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EFFECTS OF ELECTRON CORRELATIONS ON MAGNON ENERGY IN IRON AND ITS ALLOYS

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Abstract. — The magnon stiffness constant is calculated within the multiband itinerant electron model taking into account local charge and exchange correlations in the Gutzwiller variational approach. Computations are based upon the parametrized tight binding band structure of iron.

1. Introduction

A previous study [1] of the effect of electron correlations on magnon energy in itinerant electron ferromagnets indicated that correlations contribute corrections to the magnon energy which are quite significant. Results of reference [1] were based on a single tight-binding model and provided only qualitative hint on the role of correlations in the magnon energy. Effects of correlations are sensitive to the band structure and the position of the fermi level for the majority and minority spin electrons. The aim of the present work is to calculate the leading correlation corrections to the magnon stiffness constant for a multiband model approximating the band structure of iron. Arguments based upon the virtual crystal approximation are used to estimate the correlation corrections for iron-based b.c.c. alloys. For iron which is a weak itinerant ferromagnet in the sense that both the majority and minority spin bands are partially filled the effect of correlation should be pronounced [1].

2. Model

The general multiband Hamiltonian with only intratonic interactions of Coulomb origin taken into account can be written in the form [2]

\[ H = \sum_{ij\sigma} t_{ij}^{\sigma} a_{i\sigma}^\dagger a_{j\sigma} + (U + J) \sum_{j} n_{j\uparrow} + n_{j\downarrow} + \frac{1}{2} \left( U - \frac{1}{2} J \right) \sum_{j,l,i',\sigma'} n_{j\sigma} n_{l\sigma'} - J \sum_{j,l,\#i',\sigma'} S_{jl}\cdot S_{ij'}, \quad (1) \]

which is explicitly rotationally invariant. The notation is standard, \( a_{i\sigma}^\dagger \) creates an electron in the Wannier state at the lattice site \( j \), \( l \) and \( \sigma \) are the band and spin indices, respectively. \( U \) is the intraatomic Coulomb energy integral, the same value is assumed for both the intraband and interband integrals, \( J \) is the Hund rule exchange integral. As usual, \( n_{j\sigma} = a_{j\sigma}^\dagger a_{j\sigma} \) and the components of \( S_{jl} \) are defined by \( S_{jl}^\uparrow = a_{j\uparrow}^\dagger a_{l\uparrow} - a_{j\downarrow}^\dagger a_{l\downarrow} \), \( S_{jl}^\downarrow = (1/2)(n_{j\uparrow} - n_{j\downarrow}) \). The problem of evaluating the correlation corrections appears to require an extensive numerical effort. To make the task practical we make a simplifying assumption here replacing the hopping term in (1) by \( \sum_{k\sigma} t_{kl} a_{k\sigma}^\dagger a_{l\sigma} \) when passing to the Bloch representation. It is known [3, 4] that the interband terms play an essential role in precisely calculating the stiffness constant \( D \). For the purpose of calculating the correlation corrections, which finally appear to be of the order of magnitude of 10 percent of the uncorrected value of \( D \), such an approximation is acceptable.

3. Correlations

As indicated in [1] electron correlations are responsible for a renormalization of the interaction constants of the Hamiltonian i.e. the Coulomb and exchange integrals and for changes of the electron occupation numbers in the reciprocal space. The first effect is usually taken for granted by a proper choice of the interaction constants, e.g. by adjusting them to measurable quantities. To study the second effect we assume the Gutzwiller [5] variational ground state in the form \( \langle \psi \rangle = \Gamma |\phi\rangle \), where \( |\phi\rangle \) is the Hartree-Fock ground state and \( \Gamma = \prod_{j,\sigma} \exp (-\eta_{j}\delta_{j\sigma}) \). For the model (1) \( \Gamma \) can be constructed from the intraband charge correlations \( O^{(3)}_{jl} = n_{j\downarrow} n_{l\downarrow} (l \neq l') \) and the local spin correlations \( O^{(3)}_{jl} = S_{jl}\cdot S_{jl'}, \) see [6].

The magnon energy can be expressed [1] in terms of the electron occupation numbers calculated for the ground state \( |\psi\rangle \), \( \langle n_{kl\sigma} \rangle = \langle \phi | n_{kl\sigma} | \phi \rangle \) where \( n_{kl\sigma} = \langle \phi | n_{kl\sigma} | \phi \rangle \) is the H.-F. occupation number and \( n_{kl\sigma} = N^{-1} \sum_{\sigma} n_{kl\sigma} \),

\[ \chi_{kl\sigma} = N^{-2} \sum_{k'k''l} n_{kl\sigma} n_{k'k''l,\sigma} n_{k''l,\sigma} n_{kl,\sigma} \]

4. Magnon stiffness constant

The energy of the acoustical branch of the magnon spectrum in the longwavelengths limit is \( E_q = Dq^2 \). If the interband terms are neglected, as in the model assumed here, the stiffness constant \( D \) is given by (see,
e.g. [8])
\[ D = (6mN)^{-1} \sum_{kl} \left\{ \left( \langle n_{kl}^- \rangle + \langle n_{kl}^+ \rangle \right) \nabla^2 \epsilon_{kl}^- \right. \\
\left. - \frac{2}{\Delta_1} \left( \langle n_{kl}^- \rangle - \langle n_{kl}^+ \rangle \right) (\nabla \epsilon_{kl})^2 \right\}, \tag{4} \]

where \( m = \sum_i (n_{il}^- - n_{il}^+) \) is the magnetic moment per atom and \( \Delta_1 \) is the exchange splitting of the band \( l \). In the lowest order with respect to \( \eta_1 \) we get \( D = D_0 + \eta_1^2 / D_2 \). The formula (4) without the interband contributions is not a reliable starting point for calculating \( D_0 \), as discussed in [3, 4]. However, as shown below, the correction \( D_2 \) is small, so the accuracy in calculating \( D_2 \) is quite sufficient. The stiffness constant is calculated for ferromagnetic b.c.c. iron. Varying the Fermi energy and the exchange splitting parameter estimates of \( D_0 \) and \( D_2 \) can be done for isostructural Fe-based ferromagnetic alloys. The following approximations are used: 1) the band structure is parameterized by the expression
\[ \epsilon_{kl} = T_0 + T_1 \cos(ak_x) + T_2 \cos(ak_y) + T_3 \cos(ak_z) + T_4 \cos(\frac{1}{2}ak_x) \cos(\frac{1}{2}ak_y) \cos(\frac{1}{2}ak_z). \tag{5} \]

\( T_i \)'s are fitted to the paramagnetic band structure of iron, calculated by Wood [9]. In fitting the parameters \( T_\cdots \) for the highest band of the Wood structure the formula (5) was supplemented by a parabolic contribution. This procedure compensates to some extent the neglecting of the effects of hybridisation; 2) a single exchange splitting parameter is assumed, \( \Delta_1 = \Delta_2 \). As shown in [4] it is a good approximation for iron.

The tight-binding parametrization (5) is convenient for reducing the awkward triple sums over the Brillouin zone to combinations of products of single sums, e.g.
\[ N^{-1} \sum_{k} \chi_{kl\sigma} \cos k_x = \left( N^{-1} \sum_{k} n_{kl\sigma}^0 \cos k_x \right) \times \left( N^{-1} \sum_{k} n_{kl\cdots\sigma}^0 \cos k_x \right)^2, \text{ etc.} \]

5. Results

The Fermi energies for both spins were determined from the total number of electrons and the experimental value of magnetization per atom at zero temperature [10]. The exchange splitting \( \Delta = E_{F_\uparrow} - E_{F_\downarrow} \) was assumed 0.16 Ryd for iron, slightly larger than the value used in recent calculations [4]. The value \( \Delta = 0.16 \) Ryd corresponded to the magnetic moment \( m = 2.22 (\mu_B \text{ per atom}) \). For alloys \( \text{Fe}_{1-x}\text{Co}_x \) and \( \text{Fe}_{1-x}\text{Ni}_x \) the same effective interaction parameter was assumed so the exchange splitting \( \Delta(x) \) was scaled by the variation of the magnetic moment \( m(x) \) with the concentration \( x \); \( \Delta(x) / \Delta = m(x) / m \). Sample results are summarised in the table I.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( 0.5 )</th>
<th>( 0.3 )</th>
<th>( 0.2 )</th>
<th>( 0.1 )</th>
<th>( 0 )</th>
<th>( 0.1 )</th>
<th>( 0.2 )</th>
<th>( 0.25 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_0 )</td>
<td>222</td>
<td>198</td>
<td>168</td>
<td>137</td>
<td>108</td>
<td>69</td>
<td>40</td>
<td>21</td>
</tr>
<tr>
<td>( D_2 )</td>
<td>38</td>
<td>33</td>
<td>38</td>
<td>41</td>
<td>51</td>
<td>45</td>
<td>42</td>
<td>53</td>
</tr>
</tbody>
</table>

Since \( \eta_1 \gg \eta_2, \eta_3 \) [7] only the leading correction \( D_2 \) to the stiffness constant \( D = D_0 + \eta_1^2 / D_2 \) was evaluated. The parameter \( \eta_1 \) is of the order of 0.5 [7]. As it follows from the table I, correlations tend to diminish the stiffness constant although the correction is not large, typically it is less than ten percent.

The numerical values we got for \( D \) do not compare favourably with the experimental stiffness constant. For Fe the experimental value determined from neutron scattering is \( D = 314 \text{ meV} A^2 \) at \( T = 0 \), as quoted in [4], whereas from the table I it follows \( D = (163 - 0.25 \times 51) \text{ meV} A^2 = 150 \text{ meV} A^2 \). Recent calculations gave \( D = 280 \text{ meV} A^2 \) [4]. The reason for the discrepancy is the neglect here the effects of sp-d hybridisation and the use of the simplified formula (4) with no interband terms taken into account.

Still the dependence of \( D \) on concentration in iron alloys is qualitatively reproduced by the present data (see the experimental data quoted in [4]). Anyway, there are no reasons to believe that the relative role of the correlations corrections, determined by the ratio \( D_2 / D_0 \), would be much different if more exact treatment of the band structure is used. The conclusion of the present paper is that if the accuracy of calculated \( D \) has to be not worse than about 10%, the correlations corrections have to be taken into account.

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