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LETTER TO THE EDITOR

The excitation spectrum of the orbitally degenerate Hubbard model in one dimension: absence of Cooper pairing

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Abstract. The degenerate Hubbard chain with N internal degrees of freedom is integrable if site occupations of more than two electrons are excluded. If on average there is exactly one electron per site, the system is a Mott–Hubbard insulator. We discuss the elemental charge and spin excitations, the effects of crystalline fields quenching the orbital degrees of freedom, and the implications of hole states for superconductivity.

The discovery of ceramic high-temperature superconductors has renewed the interest in low-dimensional highly correlated systems. These compounds have very anisotropic magnetic and transport properties arising primarily from the conductivity within the Cu–O planes. Three ionic configurations of Cu are believed to play an important role, namely $3d^{10}$, $3d^9$ and $3d^8$, all other configurations being excluded by large Coulomb interactions. These configurations correspond to zero, and two holes (within the Cu 3d shell) per site, so as a first approximation the two-dimensional Hubbard model appears to be an adequate description of the Cu–O planes (Anderson 1987, Anderson *et al* 1988, Schrieffer *et al* 1988, Kane *et al* 1989).

If the Hubbard on-site Coulomb interaction U is sufficiently large, the system will be a Mott–Hubbard insulator if there is exactly one electron per site. While in three dimensions the Mott gap opens only for U-values larger than the critical value U_c, there is no Mott transition in one dimension (Lieb and Wu 1968), i.e. for a half-filled band there is a gap for all $U > 0$. It has so far not been established whether U_c is zero or finite in the relevant two-dimensional case. It is, however, assumed that the Coulomb interaction of the Cu 3d shell is sufficiently strong for there to be a Mott–Hubbard gap in half-filled Cu–O bands. It has been argued (Anderson 1987, Anderson *et al* 1988) that due to the quantum fluctuations in low dimensions, one and two dimensions may not be that different, so concepts from exact solutions in one dimension can be adapted to the two-dimensional case.

By means of a k-space renormalisation it has been shown (Bychkov *et al* 1966, Solyom 1980) that away from the Mott gap and for small coupling the one-dimensional Hubbard model is not unstable with respect to superconducting fluctuations at $T = 0$. However, a small additional retarded attractive force will drive the ground state of the system into a superconducting instability (Zimanyi *et al* 1988). A reliable way to address the question

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of superconductivity in the presence of a strong Coulomb repulsion and for a nearly half-filled band is within the framework of the exact solution by means of Bethe's *ansatz*.

In this letter we first discuss the charge and spin excitation spectrum of the degenerate Hubbard model. In order to preserve the integrability of the model the occupation of a site by more than two electrons must be forbidden. For highly correlated electron systems this also represents a physical condition, since ionic configurations of Cu $3d^n$ with less than eight electrons should be excluded. The degeneracy arises from both spin and orbital degrees of freedom. The crossover from the orbitally degenerate case to the non-degenerate (standard) Hubbard model can be achieved by quenching the orbital degrees of freedom with crystalline fields. Although the quenching gives rise to quantitative changes in the charge excitation spectrum, it does not change it qualitatively, so we arrive at the conclusion that an additional attractive mechanism is necessary to bind holes into pairs.

We consider the Hamiltonian

$$H = -\sum_{i=1}^{N_a}\sum_{s=1}^{N} P(c_{is}^{+}c_{i+1s} + c_{i+1s}^{+}c_{is})P + U\sum_{\substack{s,s' \\ (s\neq s')}} n_{is}n_{is'} \tag{1}$$

where N_a is the length of the chain, c_{is}^{+} creates an electron at the site i with a combined spin and orbital index s (s runs from 1 through to $N = 2(2l+1)$), $n_{is} = c_{is}^{+}c_{is}$, and P projects onto the subspace of states having two or fewer electrons at each site. We denote by N_e the number of electrons. Note that the number of electrons with spin and orbital index s is conserved by the Hamiltonian (1).

Model (1) has been independently diagonalised by means of Bethe's *ansatz* by Choy (1980) and Haldane (1980). The procedure is a straightforward extension of Lieb and Wu's (1968) solution of the non-degenerate Hubbard chain. Indeed, the two-particle problems are identical, but there is a difference in the three-particle solution if all three 'colour' components s are different. If the three electrons are allowed to occupy the same site, the three-particle scattering matrix cannot be reduced to a product of two-particle scattering matrices and the system is not integrable (Choy and Haldane 1982). However, if states with site occupations of more than two electrons are excluded, the factorisation condition is satisfied for all N_e and numbers of components N. On imposing periodic boundary conditions, the problem reduces to a set of eigenvalue equations, which has been solved by Sutherland (1968) for an arbitrary Young tableau by means of a sequence of additional $(N-1)$ nested Bethe *ansatz*. Each Bethe *ansatz* leads to a new eigenvalue problem with the number of 'colour' components reduced by one and gives rise to a set of rapidities. This procedure is repeated until all internal degrees of freedom are eliminated. As a result, N sets of rapidities $(\lambda_\alpha^{(m)})$, $m = 0, \ldots, N-1$, are obtained, which are self-consistently determined by the Bethe *ansatz* equations (Choy 1980, Haldane 1980). The set for $m = 0$ corresponds to $\lambda_\alpha^{(0)} = \sin k_\alpha$, where (k_α) are the moments of the electrons, while the other sets are associated with the spin and orbital degrees of freedom.

In the ground state, all the $\lambda_\alpha^{(m)}$ take real values. Due to the tight-binding band the k-values are limited to the interval $[-\pi, \pi]$, while the spin rapidities $\lambda^{(m)}$, $m = 1, \ldots, N-1$, are not constrained. All the rapidities within one set must be different. In the thermodynamic limit, the rapidities are closely spaced and may be regarded as a continuous variable. It is then usual to define a distribution density function, $\sigma^{(m)}(\lambda)$, for each set of rapidities, $m = 1, \ldots, N = 1$, and $\rho(k)$ for the momenta of the electrons

(also called charge rapidities). Minimisation of the energy yields densely and symmetrically (around $k = 0$ and $\lambda = 0$) distributed rapidities, so $\rho(k) \equiv 0$ for $|k| > Q$ ($Q \leqslant \pi$) and $\sigma^{(m)}(\lambda) \equiv 0$ for $|\lambda| > B_m$. The complementary 'hole' distribution functions are $\rho_h(k)$ and $\sigma_h^{(m)}(\lambda)$, $m = 1, \ldots, N = 1$, which vanish identically for $|k| < Q$ and $|\lambda| < B_m$, respectively. The density functions satisfy the following set of linear integral equations (Choy 1980, Haldane 1980)

$$\rho_h(k) + \rho(k) = 1/2\pi + \cos k \int_{-B_1}^{B_1} d\lambda\, a_1(\lambda - \sin k)\sigma^{(1)}(\lambda) \tag{2}$$

$$\sigma_h^{(1)}(\lambda) + \sigma^{(1)}(\lambda) + \int_{-B_1}^{B_1} d\lambda'\, a_2(\lambda - \lambda')\sigma^{(1)}(\lambda') = \int_{-Q}^{Q} dk\, a_1(\lambda - \sin k)\rho(k) + \int_{-B_2}^{B_2} d\lambda'\, a_1(\lambda - \lambda')\sigma^{(2)}(\lambda') \tag{3}$$

$$\sigma_h^{(m)}(\lambda) + \sigma^{(m)}(\lambda) + \int_{-B_m}^{B_m} d\lambda'\, a_2(\lambda - \lambda')\sigma^{(m)}(\lambda') = \int_{-B_{m-1}}^{B_{m-1}} d\lambda\, a_1(\lambda - \lambda')\sigma^{(m-1)}(\lambda') + \int_{-B_{m+1}}^{B_{m+1}} d\lambda'\, a_1(\lambda - \lambda')\sigma^{(m+1)}(\lambda') \tag{4}$$

where $m = 2, \ldots, N-1$, $\sigma^{(N)}(\lambda) \equiv 0$ and $a_n(\lambda) = (Un/4\pi)/[\lambda^2 + (Un/4)^2]$. The integration limits Q and B_m are determined from the number of electrons with each spin and orbital component, n_s, from

$$\frac{N_e}{N_a} = \int_{-Q}^{Q} dk\, \rho(k) \qquad n_1 N_a = \frac{N_e}{N_a} - \int_{-B_1}^{B_1} \sigma^{(1)}(\lambda)$$

$$\frac{n_m}{N_a} = \int_{-B_{m-1}}^{B_{m-1}} d\lambda\, \sigma^{(m-1)}(\lambda) - \int_{-B_m}^{B_m} d\lambda\, \rho^{(m)}(\lambda) \tag{5}$$

and the energy is given by

$$E/N_a = -2 \int dk \cos k\, \rho(k). \tag{6}$$

We first consider the situation of one electron per site ($1/N$-filled band) in the absence of external potentials, i.e. zero spin and orbital magnetisation as well as no higher orbital multipole moments. Then $Q = \pi$ and $B_m = \infty$ for all m, so all 'hole' distribution functions vanish, and the integral equations can be solved by Fourier transformation (for $N = 2$, see Lieb and Wu (1968), and for $N = 4$, see Choy (1980)). For arbitrary N the result is

$$\rho(k) = 1/2\pi + \cos k \int_0^{\infty} d\omega \cos(\omega \sin k) J_0(\omega) \times e^{-U\omega/4} \sinh[(N-1)U\omega/4]/\pi \sinh(NU\omega/4) \tag{7}$$

$$\sigma^{(m)}(\lambda) = \int_0^\infty \mathrm{d}\,\omega \cos(\omega\lambda) J_0(\omega) \sinh[(N-m)U\omega/4]/\pi \sinh(NU\omega/4) \tag{8}$$

and the energy is obtained from equation (6):

$$E_G = -4 \int_0^\infty \mathrm{d}\,\omega\, J_1(\omega) J_0(\omega)\, \mathrm{e}^{-U|\omega|/4} \sinh[(N-1)U\omega/4]/\omega \sinh(NU\omega/4) \tag{9}$$

where J_n denotes the Bessel function.

From the structure of the equations it follows that: (i) the superposition principle holds for any finite number of excitations (vanishing density in the thermodynamic limit), i.e. the excitations do not interfere and their energies are additive; and (ii) charge, spin and orbital excitations are decoupled from each other. For the non-degenerate case ($N = 2$) the excitation spectrum has been discussed by several authors (Ovchinnikov 1970, Takahashi 1972, Coll III 1974, Woynarovich 1982a, b, 1983). Su *et al* (1979) used these one-dimensional soliton-like features to explain the charge transfer in polyacetylene chains, and Anderson (1987) (see also Anderson *et al* 1988) invoked them to justify the resonant valence bond excitation spectrum in two dimensions.

An elemental charge excitation is obtained by removing one particle from the system, i.e. by introducing one 'hole' among the k-momenta. If the hole has momentum k_0, the momentum density $\rho(k)$ (equation (7)) is changed by the amount $\Delta\rho$:

$$\Delta\rho(k) = -\delta(k-k_0) - \cos k \int_0^\infty \mathrm{d}\,\omega \cos[\omega(\sin k - \sin k_0)] \times \mathrm{e}^{-U\omega/4} \sinh[(N-1)U\omega/4]/\pi \sinh(NU\omega/4) \tag{10}$$

where the first term is the bare hole, and the second represents the rearrangement of the other electrons due to the missing state. The corresponding change of energy is given by

$$\Delta E(k_0) = -2 \int_{-\pi}^{\pi} \mathrm{d}k \cos k\, \rho(k) = 2\cos k_0 + 4 \int_0^\infty \mathrm{d}\,\omega \cos(\omega \sin k_0) J_1(\omega) \times \mathrm{e}^{-U\omega/4} \sinh[(N-1)U\omega/4]/\omega \sinh(NU\omega/4). \tag{11}$$

$\Delta E(k_0)$ is symmetric in k_0 around $k_0 = 0$, but not necessarily monotonically decreasing for positive k_0, as shown in figure 1(*a*) for $U = 1$ and various N. For $U > 1.53$, $\Delta E(k_0)$ decreases monotonically for all N, so the minimum is at $k_0 = \pi$. In order to prove that the system is a Mott–Hubbard insulator, we have to show that the chemical potentials μ_+ and μ_- (for adding and removing an electron) are different (Lieb and Wu 1968), i.e.

$$\mu_+ \equiv E(N_a + 1) - E(N_a) \neq \mu_- \equiv E(N_a) - E(N_a - 1). \tag{12}$$

According to equation (11), $\mu_- = -\min(\Delta E(k_0))$, while μ_+ can be obtained using electron–hole symmetry,

$$E(N_e) = (N_e - N_a)U + E(2N_a - N_e) \tag{13}$$

(we assumed that the system is an orbital and spin singlet), so $\mu_+ = U - \mu_-$ for $N_e = N_a$, i.e. on average one electron per site. Since $\mu_+ - \mu_- > 0$, the system is an insulator. Note that if the band filling is other than one electron per site, $\mu_+ = \mu_-$ and the system is a metal (see Lieb and Wu (1968) for $N = 2$).

The same procedure applies if two or more holes are introduced. The energy is the sum of the energies of the individual holes. Hence the holes behave like independent

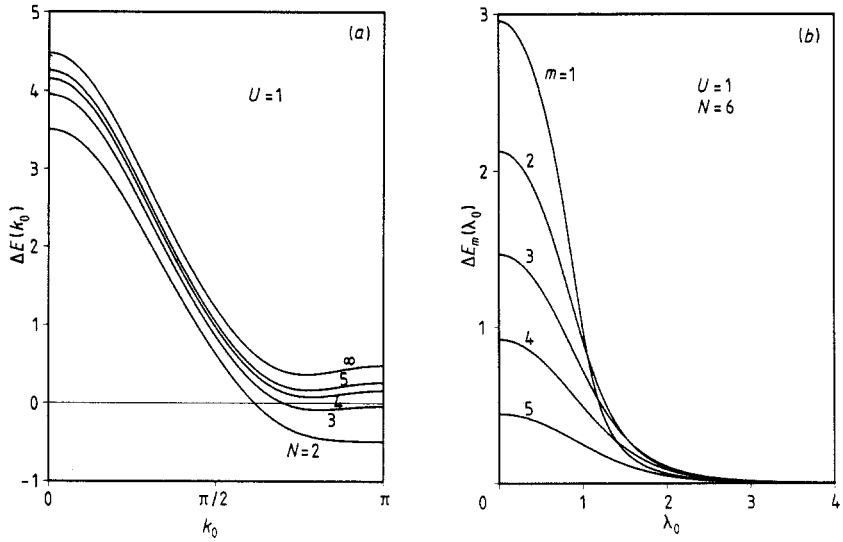

Figure 1. Elemental excitations of the degenerate Hubbard model with on average exactly one electron per site and $U = 1$. (*a*) Energy required to remove one electron from the system for various N-values (for $N = 2$ see Woynarovich 1983). Note that $\Delta E(k_0)$ is not necessarily monotonic. (*b*) The spin-excitation energies for $N = 6$ are the same as for the SU(6) Heisenberg chain. $\lambda_0 \rightarrow \infty$ corresponding to the long-wavelength limit.

soliton-like particles, which do not interact and which propagate according to the energy momentum dispersion displayed in figure 1(*a*). There are no holon bound states in the ground state. A similar picture arises if we consider a band filling of less than one electron per site, except that the dispersion relation is different (and is a function of the band filling).

Next we study excitations of spin and orbital degrees of freedom by keeping the number of particles constant. These excitations correspond to changing the 'colour' of one electron in the system. The initial state is the spin and orbital singlet and the elemental excitations are obtained by removing λ_0 from the set of rapidities $(\lambda^{(m)})$. As a consequence of the Pauli principle, the missing λ_0 modifies all the distribution functions, $\sigma^{(m)}(\lambda)$ and $\rho(k)$. The rearrangement of the momenta k (charge rapidities) is given by $\Delta\rho_m(k)$:

$$\Delta\rho_m(k) = -(\cos k)(2/NU)\sin(m\pi/N)/\{\cosh[(4\pi/NU)(\lambda_0 - \sin k)] - \cos(m\pi/N)\} \tag{14}$$

which gives rise to the excitation energies $\Delta E_m(\lambda_0)$

$$\Delta E_m(\lambda_0) = -2\int_{-\pi}^{\pi} \mathrm{d}k \cos k\, \Delta\rho_m(k)$$

$$= 4\int_0^{\infty} \mathrm{d}\omega \cos(\omega\lambda_0) J_1(\omega) \sinh[(N-m)U\omega/4]/\omega \sinh(NU\omega/4). \tag{15}$$

These excitation energy bands are shown in figure 1(*b*) for $U = 1$ and $N = 6$.

Also, these excitations are soliton-like, i.e. the excitation energy of a finite number of arbitrary excitations is the sum of the individual excitation energies. If the $N-1$ internal degree of freedom correspond to those of a spin $S=(N-1)/2$, the $\Delta E_m(\lambda_0)$ are the elemental spin-wave excitations of the SU(N) Heisenberg chain.

We now consider spin and orbital degrees of freedom in the presence of crystalline fields assuming no spin–orbit coupling. The crystalline fields quench the orbital angular momentum. For the sake of simplicity we consider only two different orbitals, i.e. $N=4$. The ionic energy levels are then split into two spin doublets (reminiscent of Kramers doublets), so in the absence of a magnetic field $B_1=B_3=\infty$, but B_2 is finite and monotonically decreasing with the crystal field splitting. We can eliminate $\sigma^{(1)}$ and $\sigma^{(3)}$ by Fourier transforming equations (2)–(4) and obtain two coupled integral equations for $\sigma^{(2)}$ and ρ:

$$\rho_h(k)+\rho(k)=1/2\pi-\cos k\int_{|\lambda|>B_2} d\lambda\,\sigma_h^{(2)}(\lambda)\{2U\cosh[\pi(\lambda-\sin k)/U]\}^{-1}$$
$$+\cos k\int_{-Q}^{Q}dk'\,\rho(k')\int_{-\infty}^{\infty}(d\omega/2\pi)\exp[-i\omega\sin k-\sin k')]$$
$$\times\exp(-U|\omega|/4)\sinh(3U\omega/4)/\sinh(\omega U) \tag{16}$$

$$\sigma^{(2)}(\lambda)+\int_{|\lambda'|>B_2}d\lambda'\,\sigma_h^{(2)}(\lambda')\int_{-\infty}^{\infty}(d\omega/2\pi)\exp[i(\lambda-\lambda')]$$
$$\times\exp(U|\omega|/4)\sinh(U\omega/2)/\sinh(3U\omega/3)$$
$$=\int_{-Q}^{Q}dk\,\rho(k)\{2U\cosh[\pi(\lambda-\sin k)/U]\}^{-1}. \tag{17}$$

For $B_2\to\infty$ all four levels are degenerate, the system is SU(4) invariant and we recover the situation discussed above. If, on the other hand, $B_2\to 0$, we see from equations (2) and (3) that ρ and $\sigma^{(1)}$ totally decouple from $\sigma^{(2)}$ and $\sigma^{(3)}$, so we recover Lieb and Wu's (1968) solution of the non-degenerate Hubbard model. The relative occupation of the two orbital bands is determined by $\int d\lambda\,\sigma^{(2)}(\lambda)$ from equations (5).

Consider a quarter-filled band, i.e. one electron per site ($Q=\pi$), and remove one charge from the system, e.g. with momentum k_0. As a consequence of the missing charge the momenta of the remaining particles are rearranged, leading to changes $\Delta\rho$ and $\Delta\sigma^{(2)}$ in the distribution functions, $\Delta\sigma^{(2)}$ satisfies the same integral equation as $\sigma^{(2)}$, namely equation (17), but with the right-hand side being replaced by

$$\{2U\cosh[\pi(\lambda-\sin k_0)/U]\}^{-1}.$$

The solution for $\Delta\sigma_h^{(2)}$ is then used to obtain $\Delta\rho(k)$. The integral equation satisfied by $\Delta\rho(k)$ is equation (16) with $\rho_h\equiv 0$, ρ being replaced by $\Delta\rho$, the driving term $1/2\pi$ being substituted by $-\delta(k-k_0)$ and $\sigma_h^{(2)}$ by $\Delta\sigma_h^{(2)}$. The excitation energy is then

$$\Delta E(k_0)=-2\int dk\cos k\,\Delta\rho(k).$$

For $Q=\pi$ the system is a Mott–Hubbard insulator, independently of the magnitude of the crystal field splitting. The same holds for any other level splitting. If $Q<\pi$ the Hubbard chain is always a metal. The energy of two or more holes is the sum of the individual excitation energies, i.e. the holes have a soliton-like behaviour.

In summary, we have analysed the elemental excitations of the degenerate Hubbard model. The system is a metal, except if there is exactly one electron per site which makes the system a Mott–Hubbard insulator. This result is independent of the level splitting, i.e. for arbitrary crystal and magnetic fields. The energies of the elemental excitations are additive, i.e. the excitations have a soliton-like behaviour. Charge excitations completely decouple from those arising from internal degrees of freedom (spin and orbit).

Finally, we would like to comment on possible implications of these results on superconductivity. Consider as a particular example one electron per site. The holes introduced by removing moments $\boldsymbol{k}_i$ move freely throughout the crystal. They do not interact with each other and a quasiparticle band picture applies, although the system is not a Fermi liquid (Lee and Schlottmann 1989). There are no bound states of holons in the ground state, i.e. no Cooper pairs. However, a small retarded attractive interaction provided by a mechanism not included in Hubbard's model (e.g. virtual transitions into another band) could lead to pairing and superconductivity at $T = 0$. Note that the formation of holons in itself overcomes the unfavourable Coulomb repulsion U among the electrons.

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