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LETTER TO THE EDITOR

On the antiferromagnetic phase in the Hubbard model

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Abstract. Using the cluster Bethe lattice method and the quasi-spin model for itinerant magnetism, we show that in a one-band model there is no metallic–antiferromagnetic phase for a half-filled band at $T = 0$.

In a recent paper published in this Journal, one of us (Brouers 1982) has discussed the influence of magnetic short-range order and electronic charge transfer on the value of the Curie temperature. In that paper based on the Bethe cluster approximation (Brouers *et al* 1973, Kittler and Falicov 1976) three 'order parameters' were introduced, the concentration of up moments, the magnetic short- and long-range order. With this description, the discussion of the phase diagram in the U/B–n plane, where U is the intra-atomic Coulomb interaction, B the half-bandwidth and n the number of electrons per atom, is more general than in previous works (Roth 1978, Liu 1978, Moran-Lopez *et al* 1981). In particular, it was shown that the introduction of magnetic short-range can reduce substantially the Curie temperature and that charge transfer between sites with up and down moments cannot be discarded.

In this Letter we want to comment on the possibility of obtaining in this model a metallic–antiferromagnetic phase for a band filling corresponding to one electron per atom. Such a phase has been observed in V_2O_3.

Cyrot and Lacour-Gayet (1972), using the coherent potential approximation, obtained two critical values for U/B, u_{AF} and u_I. For ratios smaller than u_{AF}, the local moment is zero and the system is metallic and non-magnetic. For intermediate values $u_{AF} < u < u_I$, the system becomes antiferromagnetic. There is no gap in the electron spectrum and the system remains metallic. For ratios larger than u_I the system becomes an antiferromagnetic insulator. However, this behaviour does not agree with Brinkman and Rice's (1970) theory which, on the basis of Gutzwiller's (1965) approach, states that no antiferromagnetic metallic state can exist in this model.

In the calculations of Roth (1978) which correspond to the same model, the ground state is always antiferromagnetic for any value of U/B. In the paper of Liu (1978), the published phase diagram does not allow a definite conclusion. These two authors did not discuss the metal–insulator transition.

As, moreover, a general theorem indicates that in this one-band model the appearance of two sublattices and the appearance of an insulating gap should occur simultaneously we have used the formalism described in Brouers (1982) to understand the contradictions between these various results.

We start from the single-band Hubbard Hamiltonian

$$H = \sum_{i,j,\sigma}{}' t_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where t_{ij} is the hopping integral, U is the Coulomb repulsion, the sum on i and j is over the lattice sites, and i and j are nearest neighbours. The sum on σ is over the spin states of the electrons. The number of nearest neighbours of a given site is denoted by Z. Here we have taken $Z = 12$.

The unrestricted Hartree–Fock Hamiltonian can be written

$$H_{\mathrm{HF}} = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_i \langle n_{i\downarrow} \rangle n_{i\uparrow} + U \sum_i \langle n_{i\uparrow} \rangle n_{i\downarrow} + U \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle. \tag{2}$$

We use the alloy analogy considered by Schrieffer (1970) and Cyrot and Lacour-Gayet (1972). We view the system as an Ising alloy $A_x B_{1-x}$, the A sites being occupied by up $(+)$ moments and the B sites by down $(-)$ moments. If one wants to describe antiferromagnetic states, one has to introduce two sublattices α and β. In the antiferromagnetic state, all the sites α are occupied by A atoms with up moment m_+^α and the β sites by B atoms with a down moment $m_-^\beta = -m_+^\alpha$.

The interactions corresponding to an up spin are therefore

$$\begin{aligned}
&U\langle n_+^{\alpha\downarrow} \rangle \text{ with probability } p_+^\alpha = x + \tfrac{1}{2}\eta \\
&U\langle n_+^{\beta\downarrow} \rangle \text{ with probability } p_+^\beta = x - \tfrac{1}{2}\eta \\
&U\langle n_-^{\alpha\uparrow} \rangle \text{ with probability } p_-^\alpha = 1 - x - \tfrac{1}{2}\eta \\
&U\langle n_-^{\alpha\uparrow} \rangle \text{ with probability } p_-^\beta = 1 - x + \tfrac{1}{2}\eta
\end{aligned} \tag{3}$$

and similar expressions for a down spin. Here η is the long-range order defined by

$$\begin{aligned}
&0 \leqslant \eta \leqslant 2x && \text{if } x \leqslant \tfrac{1}{2} \\
&0 \leqslant \eta \leqslant 2(1-x) && \text{if } x \geqslant \tfrac{1}{2}.
\end{aligned}$$

The eight quantities $\langle n_{+(-)}^{\alpha(\beta)\uparrow(\downarrow)} \rangle$ have been determined self-consistently and the local moments can then be calculated. We have solved this problem on a Cayley tree. The absence of closed loops allows us to express the local Green's function in the form of a continuous fraction which can be easily written in a closed form (Brouers 1982). The local Green's functions are given by

$$G_+^{\alpha\uparrow} = (z - U\langle n_{+\downarrow}^{\alpha} \rangle - Z_{++}^{\alpha\beta} t_{++}^{\alpha\beta} T_{++}^{\beta\alpha\uparrow} - Z_{+-}^{\alpha\beta} t_{+-}^{\alpha\beta} T_{-+}^{\beta\alpha\uparrow})^{-1} \text{ etc} \tag{4}$$

with the transfer matrices given by

$$T_{++}^{\alpha\beta\uparrow} = t_{++}^{\alpha\beta}(z - U\langle n_{+\downarrow}^{\alpha} \rangle - (Z_{++}^{\alpha\beta} - 1) t_{++}^{\alpha\beta} T_{++}^{\beta\alpha\uparrow} - (Z_{+-}^{\alpha\beta} - 1) t_{+-}^{\alpha\beta} T_{-+}^{\beta\alpha\uparrow})^{-1} \text{ etc} \tag{5}$$

$$Z_{+-}^{\alpha\beta} = (p_{+-}^{\alpha\beta}/p_+^\alpha) Z. \tag{6}$$

The pair probabilities are defined by

$$\begin{aligned}
&p_{++}^{\alpha\beta} = x^2 + x(1-x)\sigma && p_{-+}^{\alpha\beta} = x(1-x)(1-\sigma) - \tfrac{1}{2}\eta \\
&p_{+-}^{\alpha\beta} = x(1-x)(1-\sigma) + \tfrac{1}{2}\eta && p_{--}^{\alpha\beta} = (1-x)^2 + x(1-x)\sigma.
\end{aligned} \tag{7}$$

If we define the partial densities of states

$$g_{+(-)}^{\alpha(\beta)\uparrow(\downarrow)} = -\frac{1}{\pi} \operatorname{Im} G_{+(-)}^{\alpha(\beta)\uparrow(\downarrow)}(E + \mathrm{i}a) \tag{8}$$

the Fermi level is determined by the condition

$$n = \frac{1}{\pi}\int_{-\infty}^{E_F} \{p_{\pm}^{\alpha}[g_{\pm}^{\alpha\uparrow}(E) + g_{\pm}^{\alpha\downarrow}(E)] + \ldots\} \tag{9}$$

where n is the electron occupation number and the quantities are determined self-consistently solving the eight equations

$$n_{+(-)}^{\alpha(\beta)\uparrow(\downarrow)} = \int_{-\infty}^{E_F} g_{+(-)}^{\alpha(\beta)\uparrow(\downarrow)}(E)\,\mathrm{d}E \tag{10}$$

the local moments being

$$u_{+(-)}^{\alpha(\beta)} = \langle n_{+(-)}^{\alpha(\beta)\uparrow}\rangle - \langle n_{+(-)}^{\alpha(\beta)\downarrow}\rangle. \tag{11}$$

The total energy is given by

$$E_{\text{tot}} = \int_{-\infty}^{E_F} E\{p_{\pm}^{\alpha}[g_{\pm}^{\alpha\uparrow}(E) + g_{\pm}^{\alpha\downarrow}(E)] + \ldots\} - U[p_{\pm}^{\alpha}\langle n_{\pm}^{\alpha\uparrow}\rangle\langle n_{\pm}^{\alpha\downarrow}\rangle + \ldots]. \tag{12}$$

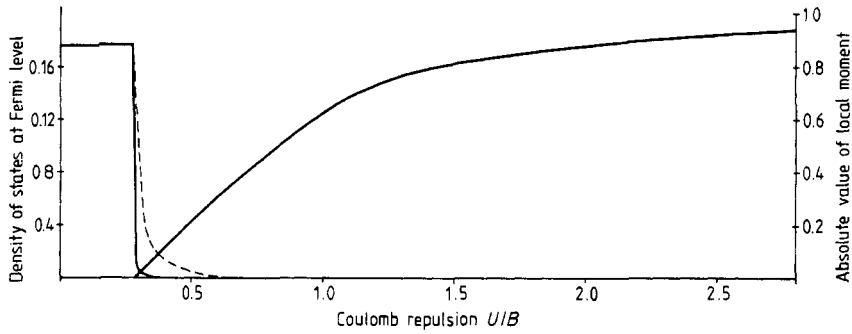

Figure 1. Absolute value of the local moment and density of states at Fermi level against U/B. The dotted line corresponds to an imaginary part of $10^{-2}t$ and the full line to $10^{-3}t$.

The results for a half-filled band ($n = 1$) are summarised in figures 1 and 2. An antiferromagnetic solution occurs for $U = 0.28$, the units being half the bandwidth $2\sqrt{12}t$. The absolute value of the local moment increases monotonically to the value 1 in the atomic limit. For $U = 0.28$ the density of states drops to zero. We have noticed that this sudden decrease, related to the appearance of a gap in the density of states, depends strongly on the presence in the denominator of the Green function of a small imaginary part which is generally introduced in the self-consistent numerical calculations to improve the convergence. The dotted line corresponds to an imaginary part of $10^{-2}t$ and the full line to $10^{-3}t$.

Using the cluster Bethe lattice method and the quasi-spin model for itinerant magnetism, we have found that for a half-filled band an antiferromagnetic solution occurs for a finite value of the interatomic Coulomb interaction $U = 0.28\ B$ where B is the half-bandwidth. Simultaneously the system undergoes a metal–insulator transition.

This result does not agree with Cyrot and Lacour-Gayet's conclusions. The fact that in their CPA calculation the two transitions do not appear simultaneously is probably due to the introduction in the numerical calculation of a small imaginary self-energy.

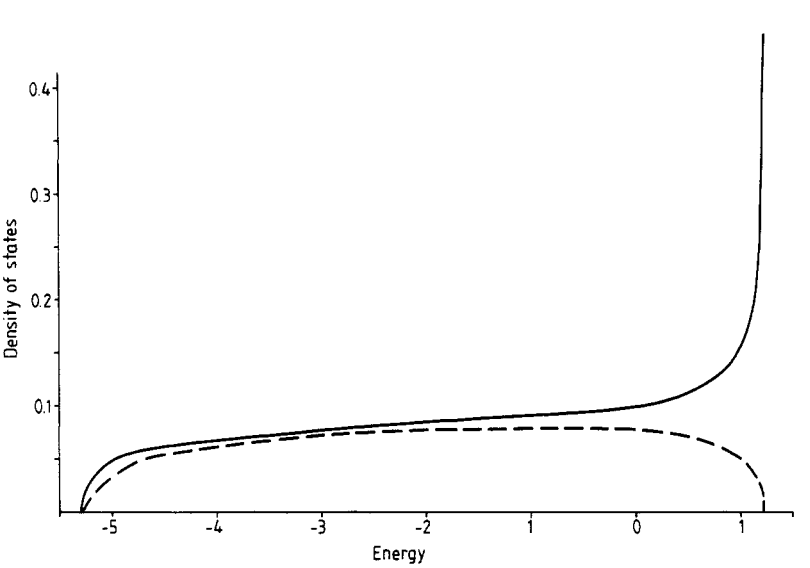

Figure 2. Density of states corresponding to up and down spin on the α sublattice. —— $g_{\uparrow}^{\alpha\uparrow}, g_{\downarrow}^{\beta\downarrow}$; ---- $g_{\uparrow}^{\alpha\downarrow}, g_{\downarrow}^{\beta\uparrow}$. $U/B = 0.4$; $n_{\uparrow}^{\alpha\uparrow} = 0.555$; $n_{\uparrow}^{\alpha\downarrow} = 0.445$; $m_{\uparrow}^{\alpha} = 0.11 = -|m_{\downarrow}^{\beta}|$.

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