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Abstract
We study two correlated electrons in a nearest-neighbour tight-binding chain,
with both on-site and nearest-neighbour interaction. Both the cases of parallel
and antiparallel spin are considered. In addition to the free electron band for two
electrons, there are correlated bands with positive or negative energy, depending
on whether the interaction parameters are repulsive or attractive. Electrons
form bound states, with amplitudes that decay exponentially with separation.
Conditions for such states to be filled at low temperatures are discussed.

Exact solutions to problems involving correlated motion of interacting particles are extremely
rare. Even simple systems such as electrons moving in a wire are usually solved only
approximately. A body of recent literature exists for the case of just two electrons moving in a
one-dimensional disordered potential [1–9]. The problem of N particles in an ordered string
of length L is conceptually simple if one ignores spin, since it is then formally equivalent to
that of a single particle in N-dimensional space, with the pair interaction acting as a defect
potential associated with the planes $x_i = x_j$, where x_i is the position of the ith particle. One
then expects a band of about L^N extended states with finite amplitude in all of space, and bands
of $L^{(N-S)}$ surface states localized about the geometrical defect where S planes intersect, or the
planes themselves if $S = 1$. In spite of this qualitative understanding of the ordered case, an
exact solution has been reported only for an $N = 2$ singlet state [10]. Thus, in reference [10],
as well as previous work [1–9] it is found that two correlated electrons exhibit a density of
states characteristic of one particle in a plane, that then has a Van Hove singularity at $E = 0$.

In this work we report on another exact solution of the two-particle problem in an ordered
lattice. It describes a paired triplet state, with an energy that may fall within the conduction
band, making it of interest to studies of superconductivity [11]. In order to see how this comes
about, we consider a chain of L sites within the tight-binding model, with up to nearest-
neighbour interaction. With the understanding that the amplitudes $c(l, m)$ represent two
electrons at sites l and m with either parallel or antiparallel spins, the equation of motion
without disorder reads

$$-tc(l-1, m) - tc(l+1, m) - tc(l, m+1) - tc(l, m-1)$$
$$+ J[\delta_{l+1,m} + \delta_{l-1,m}]c(l, m) + U\delta_{l,m}c(l, m) = Ec(l, m). \tag{1}$$

A transformation to centre-of-mass coordinates is effected by taking

$$c(l, m) = \exp(ik(l + m)a)\chi(l - m). \tag{2}$$

Here k is the centre-of-mass momentum and a is the lattice constant. Denoting by $p = l - m$ the distance between the two electrons, the equation obtained by substituting (2) into (1) is that of a single particle in an effective linear chain with sites p:

$$-2t\cos(ka)\chi(p - 1) - 2t\cos(ka)\chi(p + 1) + J[\delta_{p,1} + \delta_{p,-1}]\chi(p) + U\delta_{p,0}\chi(p) = E\chi(p) \tag{3}$$

where U is a contact Hubbard parameter [12] and J the nearest-neighbour coupling strength. A peculiar feature of this equation is that the effective hopping parameter depends on k, actually vanishing at $ka = \pm\frac{\pi}{2}$. In the absence of interactions one may set $\chi(p) = \exp(ipqa)$, obtaining the energy band

$$E(k, q) = -4t\cos(ka)\cos(qa). \tag{4}$$

This covers the range $-4t < E < 4t$. Assuming L large, equation (3) represents a lattice with impurities around the origin, and we expect expression (4) for the band to hold true even in the interacting case, save for corrections in the density of states of order $1/L$. One can easily show the dispersion (4) to be exact in the case $J = 0$ [13].

We will first work out the magnetic case of two parallel spins. The spatial wavefunction must then be antisymmetric under exchange of particles, or $\chi(p) = -\chi(-p)$. We consider equation (3) for the separate cases $p = 0, 1$, and $p \geqslant 2$, taking $\chi(0) = 0$. The equation for $p = 0$ is trivially satisfied because of the antisymmetry of the wavefunction. In looking for a solution for $p \geqslant 1$ we assume that there is some constant β such that $\chi(p + 1) = \beta\chi(p)$. From the boundary condition that the amplitudes must remain finite as p becomes large, one must have $|\beta| \leqslant 1$. Solving the equations we get

$$E = J + \left(\frac{4t^2}{J}\right)\cos^2(ka) \tag{5}$$

$$\beta = -\left(\frac{2t}{J}\right)\cos(ka). \tag{6}$$

The solution decays exponentially with exponent $\gamma = \ln|J/(2t\cos(ka))|$, having the form $\chi(p) = A_p \exp(-\gamma|p|)$ where A_p vanishes at the origin, and has the value $\frac{p}{|p|}$ if $\beta > 0$ and $(-1)^p \frac{p}{|p|}$ if $\beta < 0$, for finite p. Since the amplitude is largest when the particles are next to each other, the state represents a pair bound state moving with centre-of-mass momentum k. Notice that in equations (5) and (6), U is not involved at all, a feature already contained in the Hubbard model [14]. Therefore it was necessary to include nearest-neighbour interaction to find it. Some properties of this paired triplet state are the following. First, under a change of sign of the nearest-neighbour coupling constant, the energy just changes sign. Referring now to positive J, at a fixed value of k its energy is above those of the free electron band at the same k. The state may still be within such a band, yet with different centre-of-mass momentum. The lowest energy is J and it occurs at $|ka| = \pi/2$. In this limit state the two electrons are as close as possible, with finite amplitude as nearest neighbours only. For other values of k the energy is higher, and the pair is larger in size.

Band overlap between paired and free states occurs for $4t \geqslant J$. The energy range of overlap is $J < E < 2J$ if $2t \geqslant J$ and $J < E < 4t$ otherwise. The centre-of-mass momentum is bounded by the condition $|\cos(ka)| \leqslant \frac{J}{2t}$ in the former case, and $|\cos(ka)| \leqslant \sqrt{\frac{J}{t}(1 - \frac{J}{4t})}$ in the latter. If the Fermi energy lies above J, when band overlap occurs, it will be energetically

favourable to create bound pairs, with wavevector around $|ka| = \frac{\pi}{2}$, where the density of states has a divergence. The model thus predicts an instability in the Fermi liquid with the formation of pairs with parallel spin that coexist with other free particle states. Since the pair and the single-particle momenta are not the same at a given energy, a transfer from one state to the other requires some excitation (a phonon for example) to supply the missing momentum.

Let us go on to consider the case of antiparallel spins. In this case the U-term is involved, and if U/J is large, we can ignore the nearest-neighbour coupling and solve the model with $J = 0$, with $\chi(p) = \chi(-p)$. Again we try $\chi(p+1) = \beta\chi(p)$ with $|\beta| \leqslant 1$. Following a procedure similar to that used before, we find now

$$E = \sqrt{U^2 + 16t^2 \cos^2(ka)} \tag{7}$$

$$\beta = \sqrt{\frac{E - U}{E + U}} \tag{8}$$

giving an exponential decay rate $\gamma = \text{arcsin h}|U/4t \cos(ka)|$. The sign of the square root in equation (7) should be the same as the sign of U. This solution was already reported in [10]. Its qualitative features are similar to those of the previous one. Again, for positive (negative) U and the same wavenumber k, the values given by equation (7) are above (below) those given by equation (4). However, for $4t \geqslant U > 0$, allowing for different values of k, there may be energies in the paired band lower in energy than some in the single-electron band. For positive U the lowest-energy state for the paired band is again at $ka = \pi/2$ and the two electrons are stuck together, while as the energy increases above the band minimum U the extent of the pair increases as well.

The most likely case in a real system is $U > |J| > 0$. The paired states with lowest energy will therefore correspond to parallel spins. Different band widths for the paired states are predicted from equations (5) and (7). Effects of overscreening [15] may possibly give rise to a positive U, though a negative J. As remarked before, in the magnetic state, U does not enter, and the energies for the paired solutions lie below the energies of the single-particle band centre and, for $|J|$ sufficiently large, even below the conduction band altogether.

In conclusion, the effect of correlations on interacting electrons, taken two at a time, is to form paired states grouped in bands. In contrast to various approaches based on Green functions [16–18], our treatment is exact, though with the limitation that we only consider correlations between two electrons at a time. Correlations among more than two electrons may be important. However, the equivalent picture of a single electron moving in higher dimensions in a lattice with defects suggests that the number of such states scales as L^{-S}. The possibility of having unconventional metals has often been traced to the failure of Fermi liquid theory in correlated lower-dimensional systems [19–22]. It is obvious here that the correlated bands cannot be placed in a one-to-one correspondence with one-electron states. Thus these effects may also be traced to the possibility of correlations between two or more particles.

Acknowledgments

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