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DISPERSSIVE HYBRIDIZATION CORRELATION AND MAGNETISM IN A TWO-BAND MODEL

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Abstract. - We study a two-band Hamiltonian for hybridized and correlated bands of sc and bcc symmetry, the latter case approximating a two-dimensional band. Magnetic phase diagrams are obtained, showing in the bcc case a region of rapid phase change with filling which is absent in the sc case.

We consider a two-band system described by the following Hamiltonian in the site representation:

\[
H = \sum_{i,j,\sigma} \left( t^{aa}_{ij} a_{ij}^{+} a_{j\sigma} + t^{bb}_{ij} b_{ij}^{+} b_{j\sigma} \right) + \\
\sum_{i,j,\sigma} \left( t^{ab}_{ij} a_{ij}^{+} b_{j\sigma} + \text{h.c.} \right) + \\
\sum_{i} \left( U^{aa}_{i} n_{i\uparrow}^{a} n_{i\downarrow}^{a} + U^{bb}_{i} n_{i\uparrow}^{b} n_{i\downarrow}^{b} \right) + \\
U^{ab} \sum_{\sigma,\tau} n_{i\sigma}^{a} n_{i\tau}^{b} - J S_{i}^{a} S_{i}^{b} \right) \quad (1)
\]

The Hamiltonian is written in terms of two types of orbitals (a, b), (i, j) and (\sigma, \tau) label, respectively, the two types of sites, the sites and the spin. The remaining notation is standard. Diagonalization of H in the reciprocal (k) space is performed by treating the on-site correlation (U^{aa}, U^{bb}, U^{ab}) and exchange (J) terms in the unrestricted Hartree-Fock approximation, i.e. by allowing for nonvanishing off-diagonal expectation values \langle a_{\mathbf{k}\sigma}^{+} b_{\mathbf{k}\tau} \rangle = \langle b_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\tau} \rangle. The Green function equation-of-motion technique yields analytically the renormalized energies for para-(P), ferromagnetic (F), and antiferromagnetic (A) phases. By introducing the Fourier transforms of the hopping amplitudes \tilde{t}^{aa}_{ij}, \tilde{t}^{bb}_{ij}, \tilde{t}^{ab}_{ij}, i.e. \tilde{e}^{a}_{k}, \tilde{e}^{b}_{k}, \gamma_{k}, we can write the renormalized energies for the P and F phases as:

\[
E^{P} = \frac{1}{2} \left\{ \epsilon^{a}_{\mathbf{k}} + \epsilon^{b}_{\mathbf{k}} + A_{\mathbf{k}} + B_{\mathbf{k}} \right\} + \\
\frac{\gamma^{2}_{\mathbf{k}} + C_{\mathbf{k}}}{2} \left[ \left( \epsilon^{a}_{\mathbf{k}} - \epsilon^{b}_{\mathbf{k}} + A_{\mathbf{k}} - B_{\mathbf{k}} \right)^{2} + 4 \left( \gamma^{2}_{\mathbf{k}} + C_{\mathbf{k}} \right) \right]^{1/2} \quad (2)
\]

where

\[
A_{\mathbf{k}} \equiv U^{aa} \left\langle n_{\mathbf{k}\uparrow}^{a} \right\rangle + 2U^{ab} \left\langle n_{\mathbf{k}\downarrow}^{a} \right\rangle + 2U^{bb} \left\langle n_{\mathbf{k}\downarrow}^{b} \right\rangle;
\]

\[
B_{\mathbf{k}} \equiv U^{bb} \left\langle n_{\mathbf{k}\downarrow}^{b} \right\rangle + 2U^{ab} \left\langle n_{\mathbf{k}\uparrow}^{a} \right\rangle;
\]

\[
C_{\mathbf{k}} \equiv -2U^{aa} \left\langle a_{\mathbf{k}\uparrow}^{+} b_{\mathbf{k}\downarrow} \right\rangle.
\]

For the A case, the energies (spin independent) are the solution of the system:

\[
E^{P} + b E^{2}_{\mathbf{k}} + c E^{2}_{\mathbf{k}} + d E_{\mathbf{k}} + \epsilon = 0
\]

whose coefficients are:

\[
b \equiv -2(A_{\mathbf{k}} + B_{\mathbf{k}}) \quad (3)
\]

\[
c \equiv \left( \epsilon^{a}_{\mathbf{k}} - \epsilon^{2}_{\mathbf{k}} \right) + \left( B_{\mathbf{k}} - \epsilon^{b}_{\mathbf{k}} \right) + 4A_{\mathbf{k}}B_{\mathbf{k}} - 2(\gamma^{2}_{\mathbf{k}} + C_{\mathbf{k}}) - G^{aa} - G^{bb} \quad (4)
\]

\[
d \equiv 2 \left\{ B_{\mathbf{k}} \left( \epsilon^{a}_{\mathbf{k}} - \epsilon^{2}_{\mathbf{k}} \right) + A_{\mathbf{k}} \left( \epsilon^{b}_{\mathbf{k}} - B_{\mathbf{k}} \right) \right. + \left. (A_{\mathbf{k}} + B_{\mathbf{k}}) \left( \gamma^{2}_{\mathbf{k}} + C_{\mathbf{k}} \right) - 2\gamma_{k} C_{\mathbf{k}} \left( \epsilon^{a}_{\mathbf{k}} + \epsilon^{b}_{\mathbf{k}} \right) + B G^{a2} + A G^{b2} \right\} \quad (5)
\]

In (3-6) the spin label is actually irrelevant. The quantities \[ G^{a} = U^{aa} S^{a} + J S^{b} / 2 \]

and

\[ G^{b} = U^{bb} S^{b} + J S^{a} / 2, \]

with \[ S^{a} \text{ and } S^{b} \] the amplitudes of the antiferromagnetic moments, e.g.:

\[ S^{a} = \frac{1}{2} \sum_{k,\sigma} \sigma \left\langle a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}+\mathbf{Q}\sigma} \right\rangle \]

We take \[ Q \] half a reciprocal lattice vector, yielding a two-sublattice antiferromagnetic structure. To study concrete examples, we assume the intersite hybridization of the form \[ \gamma_{k} = \Gamma_{0} + \Gamma_{0} s_{k} \] where \[ \Gamma_{0} \] is a dispersionless part, while \[ s_{k} \] is the same canonical dispersion relation assumed to describe the bare bands:

\[ \epsilon^{a(b)}_{\mathbf{k}} \equiv W^{a(b)} s_{\mathbf{k}} + \Delta^{a(b)} s_{\mathbf{k}}, \]

with \[ \Delta^{a(b)} \] a shift with respect to the origin of the energy. The dispersive character of the hybridization has rarely been taken into account in this type of studies. However, the approximation of assuming the same dispersion relation for \[ \epsilon^{a(b)}_{\mathbf{k}} \text{ and } \gamma_{k}, \] while justified as a mean to obtain analytical results, has no pretention to
be soundly realistic. The density of states (DOS) can be obtained analytically from the renormalized energies, as discussed in [1]. The quantities to be evaluated, which characterize each phase, are $n_0^a \equiv \langle \delta n_{ka} \delta n_{ka} \rangle$; $n_{\sigma}^b \equiv \langle \delta n_{ka} \delta n_{ka} \rangle/\langle \delta n_{ka} \delta n_{ka} \rangle$; $\langle \delta n_{ka} \delta n_{ka} \rangle = \langle \delta n_{ka} \delta n_{ka} \rangle$ and the amplitude of the magnetic moments. The bare DOS (corresponding to $s_k$) we consider in the present work are s-type, of simple (sc) and body centered (bcc) cubic symmetry. The first one represents a generic featureless 3-dimensional DOS, while the second one, with its logarithmic singularity in the middle, is an approximation to the 2-dimensional tetragonal DOS of interest for the properties of the magnetic compounds related to the high $T_c$ superconductors. Due to the large number of parameters in the model, and to lack of space, we shall discuss here only the effects of varying $\Gamma$ and the numbers ($n$) of electrons in the band. A more complete study will be given elsewhere. The chosen values of the parameters, in arbitrary units of energy, are: $W^a = 2$; $W^b = W^a/2$; $\Delta_a = 0$; $\Delta_b = 0.1$; $U^{ab} = W^a/2$; $U^{bb} = 0.8 W^b$; $U^{ab} = 0.4 U^{aa}$; $J = 0.1 U^{aa}$. They represent a wider moderately correlated band (a) and a narrower, strongly correlated one (b). For the hybridization term, we take $\Gamma_0 = 0$, because its effect just adds to $C_\sigma$ a constant term, and we vary the amplitude $\Gamma$ of the dispersive part. It can be shown [1] that in the P phase, no gap due to hybridization opens provided $\Gamma \equiv \Gamma/\sqrt{W^a W^b} < 1$. As we are not interested in such effects, we take $\Gamma \leq 0.9$. The system of coupled integral equations for evaluating the various expectation values, the Fermi level ($E_F$), and finally the ground state energy ($E_{GS}$) was solved numerically by iteration. The interplay of hybridization and correlation can deeply modify the DOS already in the P phase, that in the P phase, no gap due to hybridization opens. The effects are two-fold. First, the narrower bare P band (b) is above the wider one (a), the renormalized P DOS for $n > 1$ shows the narrower band below the wider one. When magnetic effects add to the interactions, very large modifications of the magnetic DOS with respect to the P DOS are usually observed. This effect is striking in the A case. With few exceptions, the four A subbands are much narrower than in the corresponding P or F phases, and they exhibit high peaks. In many cases, some of the A subbands are so narrow that they can be considered as quasi atomic localized levels. The features of the A DOS are more sensitive to the values of the model parameters than the P or F DOS. Such properties of the DOS's in the different phases imply that the phase transitions may cause a strong modification of the DOS. This is expected for transitions to the A phase, but it is a rather unfamiliar concept for P $\rightarrow$ F transitions. As a consequence, the extension of simple single-band results (like Stoner-Wohlfarth) to two hybridized and correlated band may be misleading, in particular when local properties of the P DOS around $E_F$ are used to predict the transitions. Indeed, the magnetic phase diagrams (Fig. 1) show the F phase to set in for $n \leq 0.5$ in both cases, i.e. when $E_F$ is in a region of low P DOS. The F phase is stable up to $n$ close to 2, the exact value depending on the DOS and on $\Gamma$. For $2 \leq n \leq 3$ in the sc case, the A phase is steadily stable in a range of $n$ values which shrinks as $\Gamma$ grows. In contrast, the bcc case shows a zone (hatched in Fig. 1) where the stable phase varies very rapidly with $n$. For example, when $\Gamma = 0.1$ one has the sequence P $\rightarrow$ F $\rightarrow$ P $\rightarrow$ A $\rightarrow$ P $\rightarrow$ A $\rightarrow$ F $\rightarrow$ A as $2 \leq n \leq 3$. For larger $n$ the P phase is stable in both cases. To explain this peculiarity of the bi-dimensional case, let us recall that $E_{GS} = E_1 + E_3$, where $E_1$ is the sum of products of the average energy of each non-empty subband times the subband occupancy, while $E_3$ ($= 0$ in P state) explicitly depends on $S^{n(b)}$. Usually $|E_1| \gg |E_3|$. For small $n$, the presence of narrow peaks and gaps in the A DOS causes $E_1^A > E_3^F$. When $n \approx 2$, correlation effects raise $E_1^A$ and $E_3^F$ to values close to $E_F^A$. For $2 < n < 3$, $E_1^A$ grows with $n$ less quickly than $E_3^F$ or $E_3^P$, due both to the narrowness of A subbands, and to the pinning of $E_F$ by the A DOS peaks. This suggests that the difference between three- and two-dimensional phase diagrams for $2 < n < 3$ has to be traced to the presence of high peaks in the P or F DOS of bcc type. Their effect on $E_1$ is hence similar to that of the A DOS peaks. Then the relatively small, and strongly $n$-dependent difference $E_3^A - E_3^F$ becomes relevant to determine the stability. The sc DOS, on the contrary, has high peaks only in the A phase, so that its range of stability is mainly fixed by $E_1^A - E_3^F$, which has a more regular $n$-dependence than the difference in $E_3$.

![Fig. 1. - Magnetic phase diagram in the (n, $\Gamma$) plane.](image)