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Some exact solutions to the Hubbard model with infinite-range hopping

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Abstract. For the Hubbard model with infinite-range hopping, a sensible competition between hopping and Hubbard repulsion can only be found when U/t scales with the volume of the system. Only two electrons carry all the kinetic energy and so the variations in Hubbard repulsion are bounded by only $2U$ for an eigenstate. To be comparable with the kinetic energy this must be extensive. For this case we derive some exact eigenstates for the model. Our lowest energy solution is paramagnetic although the spin degeneracy energy scale is very small. The behaviour of this system appears to be very different to that for the shorter-range hopping systems and so little can be deduced about more physical models.

1. Introduction

Exact solutions to unphysical limits of interesting Hamiltonians often yield insight into the more physical regimes. Provided that the physical phenomena present in the unphysical limit are pertinent to the real physical problem, any real ground-state coherence may well have a transparent analogue in the unphysical system. One such unphysical limit is the classical limit of the Heisenberg model. This limit yields long range magnetic order which appears relevant to all but the most exotic quantum systems.

Perhaps the simplest model for correlated charge motion is the Hubbard model:

$$H = -\sum_{ii'\sigma} t_{ii'} c^{\dagger}_{i\sigma} c_{i\sigma} + U \sum_{i} c^{\dagger}_{i\sigma} c^{\dagger}_{i\bar{\sigma}} c_{i\bar{\sigma}} c_{i\sigma} \tag{1.1}$$

where $c^{\dagger}_{i\sigma}$ creates an electron of spin σ (complementary spin $\bar{\sigma}$) on a site i. This model has proven immensely difficult to solve in the strongly correlated limit where the Hubbard repulsion, U, dominates the chemical bonding or hopping energy, t. In this article we will study an unphysical but rather simple limit of this model: the infinite-range hopping limit, when $t_{ii'} = t$ and we have an equal matrix element for hopping to *all* sites (including no motion, $i = i'$).

We are not the first to study this model [1] but we seem to be the first to have noticed that a competition between the two contributions can only be observed if the Hubbard repulsion is chosen to be *extensive*: U/t scales with the volume of the system. We will use N to denote the number of atoms in the problem and this will be

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our extensive variable. The basic reason for choosing the Hubbard repulsion to be so large, is that at any one time there are only two mobile electrons in the system. Only these two electrons can alter the number of doubly occupied sites and so the variations in Hubbard energy are bounded by $2U$. Only if this energy is comparable with the hopping energy will it be relevant and so we must make it extensive. Although this choice ensures that the model exhibits some non-trivial behaviour, it does extend the *range* of energies over values which scale with the *square* of the volume of the system. States with significantly different numbers of doubly occupied sites are therefore well separated in energy.

Given that the fluctuations in double occupation are necessarily small, which phenomena of the physical model might have a remnant in the unphysical model? The most obvious questions relate to the spin coherence and the possible magnetic phase diagram. There are various types of magnetic state proposed for the ground state of the Hubbard model as the parameters are varied: Néel antiferromagnetism [2], Nagaoka ferromagnetism [3], Kanamori paramagnetism [4] and elementary Fermi liquid theory at weak coupling [5]. We will be concerned mainly with interpretations of the magnetism in our solutions and the physical cause of any spin-degeneracy breaking.

One major complication encountered in studying the physical Hubbard model is that the spin correlations in the vicinity of the charge carrier can be rather different from the spin correlations further away, a *spin polaron*. This effect is caused by a competition between two types of behaviour; Nagaoka ferromagnetism near the charge carrier and Heisenberg correlations at larger distances, for example. For the infinite-range hopping model, there cannot be such a length scale because two electrons are either on the same site or on different sites and there is no sense in which sites may be thought of as 'nearby'. This simplification makes the model analytically tractable but it may simultaneously eliminate the interesting physics. This will be one of the dominant considerations in our conclusions.

In section 2 we will develop some solutions to the Hamiltonian and in section 3 we will try to interpret the physical effects which lead to the stabilization of the spin correlations. In section 4 we conclude.

2. Some exact solutions

In this section we will develop some eigenstates of the infinite-range Hubbard Hamiltonian. Our solutions are *'ad hoc'* and based upon an understanding and generalization of a treatment applicable to finite systems.

The underlying mathematical structure is the full permutation group. Only the uniform phase sum is invariant under this group and so the zone centre of reciprocal space (if we arbitrarily choose a translational subgroup) plays an important role. Indeed, if we extract the two states corresponding to this sum, $c^{\dagger}_{0\sigma}$ say, then the kinetic energy becomes very simple:

$$H_0 = -Nt \sum_{\sigma} c^{\dagger}_{0\sigma} c_{0\sigma} \tag{2.1a}$$

and it is very natural to consider the state $c^{\dagger}_{0\uparrow} c^{\dagger}_{0\downarrow} |0\rangle$ *in trying to construct solutions.*

It might seem natural to expand the states in reciprocal space, since the zone centre states play such a an important role but this is in fact not so. *Any* representation of the other states is equally reasonable. Our only consideration, in deciding

upon a reasonable representation for the 'non-bonding' combinations is the Hubbard interaction:

$$H_1 = U \sum_i c^\dagger_{i\sigma} c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}} c_{i\sigma}. \tag{2.1b}$$

Since the Hubbard interaction is local in real space it seems natural to expand the non-bonding states in terms of short-range orbitals in real space.

An electron localized on a single atom is not orthogonal to the zone-centre states, and so we are forced to consider states spread across at least two atoms. If we use α as a *pair* label, describing collectively the two atoms $\{i_\alpha, j_\alpha\}$, then the operator:

$$a^\dagger_{\alpha\sigma} = (1/\sqrt{2}) \left[c^\dagger_{i_\alpha \sigma} - c^\dagger_{j_\alpha \sigma} \right] \tag{2.2}$$

creates an electron of spin σ on the pair of atoms denoted by α which is in a state orthogonal to the zone-centre states. We will use states constructed in this way.

It is clear that our chosen states are not all mutually orthogonal, since any two pairs with a common atom yield non-orthogonal states. Furthermore, our basis is rather difficult to complete, since there are $N(N-1)/2$ ways to pair up atoms and only $N-1$ *distinct* non-bonding orbitals for each spin. The reason for our arbitrary choice is that there remains a huge spatial degeneracy for the eigenstates that we construct. It happens to be more convenient to work with the local description and more exotic eigenstates can always be constructed by linear superposition.

The manner in which we enforce orthogonality is by choosing *all* our pairs to involve distinct atoms. Obviously we can only successfully describe doping levels up to a quarter filling with this constraint.

The second natural operator to emerge once we have chosen our local basis is:

$$\begin{aligned} b^\dagger_\alpha &= \frac{1}{\sqrt{2}} \left[c^\dagger_{i_\alpha \uparrow} c^\dagger_{i_\alpha \downarrow} - c^\dagger_{j_\alpha \uparrow} c^\dagger_{j_\alpha \downarrow} \right] \\ &= \frac{1}{2\sqrt{2}} \left[(c^\dagger_{i_\alpha \uparrow} + c^\dagger_{j_\alpha \uparrow})(c^\dagger_{i_\alpha \downarrow} - c^\dagger_{j_\alpha \downarrow}) + (c^\dagger_{i_\alpha \uparrow} - c^\dagger_{j_\alpha \uparrow})(c^\dagger_{i_\alpha \downarrow} + c^\dagger_{j_\alpha \downarrow}) \right] \end{aligned} \tag{2.3}$$

which creates the local configurations where the pair, α, finds one of its atoms doubly occupied, when the non-bonding electron is joined by a zone-centre electron.

The action of the Hamiltonian on this choice of basis is detailed by observing that:

$$\begin{aligned} &H_0 a^\dagger_{\alpha\sigma} c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} |0\rangle = -2Nt a^\dagger_{\alpha\sigma} c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} |0\rangle \\ &H_1 a^\dagger_{\alpha\sigma} c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} |0\rangle = -\frac{U}{\sqrt{N}} b^\dagger_\alpha c^\dagger_{0\sigma} |0\rangle + \frac{U}{N} \sum_i a^\dagger_{\alpha\sigma} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} |0\rangle \\ &H_0 a^\dagger_{\alpha\sigma} c^\dagger_{0\bar{\sigma}} |0\rangle = -Nt a^\dagger_{\alpha\sigma} c^\dagger_{0\bar{\sigma}} |0\rangle \qquad H_1 a^\dagger_{\alpha\sigma} c^\dagger_{0\bar{\sigma}} |0\rangle = \frac{U}{\sqrt{N}} \sigma b^\dagger_\alpha |0\rangle \\ &H_0 \frac{1}{\sqrt{N}} b^\dagger_\alpha c^\dagger_{0\sigma} |0\rangle = -tN \frac{1}{\sqrt{N}} b^\dagger_\alpha c^\dagger_{0\sigma} |0\rangle + t a^\dagger_{\alpha\sigma} c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} |0\rangle \\ &H_1 \frac{1}{\sqrt{N}} b^\dagger_\alpha c^\dagger_{0\sigma} |0\rangle = U \frac{1}{\sqrt{N}} b^\dagger_\alpha c^\dagger_{0\sigma} |0\rangle \\ &H_0 \frac{1}{\sqrt{N}} b^\dagger_\alpha |0\rangle = -t \sum_\sigma \sigma a^\dagger_{\alpha\sigma} c^\dagger_{0\bar{\sigma}} |0\rangle \qquad H_1 \frac{1}{\sqrt{N}} b^\dagger_\alpha |0\rangle = U \frac{1}{\sqrt{N}} b^\dagger_\alpha |0\rangle. \end{aligned} \tag{2.4}$$

We are now in a position to construct some eigenstates of the Hubbard Hamiltonian. We start out with a non-interacting eigenstate and determine the subspace that the Hamiltonian can generate. We choose the state:

$$|\psi_0\rangle = \sum_{\Sigma} S_{\Sigma} \prod_{\alpha} A^{\dagger}_{\alpha\sigma_\alpha} c^{\dagger}_{0\uparrow} c^{\dagger}_{0\downarrow} |0\rangle \tag{2.5a}$$

where $\Sigma = (\sigma_1, \sigma_2, .., \sigma_\alpha, .., \sigma_{N_\alpha})$ are the spins of the N_α non-bonding electrons, S_Σ defines the spin wavefunction that we must determine and $A^{\dagger}_{\alpha\sigma_\alpha} = a^{\dagger}_{\alpha\sigma_\alpha} \epsilon^{\dagger}_{\alpha}$ in terms of a fermionic operator $\epsilon^{\dagger}_{\alpha}$. The operators $\epsilon^{\dagger}_{\alpha}$ constitute a technical trick which enables us to define operators $A^{\dagger}_{\alpha\sigma_\alpha}$ that commute with each other, obviating minus sign complications. The reader is reminded that the pairs are chosen to be mutually distinct and therefore that $N_\alpha < N/2$.

Our task is to apply the Hamiltonian again and again until a complete subspace is generated. At first sight one might suppose that we would generate an infinite subspace but this is not so. There are only two delocalized electrons and only these two electrons can doubly occupy atoms in low energy eigenstates. Provided that we can *successfully* describe the spin degrees of freedom of states with up to two doubly occupied sites, then we ought to be able to solve the problem.

The first application of the Hamiltonian produces states where one pair has an atom which is necessarily doubly occupied:

$$H|\psi_0\rangle = -2Nt|\psi_0\rangle + U|\tilde{\psi}_0\rangle - U|\psi_1\rangle \tag{2.5b}$$

The first contribution is just the kinetic energy of the two delocalized electrons. The second term comes from the situations where both zone-centre electrons are on the same site and the third term comes from the situations where one of the zone-centre electrons resides on the same atom as a non-bonding electron. We find that:

$$|\tilde{\psi}_0\rangle = \sum_{\Sigma} S_{\Sigma} \prod_{\alpha} A^{\dagger}_{\alpha\sigma_\alpha} \frac{1}{N} \sum_{i} c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} |0\rangle \tag{2.6a}$$

is the contribution where both of the zone-centre electrons are on the same site and:

$$|\psi_1\rangle = \sum_{\Sigma} S_{\Sigma} \frac{1}{\sqrt{N}} \sum_{\beta} \prod_{\alpha\neq\beta} A^{\dagger}_{\alpha\sigma_\alpha} b^{\dagger}_{\beta} c^{\dagger}_{0\sigma_\beta} \epsilon^{\dagger}_{\beta} |0\rangle \tag{2.7a}$$

is the contribution that involves a doubly occupied atom in the pair denoted by β.

The state $|\tilde{\psi}_0\rangle$ is simple because all that can happen is that the zone-centre electrons can delocalize again:

$$H|\tilde{\psi}_0\rangle = U|\tilde{\psi}_0\rangle - 2t|\psi_0\rangle \tag{2.6b}$$

where the first term accounts for the doubly occupied site and the second term comes from the electrons delocalizing. An application of the Hamiltonian to $|\psi_1\rangle$ produces:

$$H|\psi_1\rangle = N_\alpha t|\psi_0\rangle + (U - Nt)|\psi_1\rangle - U|\psi_2\rangle \tag{2.7b}$$

where the first term finds the zone-centre electron on the same site as a non-bonding electron delocalizing again. The second term is the kinetic energy of the remaining

zone-centre electron together with the penalty for the doubly occupied site and the third term arises from the probability that the second zone-centre electron resides on the same atom as a second non-bonding electron. The new state is:

$$|\psi_2\rangle = \sum_{\Sigma} S_\Sigma \frac{1}{N} \sum_{\beta,\gamma} \prod_{\alpha \neq \beta,\gamma} A^\dagger_{\alpha\sigma_\alpha} b^\dagger_\beta \epsilon^\dagger_\beta b^\dagger_\gamma \epsilon^\dagger_\gamma |0\rangle \delta_{\bar{\sigma}_\beta \sigma_\gamma} \sigma_\beta \tag{2.8a}$$

which now has two doubly occupied sites and no zone-centre electrons. The form of this state is the most general, since the only mobile electrons are situated on the doubly occupied atoms, and if they move they become zone-centre electrons again taking us back to a state with a similar form to $|\psi_1\rangle$.

There are some subtleties associated with $|\psi_2\rangle$ these being the spin degrees of freedom. The sum of pairs involved in $|\psi_2\rangle$ are over *antiparallel* spins. If all the non-bonding electrons had parallel spins, then $|\psi_2\rangle$ would vanish and the complete situation would be described by $|\psi_0\rangle$, $|\tilde{\psi}_0\rangle$ and $|\psi_1\rangle$. The combinations relevant to $|\psi_2\rangle$ are those for which the two original spins were in a total spin singlet. The operators $b^\dagger_\alpha$ create singlet pairs of electrons, and so there is a sense in which the original spins might be thought of as *exchanging*.

Applying the Hamiltonian to the state $|\psi_2\rangle$ yields:

$$H|\psi_2\rangle = 2U|\psi_2\rangle + t|\tilde{\psi}_1\rangle \tag{2.8b}$$

where the first term describes the penalty against finding *two* atoms doubly occupied and the second term comes from the delocalization of one of the *four* electrons that are on doubly occupied atoms. It is now possible for an electron which was originally a non-bonding electron to delocalize leaving the original zone-centre electron in a non-bonding orbital in its place. It is this type of exchange that controls the spin degeneracy breaking. The new state is:

$$\begin{aligned}|\tilde{\psi}_1\rangle = \sum_{\Sigma} S_\Sigma \frac{1}{\sqrt{N}} \sum_{\beta,\gamma} \prod_{\alpha \neq \beta,\gamma} A^\dagger_{\alpha\sigma_\alpha} \Big[& A^\dagger_{\beta\sigma_\beta} b^\dagger_\gamma c^\dagger_{0\sigma_\gamma} \epsilon^\dagger_\gamma + A^\dagger_{\gamma\sigma_\gamma} b^\dagger_\beta c^\dagger_{0\sigma_\beta} \epsilon^\dagger_\beta \\ & - A^\dagger_{\beta\sigma_\gamma} b^\dagger_\gamma c^\dagger_{0\sigma_\beta} \epsilon^\dagger_\gamma - A^\dagger_{\gamma\sigma_\beta} b^\dagger_\beta c^\dagger_{0\sigma_\gamma} \epsilon^\dagger_\beta \Big] \delta_{\sigma_\gamma \bar{\sigma}_\beta} |0\rangle \end{aligned} \tag{2.9a}$$

and now the spin exchange has become transparent. Provided that the two original spins were antiparallel, the contributions involve only a simple permutation of the spin indices. We can rewrite this expression allowing the spin permutation to act on the spin wavefunction.

We can now extract the spin dependence in the form of Heisenberg operators by rewriting:

$$|\tilde{\psi}_1\rangle = \sum_{\Sigma} H_\beta S_\Sigma \frac{1}{\sqrt{N}} \sum_{\beta} \prod_{\alpha \neq \beta} A^\dagger_{\alpha\sigma_\alpha} b^\dagger_\beta c^\dagger_{0\sigma_\beta} \epsilon^\dagger_\beta |0\rangle \tag{2.10a}$$

with

$$H_\beta = \sum_{\gamma \neq \beta} 2\delta_{\sigma_\gamma \bar{\sigma}_\beta} \left[1 - P_{\beta\gamma}\right] = \sum_{\gamma \neq \beta} \left[1 - 4\boldsymbol{S}_\beta \cdot \boldsymbol{S}_\gamma\right] \tag{2.11a}$$

in terms of $P_{\beta\gamma}$ which permutes σ_β and σ_γ and the spin operators S_β which act on an equivalent Heisenberg representation. It is straightforward to show that:

$$H_\beta = N_\alpha + 2 - 4\boldsymbol{S}_\beta \cdot \boldsymbol{S}_{\text{Total}} \tag{2.11b}$$

where $\boldsymbol{S}_{\text{Total}} = \sum_\alpha \boldsymbol{S}_\alpha$ is the total spin operator. We can now observe that if the total spin of the state vanishes then the subspace has already closed, since $\boldsymbol{S}_{\text{Total}} \mapsto 0$, $H_\beta \mapsto N_\alpha + 2$ is independent of β and so $|\tilde{\psi}_1\rangle = (N_\alpha + 2)|\psi_1\rangle$.

If the total spin does not vanish then, in general, the H_β are distinct and $|\tilde{\psi}_1\rangle$ is in turn distinct from $|\psi_1\rangle$.

The Hamiltonian applied to $|\tilde{\psi}_1\rangle$ yields:

$$H|\tilde{\psi}_1\rangle = (U - Nt)|\tilde{\psi}_1\rangle - U|\tilde{\psi}_2\rangle + t\Delta(S)|\psi_0\rangle \tag{2.10b}$$

where the first term includes the kinetic energy of the remaining zone-centre electron together with the penalty from the doubly occupied site. The second term yields the contribution when the second zone-centre electron doubly occupies an atom with a non-bonding electron and the third term corresponds to the delocalization of the zone-centre electron which is doubly occupying an atom. This final term finds both of the zone-centre electrons delocalized, but the matrix element depends strongly on the total spin of the state. The two zone-centre electrons must find a pair of non-bonding electrons in a spin singlet and the probability of finding such a pair decreases as the total spin of the eigenstate is increased. The matrix element is determined from the observation that:

$$\sum_\beta H_\beta = N_\alpha(N_\alpha + 2) - 4\boldsymbol{S}_{\text{Total}} \cdot \boldsymbol{S}_{\text{Total}} \tag{2.12a}$$

$$\Delta(S) = N_\alpha(N_\alpha + 2) - 4S(S+1) \tag{2.12b}$$

where we have assumed that we have an eigenstate of total spin S.

The new state for which both the two zone-centre electrons doubly occupy atoms is:

$$|\tilde{\psi}_2\rangle = \sum_\Sigma \frac{1}{N} \sum_{\beta\gamma} H_\beta S_\Sigma \prod_{\alpha\neq\beta,\gamma} A^\dagger_{\alpha\sigma_\alpha} b^\dagger_\beta \epsilon^\dagger_\beta b^\dagger_\gamma \epsilon^\dagger_\gamma |0\rangle \delta_{\sigma_\gamma \bar{\sigma}_\beta \sigma_\beta} \tag{2.13a}$$

and the final application of the Hamiltonian yields:

$$H|\tilde{\psi}_2\rangle = 2U|\tilde{\psi}_2\rangle + t|\tilde{\psi}_1\rangle \tag{2.13b}$$

where the first term is the Hubbard penalty from the two doubly occupied atoms and the second term is where one of these *four* relevant electrons delocalizes. The final state $|\tilde{\psi}_1\rangle$ is proportional to $|\tilde{\psi}_1\rangle$. The spin degrees of freedom involve another elementary permutation which can be written in the form:

$$|\tilde{\psi}_1\rangle = \sum_\Sigma \tilde{H}_\beta S_\Sigma \frac{1}{\sqrt{N}} \sum_\beta \prod_{\alpha\neq\beta} A^\dagger_{\alpha\sigma_\alpha} b^\dagger_\beta c^\dagger_{0\sigma_\beta} \epsilon^\dagger_\beta |0\rangle \tag{2.14}$$

where:

$$\bar{H}_\beta = \frac{1}{2}\sum_{\gamma\neq\beta}\left[1-4\boldsymbol{S}_\beta\cdot\boldsymbol{S}_\gamma\right]\left[H_\beta+H_\gamma\right]$$

$$\bar{H}_\beta = \sum_{\gamma\neq\beta}\left[1-4\boldsymbol{S}_\beta\cdot\boldsymbol{S}_\gamma\right]\left(\left[1-4\boldsymbol{S}_\beta\cdot\boldsymbol{S}_\gamma\right]+\sum_{\delta\neq\beta,\gamma}\left[1-2(\boldsymbol{S}_\beta+\boldsymbol{S}_\gamma)\cdot\boldsymbol{S}_\delta\right]\right)$$

$$\bar{H}_\beta = (N_\alpha+2)H_\beta. \tag{2.15}$$

In deriving the final identity we have used $\left[1-4\boldsymbol{S}_\beta\cdot\boldsymbol{S}_\gamma\right]^2 = 4\left[1-4\boldsymbol{S}_\beta\cdot\boldsymbol{S}_\gamma\right]$ and $\left[1-4\boldsymbol{S}_\beta\cdot\boldsymbol{S}_\gamma\right](\boldsymbol{S}_\beta+\mathbf{S}_\gamma)=\mathbf{0}$, which hold for spin-$\frac{1}{2}$ systems.

We therefore conclude that $|\bar{\psi}_1\rangle = (N_\alpha+2)|\tilde{\psi}_1\rangle$ and that the complete subspace has been generated.

The full system of equations is:

$$\begin{bmatrix} -E-2Nt & U & -U & 0 & 0 & 0 \\ -2t & -E+U & 0 & 0 & 0 & 0 \\ N_\alpha t & 0 & -E+U-Nt & -U & 0 & 0 \\ 0 & 0 & 0 & -E+2U & t & 0 \\ t\Delta(S) & 0 & 0 & 0 & -E+U-Nt & -U \\ 0 & 0 & 0 & 0 & t(N_\alpha+2) & -E+2U \end{bmatrix}\begin{bmatrix} |\psi_0\rangle \\ |\tilde{\psi}_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \\ |\bar{\psi}_1\rangle \\ |\bar{\psi}_2\rangle \end{bmatrix} \tag{2.16}$$

which must be solved for the eigenvalues E. It ought to be remembered that the states involved in our analysis are *not* orthogonal and *not* necessarily linearly independent. Real solutions to this secular equation must be associated with a non-vanishing wave function.

For the limit of a macroscopic density of non-bonding electrons, the two states $|\tilde{\psi}_1\rangle$ and $|\tilde{\psi}_2\rangle$ scale with the volume while the state $|\tilde{\psi}_0\rangle$ becomes irrelevant. For the limit of finite density parameterized by $N_\alpha = nN$, $S = s(N/2)$, $U = uN$ and $E = \epsilon N$ we find the secular equation:

$$\begin{bmatrix} -\epsilon-2t & -u & 0 & 0 & 0 \\ nt & -\epsilon+u-t & -u & 0 & 0 \\ 0 & 0 & -\epsilon+2u & t & 0 \\ t(n^2-s^2) & 0 & 0 & -\epsilon+u-t & -u \\ 0 & 0 & 0 & nt & -\epsilon+2u \end{bmatrix}\begin{bmatrix} |\psi_0\rangle \\ |\psi_1\rangle \\ |\psi_2\rangle \\ |\tilde{\psi}_1\rangle/N \\ |\tilde{\psi}_2\rangle/N \end{bmatrix} = 0 \tag{2.17}$$

for the spectrum.

In order to test that the analysis presented is correct, we have numerically solved the infinite-range Hubbard model for small systems of up to twelve atoms. The secular determinant defined by equation (2.16) yields some of the eigenvalues *including* the ground-state energy for all of the situations that we have studied.

3. Solutions and interpretations

We have used the discrete formulation for finite systems to ensure that the result is correct by comparison with exact diagonalization. In this section we will study the solution to the finite density limit that is of more fundamental interest.

The determinant of the secular equation can be expanded into the form:

$$(\epsilon - 2u)\left\{(\epsilon + t - u)^2\left[(\epsilon + 2t)(\epsilon - 2u) + 2ntu\right] + t^2u^2s^2\right\} = 0. \tag{3.1}$$

The solution at $\epsilon = 2u$ is unphysical and corresponds to a situation where there are no zone-centre electrons. The remaining quartic equation contains the relevant solutions and surprisingly can be completely solved. If we reparameterize with:

$$\epsilon = u - t - (u + t)\Gamma(x) \tag{3.2a}$$

$$x = ut/(u + t)^2 \tag{3.2b}$$

then we find that:

$$\Gamma^2\left[\Gamma^2 - 1 + 2nx\right] + s^2x^2 = 0 \tag{3.3a}$$

and hence that:

$$\Gamma^2 = \tfrac{1}{2} - nx \pm \left[\left(\tfrac{1}{2} - nx\right)^2 - s^2x^2\right]^{1/2}. \tag{3.3b}$$

The corresponding wavefunction is:

$$\begin{aligned}|\psi\rangle \;=\; & |\psi_0\rangle + [u/(u+t)](1/\Gamma)\left[|\psi_1\rangle - [x/N(\Gamma(\Gamma+1)+nx)]|\tilde{\psi}_1\rangle\right] \\ & + [u/(u+t)]^2[1/\Gamma(\Gamma+1)]\left[|\psi_2\rangle - [x/N(\Gamma(\Gamma+1)+nx)]|\tilde{\psi}_2\rangle\right]\end{aligned} \tag{3.4}$$

in terms of the states defined in section 2.

Our solution is only known to be valid when $n < 1/2$, and furthermore $x < 1/4$, so it is a good approximation to expand in powers of x. We find that:

$$\epsilon = -2t + (u + t)[nx + (x^2/2)(n^2 + s^2) + O(x^3)] \tag{3.5a}$$

and so:

$$\epsilon = -2t + nu + (u^2/2t)(s^2 + n^2 - 2n) + O(u^3/t^2) \tag{3.5b}$$

as $u/t \mapsto 0$ and

$$\epsilon = -2t + nt + (t^2/2u)(s^2 + n^2 - 2n) + O(t^3/u^2) \tag{3.5c}$$

as $t/u \mapsto 0$.

The preferred magnetic state is a total spin singlet for all cases. This agrees with the results of Kanamori [4] for low densities of electrons in Hubbard models. However, the energy scale for the effect is *not* reminiscent of the result for the physical limits of the Hubbard model. For finite-range hopping, Pauli exclusion makes magnetic states unstable on a hopping energy scale, both in the weak coupling *and* strong coupling limits. This result occurs because *all* electrons take a share of the kinetic energy and so the 'exchange' of any two electrons is energetically significant. We would only obtain a similar result if we prohibited occupation of one of the zone-centre states, which would then give up half of the kinetic energy. To leading order in our calculations the degeneracy remains. This can be understood if we observe that whatever the spin

of a non-bonding electron, *one* of the two zone-centre electrons will be parallel to it and hence be Pauli excluded from being on the same atom with it. The degeneracy is broken at a higher order for infinite-range hopping.

It is easy to see that the spin degeneracy breaking *requires* a contribution from the situation where both zone-centre electrons are localized on pairs with non-bonding electrons. When only one electron becomes 'localized', it originates from the state with the opposite spin to the remaining 'delocalized' electron and can always delocalize back again; there is no intrinsic spin restriction.

The degeneracy breaking is best understood in the strong-coupling regime, by considering two pairs of atoms with four electrons on them. Since the number of non-bonding electrons is macroscopic, there is a finite probability of finding two pairs of atoms doubly occupied, with both the zone-centre electrons on the unoccupied atom of the pair. This probability is sizeable even as $u \mapsto \infty$, since there is no implied double occupancy of an *atom*, only a pair. If we focus on one pair of atoms, then the two electrons *necessarily* have parallel spins; this is a symmetry requirement based upon the necessity for one non-bonding and one bonding orbital being occupied. Each mobile electron can hop to each other occupied atom in principle but in practice the electrons can only hop into states in which they arrive in a spin singlet with the electron already present. The cause of the spin-degeneracy breaking can be traced to the *correlations* between the electrons. For non-interacting electrons the spin of the zone-centre electron is conserved:

$$H_0(c^\dagger_{i_\alpha\sigma} - c^\dagger_{j_\alpha\sigma})(c^\dagger_{i_\alpha\tau} + c^\dagger_{j_\alpha\tau})|0\rangle = -2t\sqrt{N}(c^\dagger_{i_\alpha\sigma} - c^\dagger_{j_\alpha\sigma})c^\dagger_{0\tau}|0\rangle \qquad (3.6a)$$

whereas for highly correlated electrons for which the double occupation of *atoms* has been eliminated

$$H_0(c^\dagger_{i_\alpha\sigma}c^\dagger_{j_\alpha\tau} - c^\dagger_{j_\alpha\sigma}c^\dagger_{i_\alpha\tau})|0\rangle = -t\sqrt{N}(c^\dagger_{i_\alpha\sigma} - c^\dagger_{j_\alpha\sigma})c^\dagger_{0\tau}|0\rangle - t\sqrt{N}(c^\dagger_{i_\alpha\tau} - c^\dagger_{j_\alpha\tau})c^\dagger_{0\sigma}|0\rangle \qquad (3.6b)$$

and so either electron can become the zone-centre electron and the spin can be exchanged. Perturbative hopping onto *occupied* atoms is optimized in a low spin state for which the simultaneous probability of finding electrons in relative singlets is maximized. It should be remembered that the two electrons which singly occupy the two atoms of a pair are *necessarily* in a spin triplet and so the strong singlet correlations which enhance double-occupying hops are *between* pairs. The triplet character is enforced by the spatial antisymmetry of a non-bonding and zone-centre pair. The electrons hop *between* triplets doubly occupying atoms.

Perhaps the simplest way to understand our result is by observing that the correlations induced by the Hubbard interaction allow exchange between the spins on localized and conduction electrons. The low spin energy gain comes from passive singlets in the non-bonding background becoming the active singlet between the two delocalized electrons. This interpretation does have an analogue in physical systems.

Non-interacting electrons are not subject to the spin-degeneracy breaking since for this case the spin of a zone-centre electron is conserved. Only to the extent to which there is an enhanced probability of finding two pairs with two singly occupied atoms over finding two pairs with one doubly occupied atom each is the spin degeneracy broken. This occurs to order u^2/t and is best interpreted as a residual strong-coupling interaction.

In the theory the relevant correlations are controlled by $|\psi_2\rangle$. A small addition of $|\psi_2\rangle$ to $|\psi_0\rangle$ reduces the probability of finding pairs of pairs with doubly occupied atoms. The configurations with all four atoms singly occupied but in a total spin singlet remain. For such a quartet the simultaneous probability of finding a spin on one pair in a singlet with a spin on the other pair is three quarters for each combination. This is to be compared with a simultaneous probability of one half when the total spin is one and zero when the total spin is two, although this eventuality is never reached.

4. Conclusions

We have found some exact eigenstates of the infinite-range hopping Hubbard model for the restricted case of less than a quarter band filling. We have not demonstrated that the ground state is among our solutions although we believe that it is. In order to obtain a remnant competition between the kinetic energy and Hubbard repulsion we were forced to make the Hubbard repulsion extensive. This choice is not without unphysical consequences but we have ignored the problems and studied the model with regard to its magnetic content.

In agreement with Kanamori [4] we find that the total spin singlet is stabilized from amongst the magnetic possibilities. The energy scale on which it is stabilized is rather smaller than that found in shorter-range versions of the Hubbard model. The source of the paramagnetism was found to be directly attributable to the correlations between the delocalized zone-centre and localized non-bonding electrons. These correlations allow a form of strong-coupling exchange between the two types of electron that promotes paramagnetism. A singlet correlation between two non-bonding electrons can be turned into an additional hybridization into a state in which the singlet is contracted onto a single atom. In order for the phenomenon to occur *both* of the zone-centre electrons must be involved and this fact combined with the necessity of using a doubly occupied site ensures that the spin-degeneracy energy scale is small.

The analysis presented in this article is only valid for band fillings up to a quarter. Numerical simulations show that it is *not* valid above a quarter filling. One can ask questions about higher band fillings and there are ways to generalize the present ideas to higher doping levels. This generalization is in progress and involves non-bonding clusters with higher values of total spin but unless a more interesting physical idea develops the analysis will be academic.

The final and perhaps most important question is to ask whether the phenomena found in this simple but unphysical limit yield any insight into the physical systems. Unfortunately the solution yields very little insight. For the infinite-range hopping model there are two types of electrons: the mobile zone-centre electrons and the immobile non-bonding electrons. The physics of the model is dominated by the interplay between these two types. For the shorter-range models *all* electrons play a similar role and the physics is truely many-body. It is conceivable that this model could be used to study systems in which there are two types of electrons, one light and one heavy, both of which simultaneously have Fermi surfaces and in which all the electrons are subject to strong Coulomb interactions. This is perhaps a bit far fetched.

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References

[1] van Donge P and Vollhardt D 1989 *Phys. Rev.* B **40** 7252

[2] The likelihood of long-range antiferromagnetism at half filling for all but one-dimensional and pathological systems follows directly from an exact mapping onto the Heisenberg model. For the infinite-range Heisenberg Hamiltonian the solution is known, because the Hamiltonian is proportional to the total spin of the system. The ground state is any total spin singlet and is therefore multiply degenerate.

[3] Nagaoka Y 1966 *Phys. Rev.* **147** 392

The present model is expected to be atypical as far as Nagaoka ferromagnetism is concerned. Since every atom is connected to every other atom the geometry is *not* bipartite. There is even a sense in which it is the worst example of topological frustration possible. Nagaoka ferromagnetism is known to be unstable in frustrated systems and so it is unlikely to be relevant in this case.

[4] Kanamori J 1963 *Prog. Theor. Phys.* **30** 275

[5] Weak-coupling Fermi liquid theory is also rather pathological for the present model because of the huge degeneracy involved in the non-bonding states. The lack of a non-interacting Fermi surface could well cause interpretational problems even in this usually simple limit.