ON THE SINGLE SITE APPROXIMATION IN THE HUBBARD MODEL

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The Alloy Analogy Approximation in the Hubbard model is improved by the decoupling scheme which includes the band shift. The condition for the ferromagnetic instability of the system is derived. In the strong correlation limit, our solution does not reproduce Roth's result.

1. Introduction

The Hubbard model [1, 2] is commonly employed to describe the magnetic properties of metals and alloys and the metal-insulator transition. Up to now, several sorts of Green's function decoupling schemes have been proposed (for review see e.g. [3]) but they are usually correct only in limiting cases. The original approach by Hubbard [2] explains to some extent, the mechanism of the metal-insulator transition but does not preserve the Harris-Lange sum rules [4]. This approach does not give ferromagnetic solutions of the model for any level of band filling, as it was argued by Bartel and Jarrett [5]. In the simplified version of the Hubbard III approximation (the so called Alloy Analogy Approximation (AAA)) ferromagnetic instability does not occur either [6].

However, there exists another approach to the Green's function decoupling procedure due to Roth [7] and Tahir-Kehli and Jarrett [8], which postulates that the more moments of the spectral function any approximation reproduces, the better it is. In Roth's scheme of decoupling the ferromagnetic solutions does exist in the limit of strong Coulomb correlations [7, 9]. But this approximation does not describe the metal-insulator transition.

In this paper we consider a possibility of improving the AAA. The proposed solution has a single site character. It is examined in the limit of low density. In Section 3 the single site approximation is introduced. The criterion for ferromagnetic instability is derived.

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The stability of the strongly ferromagnetic ground state against Stoner excitations is also investigated. It is found that for an elliptic density of states and $n \lesssim 1$ only the paramagnetic solution exists.

In Section 4 the results are discussed.

2. 2. *Effective Hamiltonian and the simplest treatment of scattering with spin inversion*

The Hubbard Hamiltonian is

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

where t_{ij} is the hopping integral between the i and j sites, U describes the repulsion between electrons of opposite spins in the same Wannier state i and the operator $a_{i\sigma}^{+}$ ($a_{i\sigma}$) creates (destroys) an electron with the diagonal spin component $\sigma/2$ on site i.

The first two equations of motion in Zubariev's scheme [10] are

$$E\langle\langle a_{i\sigma} | a_{l\sigma}^{+} \rangle\rangle_E = \frac{1}{2\pi} \delta_{i,l} + \sum_{m(i)} t_{im} \langle\langle a_{m\sigma} | a_{l\sigma}^{+} \rangle\rangle_E + U \langle\langle n_{i-\sigma} a_{i\sigma} | a_{l\sigma}^{+} \rangle\rangle_E \tag{2}$$

$$E\langle\langle n_{i-\sigma} a_{i\sigma} | a_{l\sigma}^{+} \rangle\rangle_E = \frac{1}{2\pi} \langle n_{i-\sigma} \rangle \delta_{i,l} + U \langle\langle n_{i-\sigma} a_{i\sigma} | a_{l\sigma}^{+} \rangle\rangle_E$$

$$+ \sum_{m(i)} t_{im} \langle\langle n_{i-\sigma} a_{m\sigma} | a_{l\sigma}^{+} \rangle\rangle_E + \sum_{m(i)} t_{im} \langle\langle (a_{i-\sigma}^{+} a_{m-\sigma} - a_{m-\sigma}^{+} a_{i-\sigma}) a_{i\sigma} | a_{l\sigma}^{+} \rangle\rangle_E. \tag{3}$$

The new Green's functions on the right hand side of (3) describe the scattering of electrons: the first function is connected with the scattering of σ-spin electrons on $-\sigma$-spin electrons; the second one expresses the scattering of σ-spin electrons into a $-\sigma$-spin hole and the spin-flip scattering.

Hubbard introduced a rather elaborate decoupling scheme in his third paper [2] in order to describe qualitatively the metal-insulator transition. Now, we propose another treatment of the scattering processes described by the second function in (3).

Let us assume that the two-body potential is replaced by the one-body coherent potential $V_\sigma(E)$ in all lattice sites except in $i = 0$

$$U n_{i\uparrow} n_{i\downarrow} \to V_\uparrow(E) n_{i\uparrow} + V_\downarrow(E) n_{i\downarrow}, \qquad i \neq 0, \tag{4}$$

and thus the effective Hamiltonian is of the form

$$\mathscr{H}_{\text{eff}}(E) = \sum_{ij\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} + \sum_{i\sigma} V_\sigma(E) n_{i\sigma} + U n_{0\uparrow} n_{0\downarrow} - \sum_{\sigma} V_\sigma(E) n_{0\sigma}. \tag{5}$$

The coherent potential $V_\sigma(E)$ will be chosen in such a way that on the average a single site will produce no further scattering.

On applying the effective Hamiltonian (5) we obtain equations of motion for the Green functions

$$E\langle\langle a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E = \frac{1}{2\pi}\delta_{i,l} + \sum_{m(i)} t_{im}\langle\langle a_{m\sigma}|a_{l\sigma}^{+}\rangle\rangle_E + V_\sigma(E)\,\langle\langle a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E$$

$$+\delta_{i,0}(U\langle\langle n_{0-\sigma}a_{0\sigma}|a_{l\sigma}^{+}\rangle\rangle_E - V_\sigma(E)\,\langle\langle a_{0\sigma}|a_{l\sigma}^{+}\rangle\rangle_E), \tag{6}$$

and

$$E\langle\langle n_{0-\sigma}a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E = \frac{1}{2\pi}\langle n_{0-\sigma}\rangle\delta_{i,l} + \sum_{m(i)} t_{im}\langle\langle n_{0-\sigma}a_{m\sigma}|a_{l\sigma}^{+}\rangle\rangle_E$$

$$+V_\sigma(E)\,\langle\langle n_{0-\sigma}a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E + \delta_{i,0}(U - V_\sigma(E))\,\langle\langle n_{0-\sigma}a_{0\sigma}|a_{l\sigma}^{+}\rangle\rangle_E$$

$$+\sum_{m(0)} t_{0m}\langle\langle (a_{0-\sigma}^{+}a_{m-\sigma} - a_{m-\sigma}^{+}a_{0-\sigma})a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E. \tag{7}$$

The simplest approximation of the last term in Eq. (7) is

$$\sum_{m(0)} t_{0m}\langle\langle (a_{0-\sigma}^{+}a_{m-\sigma} - a_{m-\sigma}^{+}a_{0-\sigma})a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E \simeq 0. \tag{8}$$

In Eqs (6) and (7) we perform the Fourier transformation

$$a_{i\sigma} = N^{-1/2}\sum_k a_{k\sigma}e^{ikR_i},$$

$$\langle\langle a_{i\sigma}|a_{l\sigma}^{+}\rangle\rangle_E = N^{-1}\sum_{kk'}\langle\langle a_{k\sigma}|a_{k'\sigma}^{+}\rangle\rangle_E e^{i(kR_i - k'R_l)}, \tag{9}$$

and we obtain the Green function $\langle\langle a_{k\sigma}|a_{k'\sigma}^{+}\rangle\rangle_E$, which we make diagonal in the Bloch representation

$$\langle\langle a_{k\sigma}|a_{k'\sigma}^{+}\rangle\rangle_E = \frac{\delta_{k,k'}}{E - \varepsilon_k - V_\sigma(E)}, \tag{10}$$

where

$$\varepsilon_k = \sum_{|i-j|} t_{ij}e^{-ik(R_i - R_j)}. \tag{11}$$

The scattering term set equal to zero yields the condition which determines the coherent potential $V_\sigma(E)$

$$V_\sigma(E) = Un_{-\sigma} + V_\sigma(E)\,(U - V_\sigma(E))G_\sigma(E), \tag{12}$$

where

$$G_\sigma(E) = \frac{1}{N}\sum_k \frac{1}{E - \varepsilon_k - V_\sigma(E)}, \tag{13}$$

and $n_{-\sigma} = \langle n_{0-\sigma}\rangle$.

The approximation introduced above appears to be equivalent to the AAA in the Hubbard model. A condition, the same as (11), was also obtained by Velicky et al. [11] in the standard version of the coherent potential approximation (CPA). The qualitative aspects of this approximation were discussed by Schneider and Drchal [12]. They showed that the AAA does not give the band shift and thus saturated ferromagnetism in the limit $n \lesssim 1$ is not possible. The lack of the band shift is due to the negligence of the electron-hole scattering, expressed by the decoupling scheme adopted in the AAA (8). On the other hand, the band shift is essential in the problem of magnetic phases, as was shown by Harris and Lange [4] and by Roth [7].

Therefore, we introduce the decoupling scheme which reproduces the first two moments of the spectral function of Green's function $\ll(a^+_{0-\sigma}a_{m-\sigma}-a^+_{m-\sigma}a_{0-\sigma})a_{i\sigma}|a^+_{l\sigma}\gg_E$ instead of one:

$$\sum_{m(0)} t_{0m}\ll(a^+_{0-\sigma}a_{m-\sigma}-a^+_{m-\sigma}a_{0-\sigma})a_{i\sigma}|a^+_{l\sigma}\gg_E$$

$$\simeq \delta_{i,0}(W_{-\sigma}\ll n_{0-\sigma}a_{0\sigma}|a^+_{l\sigma}\gg_E - W_{-\sigma}\langle n_{0-\sigma}\rangle \ll a_{0\sigma}|a^+_{l\sigma}\gg_E), \tag{14}$$

where

$$\langle n_{0-\sigma}\rangle(1-\langle n_{0-\sigma}\rangle)W_{-\sigma} = -\sum_{m(0)} t_{0m}\langle a^+_{m-\sigma}a_{0-\sigma}-2a^+_{m-\sigma}a_{0-\sigma}n_{0\sigma}\rangle. \tag{15}$$

Moments of the spectral function are defined as in [8]

$$m^{(n+1)}_{ij\sigma} = \langle\{[[\ldots[a_{i\sigma}, \mathscr{H}_{\text{eff}}]\ldots], \mathscr{H}_{\text{eff}}], a^+_{j\sigma}\}\rangle. \tag{16}$$

We notice, that the decoupling scheme (14) reproduces the first two moments of the spectral function of the Green function $\ll(a^+_{0-\sigma}a_{m-\sigma}-a^+_{m-\sigma}a_{0-\sigma})a_{i\sigma})a^+_{l\sigma}\gg_E$ only if the moments are defined via the effective Hamiltonian (5).

One can solve Eqs (6) and (7) using (9) and (14) and one gets after some algebra the modified condition for the coherent potential

$$V_\sigma(E) = Un_{-\sigma}+V_\sigma(E)(U-V_\sigma(E))G_\sigma(E)+W_{-\sigma}(V_\sigma(E)-Un_{-\sigma})G_\sigma(E). \tag{17}$$

The Green function defined by Eqs (10) and (17) reproduces exactly only three moments $m^{(n)}_{0j\sigma}$ of the spectral function. The fourth moment in the Hubbard model is:

$$m^{(4)}_{0j\sigma} = 3Un_{-\sigma}\sum_{m(0)} t^2_{0m}+\delta_{0,j}U^3n_{-\sigma}+\sum_{\substack{m(0)\\n(m)}} t_{0m}t_{mn}t_{nj}$$

$$+2U^2n_{-\sigma}t_{0j}+\delta_{0,j}U^2\sum_{m(0)} t_{0m}\langle -a^+_{m-\sigma}a_{0-\sigma}+2a^+_{m-\sigma}a_{0-\sigma}n_{0\sigma}\rangle$$

$$+U^2t_{0j}(\langle n_{0-\sigma}n_{j-\sigma}\rangle-\langle a^+_{j\sigma}a^+_{0-\sigma}a_{j-\sigma}a_{0\sigma}\rangle-\langle a^+_{j\sigma}a^+_{j-\sigma}a_{0-\sigma}a_{0\sigma}\rangle). \tag{18}$$

The part connected with its scattering with the spin inversion is exactly reproduced. The second part includes in our approximation scheme, some terms proportional to $V_\sigma(E)$ and does not reproduce exact expressions.

Let us examine the approximate solution obtained in the limit of low densities. In this limit, Kanamori solved the correlation problem exactly and the Coulomb correlation

was replaced by a T-matrix describing the scattering of two electrons [13]. Then we wish to evaluate $V_\sigma(E)$ to the first order in $n_{-\sigma}$. As a result we obtain

$$V_\sigma(E) = Un_{-\sigma} + V_\sigma(E)\,(U-\varepsilon_b)\,\frac{1}{N}\sum_k \frac{1}{\varepsilon_k - \varepsilon_b}, \tag{19}$$

where

$$n_{-\sigma}(1-n_{-\sigma})W_{-\sigma} = -\varepsilon_b n_{-\sigma}, \tag{20}$$

and ε_0 is the band-edge energy. Eq. (20) can be solved with respect to $V_\sigma(E)$

$$V_\sigma(E) = \frac{Un_{-\sigma}}{1+\dfrac{U-\varepsilon_b}{N}\displaystyle\sum_k \frac{1}{\varepsilon_b-\varepsilon_k}}. \tag{21}$$

The Kanamori result, which is exact in this limit, is

$$V_\sigma(E) = \frac{Un_{-\sigma}}{1+\dfrac{U}{2N}\displaystyle\sum_k \frac{1}{\varepsilon_b-\varepsilon_k}}. \tag{22}$$

The effect of the renormalisation of the Coulomb energy U in the denominator of (21) is connected with the decoupling scheme (14).

3. The improved version of the single site approximation

The decoupling scheme (14) distinguishes the site $i = 0$. Now we will treat all sites more symmetrically

$$\sum_{m(0)} t_{0m}\langle\langle (a^+_{0-\sigma}a_{m-\sigma} - a^+_{m-\sigma}a_{0-\sigma})a_i | a^+_{i\sigma}\rangle\rangle_E$$

$$\simeq W_{-\sigma}\langle\langle n_{0-\sigma}a_{0\sigma}|a^+_{i\sigma}\rangle\rangle_E - W_{-\sigma}\langle n_{0-\sigma}\rangle\,\langle\langle a_{0\sigma}|a^+_{i\sigma}\rangle\rangle_E. \tag{23}$$

This decoupling does preserve the same number of moments as (14). The condition for the coherent potential is now:

$$V_\sigma(E) = Un_{-\sigma} + V_\sigma(E)\,(U - V_\sigma(E))G_\sigma(E - W_{-\sigma}). \tag{24}$$

In the low density limit it yields

$$V_\sigma(E) = \frac{Un_{-\sigma}}{1+\dfrac{U}{N}\displaystyle\sum_k \frac{1}{\varepsilon_k - 2\varepsilon_b}}. \tag{25}$$

This result is closer to the exact expression (22) than (21). Our single site approximation is in fact equivalent to the replacement of one of the energies ε_k in (22) by its average value.

It is also interesting to examine the spin susceptibility in the presented scheme. The condition of ferromagnetic instability is [6]

$$K = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{E_F} dE\,\frac{\partial G_\sigma}{\partial n_{-\sigma}} \leqslant -1. \tag{26}$$

From the definition of G_σ (Eq. (13)) we have

$$\frac{\partial G_\sigma}{\partial n_{-\sigma}} = S\left[1-S\left(\frac{\partial V_\sigma}{\partial G_\sigma}\right)_{n_{-\sigma}}\right]^{-1}\left[\left(\frac{\partial V_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma}+\left(\frac{\partial W_{-\sigma}}{\partial n_{-\sigma}}\right)\right], \tag{27}$$

where

$$S = \frac{1}{N}\sum_k \frac{1}{[E-\varepsilon_k-V_\sigma(E)-W_{-\sigma}]^2}. \tag{28}$$

On the other hand,

$$\frac{\partial G_\sigma}{\partial E} = -S\left[1-S\left(\frac{\partial V_\sigma}{\partial G_\sigma}\right)_{n_{-\sigma}}\right]^{-1}. \tag{29}$$

Substituting Eq. (27) into (26) and eliminating S via (29) we get

$$K = \frac{1}{\pi}\,\mathrm{Im}\int_{G_0}^{G_F} dG_\sigma\left[\left(\frac{\partial V_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma}+\left(\frac{\partial W_{-\sigma}}{\partial n_{-\sigma}}\right)\right], \tag{30}$$

where G_F and G_0 are $G_\sigma(E_F)$ and $G_\sigma(-\infty)$. We now introduce $\mathscr{L} = V_\sigma(E)/U$ and $z = UG_\sigma$ in order to evaluate the first integral in (30). Similarly as in [6] we obtain

$$\frac{1}{\pi}\,\mathrm{Im}\int_{G_0}^{G_F} dG_\sigma\left(\frac{\partial V_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma} = \frac{1}{\pi}\,\mathrm{Im}\,\ln\left[\mathscr{L}_F(1-\mathscr{L}_F)^{-1}\right], \tag{31}$$

where $\mathscr{L}_F = \mathscr{L}(E_F)$. This part of K is always negative but greater than -1. The second integral is

$$\frac{1}{\pi}\,\mathrm{Im}\int_{G_0}^{G_F} dG_\sigma\left(\frac{\partial W_{-\sigma}}{\partial n_{-\sigma}}\right) = \frac{1}{\pi}\,\mathrm{Im}\,G_F\left(\frac{\partial W_{-\sigma}}{\partial n_{-\sigma}}\right). \tag{32}$$

As the derivative $\left(\frac{\partial W_{-\sigma}}{\partial n_{-\sigma}}\right)$ is usually positive and Im G_F is always negative, the expression (32) is usually negative. Thus the condition of ferromagnetic instability

$$1+\frac{1}{\pi}\,\mathrm{Im}\,\ln\left[\mathscr{L}_F(1-\mathscr{L}_F)^{-1}\right]+\frac{1}{\pi}\,\mathrm{Im}\,G_F\left(\frac{\partial W_{-\sigma}}{\partial n_{-\sigma}}\right)\leqslant 0 \tag{33}$$

can be fulfilled for a certain band shape and band filling.

We have examined the single site approximation in the strong correlation limit $U\to\infty$ assuming the model density of states suggested by Hubbard [2]

$$\varrho^{(0)}(E)=\begin{cases}\frac{2}{\pi}(1-E^2)^{1/2}, & |E|\leqslant 1,\\ 0, & |E|>1.\end{cases} \tag{34}$$

For this density of states the condition (24) gives a cubic equation for G_σ. In the strong correlation limit this equation becomes quadratic

$$\tfrac{1}{4}G_\sigma^2-zG_\sigma+(1-n_{-\sigma})=0, \tag{35}$$

where $z=E-W_{-\sigma}$, and gives the density of states

$$\varrho_\sigma(E)=\begin{cases}\frac{2}{\pi}(1-n_{-\sigma}-z^2)^{1/2}, & |z|\leqslant\sqrt{1-n_{-\sigma}},\\ 0, & |z|>\sqrt{1-n_{-\sigma}}.\end{cases} \tag{36}$$

The usual Green's function technique yields

$$\langle n_{i\sigma}\rangle=2\int_{-\infty}^{E_F}\mathrm{Im}\,G_\sigma(E-i\varepsilon)dE, \tag{37}$$

$$\langle n_{i\sigma}\rangle(1-\langle n_{i\sigma}\rangle)W_\sigma=-\int_{-\infty}^{E_F}dE\left[E-\frac{\langle n_{i-\sigma}\rangle(W_{-\sigma}-E)}{1-\langle n_{i-\sigma}\rangle}\right]\varrho_\sigma(E). \tag{38}$$

This set of quantities was determined selfconsistently for the model density of states (34) until the difference between two successive iterates was less than 10^{-5}. It appears that the paramagnetic solution is the only solution of this set. If we assume that all electrons have the same spin direction, the center of gravity of the subband of opposite-spin electrons is pushed above the Fermi level, but the lower edge of this subband lies below the Fermi level, as is shown in Fig. 1. In Fig. 2 we present positions of the Fermi level and the lower band edge of down-spin electrons in our and Roth approximation [7]. The saturated ferromagnetism is the stable solution in Roth's approximation for the band shape (34), but it is not stable in ours.

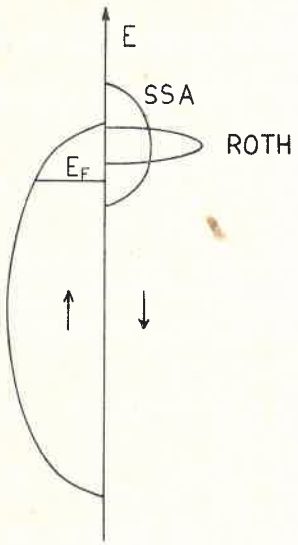

Fig. 1. Sketch of the density of states for the up- and down-spin electrons in the case of a nearly half-filled band and fully aligned spins in the presented approximation (SSA) and in that of Roth (ROTH). In the figure $n = 0.9$

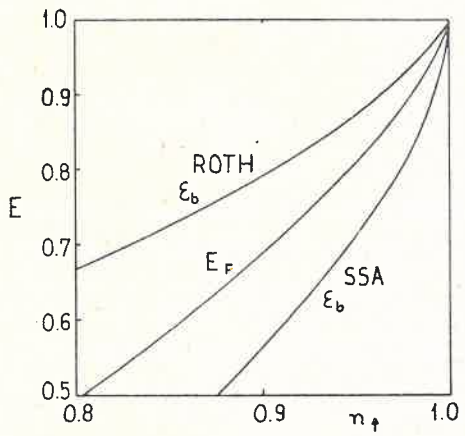

Fig. 2. Position of the Fermi level (E_F) and the lower band-edge in our decoupling scheme (ε_b^{SSA}) and in Roth's approximation (ε_b^{ROTH}) for the fully aligned spin system

4. Discussion

We have studied a certain improvement of the AAA which includes the band shift, connected with scattering with spin inversion. The decoupling scheme proposed above can be incorporated into the usual CPA for alloy systems and is more tractable in calculations than the original Hubbard's approach.

On the other hand, the theory obtained is not consistent with Nagaoka's limit [14]. Nagaoka showed that the ferromagnetic state should be stable in the limit of infinite Coulomb correlations if there are $N\pm1$ electrons. N gives the number of atoms in the crystal. It should be noted that the proof of Nagaoka holds only for $1-n = 1/N$. It was argued, however, that this result can be extended to values of n which differ by a finite amount from $n = 1$.

Our results are also not consistent with those of Roth who used the decoupling scheme conserving the first four moments of the spectral function [7]. This inconsistency is due to the fact that the width of the down-subband is proportional to $(1-n_{\downarrow})^{1/2}$ in the presented scheme and not to $(1-n_{\downarrow})$ as in Roth's scheme. We mention that the effective Hamiltonian which was derived in the strong correlation limit by the canonical transformation method [15] also gives the same $\sim(1-n_{\downarrow})$ width of the down-subband as Roth's theory. Thus we conclude that the theory of the metal-insulator transition needs further improvement in order to describe quasiparticle subspace of single-occupied sites correctly, especially in the strong correlation limit.

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