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Magnetic susceptibility, exchange interactions and spin-wave spectra in the local spin density approximation

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Abstract

Starting from exact expression for the dynamical spin susceptibility in the time-dependent density functional theory a controversial issue about exchange interaction parameters and spin-wave excitation spectra of itinerant electron ferromagnets is reconsidered. It is shown that the original expressions for exchange integrals based on the magnetic force theorem (J. Phys. F **14** L125 (1984)) are optimal for the calculations of the magnon spectrum whereas static response function is better described by the “renormalized” magnetic force theorem by P. Bruno (Phys. Rev. Lett. **90** 087205 (2003)). This conclusion is confirmed by the *ab initio* calculations for Fe and Ni.

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An efficient scheme for the first-principle calculations of exchange interaction parameters in magnets based on a so-called “magnetic force theorem” (MFT) [1, 2] in the density functional theory is frequently used for analysis of exchange parameters for different classes of magnetic materials such as dilute magnetic semiconductors [3], molecular magnets [4], colossal magnetoresistance perovskites [5], transition metal alloys [6], hard magnetic materials such as PtCo [7] and many others. Recently this method was generalized to take into account the correlation effects and successfully used for the quantitative estimation of exchange interactions in Fe and Ni [8, 9]. At the same time the formal status of this approach is still not well-defined since a general mapping of formally rigorous spin density functional to an effective classical Heisenberg Hamiltonian can be done only approximately. It was noticed already in the first work on the MFT [1] that only the expression for spin wave stiffness constant D is reliable. In terms of the diagrammatic many-body approach it means that the exchange integrals (J_{ij}) in general should contain vertex corrections [10] which are neglected in the simple expression [1, 2] (see Ref. 9). At the same time, using a general expression for spin-wave stiffness due to Hertz and Edwards [11] one can prove that the vertex corrections to D are cancelled for any local approximation for the self-energy (or, in the density functional method, for the local exchange correlation potential) [12]. Recently P. Bruno has suggested [13] corrections to the MFT and consequently to the expressions for J_{ij} (see also Ref. 14). It is important to note that, first, the new expression for D coincides with the old one and, second, that these corrections for the case of itinerant electron magnets are formally small in adiabatic parameter $\eta = \varpi/\Delta$ where ϖ is a characteristic magnon frequency and Δ is the Stoner spin splitting. At the same time, mapping of the local spin density approximation (LSDA) onto the classical Heisenberg model itself is valid only in the adiabatic approximation $\eta \rightarrow 0$ [1, 2, 16]. If we are interested in higher order effects in the η it might be needed different effective exchange parameters for different physical properties. We will show on few examples that this is exactly the case. It turns out that the spin-wave excitation spectrum should be calculated in terms of “old” exchange integrals [1, 2] whereas for static properties “new” exchange integrals [13, 14] are more appropriate.

The most reliable way to consider spin-wave properties of itinerant electron magnets in the framework of the spin density functional theory is the use of frequency dependent magnetic susceptibility [17, 18, 19]. One should start from the time-dependent density functional theory in the adiabatic approximation (ADA-TDDFT) [20, 21]. We proceed with

the Schrödinger-like equation within the self-consistent ADA-TDDFT potential

$$\begin{aligned}
i\frac{\partial\psi}{\partial t} &= H\psi \\
H &= -\nabla^2 + V(\mathbf{r}) - \frac{1}{2}(\mathbf{B}_{xc}(\mathbf{r}) + \mathbf{B}_{ext}(\mathbf{r}))\sigma
\end{aligned}
\tag{1}$$

(Slater's units are used here) where $V(\mathbf{r})$ is an effective potential, $\mathbf{B}_{ext}(\mathbf{r})$ and $\mathbf{B}_{xc}(\mathbf{r})$ are external magnetic field acting on spin and exchange-correlation field, respectively. The adiabatic approximation means that the functional dependences of exchange-correlation potential and field on the charge and spin density are supposed to be the same as in the stationary case. In LSDA one has

$$\begin{aligned}
V(\mathbf{r}) &= V_{ext}(\mathbf{r}) + \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\partial}{\partial n}[n\varepsilon_{xc}] \\
\mathbf{B}_{xc} &= -2\frac{\mathbf{m}}{m} \frac{\partial}{\partial m}[n\varepsilon_{xc}]
\end{aligned}
\tag{2}$$

where n and \mathbf{m} are charge and spin density, ε_{xc} is the exchange-correlation energy per particle, V_{ext} is the external potential, i.e. the Coulomb potential of nuclei. To calculate the spin susceptibility we will assume $\mathbf{B}_{ext}(\mathbf{r}) \rightarrow 0$. It leads to the effective complete “non-equilibrium” field

$$\delta B_{tot}^\alpha = \delta B_{ext}^\alpha + \frac{\delta B_{xc}^\alpha}{\delta m^\beta} \delta m^\beta
\tag{3}$$

where $\alpha\beta$ are Cartesian indices and the sum over repeated indices is assumed.

By definition of the exact non-local frequency-dependent spin susceptibility $\hat{\chi}^{\alpha\beta}$ the variation of the spin density is equal to

$$\delta m^\alpha = \hat{\chi}^{\alpha\beta} \delta B_{ext}^\beta
\tag{4}$$

Operator product is defined here as usual:

$$(\hat{\chi}\varphi)(\mathbf{r}) = \int d\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}') \varphi(\mathbf{r}')
\tag{5}$$

On other hand, it was shown in Ref. 20 that in the time-dependent density functional theory we should have exactly

$$\delta m^\alpha = \hat{\chi}_0^{\alpha\beta} \delta B_{tot}^\beta
\tag{6}$$

where $\hat{\chi}_0^{\alpha\beta}$ is the susceptibility of an auxiliary system of free Kohn-Sham particles. It has been demonstrated originally for the charge excitations but the generalization of TDDFT

for the spin-polarized case [21], shows that the equation (6) holds also for spin excitations. Comparing two expressions for δm^α we have the following equation

$$\widehat{\chi}^{\alpha\beta} = \widehat{\chi}_0^{\alpha\beta} + \widehat{\chi}_0^{\alpha\gamma} \frac{\delta B_{xc}^\gamma}{\delta m^\delta} \widehat{\chi}^{\delta\beta} \quad (7)$$

This ‘‘RPA-like’’ equation is formally exact in ADA-TDDFT. For the *local* spin density approximation (Eq.(2)) one has

$$\frac{\delta B_{xc}^\gamma}{\delta m^\delta} = \frac{B_{xc}}{m} \left(\delta_{\gamma\delta} - \frac{m^\gamma m^\delta}{m^2} \right) + \frac{m^\gamma m^\delta}{m^2} \frac{\partial B_{xc}}{\partial m} \quad (8)$$

The first term in Eq.(8) is purely transverse and the second one is purely longitudinal with respect to the local magnetization vector. In collinear magnetic structures there are no coupling between the longitudinal and transverse components and for the transverse spin susceptibility we have the following equation:

$$\chi^{+-}(\mathbf{r}, \mathbf{r}', \omega) = \chi_0^{+-}(\mathbf{r}, \mathbf{r}', \omega) + \int d\mathbf{r}'' \chi_0^{+-}(\mathbf{r}, \mathbf{r}'', \omega) I_{xc}(\mathbf{r}'') \chi^{+-}(\mathbf{r}'', \mathbf{r}', \omega) \quad (9)$$

where

$$I_{xc} = \frac{B_{xc}}{m} \quad (10)$$

is an exchange-correlation ‘‘Hund’s rule’’ interaction, the magnetic and charge electron density being defined as usual

$$\begin{aligned} m &= \sum_{\mu\sigma} \sigma f_{\mu\sigma} |\psi_{\mu\sigma}(\mathbf{r})|^2 \\ n &= \sum_{\mu\sigma} f_{\mu\sigma} |\psi_{\mu\sigma}(\mathbf{r})|^2 \end{aligned} \quad (11)$$

The bare susceptibility has the following form:

$$\chi_0^{+-}(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi_{\mu\uparrow}^*(\mathbf{r}) \psi_{\nu\downarrow}(\mathbf{r}) \psi_{\nu\downarrow}^*(\mathbf{r}') \psi_{\mu\uparrow}(\mathbf{r}') \quad (12)$$

where $\psi_{\mu\sigma}$ and $\varepsilon_{\mu\sigma}$ are eigenstates and eigenvalues for the Kohn-Sham quasiparticles

$$\begin{aligned} \left(H_0 - \frac{1}{2} \sigma B_{xc} \right) \psi_{\mu\sigma} &= \varepsilon_{\mu\sigma} \psi_{\mu\sigma} \\ H_0 &= -\nabla^2 + V(\mathbf{r}) \end{aligned} \quad (13)$$

and $f_{\mu\sigma} = f(\varepsilon_{\mu\sigma})$ is the Fermi distribution function.

Although the longitudinal spin susceptibility is not necessary to consider the exchange interactions it is instructive to write also an explicit expression for it. The derivation is

similar to those presented above with a small complication, since we have to consider separately the response of spin-up and spin-down electrons. Suppose we have an external perturbation δV_{ext}^σ . It leads to the change of the exchange correlation potential $V_{xc}^\sigma = \frac{\partial(n\varepsilon_{xc})}{\partial n_\sigma}$ ($n_\sigma = \frac{1}{2}(n + \sigma m)$), namely,

$$\begin{aligned}\delta V_{xc}^\sigma &= U_{\sigma\sigma'} \delta n_{\sigma'}, \\ U_{\sigma\sigma'} &= \frac{\partial^2(n\varepsilon_{xc})}{\partial n_\sigma \partial n_{\sigma'}}\end{aligned}\tag{14}$$

which gives the total perturbation $\delta V_{tot}^\sigma = \delta V_{ext}^\sigma + \delta V_{xc}^\sigma$. One can introduce the response functions $K^{\sigma\sigma'}$ by the formal expression

$$\delta n^\sigma = K^{\sigma\sigma'} \delta V_{ext}^{\sigma'}\tag{15}$$

Then the longitudinal spin susceptibility can be expressed in terms of the K -functions as

$$\chi^{zz} = \frac{1}{4} (K^{\uparrow\uparrow} + K^{\downarrow\downarrow} - K^{\uparrow\downarrow} - K^{\downarrow\uparrow})\tag{16}$$

At the same time, according to the general scheme of TDDFT, we have

$$\delta n^\sigma = \hat{X}_\sigma \delta V_{tot}^\sigma\tag{17}$$

where

$$X_\sigma(\mathbf{r}, \mathbf{r}') = \sum_{\mu\nu} \frac{f_{\mu\sigma} - f_{\nu\sigma}}{\omega - \varepsilon_{\mu\sigma} + \varepsilon_{\nu\sigma}} \psi_{\mu\sigma}^*(\mathbf{r}) \psi_{\nu\sigma}(\mathbf{r}) \psi_{\mu\sigma}(\mathbf{r}') \psi_{\nu\sigma}^*(\mathbf{r}')\tag{18}$$

Comparing these two expressions for δn^σ one obtains

$$\begin{aligned}K^{\uparrow\uparrow} &= X_\uparrow + X_\uparrow U_{\uparrow\uparrow} K^{\uparrow\uparrow} + X_\uparrow U_{\uparrow\downarrow} K^{\downarrow\downarrow} \\ K^{\downarrow\downarrow} &= X_\downarrow + X_\downarrow U_{\downarrow\downarrow} K^{\downarrow\downarrow} + X_\downarrow U_{\downarrow\uparrow} K^{\uparrow\uparrow} \\ K^{\uparrow\downarrow} &= X_\uparrow U_{\uparrow\downarrow} K^{\downarrow\downarrow} + X_\uparrow U_{\uparrow\uparrow} K^{\uparrow\uparrow} \\ K^{\downarrow\uparrow} &= X_\downarrow U_{\downarrow\uparrow} K^{\uparrow\uparrow} + X_\downarrow U_{\downarrow\downarrow} K^{\downarrow\downarrow}\end{aligned}\tag{19}$$

Similar expressions have been obtained in the RPA for the Hubbard model in Ref 22. A coupling between the longitudinal spin and density degrees of freedom is important also for the electronic structure calculations which take into account correlation effects [9, 23].

Let us continue the derivation of useful expression for the transverse susceptibility (Eq.(9)). In order to consider the case of small ω it is useful to make some identical transformations of the kernel (12) similar to the Hubbard model consideration [24]. Using Eq.(13)

one can find

$$B_{xc}\psi_{\mu\uparrow}\psi_{\nu\downarrow}^* = (\varepsilon_{\nu\downarrow} - \varepsilon_{\mu\uparrow})\psi_{\nu\downarrow}^*\psi_{\mu\uparrow} + \nabla(\psi_{\mu\uparrow}\nabla\psi_{\nu\downarrow}^* - \psi_{\nu\downarrow}^*\nabla\psi_{\mu\uparrow}) \quad (20)$$

Substituting Eq.(20) into Eq.(12) we obtain

$$(\chi_0^{+-}B_{xc})(\mathbf{r}, \mathbf{r}', \omega) = m(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') - \omega\chi_0^{+-}(\mathbf{r}, \mathbf{r}', \omega) \quad (21)$$

where we used the completeness condition

$$\sum_{\mu} \psi_{\mu\sigma}^*(\mathbf{r})\psi_{\mu\sigma}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (22)$$

Substituting Eq.(21) into Eq.(12) we can transform the latter expression to the following form

$$\widehat{\chi}^{+-} = \widehat{\chi}_0^{+-} + \widehat{\chi}_0^{+-}\frac{B_{xc}}{m}\widehat{\chi}^{+-} = \widehat{\chi}_0^{+-} + \widehat{\chi}^{+-} - \omega\widehat{\chi}_0^{+-}\frac{1}{m}\widehat{\chi}^{+-} + \frac{\widehat{\Lambda}}{m}\widehat{\chi}^{+-} \quad (23)$$

or, equivalently,

$$\widehat{\chi}^{+-} = m \left[\omega - (\widehat{\chi}_0^{+-})^{-1} \widehat{\Lambda} \right]^{-1} \quad (24)$$

where

$$\Lambda(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi_{\mu\uparrow}^*(\mathbf{r})\psi_{\nu\downarrow}(\mathbf{r}) \nabla [\psi_{\mu\uparrow}(\mathbf{r}')\nabla\psi_{\nu\downarrow}^*(\mathbf{r}') - \psi_{\nu\downarrow}^*(\mathbf{r}')\nabla\psi_{\mu\uparrow}(\mathbf{r}')] \quad (25)$$

Using Eqs.(12),(24) one has finally

$$\widehat{\chi}^{+-} = (m + \widehat{\Lambda}) \left(\omega - I_{xc}\widehat{\Lambda} \right)^{-1} \quad (26)$$

which is exactly equivalent to Eq.(9) but much more suitable for investigation of the magnon spectrum. Spin wave excitations can be separated from the Stoner continuum (e.g., paramagnons) only in the adiabatic approximation, which means the replacement $\Lambda(\mathbf{r}, \mathbf{r}', \omega)$ by $\Lambda(\mathbf{r}, \mathbf{r}', 0)$ in Eq.(26). Otherwise one should just find the poles of the total susceptibility, and the whole concept of “exchange interactions” is not uniquely defined. Nevertheless, *formally* we can introduce the effective exchange interactions via the quantities

$$\Omega(\mathbf{r}, \mathbf{r}', \omega) = I_{xc}\Lambda(\mathbf{r}, \mathbf{r}', \omega). \quad (27)$$

Substituting Eq.(20) into Eq.(26) we get

$$\Lambda(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi_{\mu\uparrow}^*(\mathbf{r})\psi_{\nu\downarrow} [B_{xc}(\mathbf{r}') - \varepsilon_{\nu\downarrow} + \varepsilon_{\mu\uparrow}] \psi_{\nu\downarrow}^*(\mathbf{r}')\psi_{\mu\uparrow}(\mathbf{r}') \quad (28)$$

Therefore

$$\Omega(\mathbf{r}, \mathbf{r}', \omega) = \frac{4}{m(\mathbf{r})} J(\mathbf{r}, \mathbf{r}', \omega) + I_{xc}(\mathbf{r}) \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} (\varepsilon_{\mu\uparrow} - \varepsilon_{\nu\downarrow}) \psi_{\mu\uparrow}^*(\mathbf{r}) \psi_{\nu\downarrow}(\mathbf{r}) \psi_{\nu\downarrow}^*(\mathbf{r}') \psi_{\mu\uparrow}(\mathbf{r}') \quad (29)$$

where an expression for frequency dependent exchange interactions has the following form

$$J(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{4} \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi_{\mu\uparrow}^*(\mathbf{r}) B_{xc}(\mathbf{r}) \psi_{\nu\downarrow}(\mathbf{r}) \psi_{\nu\downarrow}^*(\mathbf{r}') B_{xc}(\mathbf{r}') \psi_{\mu\uparrow}(\mathbf{r}') \quad (30)$$

The later coincides with the exchange integrals [1, 2, 25] if we neglect the ω - dependence. Since $B_{xc} \sim m$ we have $J \sim m^2$ and the expression (29) vanishes in non-magnetic case, as it should be. Using the identity (22) one can show that

$$\Omega(\mathbf{r}, \mathbf{r}', 0) = \frac{4}{m(\mathbf{r})} J(\mathbf{r}, \mathbf{r}', 0) - B_{xc}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \quad (31)$$

Note that for $\omega = 0$ we have exactly:

$$-I_{xc} \hat{\Lambda} = \hat{\Omega}$$

and the static susceptibility $\hat{\chi}^{+-}(0)$ can be represented in the form

$$\hat{\chi}^{+-}(0) = m \left(\hat{\Omega}^{-1} - B_{xc}^{-1} \right) \quad (32)$$

which is equivalent to the result of Ref. 13

$$\hat{\tilde{\Omega}} = \hat{\Omega} \left(1 - B_{xc}^{-1} \hat{\Omega} \right)^{-1} \quad (33)$$

for the renormalized exchange interaction if one define them in terms of inverse *static* susceptibility [14, 15].

As it was stressed above for a generic case of an itinerant electron magnet it is impossible to introduce the effective exchange integrals and one should to work with the generalized spin susceptibility. Any definition of the exchange integrals assume the adiabatic approximation somewhere. For the spin-wave spectrum which is determined by the pole of the transverse susceptibility it is natural to formulate “exchange concept” as neglecting of the ω -dependence in $\hat{\Omega}$. Then, in virtue of Eq.(26) the magnon frequencies are just eigenstates of the operator $\hat{\Omega}(0)$ which exactly corresponds to the expression from the “old” MFT exchange interactions [1, 2]. Note that for the long-wavelength limit $\mathbf{q} \rightarrow 0$ this result turns out to be exact which proves the above statement about the stiffness constant D : in the framework of the local

approximation it is rigorous. Corrections to D from a *nonlocality* of the exchange-correlation potential have been estimated recently [26] for Fe and Ni and turned out to be small.

At the same time, if we are interested in the computations of the thermodynamic properties such as the Curie temperature T_C the renormalized exchange integrals can really give more accurate results. One can introduce for the itinerant electron magnets a magnon-like operators

$$b_{\mathbf{q}} = \frac{1}{\sqrt{m_0}} S_{\mathbf{q}}^-, \quad b_{\mathbf{q}}^\dagger = \frac{1}{\sqrt{m_0}} S_{\mathbf{q}}^+ \quad (34)$$

where $m_0 = 2\bar{S}$ is the ground-state magnetization and write for the temperature dependence of the magnetization the Bloch-like expression

$$m(T) = m_0 - \sum_{\mathbf{q}} \langle b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \rangle = m_0 + \frac{1}{m_0} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} d\omega \frac{\text{Im} \chi^{+-}(\mathbf{q}, \omega)}{\exp(\omega/T) - 1} \quad (35)$$

(a similar approximation for the Hubbard model has been proposed in Ref. 24). If we will use the classical-spin approximation usually exploited for first-principle estimations of the Curie temperature one should replace the Planck function in Eq.(35) by its classical limit T/ω which immediately gives (taking into account the Kramers-Kronig relations) the following expression for the Curie temperature

$$\frac{1}{T_C} = \frac{1}{m_0^2} \sum_{\mathbf{q}} \chi^{+-}(\mathbf{q}, \omega = 0) \quad (36)$$

which is identical to the expression from Ref. 13 in terms of the *renormalized* exchange interactions. Note, however, that the quantum character of the spin (which can be taken into account only beyond the LSDA) is probably very essential for proper description of high-temperature magnetism of transition metals [27] which makes a problem of an improvement of *classical* estimations of T_C less important.

In order to test different approximations to the exchange interactions we calculated spin-wave spectrum for iron and nickel using the LMTO-TB method [28]. The orthogonal LMTO representation was used and the calculation scheme was the following.

The matrix of Green function in s,p,d-basis set is equal to

$$G_{\sigma}(\mathbf{k}, \omega_n) = [i\omega_n + \mu - H_{LDA}^{\sigma}(\mathbf{k})]^{-1} \quad (37)$$

where μ is the chemical potential, ω_n are Matsubara frequencies and H_{LDA} is the orthogonal LSDA Hamiltonian. We use the following approximation for the matrix I_{xc} :

$$V_{xc} \equiv mI_{xc} = H_{LDA}^\dagger(0) - H_{LDA}^\downarrow(0) \quad (38)$$

The matrix of the LDA-susceptibility has been calculated using the fast Fourier transform technique with $k = (\mathbf{k}, \omega_n)$

$$\chi_0^{+-}(q) = - \sum_k G_\uparrow(k) * G_\downarrow(k+q) \quad (39)$$

The Fourier transforms of the “bare” exchange interactions $\hat{J}(0)$ (30) is defined as

$$J(\mathbf{q}) = \frac{1}{4} V_{xc} \chi_0^{+-}(\mathbf{q}, \omega = 0) V_{xc} \quad (40)$$

whereas for the “renormalized” exchange integrals [13, 14] one has

$$\begin{aligned} \tilde{J}(0) - \tilde{J}(\mathbf{q}) &= \frac{1}{4} Tr_L \left[m (\chi^{+-}(\mathbf{q}, \omega = 0))^{-1} m \right] \\ &= \frac{1}{4} Tr_L \left[m \left((\chi_0^{+-}(\mathbf{q}, \omega = 0))^{-1} - (\chi_0^{+-}(\mathbf{q} = 0, \omega = 0))^{-1} \right) m \right] \end{aligned} \quad (41)$$

The magnon spectrum is determined via the exchange integrals as

$$\omega(\mathbf{q}) = \frac{4}{M} [J(0) - J(\mathbf{q})], \quad (42)$$

where $M = Tr_L m$ is the total magnetic moment. One can see from Fig.1 and Fig.2 that the LDA “bare” exchange parameter better describe the spin-wave spectrum in Fe and Ni, while thermodynamics (e.g. the Curie temperature - see Table. I) are more reasonable with the exact static LDA-exchange (which is the “RPA”-like expression). This confirms a general consideration presented above.

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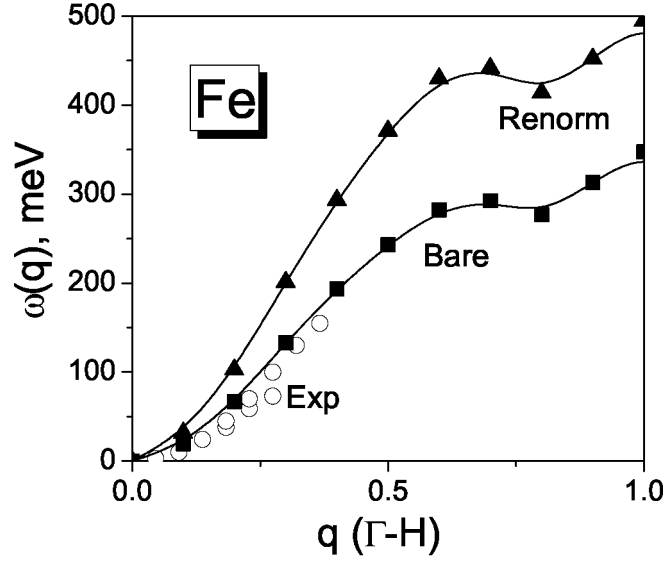


FIG. 1: The spin-wave spectrum for ferromagnetic iron in the bare exchange (Eq.(40)) and renormalized exchange (Eq.(41)) scheme in comparison with experimental data (from Ref.[29]).

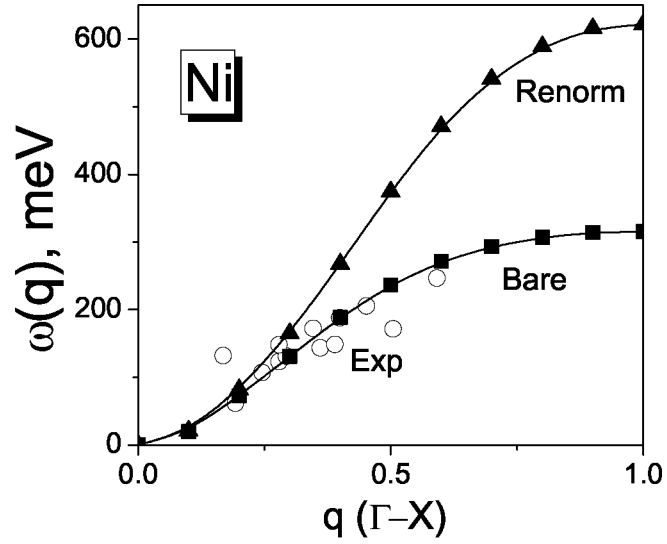


FIG. 2: The spin-wave spectrum for ferromagnetic nickel in the bare exchange (Eq.(40)) and renormalized exchange (Eq.(41)) scheme in comparison with experimental data (from Ref.[29]).

TABLE I: Curie temperature (in K) for Fe and Ni calculated with the bare (Eq.(40)) and renormalised (Eq.(41)) LDA exchange interactions; “M” is the mean-field approximation $T_c = 2/3J(0)$ and “T” is the Tjablikov, or RPA, approximation for T_c , similar to Eq.(36)

$T_c(K)$	Exp	Bare-M	Renorm-M	Bare-T	Renorm-T
Fe	1045	1060	1620	820	1280
Ni	631	310	760	285	630

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