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Spin-Singlet Solutions of the Hubbard Model

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Abstract :

We find spin-singlet solutions of the Hubbard model for all U. These solutions, called the coherent bond states and denoted by $|Z\rangle$, lie in the middle of the Mott-Hubbard or the SDW gap. The significance of these solutions is explored.

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The states of the Hubbard Model are of interest for a number of reasons[1]. In these systems a Mott-Hubbard gap exists at halffilling. In a mean field sense a spin density wave gap is there for all values of on-site repulsion, U. In this work we explore alternate spin-singlet soliton type modes of these systems. Starting with a simpler system, we build towards the Hubbard model.

A simple hamiltonian that has soliton solutions is the hopping hamiltonian, often also called the tight-binding model[2]. These states were illustrated in our earlier work, now on referred to as I. The soliton states, also called the coherent bond states (CBS), arise from an underlying infinite dimensional symmetry.

The hopping hamiltonian has recently been the subject of intense work in conjunction with the antiferromagnetic (AF) hamiltonian. The resulting system, the so called t-J model, at the mean field level, may have spin-singlet states[3]. The gauge symmetry of the AF system leads to fluctuations that are much too large and destroy these states; instead flux states[4], containing singlet variables gauge invariantly configured on a plaquette, are stable. On a t-J system it is also known that commensurate flux phases are stable.[5] This, however, requires $t \gtrsim U$, where U is the Hubbard on-site repulsion. The importance of the t term, i.e., the hopping hamiltonian in this instance is evident.

Solitons, or collective many-body states exist in numerous systems, including weakly interacting ones[6]. In the case of the hopping hamiltonian the usual single particle states are the bloch functions. One constructs a determinant of these bloch functions to get an N particle state. The excitations are single particle states over the fermi sea[7].

The exchange hamiltonian is essentially square of the hopping, projected onto a space that does not allow double occupancy[8]. The states of the exchange, i.e, the AF solutions, appear to differ significantly from the usual band states, which have a paramagnetic character. A question naturally is : is it only the constraint of non-double occupancy that leads to this difference? Or, does the hopping hamiltonian have other states?

It is our assumption that the soliton states of hopping provide some of the answers. So far we have constructed the generators of symmetries of hopping and shown they lead to the soliton configurations[9]. We have also analysed the possible excitations[2]. On that trail we reanalyse here the spectrum of excitations and obtain two other types of states that are in the spectrum of these states. So far much of these states were written in the Wannier basis, but here we rewrite them in terms of the Bloch functions. Further we analyse the suitability of

these states in the context of the Hubbard model. And just as in I, even though we discuss the scenario in one dimension, the results generalize to higher dimensions.

To recall, briefly, the hamiltonian of interest is :

$$H = - t \sum_{\substack{\langle i,j \rangle \\ \alpha}} (C^{+}_{i\alpha} \; C_{j\alpha} + h.c.) \qquad \ldots (1)$$

The generators of symmetry are[2] (Fig 1) :

h_1, the global number

h_2, translation by two lattice units

h_3, translation by four lattice units

etc.

and $e_{\pm}$ type generators ... (A)

$$e_{+1} = \sum_{\text{links}} T^{+}_{ij}(n)$$

$$e_{-1} = (e_1)^{+}$$

$$e_{+2} = T^{+}_{14}(+) + T^{+}_{25}(-) + T^{+}_{36}(+) + T^{+}_{47}(-) + \ldots$$

$$e_{-2} = (e_2)^{+}$$

etc.

From these generators we can construct the soliton states:

$$|Z\rangle = \{\exp[\sum_{\beta}(Z_\beta e_\beta - h.c.)]\}|0\rangle, \qquad \ldots (2)$$

where $|0\rangle$ is the state of h_1 containing no particles[10].

In Bloch Basis :-

It is important to observe the generator $e_\pm$ in that they have bond lengths that are odd in units of the lattice spacing, i.e, e_{+1} have elementary bond length of a (the lattice spacing); $e_{\pm 2}$ have bond lengths of 3a and so on. The generators of generation of even bond lengths are not in the algebra. The reason is the boundary conditions. In fig 2 we have drawn a small lattice of five points. The assignment of signs + and - on the bonds is such that if the periodic boundary conditions (p.b.c) can be satisfied for odd bond lengths they cannot be satisfied with even bond lengths and vice versa. This topological feature has consequences that we discuss later.

So far we have represented the generators and the states in the Wannier basis. Of course, they may equally well be represented in terms of the Bloch states. For instance the $|Z\rangle$ of eqn. (2) in Bloch basis is

$$|Z\rangle = \{\exp\{\sum_{\alpha=0}^{\infty} Z_\alpha \sum_k 2\cos[(2\alpha+1)ka]\,[C^+_{k\uparrow}C^+_{\pi-k\downarrow} - C^+_{k\downarrow}C^+_{\pi-k\uparrow}] - h.c.\}\}|0\rangle \qquad \ldots (3)$$

Each pair has zero energy because $\varepsilon_k + \varepsilon_{\Pi-k} = 0$. In that sense this sector of the hamiltonian is obtained from the bloch states by appropriate pairing. The cosine factors are arranged to yield odd bond lengths and the c.m. momentum Π of pairs ensures the sign on bonds alternate on links.

The Ground state and The Excitations :-

In I we outlined possible excitations of the $|Z\rangle$ states. Here we take up the issue again. The excitations discussed in I were of three types :

1. e_α - walls : where two states $|Z_1\rangle$ and $|Z_2\rangle$ form a boundary.

2. Phase defects : formed of fluctuations in sign on of the bonds.

3. Bond Excitations : Where a sea of singlet bonds have a few triplets in them.

This list needs updating on two counts. First, the e_α - walls do not appear as excitations because Z_α are continuous parameters. It is, therefore, difficult to argue energy is required to change the Z values.

Second, there are two other types of excitations that need to be included in the list. One, of them is a soliton excitation shown in Fig 3. A single charge remains unpaired, and is surrounded on both sides by ground state of the system.

The other excitation is obtained as follows : We have seen that in $|Z\rangle$ [eqn. 3] only odd-bond lengths appear . The reason is topological and is explained in Fig 2. However, instead of starting with e_1 we could have equally well started with a generator E_1 that has pairs of bond lengths 2a. The algebra will once again close and we would have a new state $|Z_{even}\rangle$ made up of pairs obtained by operating on $|0\rangle$ by generators of the E type. In contrast the $|Z\rangle$ of eqn. 2 let us rename $|Z_{odd}\rangle$. A boundary wall excitation is now possible when $|Z_{odd}\rangle$ meets $|Z_{even}\rangle$. These we call odd-even excitations.

Thus, the possible excitations are :

(1) Phase Defects

(2) Bond excitations,

(3) Single particle solitons, and

(4) Odd-even excitations.

Since the $|Z\rangle$ configurations are at the same energy as the state $|0\rangle$, the usual band states, at least upto half-filling, lie lower in energy than the $|Z\rangle$ solitons. In I we argued that a Peierl's type gap may come about for fermi surface nesting due to the phase assignments on bonds. A closer examination of the argument is given in Fig 1. A translation by a can be compensated by an overall change of sign. A Peierl's type possibility, therefore, appears ruled out.

The question naturally is, if charge carriers are introduced on a half-filled fermi surface could they go into $|Z\rangle$ type states?

For many reasons in a realistic system there may be a gap at half-filling such as due to a Mott-Hubbard type of interaction. We investigate now if $|Z\rangle$ type states are solutions of the hubbard model.

<u>$|Z\rangle$ are zero-modes of the Hubbard Model</u> :-

We show now that the $|Z\rangle$ states, at the mean-field level, are solutions of the Hubbard model.

For this let us recast the Hubbard model, usually written as :

$$H = -t \sum_{\substack{\langle i,j\rangle \\ \sigma}} (C^{+}_{i\sigma} C_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \quad , \qquad \ldots (4)$$

in terms of the spin variables. The spin operator is represented as :

$$\vec{S}_i = \tfrac{1}{2}.C^{+}_{i\sigma} \vec{\tau}_{\sigma\sigma} , C_{i\sigma} , \qquad \ldots (5)$$

where, $\vec{\tau}$ are the Pauli matrices. By simple algebra, we find,

$$S_1^2 = S_2^2 = S_3^2 = \tfrac{1}{4}\,[\, n_\uparrow + n_\downarrow - 2n_\uparrow n_\downarrow \,] \qquad \ldots (6)$$

Therefore, the Hubbard Model may be rewritten as :[11]

$$H = -t \sum_{\substack{\langle i,j\rangle \\ \sigma}} (C^{+}_{i\sigma}\, C_{j\sigma} + h.c.\,) - \frac{2}{3}\, U \sum \vec{S}_i^{\,2} \qquad \ldots (7)$$

Using, $\vec{S}_i = \langle \vec{S}_i \rangle + (\, \vec{S}_i - \langle \vec{S}_i \rangle \,)$, ... (8)

the meanfield hamiltonian becomes,

$$H_{MF} = -t \sum_{\substack{\langle i,j\rangle \\ \sigma}} (C^{+}_{i\sigma}\, C_{j\sigma} + h.c.\,) + \frac{2U}{3} \sum_i \langle S_i \rangle^2 - \frac{4U}{3} \sum_i \langle \vec{S}_i \rangle . \vec{S}_i \,. \qquad \ldots (9)$$

Assume the average field $\langle S_i \rangle$ is independent of i (this assumption is strictly not necessary, as we explain later), thus, $\langle \vec{S}_i \rangle$ may be taken outside the sum in the last term, which now becomes proportional to the total spin operator. Since the $|\,Z\rangle$ states are precise spin-singlets, they are eigenstates of the total spin operator with eigenvalue zero[F 1]. Thus $|\,Z\rangle$ is an exact eigenstate of (9) with eigenvalue zero, i.e, $|\,Z\rangle$ are the zero-modes[12]. Ofcourse,

we know the equation (9) has other mean-field solutions like the SDW. For half-filling there is a gap at the fermi surface for these SDW states, and , of course, sitting in the middle of this gap are the $|\,Z\rangle$ states.

Therefore, one might not like to worry about the $|Z\rangle$ states, because they have higher energy than the SDW ground state. But, that would be wrong for two reasons.

1. The SDW instability is precisely at half-filling[11]. Thus, if charge carriers (particles or holes) are introduced onto nested fermi surfaces, they could go into the $|\,Z\rangle$ states.

2. More importantly, for the $|\,Z\rangle$ states, not only are they eigenstates of $\sum \vec{S}_i$, but because they are singlets, $\langle S_i \rangle = 0$. That means, no matter what ansatz (SDW, ferromagnet . . .) we choose for $\langle S_i \rangle$ in equation (9), the $|\,Z\rangle$ state come mixed with all of them. Thus, the usual SDW ansatz carries in it some mixture of $|\,Z\rangle$. The $|\,Z\rangle$ are precise zero modes; no states of the system are free from them.

Conclusions:

Starting with the tight-binding system we constructed a zero energy solution. These solutions, the coherent bond states, are denoted by $|\,Z\rangle$. They are precise spin-singlets. Their excitations are of four types :

1. Phase defects, 2. Bond Excitations, 3. Single particle solitons and 4. Odd-even excitations.

Recasting the Hubbard model in terms of the spin variables, the on-site repulsion term is written in terms of the spins. Since the $|Z\rangle$ states are singlets they satisfy the conditions :

1. $\{ \sum \vec{S}_i \} \, |Z\rangle = 0$, and
2. $\langle \vec{S}_i \rangle$ in the $|Z\rangle$ states is zero.

Taken together we conclude that $|Z\rangle$ are zero modes of the mean-field Hubbard model. Following are the consequences :

1. Pure $|Z\rangle$ states lie in the middle of the SDW gap.

2. If charge carriers are introduced onto a half-filled fermi surface, they could go to $|Z\rangle$.

3. Because these are zero-modes, they mix with all other states of the system. In particular, the SDW state has $|Z\rangle$ in them .

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Footnotes:

F1 : Note that since h_1, the global number, is one of the generators of the algebra (A) represented by the $|Z\rangle$, the expectation value of h_1 is a constant in the $|Z\rangle$ states. Further, projections of $|Z\rangle$ onto states of definite h_1 are also eigenstates of (1).

Figure Caption:

Fig.1 : The phases η on links that make $e_1 = \sum T_{ij}(\eta)$, (where $T_{ij} = C^+_{i\uparrow} C^+_{j\downarrow} - C^+_{i\downarrow} C^+_{j\uparrow}$; $T_{ij}(\eta) = T_{ij}(\pm) = \pm T_{ij}$) an invariant generator. Notice that a translation by one lattice unit corresponds to an overall change of phase.

Fig.2 : For a lattice of five units, even bond lengths do not satisfy periodic boundary conditions.

Fig.3 : A single particle soliton excitation located at site 3.

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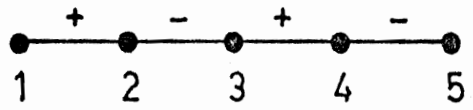

Fig. 1

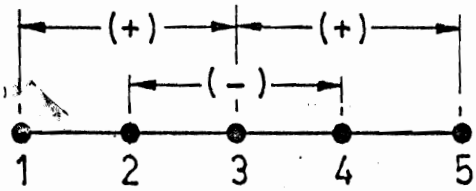

Fig. 2

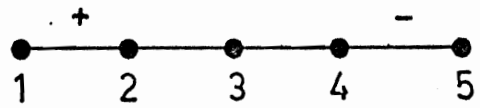

Fig. 3