

## Metallic ferromagnetism from kinetic-energy gain: The case of $\text{EuB}_6$

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A recently proposed band model to describe metallic ferromagnetism predicts a lowering of the carrier's effective mass upon spin polarization, leading to a gain in kinetic energy. The effect arises from a reduction in bond-charge Coulomb repulsion when spin polarization develops. Recent optical experiments in  $\text{EuB}_6$  show clear evidence for this effect. Related manifestations of this physics are large negative magnetoresistance, anomalously large decrease in resistivity as the temperature is lowered, and positive pressure dependence of  $T_c$ , also seen in  $\text{EuB}_6$ . We explore parameters in the model that can give rise to these effects of the magnitude seen in  $\text{EuB}_6$ , and suggest that qualitatively similar effects should be seen to varying degrees in all ferromagnetic metals. In particular, similar effects of large magnitude are seen in  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ . Photoemission experiments should be able to shed light on the validity of different possible explanations for the observed effects. [S0163-1829(99)06701-6]

The origin of ferromagnetism in metals remains a controversial question. In particular, it is not known whether a single mechanism can describe metallic ferromagnetism in the wide range of manifestations that it exhibits in nature, for example: the ferromagnetic transition metals Fe, Co, and Ni and their alloys,<sup>1</sup> weak metallic ferromagnets such as  $\text{ZrZn}_2$  and  $\text{ScIn}_3$ ,<sup>2</sup> colossal magnetoresistance (CMR) manganites such as  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ,<sup>3</sup> and rare earth hexaborides such as  $\text{EuB}_6$ .<sup>4</sup> It would be useful to identify the simplest model that exhibits the essential physics of the phenomenon in each situation. For example, it has been argued that orbital degeneracy is essential to the understanding of ferromagnetism of the transition metals,<sup>5</sup> that the electron-lattice interaction plays an essential role in the CMR manganites,<sup>6</sup> that spin fluctuations explain the weak ferromagnetism of  $\text{ZrZn}_2$  and  $\text{ScIn}_3$ ,<sup>7</sup> and that the RKKY interaction accounts for ferromagnetism in  $\text{EuB}_6$ .<sup>8</sup>

Important theoretical progress has been recently achieved by Vollhardt and co-workers,<sup>9,10</sup> who in a series of papers have investigated the conditions favoring itinerant ferromagnetism in a variety of microscopic models. They as well as others<sup>11</sup> have provided strong evidence that ferromagnetism is stable in the single band Hubbard model with a properly tuned density of states, and found also that the Hund's rule coupling between electrons in degenerate atomic orbitals provides an effective mechanism for ferromagnetism in a broad range of parameters.<sup>10</sup> They conclude that the question of which of those mechanisms drives ferromagnetism in the transition metals remains open. More generally, there has been a consensus over the years starting with the work of Slater and Van Vleck<sup>5</sup> that band degeneracy is essential to explain the physics of most if not all ferromagnetic metals.

Traditionally, metallic ferromagnetism has been understood as a competition between kinetic energy of single particles, favoring the paramagnetic state, and "exchange energy" originating in the Coulomb interaction, favoring the spin-polarized state.<sup>12</sup> It is argued that in ferromagnets the gain in exchange energy overcomes the cost in kinetic energy that arises from the Pauli principle that forbids double occupancy of low kinetic energy states for parallel spins.

We have recently proposed an alternative point of view, in a sense opposite: that in fact metallic ferromagnetism is driven by band broadening, or equivalently an effective mass reduction, that occurs upon spin polarization.<sup>13,14</sup> This leads to a gain (i.e., a decrease), rather than a cost, in kinetic energy. Certain phenomena in the conventional ferromagnets Fe, Co, and Ni, such as negative magnetoresistance and anomalously large drop in resistivity below the Curie temperature, may be interpreted as manifestations of this physics (instead these observations have usually been interpreted as arising from a decrease in the scattering rate upon spin polarization<sup>15</sup>). The origin of this effect is the bond-charge Coulomb repulsion, which in a tight binding formulation is described by "off-diagonal" nearest neighbor exchange and pair hopping matrix elements of the Coulomb interaction.<sup>16</sup> This interaction is present in all metals and thus could be the driving force for ferromagnetism in all cases. This point of view implies in particular that atomic orbital degeneracy is *not* an essential ingredient to metallic ferromagnetism.<sup>17</sup>

The material  $\text{EuB}_6$  presents a particularly interesting example.<sup>4,8,18-20</sup>  $\text{EuB}_6$  exhibits semimetallic behavior in the resistivity above the Curie temperature  $T_c \sim 16$  K, and the resistivity drops very rapidly below  $T_c$ . In a magnetic field the resistivity is sharply lowered both above and below  $T_c$ .<sup>18,19</sup> Optical experiments show a dramatic shift of spectral weight in optical absorption towards low frequency, resulting in a large increase in the Drude part of the optical conductivity as spin polarization develops.<sup>20</sup> Degiorgi and co-workers have fitted the frequency-dependent conductivity to a Drude form and obtain a temperature-dependent plasma frequency that increases by approximately a factor of 3 upon spin polarization. Furthermore the plasma frequency shows a small increase as the temperature is lowered from 300 K down to  $T_c$ . It is concluded in Ref. 20 that the increase in plasma frequency below  $T_c$  indicates an increase in itinerant carrier concentration, a reduction in effective mass, or a combination of both. Here we take the point of view that the dominant effect is an effective mass shift, although we cannot rule out an accompanying change in carrier concentration.

The simplest model of magnetism of itinerant electrons, the Stoner model,<sup>21</sup> cannot describe the above-discussed physics. In particular it does not describe *any* variation in properties due to magnetism above  $T_c$ , and has to be supplemented with other ingredients, e.g., inclusion of magnetic short range order above  $T_c$ , to describe that regime.<sup>22</sup> The model discussed here is a natural extension of the Stoner model to include basic interactions that occur in nature. In addition to providing a better description of phenomena described by the Stoner model it naturally describes observed properties that the Stoner model cannot account for.<sup>13</sup> We believe it is a natural starting point for the description of metallic magnetism, and other effects such as electron-lattice interactions, spin fluctuations or band degeneracy effects should only be included after the consequences of this simplest model have been explored, to explain remaining discrepancies with experiment.

The model of interest arises from writing the Hamiltonian for electrons in a band in a Wannier representation and keeping certain matrix elements of the Coulomb interaction between nearest neighbor sites. The Hamiltonian is

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{J}{2} \sum_{\langle ij \rangle} \left[ \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) \right]^2, \quad (1)$$

where  $c_{i\sigma}^\dagger$  creates an electron in the  $i$ th local state (atomic orbital or Wannier state).  $U$  is the on-site repulsion and  $J$  is the bond-charge repulsion, given by the Coulomb matrix element

$$J = \int d^3r d^3r' \varphi_i^*(r) \varphi_j^*(r') \frac{e^2}{|r-r'|} \varphi_i(r') \varphi_j(r) \quad (2)$$

with  $\varphi_i$ ,  $\varphi_j$  Wannier orbitals at neighboring sites  $i$  and  $j$ . On expanding the  $J$  term in Eq. (1) we obtain two types of terms, describing nearest neighbor exchange and pair hopping:

$$H_J = J \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{i\sigma'} c_{j\sigma} + J \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} + \text{H.c.}). \quad (3)$$

The Hamiltonian Eq. (1) will be used as an effective model to describe the physics of ferromagnetism in  $\text{EuB}_6$ . It may be asked whether the model is consistent with the electronic structure of  $\text{EuB}_6$ . In particular, whether the  $f$  electrons of Eu, which are clearly involved in the magnetism, are also involved in the transport, or whether they should instead be regarded as localized. In fact, early band structure calculations by Longuet-Higgins and Roberts<sup>23</sup> completely neglected the rare-earth orbitals in calculating the band structure around the Fermi level. However, later band structure calculations by Hasegawa and Yanase<sup>24</sup> found that in fact there is appreciable hybridization between B-2*p* and Eu-4*f* orbitals, giving an itinerant character to the  $f$  bands (see Fig. 1 of Ref. 24). The Hamiltonian Eq. (1) is proposed as an effective model to describe these narrow bands of predominant 4*f* character that are close to the Fermi energy.<sup>24</sup>

Still, the question remains whether the parameter  $J$  in the Hamiltonian, which involves orbital overlaps between neighboring sites [Eq. (2)], would be sufficiently large in view of the fact that  $f$  orbitals are well localized. We have not performed a detailed quantitative estimate. However, it should be noted that the Wannier orbitals in Eq. (2) should be hybridized orbitals involving Eu-4*f* and B-2*p* atomic orbitals, and thus will have larger overlaps than pure 4*f* orbitals. Hasegawa and Yanase estimate the overlap between B-2*p* and Eu-4*f* orbitals to be as large as 0.68 eV.<sup>24</sup> As we will see in the following, the model Eq. (1) requires parameters of order  $zJ/T_c \sim 25$  to describe  $\text{EuB}_6$ , with  $z$  the number of nearest neighbors to a site. With  $z=6$  and  $T_c \sim 15$  K this yields  $J \sim 0.005$  eV, which is so small that it is well possible that it could arise from rather localized orbitals of predominantly 4*f* character.

In the presence of an external vector potential  $\mathbf{A}$ , the phases of the Wannier orbitals giving rise to the tight binding model are modified as

$$\varphi_i \rightarrow \varphi_i \exp(-ie\mathbf{R}_i \cdot \mathbf{A}/\hbar c), \quad (4)$$

which leads to a modification of the single-particle hopping amplitude between sites  $i$  and  $i+\delta$

$$t_{i,i+\delta} = t \exp[(-ieA_\delta/\hbar c)\delta] \quad (5)$$

and of the interaction  $J$  that enters in the pair hopping term in Eq. (3):

$$J_{i,i+\delta} = J \exp[(-2ieA_\delta/\hbar c)\delta]. \quad (6)$$

The paramagnetic (intra-band) current operator is obtained by taking the derivative of the Hamiltonian with respect to the vector potential and yields

$$J_{1\delta} = \frac{ie}{\hbar} t \sum_{i,\sigma} (c_{i+\delta,\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{i+\delta,\sigma}) - \frac{2ie}{\hbar} J \sum_{i,\sigma,\sigma'} [c_{i+\delta,\sigma}^\dagger c_{i+\delta,\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} - c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i+\delta\sigma'} c_{i+\delta\sigma}] \quad (7)$$

and one can derive a conductivity sum rule for the optical conductivity arising from intra-band processes  $\sigma_1(\omega)$ , following the same steps as in Maldague's derivation<sup>25</sup> with the single particle hopping term

$$\int_0^{\omega_m} d\omega \sigma_1(\omega) = \frac{\pi a_\delta^2}{2\hbar^2} [e^2 \langle -T_\delta^t \rangle + (2e)^2 \langle -T_\delta^J \rangle] \quad (8)$$

with

$$T_\delta^t = - \sum_{i,\sigma} [t(c_{i+\delta,\sigma}^\dagger c_{i\sigma} + \text{H.c.})], \quad (9)$$

$$T_\delta^J = J \sum_{i,\sigma'} (c_{i+\delta,\sigma}^\dagger c_{i+\delta\sigma'}^\dagger c_{i\sigma'} c_{i\sigma} + \text{H.c.}), \quad (10)$$

the kinetic energies arising from single particle and pair hopping processes. When spin polarization develops the contribution of pair hopping processes to the kinetic energy decreases, the second term in Eq. (8) becomes smaller in

magnitude and the total spectral weight from intraband processes increases as given by Eq. (8) due to the decreased kinetic energy.

A mean field treatment of the interactions in this Hamiltonian leads to the following form for the quasiparticle energies:<sup>13</sup>

$$\epsilon_{\sigma}(\epsilon) = [1 - 2j(I_{\uparrow} + I_{\downarrow}) - 2j'I_{-\sigma}] \epsilon - \sigma D \left[ \frac{k}{2} m + h \right] - \mu. \quad (11)$$

Here,  $\mu$  is the chemical potential,  $D$  the bandwidth, and

$$h = \mu_B H / D, \quad (12)$$

with  $H$  the applied magnetic field and  $\mu_B$  the Bohr magneton ( $\mu_B = 0.579 \times 10^{-5}$  eV/G). The magnetization  $m$  and occupation  $n$  per site are given by

$$n = \int_{-D/2}^{D/2} d\epsilon g(\epsilon) \{f[\epsilon_{\uparrow}(\epsilon)] + f[\epsilon_{\downarrow}(\epsilon)]\}, \quad (13a)$$

$$m = \int_{-D/2}^{D/2} d\epsilon g(\epsilon) \{f[\epsilon_{\uparrow}(\epsilon)] - f[\epsilon_{\downarrow}(\epsilon)]\} \quad (13b)$$

with  $f$  the Fermi function and  $g(\epsilon)$  the density of states. The band narrowing parameters  $I_{\sigma}$  are the expectation values of the bond charge density between nearest neighbor sites, given by  $I_{\sigma} = \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle$ , or equivalently

$$I_{\sigma} = \int_{-D/2}^{D/2} d\epsilon g(\epsilon) \left[ \frac{-\epsilon}{D/2} \right] f[\epsilon_{\sigma}(\epsilon)]. \quad (14)$$

The free energy per site is given by

$$F = F_0 + \frac{D}{4} k m^2 - \frac{Dj}{2} (I_{\uparrow} + I_{\downarrow})^2 - Dj' I_{\uparrow} I_{\downarrow}, \quad (15a)$$

$$F_0 = -k_B T \sum_{\sigma} \int d\epsilon g(\epsilon) \ln(1 + e^{-\epsilon_{\sigma}(\epsilon)/k_B T}) + \mu n. \quad (15b)$$

The interaction parameters in Eq. (11) are given in terms of the parameters in the Hamiltonian Eq. (1) by

$$k = u + j, \quad (16a)$$

$$u = U/D, \quad (16b)$$

$$j = zJ/D, \quad (16c)$$

$$j' = zJ'/D, \quad (16d)$$

with  $z$  the number of nearest neighbors to a site. Following previous work<sup>13</sup> we have denoted the interactions arising from exchange and pair hopping as  $J$  and  $J'$  to keep their effect separate, even though they are equal according to Eq. (3).

The mean field treatment is an approximation, and it is well known that for the Stoner model [Eq. (1) with  $J=0$ ] it yields qualitatively incorrect results. However, exact diagonalization results<sup>26</sup> show that the effect of  $J$  on the tendency to ferromagnetism, including the regimes of both partial and full spin polarization, is well described by mean field theory

[see, e.g., Ref. 26(a) Figs. 8, 10, and 11; Ref. 26(b) Figs. 3 and 4], including the regime of large  $J$ . Furthermore the mean field results for our model concerning the effect of  $J$  on ferromagnetism are consistent with exact results by Strack and Vollhardt<sup>9</sup> as well as the exact results in Ref. 27. While exact results at finite temperature do not exist, we believe that the effectiveness of mean field theory in describing both the onset and the regimes of partial and full spin polarization at zero temperature make it plausible that it may also provide a good description of the development of ferromagnetism as a function of temperature.

On the other hand, comparison of mean field theory with exact diagonalization<sup>26</sup> has shown that it is also defective in some respects: it greatly overestimates the effect of the on-site repulsion  $U$ , and it also overestimates the effect of the pair hopping term, which exact diagonalization shows to be small when the on-site repulsion is large. Nevertheless, for the reasons stated above we believe that the *structure* of the mean field equations (11)–(15) is correct in capturing the essential physics of the problem. Hence we will regard the mean field equations as the fundamental equations of the theory, with the band-narrowing parameters  $j$  and  $j'$  and the exchange interaction  $k$  as phenomenological parameters, to be determined to fit experimental observations. This will not necessarily correspond to physically plausible values of the parameters  $U$  and  $J$  in Eqs. (16), (1). As mentioned above, the relation Eq. (16) is likely to be inaccurate due to correlation effects, and furthermore other interaction parameters not included in the initial Hamiltonian Eq. (1) could further contribute to the renormalization of the effective interaction parameters  $j$ ,  $j'$ , and  $k$ .

We consider for simplicity a constant density of states  $g(\epsilon)$  and the particle-hole symmetric case,  $\mu=0$ . This corresponds to  $n=1$ , a half-filled band. Figure 1 shows the temperature dependence of the effective hopping amplitude ratio

$$t_{\text{eff}}/t = 1 - 3j(I_{\uparrow} + I_{\downarrow}) \quad (17)$$

and the corresponding effective mass enhancement  $m^*/m = t/t_{\text{eff}}$  for various values of  $j$ . For the particular case studied, effective masses for majority and minority spins remain equal to each other when spin polarization develops. We have also assumed  $j'=j$ . As the temperature decreases above  $T_c$  the bond-charge density  $I_{\sigma}$  increases, leading to an effective mass enhancement. As the temperature decreases below  $T_c$  and spin polarization develops the bond-charge density decreases and the mass enhancement is rapidly suppressed. Note that the model can give rise to large changes in the effective mass versus temperature for appropriate parameters. The Drude formula for the optical conductivity

$$\sigma_1(\omega) = \frac{ne^2}{m^*} \frac{\tau}{1 + \omega^2 \tau^2} \quad (18)$$

( $\tau$ =relaxation time) implies that large changes in optical absorption will occur in those cases.

For the case of  $\text{EuB}_6$ , Degiorgi and co-workers find the plasma frequency to increase by approximately a factor of 2.5 below  $T_c$ .<sup>20</sup> From  $\omega_p^2 \sim n/m^*$  this corresponds to approximately the case  $j=6$  in Fig. 1. Degiorgi *et al.* also found a small increase in the plasma frequency as the tem-

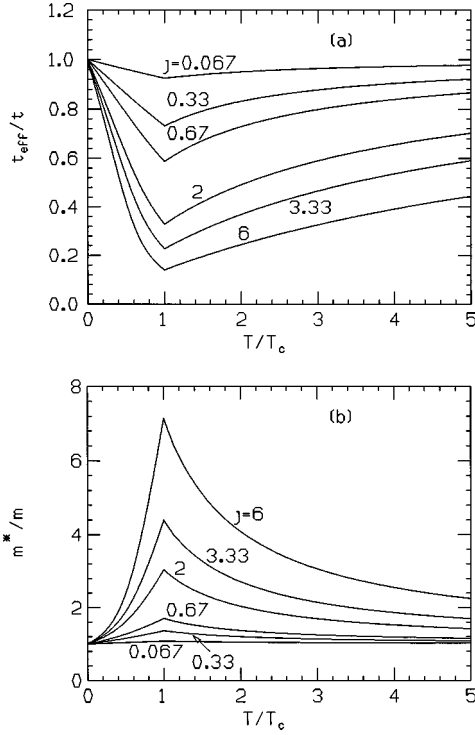


FIG. 1. Effective hopping amplitude [Eq. (17)] (a) and effective mass enhancement (b) versus temperature, for exchange parameter  $k=1$  and various values of  $j$  (numbers next to the curves), with  $j'=j$ . The effective hopping amplitude should be proportional to  $\omega_p^2$ , with  $\omega_p$  the plasma frequency.

perature is increased for  $T > T_c$ . Our model also yields such an increase, but of larger magnitude than observed by Degiorgi *et al.*

Figure 2 shows the effective magnetic moment, defined by

$$\chi(T) = \frac{p_{\text{eff}}^2(T)}{3(T - T_c)}, \quad (19)$$

where  $\chi$  is the magnetic susceptibility. Note that  $p_{\text{eff}}$  is almost temperature independent, except for very small values of  $j$ . Measurement of the magnetic susceptibility of  $\text{EuB}_6$  (Ref. 19) shows good agreement with Curie-Weiss behavior over a wide temperature range, which implies a constant effective moment with temperature. In contrast, the Stoner

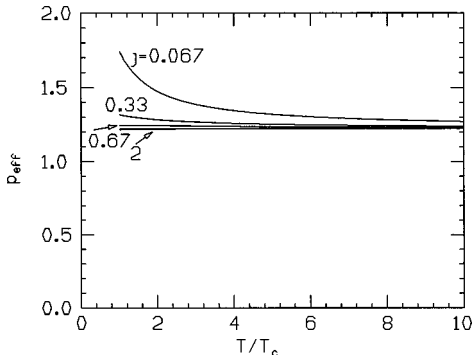


FIG. 2. Effective moment versus temperature for the parameters used in Fig. 1. The curves for  $j \geq 2$  are indistinguishable from one another.

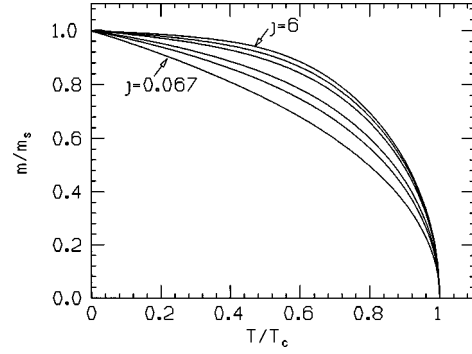


FIG. 3. Magnetization versus temperature for exchange parameter  $k=1$  and the same values of  $j$  as in Fig. 1. As  $j$  increases, the magnetization curves become steeper.

model would predict an effective moment that increases substantially as  $T$  approaches  $T_c$ .<sup>13</sup>

The magnetization versus temperature is shown in Fig. 3. Note that the magnetization curves become steeper as the band narrowing parameter increases, that is for parameters that would give rise to larger spectral weight transfer in optical properties. We are not aware of measurements of magnetization versus temperature in  $\text{EuB}_6$  to compare with our results.

From the Drude formula for the electrical resistivity

$$\rho = \frac{m^*}{ne^2\tau} \propto \frac{1}{t_{\text{eff}}} \frac{1}{ne^2\tau} \quad (20)$$

we conclude that our model will exhibit a decrease in resistivity as the system develops spin polarization, both as a function of temperature and of applied magnetic field, due to the effective mass reduction. We will assume for simplicity that the relaxation time  $\tau$  is independent of spin polarization. That is, we assume that the dominant scattering mechanism is *not* spin-disorder scattering as usually assumed, because the itinerant carriers are themselves magnetic. The magnetoresistance is then given by

$$\frac{\Delta\rho}{\rho} = \frac{\rho(H) - \rho(0)}{\rho(0)} = 3j \frac{I[T, m(h)] - I[T, m(0)]}{1 - 3jI[T, m(h)]}. \quad (21)$$

We will not attempt to model the scattering processes that give rise to the relaxation time  $\tau$ . In fact, the carrier concentration  $n$  may also have a temperature dependence. Rather, we will take a temperature dependence of  $n\tau$  such that the results resemble experimental observations. Assuming a temperature dependence  $n\tau \propto T^{-0.75}$ , Fig. 4 shows the resistivity versus temperature, which yields a small upturn of  $\rho$  as  $T$  approaches  $T_c$  and a cusp at  $T_c$ , as seen experimentally. When a magnetic field is applied the resistivity decreases smoothly through  $T_c$  as seen experimentally.

In the experimental results of Guy *et al.*,<sup>18</sup> the effect of a magnetic field of 15T resembles the effect we find in Fig. 4 for  $h \sim 0.2$ . If we assume that the effect of the magnetic field is due to the coupling with the Eu moment, we should replace Eq. (5) by

$$h = \mu_{\text{Eu}} \frac{H}{D} \quad (22)$$

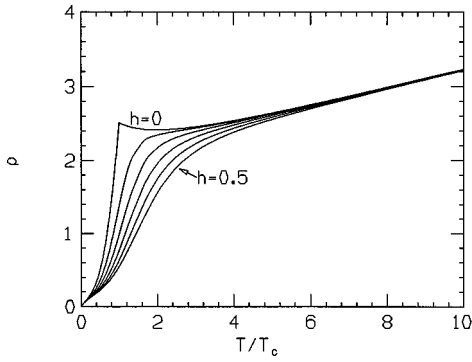


FIG. 4. Resistivity (arbitrary units) versus  $T/T_c$  for parameters  $k=1$ ,  $j=6$  and applied magnetic fields  $h=0, 0.1, 0.2, 0.3, 0.4, 0.5$ . The resistivity decreases monotonically with applied magnetic field.

with  $\mu_{\text{Eu}}$  the magnetic moment of the  $\text{Eu}^{++}$  atom, approximately 8 Bohr magnetons. Hence,

$$h = \frac{8\mu_B H}{D} = \frac{0.54H(\text{kG})}{T_c(\text{K})} \frac{T_c}{D}. \quad (23)$$

For  $H=15$  kG and  $T_c \sim 15$  K we have then  $h=0.54T_c/D$ . For the parameters in Fig. 4, our model yields  $T_c/D=0.248$ , hence  $h=0.13$ . (Note that  $T_c/D=0.248$  and  $j=zJ/D=6$  yields  $zJ/T_c \sim 25$ , consistent with our earlier discussion.) We conclude that the model yields approximately the correct order of magnitude for the effect of magnetic field on the transport properties, without necessitating to invoke a large change in the scattering rate with magnetization. Similar effects of large magnitude should be seen in optical properties when measured in the presence of a magnetic field, reflecting the change in effective mass with magnetization.

In Fig. 5 we plot the magnetoresistance predicted by this model. It can be seen that negative magnetoresistance occurs for temperatures substantially larger than  $T_c$ , which is also observed experimentally.<sup>18</sup> The order of magnitude and qualitative behavior resemble experimental observations in  $\text{EuB}_6$ .<sup>28</sup> It should be emphasized that the negative magnetoresistance in our model arises purely from the effective mass dependence on spin polarization.

Finally we consider the effect of pressure in this model. Because the driving force for ferromagnetism is the Coulomb matrix element Eq. (2) that depends on wave function overlaps we expect a strong dependence on pressure. The

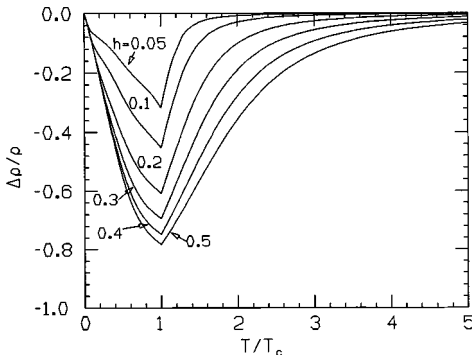


FIG. 5. Magnetoresistance versus temperature for  $k=1$ ,  $j=6$  and various values of applied magnetic field (numbers next to the curves).

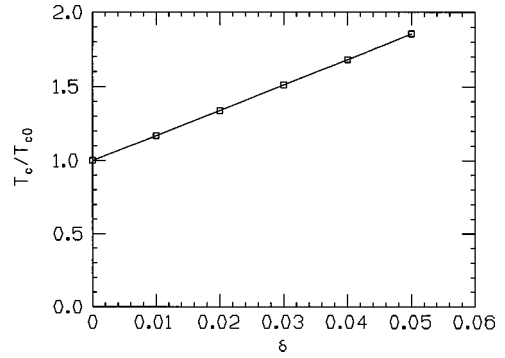


FIG. 6. Dependence of critical temperature on lattice spacing contraction parameter  $\delta$  for  $k=1$ ,  $j=6$ .  $T_{c0}$  is the critical temperature for  $\delta=0$ .

hopping matrix element  $t$  in Eq. (1) will depend exponentially on interatomic distance  $R$  as

$$t = t_0 e^{-\alpha R} \quad (24)$$

while the matrix element Eq. (2), involving two overlaps, should behave as

$$J = J_0 e^{-2\alpha R}. \quad (25)$$

Thus, for a small change in interatomic distance  $\Delta R \equiv \alpha \delta$ , the bandwidth and interactions will change as

$$D \rightarrow D(1 + \delta), \quad (26a)$$

$$j \rightarrow j(1 + \delta), \quad (26b)$$

$$u \rightarrow u(1 - \delta), \quad (26c)$$

$$k \rightarrow k(1 - \delta) + 2j\delta, \quad (26d)$$

assuming that the on-site repulsion  $U$  is unchanged by interatomic distance changes. The critical temperature in our model within the Sommerfeld expansion is given by<sup>13</sup>

$$k_B T_c = \left( \frac{3}{4\pi^2} \right)^{1/2} D k m_0 \quad (27)$$

with  $m_0$  the zero-temperature magnetization.  $m_0$  can increase or decrease with pressure depending on the parameters,<sup>13</sup> while  $T_c$  will generally increase with pressure unless the interaction parameter  $j$  is very small. In general the model predicts a positive pressure derivative of both  $T_c$  and  $m_0$ , with the pressure dependence of  $T_c$  being larger than that of  $m_0$ .

The positive dependence of  $T_c$  on pressure in our model arises from the increase in the magnitude of the parameter  $J$  when the interatomic distance decreases due to increased wave function overlap. From the agreement of exact diagonalization and mean field results for the effect of  $J$  in our model<sup>26</sup> we are confident that mean field theory correctly accounts for this effect even if the parameter  $J$  is not small. This is in contrast to what occurs in the Stoner model ( $U$  only) which predicts a negative pressure derivative of the critical temperature for any  $U$ , due to the decreasing density of states, which is certainly incorrect in the large  $U$  limit

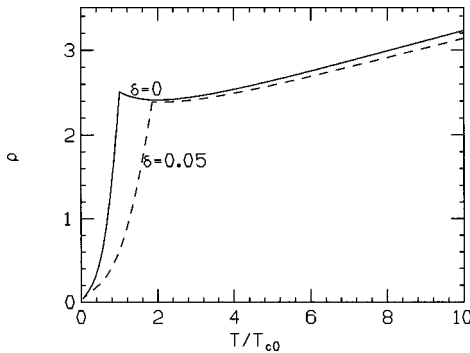


FIG. 7. Resistivity versus temperature for  $k=1$ ,  $j=6$  and lattice contraction parameter  $\delta=0$  and  $\delta=0.05$ .  $T_{c0}$  is the critical temperature for  $\delta=0$ .

where the superexchange parameter  $t^2/U$  increases with pressure due to increasing wave function overlap.

For the parameters used in the previous figures to describe  $\text{EuB}_6$ , Fig. 6 shows the dependence of  $T_c$  on interatomic distance and Fig. 7 the temperature dependence of resistivity with and without pressure. Measurements in  $\text{EuB}_6$  (Ref. 8) show a large positive pressure derivative of  $T_c$  initially, which saturates for larger pressures. The difference with the almost linear behavior seen in Fig. 6 could be due to a non-linear dependence of interatomic distance on pressure. For the resistivity, experiments show a substantially larger decrease with pressure than found in Fig. 7 for a corresponding change in  $T_c$ , which is, however, very sample dependent.<sup>8</sup> The difference with the results in Fig. 7 could be due to pressure dependence of carrier concentration or relaxation time, which are not taken into account in the present treatment. The possibility that the number of conduction electrons in  $\text{EuB}_6$  increases with increasing pressure is discussed in Ref. 8. It would be of interest to measure the Hall effect under pressure to be able to differentiate between behavior originating in carrier concentration changes versus changes in other parameters.

In summary, the model discussed here can qualitatively account for several of the anomalous properties seen in  $\text{EuB}_6$ . The model was introduced to describe metallic ferromagnetism in general,<sup>13</sup> and for most of its parameter range these anomalous properties would be of much smaller magnitude. In this paper we have shown that for appropriate parameters the model can give rise to effective masses changing by large factors, thus giving rise to very large changes in observable properties with temperature and magnetization, as seen in  $\text{EuB}_6$ . However, we argue that the underlying physics described by this model is the same for all metallic ferromagnets, even when these effects are much smaller or not even evident: a variation of the carrier effective mass with temperature and with magnetic ordering, arising from the ubiquitous bond-charge Coulomb repulsion. The variation is always such that the effective mass increases as the temperature is lowered in the paramagnetic state, and decreases with onset of spin polarization. In some materials this physics will be almost invisible, in others such as  $\text{EuB}_6$  it will show up dramatically. We have shown before that the model can also describe many of the properties of the weak ferromagnet  $\text{Sc}_3\text{In}$  for appropriate parameters.<sup>29</sup>

It is of interest to contrast the physics of our model with that of the double exchange model<sup>30</sup> that has been used to describe the manganites exhibiting colossal magnetoresistance. In that model there is also a hopping amplitude enhancement (effective mass reduction) as the system orders magnetically, arising from the Hund's rule interaction in degenerate orbitals. One key difference is that our model describes the physics of a single band, and is thus applicable to both degenerate and nondegenerate orbitals. Another key difference, from an experimental point of view, is that our model predicts an effective mass *decrease* as the temperature increases above  $T_c$ , while the double-exchange model predicts effective mass *enhancement*, arising from increasing spin disorder, leading eventually to a bandwidth collapse.<sup>32</sup> It should be possible experimentally to distinguish between the two behaviors in optical properties above  $T_c$ . For  $\text{EuB}_6$ , the qualitative behavior<sup>20</sup> is in agreement with our model. While there are optical experiments below  $T_c$  in the manganites<sup>31</sup> that show qualitatively similar behavior to  $\text{EuB}_6$ , we are not aware of optical experiments above  $T_c$ . We will use our model to describe the manganites in future work.

The model discussed here ascribes the changes observed in resistivity with magnetization in ferromagnets to changes in effective mass rather than in scattering rate. Further information concerning the validity of this concept could be obtained from measurement of optical properties in the presence of a magnetic field. For  $\text{EuB}_6$ , such experiments are apparently in progress.<sup>33</sup> Other useful information for the understanding of  $\text{EuB}_6$  could be obtained from measurement of the Hall coefficient as function of temperature, pressure and magnetic field, to detect possible changes in carrier concentration. More generally, angle-resolved photoemission experiments could yield direct information on the existence of band broadening effects as function of temperature and magnetization, as predicted by our model; the quasiparticle dispersion should exhibit a strong dependence on applied magnetic field or spontaneous magnetization. We are not aware of such experiments for either  $\text{EuB}_6$  or the manganites. Such experiments would yield valuable insight on the applicability of the model discussed here as well as of other models to the understanding of these and other ferromagnetic metals.

The concept of effective mass reduction, or kinetic energy gain, driving the transition to an ordered electronic state at low temperatures, has recently been discussed in another context, that of superconductivity. There, certain models<sup>34,35</sup> also predict that the energy gain leading to order arises from kinetic energy, which also leads to a transfer of spectral weight in optical absorption from high to low frequencies as the ordered state develops. In the case of superconductivity we have suggested where the high-energy spectral weight is coming from;<sup>36</sup> the corresponding question in the case of ferromagnetism remains open. It would be of great interest if the two most common examples of collective effects in metals, superconductivity and ferromagnetism, could be understood as having a common physical origin.<sup>14</sup>

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