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Ferromagnetism in two band metals: The very strong coupling limit ☆

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ABSTRACT

The main purpose of this paper is to examine the occurrence of ferromagnetism in metals at the very strong coupling regime ($U \to \infty$) in the single-site approximation (SSA). The metal is described by a realistic two hybridized bands (V), one including Hubbard correlation and the other an uncorrelated one. We parametrize the ratio of the band widths and their centers as well. In this method the Hamiltonian is approximated by an effective and simpler one in which only one site retains the full correlation (U) while in the others acts an internal field, the self-energy. This field does not depend on the wave vector and is self-consistently determined by imposing the translation invariance of the problem, a coherent potential approximation (CPA) procedure. We also introduce Roth's wave vector dependent band shift $\mathcal{W}_{k,\sigma}$. For several total electronic occupation numbers (n_{tot}) we compare the spin dependent free energies with the corresponding paramagnetic ones at $T=0$. We conclude making a critical analysis of Roth's method for this problem arguing that the existence of a stable ferromagnetic state in this regime depends on a strong competition among $\mathcal{W}_{k,\sigma}$, the limit $U \to \infty$ and V.

1. Introduction

Magnetism in itinerant ferromagnets still attracts great interest [1–11]. It is then relevant to propose, use and test models on this subject and analyze their effectiveness, what we do in this paper for a specific model.

The model consists of a Hubbard like narrow band (band a) with intra-site Coulomb interaction U, hybridized with another band, which is broad and uncorrelated (band b), through a hybridization coupling V_{ab}. We now include the k-dependent band shift $\mathcal{W}_{k,\sigma}$ in the Green function of the a band (see below), proposed by Roth [12,13], in order to enhance the possibility of the ferromagnetic state in the metal. We comment more on that later. In this approach (Ref. [12], see also Refs. [14,15]) the single-site approximation (SSA) is introduced; it assumes that the correlation exists only in one site (say, the origin), while in the others acts an effective spin and energy dependent but wave vector independent field, the (complex) self-energy $\Sigma^{\sigma}(\omega)$. This self-energy is self-consistently determined by imposing the vanishing of the scattering T matrix associated to the origin and then restoring the translational invariance of the host. The starting point of the formalism is the Hubbard III approximation; it includes the so-called scattering correction which turns out to be a CPA (single-site approach). It generates a k-dependent band shift $\mathcal{W}_{k,\sigma}$ [12]. In this paper we are concerned about the occurrence of ferromagnetic order in metals at the very strong coupling regime ($U \to \infty$) using the above model in its single-site approximation (SSA) version. (The absence of ferromagnetic solution in the so-called Hubbard III approximation has been proved [16] for the one band model without $\mathcal{W}_{k,\sigma}$.)

The effective Hamiltonian in conventional notation is

$$\mathcal{H}_{eff} = \sum_{i,j,\sigma} t_{ij}^{a} a_{i\sigma}^{+} a_{j\sigma} + \sum_{i,j,\sigma} t_{ij}^{b} b_{i\sigma}^{+} b_{j\sigma} + \sum_{i\neq 0,\sigma} n_{i\sigma}^{a} \Sigma^{\sigma} + U n_{0\uparrow}^{a} n_{0\downarrow}^{a} + \sum_{i,j,\sigma} (V_{ab} b_{i\sigma}^{+} a_{j\sigma} + h.c.) \quad (1)$$

where $n_{i\sigma}^{a} = a_{i\sigma}^{+} a_{i\sigma}$ and σ denotes spin. $t_{ij}^{a,b}$ denotes the tunneling amplitudes between neighboring sites i and j, in each band. Here $a_{i\sigma}(b_{i\sigma})$ is the destruction operator for electrons in the $a(b)$ band.

We review briefly the main equations we obtained in [15] for the a band Green function, now with Roth's band shift:

$$G_{kk',\sigma}^{a}(w) = \frac{\delta_{kk'}}{w - \tilde{\epsilon}_{k}^{a} - \Sigma^{\sigma}(w) - \mathcal{W}_{k,\sigma}}, \quad (2)$$

where

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$$\mathcal{W}_{k,\sigma} = \frac{(2n^a_{k,-\sigma} - 1)\sum_{k'} \epsilon_{k'} n^a_{k',\sigma}}{n^a_\sigma(1 - n^a_\sigma)}, \tag{3}$$

$$\tilde{\epsilon}^a_k = \epsilon^a_k + \frac{|V_{ab}|^2(k)}{w - \epsilon^b_k}, \tag{4}$$

the latter is the recursion relation of the partially renormalized (only by V_{ab}) a band, ϵ^a_k and ϵ^b_k being the bare bands, with

$$\epsilon^a_k = \frac{t_a(\cos(k_x a) + \cos(k_y a) + \cos(k_z a))}{A}. \tag{5}$$

In (3) $n^a_{k,-\sigma}$ is the number of states in the mode k of the a band and n^a_σ is the occupation per site of the a band. The sum of k' is divided by N the total number of sites in the $d=3$ simple cubic lattice we use. In this paper we use $t_a=1$ and $A=1$, in arbitrary energy units. All energy magnitudes are taken in units of t_a, making them dimensionless. The bare a band width is then $W_a=6$. Here we also use homothetic bands [14,15]

$$\epsilon^b_k = \epsilon_s + \alpha\epsilon^a_k. \tag{6}$$

ϵ_s is the center of the b band and represents a shift in the bands. $\alpha > 1$ is a phenomenological parameter describing the ratio of the effective masses of the a and the b electrons. From now on we take the lattice constant equal to 1, $k_i a \to k_i$, $i = x, y, z$ and $V_{ab} = V_{ba} \equiv V =$ real and constant independent of k_i. In Fig. 1 the density of states (DOS) of the bare bands for $\alpha = 2.7$ and $\epsilon_s = -1.5$ is plotted.

The vanishing of the T-matrix [15] gives the self-consistent equation for the self-energy which, in the limit $U \to \infty$, reduces to

$$\Sigma^\sigma = -\frac{n^a_{0-\sigma}}{F^\sigma(w, \Sigma^\sigma)} \tag{7}$$

with

$$F^\sigma(w, \Sigma^\sigma) = N^{-1}\sum_k G^a_{kk,\sigma}, \tag{8}$$

where $n^a_{0-\sigma}$ is an initial guess for the a-band occupation number. The Green function of the b band is

$$G^{bb}_{k,\sigma}(w) = G^b_{k,\sigma}(w) + V^2 G^b_{k,\sigma}(w) G^a_{k,\sigma}(w) G^b_{k,\sigma}(w), \tag{9}$$

where $G^b_{k,\sigma}(w) = 1/(w - \epsilon^b_k)$ is the Green function of the bare b band.

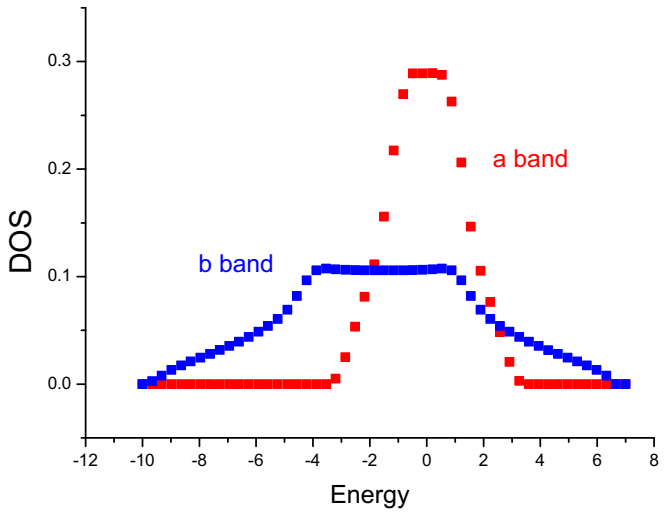

Fig. 1. DOS of the bare a and b bands ($U=0$, $V=0$) for $\alpha = 2.7$ and $\epsilon_s = -1.5$. The width of the a band is 6 and that of the b band is 16.2.

2. The method and numerical results

The self-consistency is performed in Σ^σ and in n^a_σ as well, for each total occupation $n_{tot} = n^a + n^b$. The total number of electrons per site is a constant of motion but n^a and n^b are not. It is the self-consistency and the dynamics that distribute the electrons among $n^a_\uparrow$, $n^a_\downarrow$ and n^b, eventually producing a ferromagnetic state (the b-band contribution to the magnetization is very small, that is, $n^b_\uparrow \simeq n^b_\downarrow$). As a result, in this method the density of state (DOS) of each band and their areas depend strongly on n_{tot}. We now want to exhibit the combined effect of V, α and ϵ_s in this process at $T=0$ K, for each n_{tot}. Schwieger and Nolting [3] address the same problem using methods similar to ours, the Spectral density approach (SDA) and the Modified Alloy analogy (MAA) both giving rise to a band shift. There are nevertheless some differences: their methods do not arrive at a self-consistency equation so they make an expansion in V and $1/w$ and find the self-energy analytically in some approximation.

The area per spin of the b band is 1 but the area of the a band is reduced, a reminiscence of the exclusion of double occupation states in the original Hamiltonian. The occupation number per site in the a band reduces to 1 (see Fig. 2), giving a maximum $n_{tot} = 3$ electrons per site in the metal in this very strong coupling limit. But notice that we have a electrons with both polarizations (see Fig. 3).

The renormalized density of states is displayed in Fig. 3. Notice the dip on the a band around its center and E_F. Although, as shown in Fig. 4, there is a net transfer from b to a band as n_{tot} grows, for a given n_{tot} and as a function of energy, this transfer is such that the large b band does not change in an appreciable way and the a band DOS is reduced around the Fermi energy.

In Fig. 4 we show how $n_{tot} = n^a + n^b$ is distributed between the two bands for $V=0.2$ and $V=0.6$. The fractional occupation of the b band decreases with n_{tot} while that of the a increases, for each V. For the values of the parameters (α,ϵ_s) used, the low energy states involved in small occupation are predominantly from the b band. There is then a transference of electrons from b to a as n_{tot} increases. But the difference between the two V's is small. The magnetization however involves the difference between the up and the down a band occupations rather than their sum and is more sensitive to the hybridization as shown in Fig. 5.

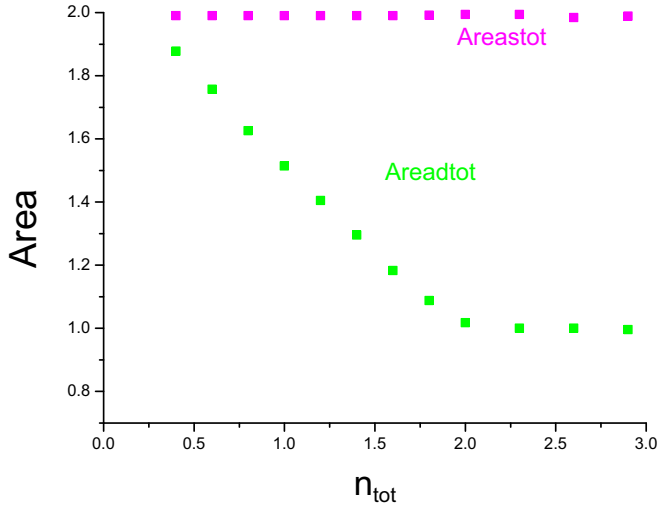

Fig. 2. Total (up+down) area for each band versus n_{tot}. The b band area is practically constant and equal to 2 while the a band area decreases to 1 as n_{tot} approaches 3. Here $\alpha = 2.7$ and $\epsilon_s = -1.5$ and $V=0.6$.