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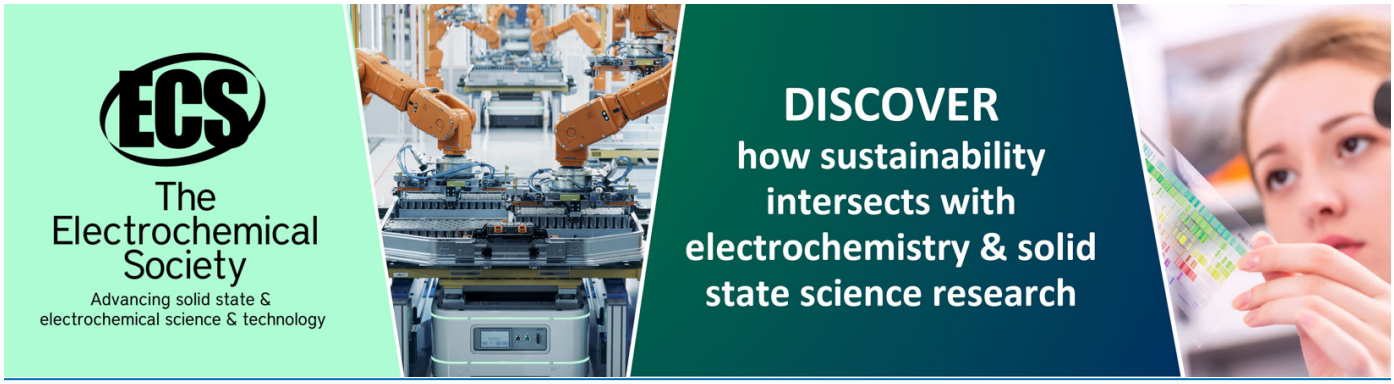

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Magnetic properties of correlated one-band metals: the effect of the Roth band shift in the single site approximation

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Abstract. The magnetic properties of one-band metals are discussed within the single site approximation, which is a picture to take into account electron correlations beyond the standard mean-field approach. The metal is described by a Coulomb correlated band. The Roth band shift arising from a two pole approximation is included. Here we present results for the infinite Coulomb correlation limit.

1. Introduction

In his pioneering paper on electron correlation in narrow one-band metals, Hubbard [1], now referred to as Hubbard I, proposed a model that reduces to the exact solution in the zero bandwidth limit. This model however, contrary to what is observed for real metals, found that at low temperatures, for any finite value of the correlation parameter U, the metal would be in a insulating state. In order to correct this, he proposed[2] another approximation, now referred to as Hubbard III. It consists of freezing say, the down spins, and let the up spins move and be scattered by this background (scattering correction). As these ideas were to become later the coherent potential approximation (CPA) , the approximation in Hubbard III became also known as alloy analogy [3].

Following Roth [4] we include scattering correction but allow the dynamics of the down spin electrons through the single site approximation (SSA). In this formulation the full Coulomb correlation exists in only one site, say the origin; in the others there is a sort of 'external field', the site independent but spin and energy dependent self-energy Σ^σ. Σ^σ is self-consistently determined by imposing the vanishing of the scattering T matrix associated to the given site that exhibits the full Coulomb interaction.

The metal is described by one non-degenerate conventional Hubbard-like narrow band with in-site interaction U:

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

where $n_{i\sigma} = a^+_{i\sigma} a_{i\sigma}$; σ denotes spin. t_{ij} is the tunneling amplitude between neighboring sites i and j. The single site approximation (SSA) [4] adopts instead the following effective

Hamiltonian:

$$\mathcal{H}_{eff} = \sum_{i,j,\sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma} + \sum_{i\neq 0,\sigma} n_{i,\sigma}\Sigma^{\sigma} + U n_{0\uparrow} n_{0\downarrow} \tag{2}$$

The method then replaces a translationally invariant problem, as defined by (1), by an impurity problem where only the origin incorporates the Coulomb interaction, the other sites being acted by the field Σ^{σ}. But the effective Hamiltonian (2) is far from being simple due to the presence of the Coulomb intra-atomic term at the origin and we have to resort to some approximation.

We use the two-pole approximation developed by Roth [4]; after some calculation we end up with the following Green's function (in this paper we'll be working at temperature $T = 0$):

$$G_{kk',\sigma}(w) = \frac{\delta_{kk'}}{w - \epsilon_k - \Sigma^{\sigma}(w) - \mathcal{W}_{k,-\sigma}}. \tag{3}$$

In this expression

$$\epsilon_k = \frac{t(cos(k_x a) + \cos(k_y a) + \cos(k_z a))}{A}, \tag{4}$$

is the recursion relation of the bare band . We use $t = 1$ and $A = 3$, in arbitrary energy units. All energy magnitudes are taken in units of t, making them dimensionless. The bare band width is then $W = 2$. On the other hand the band shift $\mathcal{W}_{k,\sigma}$ is

$$\mathcal{W}_{k,\sigma} = \frac{(2n_{k,-\sigma} - 1)\sum_{k'} \epsilon_{k'} n_{k',\sigma}}{n_{\sigma}(1 - n_{\sigma})}, \tag{5}$$

The vanishing of the T-matrix gives a self-consistent equation for the self-energy:

$$\Sigma^{\sigma}(w) = U < n_{0-\sigma} > + \Sigma^{\sigma}(w)(U - \Sigma^{\sigma}(w))F^{\sigma}(w, \Sigma^{\sigma}(w)), \tag{6}$$

with

$$F^{\sigma} = \sum_{k} G_{kk,\sigma} \tag{7}$$

The self-consistency is implemented as follows: we start giving initial values for $< n_{0\sigma} >$ and take for Σ^{σ}, the Hartree-Fock(HF) expression $U < n_{0-\sigma} >$ and $\mathcal{W}_{k,\sigma} = 0$. Then F is calculated (eq(7)) and a new Σ^{σ} is found through eq(6). Now it is possible to calculate the density of states (DOS), the Fermi energy and $\mathcal{W}_{k,\sigma}$ and new $< n_{\sigma} >$. This proceeds until a prescribed convergence in Σ^{σ} is reached ; in our case the absolute value of the difference between the input and the output values differs by less than $\epsilon = 5\times 10^{-3}$. The self-consistency applies for $< n_{\sigma} >$ as well. The total $< n >=< n_{\uparrow} > + < n_{\downarrow} >$ is preserved but the dynamics and the self-consistency redistribute the down and up spins.

2. Numerical results and conclusions

We focus on the very strong coupling limit, namely, $U = \infty$. In fig (1) the total area of the density of states (DOS) is displayed versus $< n >$. It is seen that the total area decreases with $< n >$ *linearly*, a consequence of the elimination of states involving double occupied sites (Hubbard-like contraction [1]). In the present method, as in alloy analogy approaches, there is a strong dependence of DOS -and so of other physical quantities- on $< n_{\sigma} >$. Fig (2) displays the zero temperature magnetization versus $< n >$; magnetization grows with higher electron occupancy, but not monotonically since we are dealing with renormalized CPA DOS; fig(3)compares the energy of the paramagnetic and of the ferromagnetic states.

Ferromagnetism is more favorable for $< n >\geq 0.4$. As fig (4)shows the strong correlation distorts the bands considerably; the initial bare bands were just the conventional d-band DOS of (4).

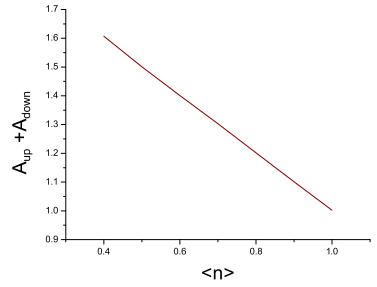

Figure 1. (Color online) Plot of DOS total area $A_{up} + A_{down}$ versus $< n >$. The decrease with $< n >$ is due to elimination of states involving double occupied sites; the number of these states increases with $< n >$.

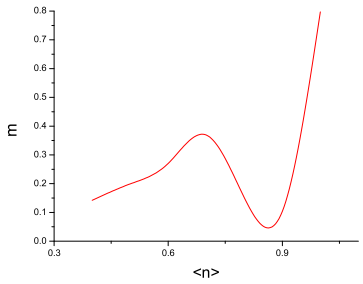

Figure 2. (Color online) Magnetization m versus $< n >$. The non-monotonic behavior is due to the strong dependence of DOS on $< n >$.

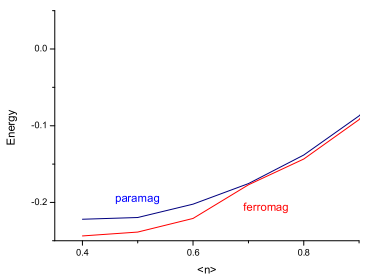

Figure 3. (Color online) Energy of the paramagnetic and of the ferromagnetic states versus $< n >$.

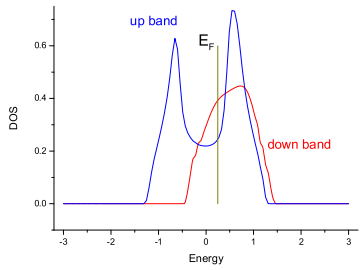

Figure 4. (Color online) Density of states for $< n >= 0.6$. The Fermi level is at $E_F = 0.247$ giving a magnetization $m = 0.276$.

A more complete calculation for finite U in the strong limit regime ($U/W > 1$) as well as including one-electron hybridization in a two band model, suitable to describe transition metals, is in progress.

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