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(Received 24 July 2002; published 27 February 2003)

The “magnetic force theorem” is frequently used to compute exchange interaction parameters and adiabatic spin-wave spectra of ferromagnets. The interest of this approach is that it allows one to obtain these results from a non-self-consistent calculation of the (single-electron) band energy only, which greatly reduces the computational effort. However, as discussed by various authors, this approach entails some systematic error. Here, a “renormalized magnetic force theorem” allows us to remove this systematic error without significantly increasing the computational effort involved. For systems with one atom per unit cell, it amounts to a simple renormalization of the spin-wave spectrum.

DOI: 10.1103/PhysRevLett.90.087205

PACS numbers: 75.30.Et, 75.10.–b, 75.10.Lp, 75.30.Ds
energy is then given by
\[ E = \sum_{i=1}^{N_{\text{d}}} (\epsilon_i w_{\text{eff}}[\rho, \mathbf{B}^\perp]) = \frac{\delta (E_{\text{ext}}[\rho] + E_H[\rho] + E_{\text{xc}}[\rho] + E_{\text{con}}[\rho, \mathbf{B}^\perp])}{\delta (\rho(r))}, \]

where the functional derivative is taken at the \textit{a priori} prescribed spinor density. This essential difference between \( w_{\text{eff}}'[\rho, \mathbf{B}^\perp] \) and \( w_{\text{eff}}[\rho] \) allows us to calculate explicitly the value of the HF for a spinor density \( \rho \) and constrains \( \mathbf{B}^\perp \) chosen \textit{a priori} (provided we know some suitable approximation of \( E_{\text{xc}}[\rho] \)), which constitutes a great advantage with respect to the CHKF. In view of the Kohn-Sham theorem [8], the HF and CHKF obviously take the same value \( E_0 \) for the density \( \rho_0 \) and constrains \( \mathbf{B}^\perp \) corresponding to the constrained ground state (solution of the constrained Kohn-Sham equation). In addition, the HF can be shown to be \textit{stationary}, but not necessarily \textit{minimal}, in contrast to the CHKF with respect to \( \rho \) and \( \mathbf{B}^\perp \) in the vicinity of the constrained ground state \( (\rho^*, \mathbf{B}^\perp) \). The properties of the HF have been studied by various authors who found that, in fact, it often yields a better approximation of the ground state energy, in the vicinity of \( (\rho^*, \mathbf{B}^\perp) \), than the corresponding HKF [10].

Starting from the ferromagnetic state (with \( \mathbf{u}_\mathbf{R}^0 = \mathbf{u}_0 \) for all sites \( \mathbf{R} \)), for which we assume the self-consistent density \( \rho_0 = n_0 \sigma_0 + m_0 \mathbf{u}_0 \cdot \sigma \) to be known, we perform some infinitesimal rotations: \( \mathbf{u}_\mathbf{R} = \mathbf{u}_0^0 + \delta \mathbf{u}_\mathbf{R} \). For the ferromagnetic state, the constraining field vanishes everywhere. For the rotated state, we approximate the energy by using the HF \( J_{\text{Harris}}[\rho, \mathbf{B}^\perp] \), evaluated for a trial input density equal to \( \rho_\text{in} = n_0 \sigma_0 + m_0 (\mathbf{u}_0 + \delta \mathbf{u}) \cdot \sigma \), and for some trial input constrain \( \mathbf{B}_\mathbf{m}^\perp \) (to be specified later).

If we use the local density approximation (LDA) for the exchange-correlation term (as is almost always done), the only term in our trial evaluation of the HF which varies with \( \delta \mathbf{u} = \{\delta \mathbf{u}_\mathbf{R}\} \) is the band energy (sum of eigenvalues \( \epsilon_i \)), so that the energy associated with the fluctuation \( \delta \mathbf{u} \) is

we are only able to obtain the value of the HKF for the output spinor density, which we did not know \textit{a priori}, but not for some spinor density chosen \textit{a priori}. This problem can be circumvented by using an auxiliary energy functional, first introduced by Harris [9]. The Harris functional (HF) \( J_{\text{Harris}}[\rho, \mathbf{B}^\perp] \), in the present context, has the same form as the CHKF \( J_{\text{HK}}[\rho, \mathbf{B}^\perp] \), with \( T'_0[\rho] \) replaced by

\[ T'_0[\rho, \mathbf{B}^\perp] = \sum_{i=1}^{N_{\text{d}}} \epsilon_i (w_{\text{eff}}'[\rho, \mathbf{B}^\perp]) - \int \delta (n \mathbf{v}_{\text{eff}} - m \mathbf{B}_\text{eff}) \cdot \mathbf{B}^\perp, \]

where the new effective spinor potential \( w_{\text{eff}}'[\rho, \mathbf{B}^\perp] = V_{\text{eff}}[\rho, \mathbf{B}^\perp] - \mathbf{B}^\perp \cdot \sigma \) is defined explicitly in terms of \( \rho \) and \( \mathbf{B}^\perp \) by

\[ \Delta E'(\delta \mathbf{u}) = \sum_{\mathbf{R}, \mathbf{R}'} A_{\mathbf{R} \mathbf{R}'} \Delta \mathbf{u}_\mathbf{R} \cdot \Delta \mathbf{u}_\mathbf{R}' + O_2(\delta n, \delta m, \delta \mathbf{B}^\perp), \]

with \( A_{\mathbf{R} \mathbf{R}'} = -J_{\mathbf{R} \mathbf{R}'} + \delta_{\mathbf{R} \mathbf{R}'}(\sum_{\mathbf{R}} J_{\mathbf{R} \mathbf{R}'}), \) which defines the coupling parameters \( J_{\mathbf{R} \mathbf{R}'} \). The sum rule,

\[ \sum_{\mathbf{R}} A_{\mathbf{R} \mathbf{R}'} = \sum_{\mathbf{R}} A_{\mathbf{R} \mathbf{R}'} = 0, \]

expresses the fact that the total energy remains invariant (within the nonrelativistic theory) upon a uniform rotation of the magnetization. The definition (4) for \( A_{\mathbf{R} \mathbf{R}'} \) implies that it is related to the (static) transverse susceptibility \( \chi \) by \( 2A_{\mathbf{R} \mathbf{R}'} = M_R (\chi^{-1})_{\mathbf{R} \mathbf{R}'} M_{\mathbf{R}'} \).

The bare MFT of Liechtenstein \textit{et al.} [3] amounts to make the choice \( \mathbf{B}_\mathbf{m}^\perp = 0 \) for the trial input constraining fields. They then obtain

\[ \Delta E'(\delta \mathbf{u}) = \sum_{\mathbf{R}, \mathbf{R}'} A_{\mathbf{R} \mathbf{R}'} \delta \mathbf{u}_\mathbf{R} \cdot \delta \mathbf{u}_\mathbf{R}' + O_2(\delta n, \delta m, \mathbf{B}^\perp), \]

with \( A_{\mathbf{R} \mathbf{R}'} = -J_{\mathbf{R} \mathbf{R}'} + \delta_{\mathbf{R} \mathbf{R}'}(\sum_{\mathbf{R}} J_{\mathbf{R} \mathbf{R}'}), \) and
moments. The constrains are obtained by expressing the transverse
\[ \hat{J}_{RR'} = \frac{1}{\pi} \text{Im} \int_{-\infty}^{\infty} \text{d}e \int_{\Omega_R} \text{d}r \int_{\Omega_{R'}} \text{d}r'B_{sc}(r)G^1(r, r') \times B_{sc}(r')G^1(r', r). \]  
(7)

Since \( \delta n \) and \( \delta m \) are even with respect to \( \delta u \), they are
generally of second order in \( \delta u \); however, the constrains \( B_{\perp}^\pm \) are odd with respect to \( \delta u \), and therefore generally of
first order in \( \delta u \), so that \( O_2(\delta n, \delta m, B_{\perp}^\pm) = O_2(\delta u) \),
although \( O_2(\delta n, \delta m) = O_3(\delta u) \). As a consequence, the
parameters \( \hat{J}_{RR'} \) (hereafter called the bare exchange parameters) are not equal to the true exchange parameters \( \hat{J}_{RR'} \) and entail some systematic error. Note, however, that
this problem does not occur for the case considered by Oswald et al. [2] since the constrains vanish in the case they consider.
Clearly, to calculate correctly the true exchange parameters \( \hat{J}_{RR'} \), we need to take the exact constrains \( B_{\perp}^\perp \) (which are still unknown yet) as trial input in our estimate of the HF. If we do so, we obtain, after some algebra,
\[ \Delta E(\delta u) = \sum_{R,R'} \left[ \hat{A}_{RR'} \delta u_R \cdot \delta u_{R'} + (M_{RR'}^\perp \hat{K}_{RR'}) \left( B_{\perp}^\perp \cdot \delta u_R - \frac{1}{2} \hat{K}_{RR'} B_{\perp}^\perp \cdot B_{\perp}^\perp \right) \right] + O_4(\delta u), \]  
(8)

with \( M_R = \int_{\Omega_R} \text{d}r m(r) \) is the magnetic moment of atom \( R \), and where the bare transverse susceptibility \( \hat{\chi}_{RR'} \) and
the exchange-correlation response function \( \hat{K}_{RR'} \) are given by
\[ \hat{\chi}_{RR'} = \frac{2}{\pi} \int_{-\infty}^{\infty} \text{d}e \int_{\Omega_R} \text{d}r \int_{\Omega_{R'}} \text{d}r' \text{Im}[G^1(r, r')G^2(r', r)], \]  
(9)
\[ \hat{K}_{RR'} = \frac{1}{\pi} \int_{-\infty}^{\infty} \text{d}e \int_{\Omega_R} \text{d}r \int_{\Omega_{R'}} \text{d}r' \times \text{Im}[G^1(r, r')B_{sc}(r')G^2(r', r) + G^1(r, r')B_{sc}(r')G^2(r', r)]. \]  
(10)
The constrains are obtained by expressing the transverse
moments \( M_R \delta u_R \) as resulting from the transverse exchange-correlation and constraining fields: \( M_R \delta u_R = \sum_R (\hat{K}_{RR'} \delta u_R + \hat{\chi}_{RR'} B_{\perp}^\perp) \). In order to keep the expressions compact, we introduce matrix notations: \( A, \hat{A}, \hat{K}, \hat{X}, \hat{M} \) are the matrices whose \( (RR') \) elements are, respectively, \( A_{RR'}, \hat{A}_{RR'}, \hat{K}_{RR'}, \hat{X}_{RR'}, M_{\delta RR'} \). Inserting the resulting expression of the constrains, \( B_{\perp}^\perp = \sum_R [X^{-1}(M - \hat{K})]_{RR} \delta u_R \), into the above expression of \( \Delta E(\delta u) \), we finally obtain the exact explicit expression of the renormalized exchange parameters:
\[ A = \hat{A} + \frac{1}{2} (M - \hat{K}) \hat{X}^{-1} (M - \hat{K}). \]  
(11)

One can easily prove the sum rule \( M_R = \sum_{R'} \hat{K}_{RR'} \),
which implies that the constrains \( B_{\perp}^\perp \) vanish for a coherent
rotation of all magnetic moment, and that the sum rule (5) is indeed satisfied. The above result, Eq. (11), the “renormalized magnetic force theorem,” constitutes the main result of this Letter. Its importance is that it corrects the systematic error introduced by the “bare magnetic force theorem,” without increasing significantly the computational effort. It therefore provides a general method to calculate exactly the exchange parameters \( \hat{J}_{RR'} \) which is several orders of magnitude faster than a fully self-consistent calculation.
TABLE I. Curie temperature calculated within the RPA by using the bare ($T_C^{\text{RPA}}$) and renormalized ($T_C^{\text{RRPA}}$) exchange parameters, as compared with the experimental value ($T_C^{\text{exp}}$).

<table>
<thead>
<tr>
<th>System</th>
<th>$T_C^{\text{RPA}}$ (K)</th>
<th>$T_C^{\text{RRPA}}$ (K)</th>
<th>$T_C^{\text{exp}}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe (bcc)</td>
<td>950</td>
<td>1057</td>
<td>1045</td>
</tr>
<tr>
<td>Ni (fcc)</td>
<td>350</td>
<td>634</td>
<td>621–631</td>
</tr>
</tbody>
</table>

bare (unrenormalized) spin-wave matrix. Noting that the bare parameters $\tilde{A}_{RR}$ can be expressed in terms of the Stoner parameters $(\tilde{I}_{\text{RR}}) = \delta_{RR} \Delta_R / (2M_R)$ as $2\tilde{A} = M \tilde{I}_{\text{RR}} (1 - \tilde{X}_{\text{RR}}) M$, one easily shows that the renormalization (15) can be reexpressed as

$$2\tilde{A} = M \tilde{X}^{-1} M = M \tilde{X}^{-1} - (\tilde{I}_{\text{RR}}) M.$$  \hspace{1cm} (17)

The above expression has the familiar form of the random-phase-approximation (RPA) result for the transverse susceptibility; it is important to realize, however, that in the present context (as shown by the above derivation) this result is exact within the LDA [except for the discretization approximation $u(r) \rightarrow u_R$, which as already indicated, can be removed easily]. The present approach is therefore formally equivalent to approaches based on calculations of the transverse susceptibility [5], however without the need for self-consistent total energy calculations.

For the particular case of periodic lattices, the above equations are most conveniently solved in Fourier space. For systems with a single atom per unit cell, and using the approximation (14), the renormalization of the exchange parameters leads to the simple rescaling of the spin-wave spectrum

$$\hbar \omega(q) = \frac{\hbar \tilde{\omega}(q)}{1 - \hbar \tilde{\omega}(q)/\Delta}.$$  \hspace{1cm} (18)

The above result clearly shows that the bare MFT yields correct results only in the limit of long wavelength (in particular, it yields the correct spin-wave stiffness $D$), or if the spin-wave energies remain much smaller than the exchange splitting $\Delta$. The above result is in agreement with the estimate of the error entailed by the bare MFT proposed by Grotheer [5]: $\hbar \omega \approx \hbar \tilde{\omega} \leq \hbar \tilde{\omega}/(1 - \hbar \tilde{\omega}/\Delta)^2$.

The Curie temperature can be calculated by means of the random-phase-approximation Green’s function method [11]. For periodic systems with a single atom per unit cell, one has

$$\frac{1}{k_B T_C^{\text{RPA}}} = 6 \frac{1}{M N} \sum_q \frac{1}{\hbar \omega(q)}.$$  \hspace{1cm} (19)

so that, by using approximation (14), one therefore obtains an extremely simple renormalization of the (RPA) Curie temperature:

$$k_B T_C^{\text{RRPA}} = k_B T_C^{\text{RPA}} \left(1 - 6 \frac{k_B T_C^{\text{RPA}}}{M \Delta} \right)^{-1},$$  \hspace{1cm} (20)

where $T_C^{\text{RPA}}$ is the Curie temperature obtained from the bare exchange parameters. As seen from Table I, the renormalization of the exchange parameters considerably improves the agreement between theoretical and experimental Curie temperatures of Fe and Ni.

The method discussed here provides a convenient and accurate approach to study the exchange interactions, spin-wave spectra, and Curie temperature of complex systems such as disordered alloys, ultrathin films, nanostructures, dilute magnetic semiconductors (e.g., Ga$_{1-x}$Mn$_x$As, etc).

I wish to express my thanks to Helmut Eschrig for some very stimulating discussions which motivated me to address this problem. I am grateful to Josef Kudrnovsky, Leonid Sandratskii, and Valeri Stepanyuk for their helpful remarks on this work.