘independent-hole’-like. The result is that

$$H|\mathbf{R} = \mathbf{n}_p\rangle = -2Z\lambda t|\mathbf{R}\rangle + 2\sqrt{2}t|0\rangle + 2t \sum_{j \neq p} |\mathbf{R} + \mathbf{n}_j\rangle. \quad (18)$$

Now that we know all the matrix elements, it can be seen that they deviate from a perfectly periodic Hamiltonian in just two ways: (i) the coupling between $|0\rangle$ and the ‘nearest-neighbour’ states $|\mathbf{n}_j\rangle$ is enhanced by a factor of $\sqrt{2}$, and (ii) the intra-pair energy $2Z\lambda t$ is *not* gained by $|0\rangle$. We can write the Hamiltonian as the sum of a periodic term, H_0 , and a ‘local’ term H_1 , where the matrix elements of these two terms are given by

$$H_0|\mathbf{R}\rangle = -2Z\lambda t|\mathbf{R}\rangle + 2t \sum_{j=1}^Z |\mathbf{R} + \mathbf{n}_j\rangle \quad (19)$$

and

$$H_1 \begin{bmatrix} |0\rangle \\ |\mathbf{n}_1\rangle \\ |\mathbf{n}_2\rangle \\ \vdots \\ |\mathbf{n}_Z\rangle \end{bmatrix} = 2t \begin{bmatrix} Z\lambda & \sqrt{2}-1 & \sqrt{2}-1 & \dots & \sqrt{2}-1 \\ \sqrt{2}-1 & 0 & 0 & \dots & 0 \\ \sqrt{2}-1 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sqrt{2}-1 & 0 & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} |0\rangle \\ |\mathbf{n}_1\rangle \\ |\mathbf{n}_2\rangle \\ \vdots \\ |\mathbf{n}_Z\rangle \end{bmatrix}. \quad (20)$$

It is convenient to rescale the Hamiltonian so that all energies are ‘per hole’ in units of Zt : the rescaled two-hole Hamiltonian, \mathcal{H} , is defined by $H = 2Zt\mathcal{H}$. In order to exactly

solve this eigenproblem we will make use of the Greens function for the entire Hamiltonian, $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, which can be written as

$$\mathcal{G}(z) = \mathcal{G}_0(z) + \mathcal{G}_0(z)\Sigma(z)\mathcal{G}_0(z) \tag{21}$$

where $\mathcal{G}_0(z)$ is the Greens function for \mathcal{H}_0 , the periodic part of the Hamiltonian,

$$\mathcal{G}_0(z) = [z - \mathcal{H}_0]^{-1} = \frac{1}{z + \lambda - \gamma_k} \tag{22}$$

and

$$\Sigma(z) = [1 - \mathcal{H}_1\mathcal{G}_0(z)]^{-1}\mathcal{H}_1. \tag{23}$$

The energy eigenvalues of the periodic case alone are found at the poles of $\mathcal{G}_0(z)$. If we anticipate that the inclusion of \mathcal{H}_1 generates a new state, then its pole must be present in $\Sigma(z)$. Hence the pole is found at $z = \epsilon$ such that

$$\det[1 - \mathcal{H}_1\mathcal{G}_0(\epsilon)] = 0. \tag{24}$$

Equation (20) shows how the local term of the Hamiltonian, \mathcal{H}_1 , can be represented by a $(Z + 1) \times (Z + 1)$ matrix; the above determinant equation involves the product $\mathcal{H}_1\mathcal{G}_0$, hence the relevant part of the matrix $\mathcal{G}_0(z)$ is simply

$$\mathcal{G}_0(z) = \begin{bmatrix} \mathcal{G}_{00}(z) & \mathcal{G}_{01}(z) & \mathcal{G}_{02}(z) & \cdots & \mathcal{G}_{0Z}(z) \\ \mathcal{G}_{10}(z) & \mathcal{G}_{11}(z) & \mathcal{G}_{12}(z) & \cdots & \mathcal{G}_{1Z}(z) \\ \mathcal{G}_{20}(z) & \mathcal{G}_{21}(z) & \mathcal{G}_{22}(z) & \cdots & \mathcal{G}_{2Z}(z) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathcal{G}_{Z0}(z) & \mathcal{G}_{Z1}(z) & \mathcal{G}_{Z2}(z) & \cdots & \mathcal{G}_{ZZ}(z) \end{bmatrix} \tag{25}$$

where, if we conveniently let $\mathbf{n}_0 = 0$, these real-space elements are defined by

$$\mathcal{G}_{ij}(z) = \frac{1}{N} \sum_k \frac{\exp[i\mathbf{k} \cdot (\mathbf{n}_i - \mathbf{n}_j)]}{z + \lambda - \gamma_k}. \tag{26}$$

Extracting the point-symmetry of the superlattice reduces the matrices to 2×2 ,

$$\mathcal{H}_1 = \begin{bmatrix} \lambda & \sqrt{2} - 1 \\ \sqrt{2} - 1 & 0 \end{bmatrix} \quad \text{and} \quad \mathcal{G}_0 = \begin{bmatrix} \mathcal{G}_{00}(z) & \mathcal{G}'(z) \\ \mathcal{G}'(z) & \tilde{\mathcal{G}}(z) \end{bmatrix} \tag{27}$$

where

$$\mathcal{G}'(z) = \frac{1}{N} \sum_k \frac{\gamma_k}{z + \lambda - \gamma_k} \quad \text{and} \quad \tilde{\mathcal{G}}(z) = \frac{1}{N} \sum_k \frac{\gamma_k^2}{z + \lambda - \gamma_k}. \tag{28}$$

Evaluating the determinant equation (24) to find the pole at $z = \epsilon$ gives

$$1 = \lambda\mathcal{G}_{00}(\epsilon) + 2(\sqrt{2} - 1)\mathcal{G}'(\epsilon) + (\sqrt{2} - 1)^2[\mathcal{G}_{00}(\epsilon)\tilde{\mathcal{G}}(\epsilon) - \mathcal{G}'^2(\epsilon)] \tag{29}$$

which can be further simplified using the identities

$$\mathcal{G}'(\epsilon) = (\epsilon + \lambda)\mathcal{G}_{00}(\epsilon) - 1 \quad \text{and} \quad \tilde{\mathcal{G}}(\epsilon)\mathcal{G}_{00}(\epsilon) - \mathcal{G}'^2(\epsilon) = \mathcal{G}'(\epsilon) \tag{30}$$

to give the self-consistent equation

$$\frac{2}{\epsilon + 2\lambda} = \frac{1}{N} \sum_k \frac{1}{\epsilon + \lambda - \gamma_k}. \tag{31}$$

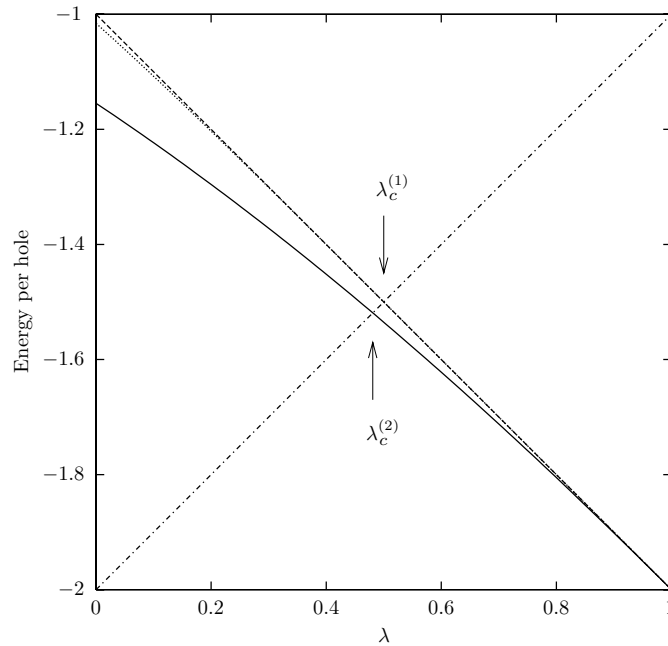


Figure 2. The energy *per hole* of various states as a function of the model parameter λ . Whether we are considering the linear chain, square, or cubic superlattice, the one-hole ferromagnetic Nagaoka state (— · —) and one-hole low-spin state (- - -) are degenerate at $\lambda_c^{(1)} = 1/2$. The two-hole bound-pair low-spin state on the linear chain (—) is degenerate with the two-hole Nagaoka state at $\lambda_c^{(2)} = 0.4809(6)$. The binding energy of the two-hole low-spin state on the square superlattice (· · · · ·) is an order of magnitude smaller than the linear chain case; in both 1d and 2d the binding energy vanishes at $\lambda = 1$.

In one and two dimensions this equation has a solution in the parameter range $0 \leq \lambda < 1$. For example, the energy per hole of the linear-chain superlattice state is given exactly by

$$\epsilon = -\frac{2}{3} \left[\lambda + \sqrt{\lambda^2 + 3} \right] \equiv -1 - \lambda - \delta \tag{32}$$

where we have parametrized the binding energy per hole as δ : this energy is compared with the independent-hole low-spin and high-spin energies in figure 2. Equation (31) can be solved numerically for the case of the square superlattice; the binding energy is about an order of magnitude smaller than the 1d binding energy, and hence the 2d bound state curve is barely visible below the independent-hole line in figure 2.

The Greens function contains the eigenvalue *and* eigenvector information, so this technique allows us to determine the ‘size’ of the bound-state pair as a function of binding energy. Provided that $\delta \neq 0$, the amplitude of the real-space wavefunction when the holes are separated by \mathbf{R}_i is proportional to

$$\mathcal{G}_{i0}(\epsilon) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\exp[i \mathbf{k} \cdot \mathbf{R}_i]}{\epsilon + \lambda - \gamma_{\mathbf{k}}} \tag{33}$$

In the one-dimensional example, this quantity is

$$\mathcal{G}_{i0}(\epsilon) \propto \frac{(-1)^{|i|}}{2\lambda - \sqrt{\lambda^2 + 3}} \left[\frac{1}{3} \left(\lambda + \sqrt{\lambda^2 + 3} \right) \right]^{|i|} \tag{34}$$

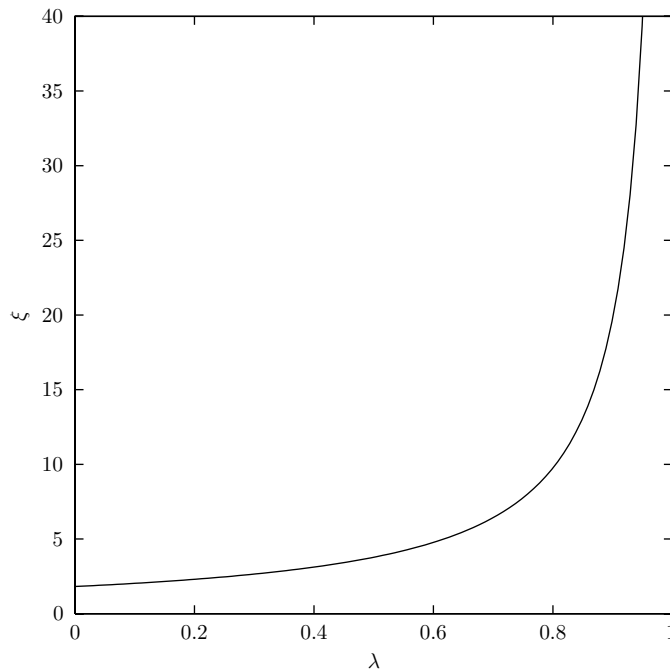


Figure 3. The size of the bound-state hole pair ξ (in units of the lattice parameter) on the one-dimensional chain, as a function of the model parameter, λ . The binding energy vanishes as $\lambda \rightarrow 1$, with a concomitant divergence in the real-space size of the bound pair.

which means that, for $\lambda < 1$, the magnitude of the real-space wavefunction decays exponentially with a length scale ξ defined by

$$\frac{1}{\xi} = -\ln \left[\frac{1}{3} (\lambda + \sqrt{\lambda^2 + 3}) \right]. \quad (35)$$

The variation of this length scale with λ is plotted in figure 3.

5. Discussion and conclusions

We have shown that, for a restricted range of λ , pairs of holes in our strong-coupling Hubbard model bind together to form the real-space analogue of Cooper pairs. The background spins are induced into an RVB state by the motion of these holes. We have not addressed the important issue of the relevance of these results to superconductivity in CuO_2 planes, and whether or not one would anticipate superconductivity in our model at finite doping [6].

It is important to realize that the demands of superconductivity are less stringent than that of binding holes into pairs. In one and two dimensions any magnitude of net attraction between two holes guarantees a bound state, but in three dimensions there is a non-zero threshold that must be exceeded. Consequently, we can achieve the bound state for the linear chain and square superlattice, but in the cubic superlattice case the bound state is irrelevant as it only forms for values of λ for which the groundstate is ferromagnetic.

Superconductivity, on the other hand, involves macroscopic doping. When the number of holes is of the same order as the number of lattice sites, the holes are forced to be near

each other, and then can always make use of an attraction to form a ‘collective’ paired state: attraction guarantees a pairing instability of a Fermi surface. It is possible that in one dimension a Luttinger liquid might arise, with power-law pairing correlations and no long-range order, but inter-layer coupling stabilizes the superconductor.

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