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FINITE-TEMPERATURE MAGNETISM IN THE
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VARIATIONAL APPROACH TO FINITE-TEMPERATURE MAGNETISM IN THE DEGENERATE NARROW BANDS

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Abstract. — The variational approach which describes the local electron correlations at finite temperatures has been extended to the degenerate-band case. It reduces $T_C$ in the static approximation by a factor of two, gives realistic $T_C$ between the observed value $T_C$ (Obs) and $2T_C$ (Obs), and suppresses the temperature independent charge fluctuation in Fe and Ni.

The finite-temperature theories of magnetism which interpolate between the weak and strong interaction limits have extensively been applied to the narrow band systems to understand the local vs. itinerant behavior of magnetism [1]. Among them the variational approach (VA) developed by Kakehashi and Fulde [2] reduces to the Gutzwiller-type energy at the ground state, therefore takes into account the local electron correlations missing in the static approximation (SA) which has been adopted in the most of other theories. Recent numerical investigations to the simple-cubic Hubbard model with half-filled band [3] have shown that the calculated ground-state energy and sublattice magnetization quantitatively agree with those in the variational Monte-Carlo method [4] in which the ground state quantities are exactly obtained for a given Gutzwiller wave function. Furthermore the Néel temperatures calculated from the VA are expected to be much better than those obtained from the $4 \times 4 \times 4$ Monte-Carlo simulation by Hirsch [5]. Thus we believe that among various theories the VA describes best the finite temperature magnetism in the intermediate regime.

So far the VA is limited to the single-band Hubbard model, thus it was impossible to argue the correlation effects at finite temperatures in realistic systems. We present in this paper an extension of the VA to the degenerate bands and clarify the role of the local electron correlations in Fe and Ni.

The Hamiltonian which we adopt here is the degenerate-band Hubbard model with the following electron-electron interactions

$$H_1 = \frac{1}{4}U \sum_i n_i^2 - J \sum_i S_i^2.$$  \hspace{1cm} (1)

Here $U$ and $J$ are Coulomb and exchange energy parameters respectively, $n_i$ and $S_i$ denote the total charge- and spin-density operators on site $i$. According to the functional integral method the free energy $F$ is exactly expressed by means of an energy functional $E(\xi, T)$ projected onto the longitudinal field variables $\{\xi_i\}$.

$$F = -\beta^{-1} \ln \int \left[ \prod_i \left( \frac{\beta J}{4\pi} \right)^{\frac{1}{2}} d\xi_i \right] \times e^{-\beta E(\xi, T)}. \hspace{1cm} (2)$$

Here $\beta$ denotes the inverse temperature, and $\bar{J} = U/2D + J (1 + 1/2D)$, $D$ being the degeneracy of the bands. Feynmann inequality to the free energy (2) is then written as

$$F \leq F_t + \langle E(\eta, T) - E_t(\eta, T) \rangle_\xi. \hspace{1cm} (3)$$

Here $F_t$ is the trial free energy with the trial energy functional $E_t(\eta, T)$, and the average $\langle \cdot \cdot \cdot \rangle_\xi$ means a classical average with respect to $E_t(\eta, T)$.

Since the characteristic temperature associated with the correlated motion of electrons is much higher than the Curie temperature $T_C$, most of the local electron correlations persist even above $T_C$. We therefore take them adiabatically into account assuming the following trial energy functional.

$$E_t(\eta, \xi(T), T) = E_{st}(\xi, T) + \langle Q(\eta) \bar{H}Q(\eta) \rangle_0. \hspace{1cm} (4)$$

Here $E_{st}(\xi, T)$ is the energy functional to the SA which reduces to the Hartree-Fock energy at $T = 0$. The second term is the Gutzwiller-type correlation energy [6] in the random exchange fields $\{\xi_i\}$. $\bar{H} = H - \langle H \rangle_0$, and $\langle \cdot \cdot \cdot \rangle_0$ means the average with respect to the independent electrons in the random exchange fields $\{\xi_i\}$. The operator $Q(\eta)$ is defined by

$$Q(\eta) = N \prod_i (1 - \eta_i c_i O_{ic} - \eta_i a_i O_{ia}). \hspace{1cm} (5)$$

Here $N$ is a normalization factor. $\{Q_{ic}\}$ and $\{Q_{ia}\}$ are the local operators which create the Hilbert space expanded by the scattering from the Hartree-Fock state. The parameters $\eta_i(\xi, T)$ and $\eta_i(\xi, T)$ describe the correlated motion of electrons at finite temperatures as well as the ground state. They are determined from the variational principle (3).

The present theory reduces to that proposed by Kakehashi and Fulde when $D = 1$. The free energy reduces to the Gutzwiller-type energy for the degenerate bands when $T = 0$. 

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We have performed the numerical calculations within the single-site approximation. Calculated Curie temperatures \( T_C \) (VA) are 1520 K, 2600 K, and 1000 K for Fe, Co, and Ni respectively. The ratios of \( T_C \) (VA) to the observed values \( T_C \) (Obs) are 1.5, 1.9, and 1.6 respectively. The discrepancy between the theory and the experiment seems to be explained by two sources: the neglects of the transverse degree of freedom in the local moments and the magnetic short range order. Both effects overestimate \( T_C \). In the insulator regime the ratio \( T_C \) (VA) / \( T_C \) (Obs) is estimated as \[ \frac{T_C \text{(MF)}}{T_C \text{(Exact)}} \times \frac{\ln (2S+1)}{\ln 2} \], where \( T_C \) (MF) and \( T_C \) (Exact) are the Curie temperature in the molecular field approximation and the exact value, and \( S \) denotes the total spin of an atom. The formula gives 2.2 for Fe (\( S = 1 \)), 1.9 for Co (\( S = 0.8 \)), and 1.4 for Ni (\( S = 0.5 \)) respectively.

Figure 1 a shows the numerical results for Fe. A remarkable point is that \( T_C \) in the SA is reduced by a factor of two due to the electron correlations even in the degenerate-band case. This is because the SA overestimates the magnetic energy. A conventional method to avoid this difficulty is to reduce phenomenologically the Coulomb and exchange energy parameters \( U \) and \( J \), which we call the \( U_{\text{eff}} \) SA. This method can describe the magnetization-temperature curve as well as the paramagnetic susceptibility as shown in figure 1a. The phenomenological reduction of \( U \) and \( J \) however enhances the delocalized character, so that the charge fluctuations \( \sqrt{\langle (\delta n)^2 \rangle} \) and the temperature dependence of the amplitude of the local moments are overestimated. (See Fig. 1a). In particular the former difficulty becomes serious in Ni as shown in figure 1b; the \( U_{\text{eff}} \) SA hardly suppresses the charge fluctuations, while the VA reduces it by a factor of three. This discrepancy must correspond to the fact that the density of states in the \( U_{\text{eff}} \) SA does not explain the formation of the two hole bound state in the photoemission spectra [7]. We also found the strong electron correlation effects in Ni in the pressure dependence of \( T_C \): \( \delta T_C / \delta P = 0.49 \) (K/kbar) in the VA, \(-0.62 \) (K/kbar) in the \( U_{\text{eff}} \) SA, while the experimental value is 0.35 (K/kbar).

In summary we have developed the VA to the degenerate bands which leads to the Gutzwiller-type energy at \( T = 0 \). Numerical results for Fe and Ni have shown that the local electron correlations certainly play an important role at finite temperatures even in the degenerate band case.