An effective quantum parameter for strongly correlated metallic ferromagnets

Bhaskar Kamble\textsuperscript{1} and Avinash Singh\textsuperscript{2}

\textsuperscript{1} Theoretical Physics III, Ruhr-University Bochum, 44801 Bochum, Germany
\textsuperscript{2} Department of Physics, Indian Institute of Technology, Kanpur-208016, India

E-mail: avinas@iitk.ac.in

Received 11 October 2011, in final form 27 December 2011
Published 26 January 2012
Online at stacks.iop.org/JPhysCM/24/086004

Abstract

The correlated motion of electrons in metallic ferromagnets is investigated in terms of a realistic interacting-electron model with $N$-fold orbital degeneracy and intra-orbital ($U$) and inter-orbital ($J$) Coulomb interactions. Correlation-induced self-energy and vertex corrections are incorporated systematically to provide a non-perturbative Goldstone-mode-preserving scheme. An effective quantum parameter $\frac{U^2+(N-1)J^2}{U+(N-1)J}$ is obtained which determines, in analogy with $1/S$ for quantum spin systems and $1/N$ for the $N$-orbital Hubbard model, the strength of correlation-induced quantum corrections to magnetic excitations. The rapid suppression of this quantum parameter with Hund’s coupling $J$, especially for large $N$, provides fundamental insight into the phenomenon of strong stabilization of metallic ferromagnetism by orbital degeneracy and Hund’s coupling. Correlation effects are investigated for spin stiffness, magnon dispersion, electronic spectral function, density of states, and finite-temperature spin dynamics using realistic bandwidth, interaction, and lattice parameters for iron.

(Some figures may appear in colour only in the online journal)

1. Introduction

Dramatic improvements in experimental techniques such as angle-resolved photoemission spectroscopy [1] have led to important insights into the origin and role of correlation effects in itinerant ferromagnets such as iron, highlighting the coupling of electrons with magnons as playing a major role in the electron self-energy renormalization and scattering rates. Correlation effects also play an important role in the observed zone boundary magnon softening and damping in ultra-thin films of iron, as observed in recent spin-resolved electron energy loss spectroscopy experiments [2]. where the zone boundary magnon energies are much lower than those predicted within the random phase approximation, and the magnon energies were observed to depend non-monotonically on the film thickness [3]. Further evidence of correlation effects is provided by \textit{ab initio} band structure calculations of half-metallic Heusler alloys showing emergence of non-quasiparticle minority-spin states near the Fermi energy at finite temperatures, which has been suggested to be responsible for the strong suppression of tunneling magnetoresistance ratio with temperature in Co$_2$MnSi-based magnetic tunneling junctions observed in tunneling conductance measurements [4]. These experiments highlight the importance of incorporating electron–magnon coupling effects in the correlated electron spin dynamics in metallic ferromagnets.

Owing to its intrinsically strong-coupling nature, band ferromagnetism has been recognized as a fairly challenging problem, particularly with respect to the estimation of Curie temperature for the Hubbard model, although considerable progress has been achieved in the recent past [5]. A considerable amount of work has been devoted recently to understanding the electronic band structure of these metallic ferromagnets [6], starting from the local spin density approximation (LSDA) within the density functional theory, which accounted for correlations only in a limited way. The development of several extensions [7–9] has led to considerable progress in incorporating correlation effects in realistic band structure calculations. However, here the
correlation term is incorporated either at the mean-field level (LDA + \( U \) and LDA ++) or within a local self-energy approximation of the dynamical mean-field theory (LDA + DMFT) which neglects the momentum dependence. These methods therefore cannot be used to directly address spin-wave excitations as they do not explicitly preserve the spin rotation symmetry, for which vertex corrections must also be included systematically \([10, 11]\), and also predict much higher Curie temperatures \([9]\) than observed experimentally due to neglect of long wavelength spin-fluctuation modes.

Since metallic ferromagnets are characterized by intermediate to strong correlations, a proper description of spin waves must incorporate correlation effects non-perturbatively and simultaneously preserve the Goldstone mode. Spin-wave excitations in itinerant ferromagnets with realistic band structure have been mainly studied in the past using two theoretical approaches—the random phase approximation (RPA) \([12–14]\) and mapping to an equivalent Heisenberg model of localized spins by using the magnetic force theorem and its generalization to compute the exchange interaction parameters \([15–17]\). Due to neglect of correlation effects, the RPA is well known to overestimate the spin stiffness, magnon energies, and stability of the ferromagnetic state \([10]\). On the other hand, mapping to an effective Heisenberg model does not capture typically itinerant features such as zero-temperature magnon damping. The adiabatic approximation has been used to investigate spin dynamics of ultra-thin films \([15]\), but it has been pointed out that this approach breaks down for large wavevector modes \([13]\). The localized spin model has also proved unsatisfactory in explaining the doping dependence of the anomalous softening and damping of zone boundary spin-wave modes in the ferromagnetic manganites \([18]\). Although linear response density functional theory based studies of spin dynamics of iron \([19, 20]\) and the Heusler alloys \([21]\) account for damping of high-energy magnon modes due to decay into Stoner excitations, it has been pointed out that spin–charge coupling in a band ferromagnet results in significant magnon damping for modes lying even within the Stoner gap \([22]\).

In this situation, it will be useful to have a scheme which could incorporate some realistic features of multi-orbital metallic ferromagnets and simultaneously take into account the most important correlation effects within a non-perturbative and Goldstone-mode-preserving approach. Recently, correlation effects in metallic ferromagnets have been investigated within a \( N \)-orbital Hubbard model using a non-perturbative, inverse-degeneracy expansion scheme in which self-energy and vertex corrections are included systematically so that the spin rotation symmetry and the Goldstone mode are explicitly preserved order by order \([23, 24, 22]\). The \( N \)-orbital Hubbard model considered in these earlier studies involved the orbital symmetric case with identical intra-orbital and inter-orbital Coulomb interactions, and the focus was on how the geometrical factors (dimensionality, lattice, band filling, saddle points in energy-band dispersion, peaked spectral distribution) control the correlation-induced quantum corrections and thus the ferromagnetic stability. The present study will be concerned more with the role of the atomic factors (orbital degeneracy, intra-orbital and inter-orbital Coulomb interactions).

In this paper, we shall extend this spin rotationally symmetric Goldstone-mode-preserving approach to the general orbitally asymmetric case with orbital degeneracy \( \mathcal{N} \) and arbitrary intra-orbital \( (U) \) and inter-orbital \( (J) \) Coulomb interactions. We will derive an effective quantum parameter \( [U^2 + (\mathcal{N} - 1)J^2]/[U + (\mathcal{N} - 1)J]^2 \) which determines, in analogy with \( 1/S \) for quantum spin systems and \( 1/N \) for the orbitally symmetric Hubbard model, the strength of the correlation-induced quantum corrections in a realistic multi-orbital metallic ferromagnet. The diagrammatic approach presented here draws from our recent study of the two-orbital model \([25]\). However, as we shall see, there are several new diagrammatic contributions in the general \( \mathcal{N} \)-orbital case with coefficient \( (\mathcal{N} - 2) \) which are absent in the two-orbital case, and the presence of which in the exact Goldstone-mode cancelation shown in section 4 highlights the non-trivial nature of the extension from two to \( \mathcal{N} \) orbitals.

The inclusion of long wavelength spin-fluctuation modes in the finite-temperature spin dynamics is a distinct advantage of our Goldstone-mode-preserving approach, and it provides a quantitative measure of the Curie-temperature overestimate in local self-energy based calculations (for example, the LDA + DMFT) which neglect the contribution of long wavelength modes.

The importance of vertex corrections in restoring the spin rotation symmetry and Goldstone mode has been recognized at a formal level in the context of self-energy corrections in a band ferromagnet, and a Ward identity connecting vertex corrections to self-energy corrections has been derived \([10, 11]\). Correlation-induced magnon and electronic spectral function renormalizations have also been studied using the equation of motion approach \([26]\), where various electronic and magnetic properties were discussed, including non-quasiparticle states in the electronic spectrum near the Fermi energy, consideration of which has also been generalized to a multi-orbital model \([27]\). The role of electron–magnon interaction on magnetic, spectral, thermodynamic, and transport properties of half-metallic ferromagnets has been recently reviewed \([28]\), highlighting the interpolation from band structure to many-body effects.

The outline of this paper is as follows. After introducing the orbitally asymmetric \( \mathcal{N} \)-orbital interacting-electron model in section 2, the transverse spin-fluctuation propagator is studied in section 3. The effective quantum parameter is derived in section 4 from the first-order quantum correction diagrams for the irreducible particle–hole propagator, and quantum corrections to spin stiffness are studied in section 5. Using realistic bandwidth, interactions, and lattice parameters, the effective quantum parameter approach is illustrated in section 6 with evaluation of renormalized spin stiffness, magnon dispersion, density of states, electronic spectral function, and finite-temperature spin dynamics using realistic bandwidth, interaction, and lattice parameters for iron. Our conclusions are presented in section 7.
2. \(\mathcal{N}\)-orbital interacting-electron model with Hund’s coupling

We consider the following orbitally asymmetric \(\mathcal{N}\)-orbital interacting-electron model:

\[
\mathcal{H} = - \sum_{\langle ij \rangle, \sigma, \mu} t_{ij} (a_{i\sigma \mu}^\dagger a_{j\sigma \mu} + a_{j\sigma \mu}^\dagger a_{i\sigma \mu}) - U \sum_{i, \mu} S_{i\mu} \cdot S_{i\mu} - J \sum_{i, \mu \neq \nu} S_{i\mu} \cdot S_{i\nu}
\]

with arbitrary intra-orbital (\(U\)) and inter-orbital (\(J\)) Coulomb interactions. Here \(\mu\) and \(\nu\) refer to the \(\mathcal{N}\) degenerate orbitals at each lattice site \(i\), and \(S_{i\mu} = \psi_{i\mu}^\dagger(a_{i\mu}^\dagger a_{i\mu})\) is the local spin operator in terms of the fermion operators \(\psi_{i\mu}^\dagger = (a_{i\mu}^\dagger a_{i\mu})\) for the electron in the \(\mu\) orbital. For \(J = U\), the model reduces to the orbitally symmetric case considered earlier [23]. The inter-orbital density interaction term \(V_{i\mu}H_{i\nu}\) is not included here as this charge term has no leading order effect on magnetism and only weak effects on spin dynamics when quantum corrections are included away from the onset of staggered orbital ordering. The role of orbital fluctuations on spin dynamics due to this inter-orbital density interaction term has been studied recently [29, 30] in the context of the observed zone boundary anomalies in manganites.

The continuous spin rotation symmetry of the above Hamiltonian implies the existence of Goldstone modes in the spontaneously broken-symmetry state. In the following we will present a non-perturbative scheme in which the correlation-induced self-energy and vertex corrections are incorporated systematically so that the Goldstone mode is explicitly preserved order by order.

3. Transverse spin fluctuations

We assume a ferromagnetic ground state with magnetization in the \(z\) direction and examine transverse spin fluctuations representing both collective (spin-wave) and single-particle (Stoner) excitations. For simplicity, we consider a saturated ferromagnetic state which considerably simplifies the diagrammatic analysis for quantum corrections. We consider the time-ordered transverse spin-fluctuation propagator in this broken-symmetry state:

\[
\chi_{\mu\nu}^{++}(q, \omega) = i \int dt e^{i\omega t} \left\langle \left\{ S_{i\mu}(t)S_{i\mu}(t') \right\} \right\rangle | \psi_0 \rangle
\]

where \(S_{i\mu} = \psi_{i\mu}^\dagger(\sigma^z/2)| \psi_{i\mu} \rangle\) are the spin-lowering and spin-raising operators for the electron at lattice site \(i\) in orbital \(\mu\). In terms of the irreducible particle–hole propagator \(\phi_{\mu\nu}(q, \omega)\), the above spin-fluctuation propagator can be written exactly as:

\[
\chi_{\mu\nu}^{++}(q, \omega) = \phi_{\mu\nu}(q, \omega) + \phi_{\mu\nu}(q, \omega)U_{\mu\nu} \chi_{\mu'\nu'}^{++}(q, \omega),
\]

where the interaction term \(U_{\mu\nu} = U\) for \(\mu = \nu\) and \(U_{\mu\nu} = J\) for \(\mu \neq \nu\); summation over repeated indices is implied. It is physically relevant to consider the total transverse spin-fluctuation propagator as external probes such as magnetic field or neutron magnetic moment couple equally to the electron moment for all orbitals. It is particularly convenient to solve the coupled equations then to obtain:

\[
\chi_{\mu\nu}^{++}(q, \omega) = \frac{\sum_{\mu} \chi_{\mu\mu}^{++}(q, \omega)}{1 - U^+ \phi(q, \omega)}
\]

where the interaction term \(U^+ = U + (\mathcal{N} - 1)J\), and the total irreducible particle–hole propagator:

\[
\phi(q, \omega) = \sum_{\mu} \phi_{\mu\mu}(q, \omega).
\]

In analogy with the \(1/N\) expansion for the orbitally symmetric \(N\)-orbital Hubbard model, we consider a systematic expansion:

\[
\phi = \phi^{(0)} + \phi^{(1)} + \phi^{(2)} + \cdots
\]

for the irreducible propagator \(\phi(q, \omega)\) in terms of fluctuations. The zeroth-order term \(\phi^{(0)}\) is the bare particle–hole propagator, and higher-order terms \(\phi^{(1)}, \phi^{(2)}\) etc represent correlation-induced quantum corrections involving self-energy and vertex corrections, as discussed below.

Retaining only the zeroth-order term \(\phi^{(0)}\) in the expansion yields the random phase approximation (RPA), amounting to a ‘classical-level’ description of non-interacting spin-fluctuation modes. As the hopping term is diagonal in orbital indices, the zeroth-order term involves only the intra-orbital contribution:

\[
\phi^{(0)}_{\alpha\alpha}(q, \omega) = \sum_{k} \frac{1}{\epsilon_{k} - \sigma \Delta + \omega - i\eta},
\]

where the Hartree–Fock (HF) level band energies \(\epsilon_{k} = \epsilon_{k} - \sigma \Delta\) involve the exchange splitting:

\[
2\Delta = [U + (\mathcal{N} - 1)J]m
\]

between the two spin bands. The superscripts \((-\) refer to particle (hole) states above (below) the Fermi energy \(\epsilon_F\). Here the magnetization \(m = 2(S_{\mu}^z)\) is identical for all \(\mathcal{N}\) orbitals in the orbitally degenerate ferromagnetic state. For the saturated ferromagnet, the magnetization \(m\) is equal to the particle density \(n\) for each orbital.

Due to orbital degeneracy, there are only two independent cases of interest corresponding to \(\mu = \nu\) and \(\mu \neq \nu\). Following equation (3), the two corresponding coupled equations at the RPA level are:

\[
\chi_{\alpha\alpha}^{++} = \chi_{0} + \chi_{0}U\chi_{\alpha\alpha}^{--} + (\mathcal{N} - 1)\chi_{0}\chi_{\beta\alpha}^{--},
\]

\[
\chi_{\beta\alpha}^{++} = \chi_{0}\chi_{\alpha\alpha}^{--} + \chi_{0}\chi_{\beta\alpha}^{--} + (\mathcal{N} - 2)\chi_{0}\chi_{\beta\alpha}^{--},
\]

solving which, we obtain

\[
\chi_{\alpha\alpha}^{++} = \frac{1}{\mathcal{N}} \left( \frac{\chi_{0}}{1 - U^+ \chi_0} + \left( \frac{\mathcal{N} - 1}{\mathcal{N}} \right) \left( \frac{\chi_{0}}{1 - U^+ \chi_0} \right) \right),
\]

\[
\chi_{\beta\alpha}^{++} = \frac{1}{\mathcal{N}} \left( \frac{\chi_{0}}{1 - U^+ \chi_0} - \frac{\chi_{0}}{\mathcal{N}} \left( \frac{\chi_{0}}{1 - U^+ \chi_0} \right) \right).
\]
where the two interaction terms above are $U^+ = U + (N - 1)J$ and $U^- = U - J$. The propagators involve linear combinations of in-phase and out-of-phase modes with respect to the orbitals, representing gapless (acoustic) and gapped (optical) branches, respectively. The in-phase mode with effective interaction $U^+$ corresponds to the usual Goldstone mode (acoustic branch), while the out-of-phase mode with effective interaction $U^-$ yields gapped excitations (optical branch [31]).

4. Quantum corrections and effective quantum parameter

Diagrammatic contributions to the first-order quantum correction $\phi^{(1)}$ for the orbitally asymmetric Hamiltonian (1) are shown in figure 1. Structurally, they are similar to the $O(1/N)$ diagrams in the orbitally symmetric case [23], but the different orbital components with appropriate interaction terms are now considered separately. Diagrams (a) and (d) represent corrections to the irreducible propagator due to self-energy corrections, whereas diagrams (b) and (c) represent vertex corrections. The corresponding expressions are as below:

$$
\phi^{(a)}(q, \omega) = \sum_Q \int \frac{d\Omega}{2\pi} \left\{ \left[ U^2 + (N - 1)J^2 \right] \chi^{++}_{\alpha\alpha}(Q, \Omega) + 2(N - 1)UJ \chi^{+}_{\beta\alpha}(Q, \Omega) + (N - 1)(N - 2)J^2 \chi^{+}_{\beta\alpha}(Q, \Omega) \right\},
$$

$$
\phi^{(b)}(q, \omega) = -2 \sum_Q \int \frac{d\Omega}{2\pi} \left\{ \left[ U^2 + (N - 1)J^2 \right] \chi^{++}_{\alpha\alpha}(Q, \Omega) + 2(N - 1)UJ \chi^{+}_{\beta\alpha}(Q, \Omega) + (N - 1)(N - 2)J^2 \chi^{+}_{\beta\alpha}(Q, \Omega) \right\},
$$

$$
\phi^{(c)}(q, \omega) = \sum_Q \int \frac{d\Omega}{2\pi} \left\{ \left[ U^2 + (N - 1)J^2 \right] \chi^{++}_{\alpha\alpha}(Q, \Omega) + 2(N - 1)UJ \chi^{+}_{\beta\alpha}(Q, \Omega) + (N - 1)(N - 2)J^2 \chi^{+}_{\beta\alpha}(Q, \Omega) \right\},
$$
\[
\times \left(\frac{1}{\epsilon_{k^-} - \epsilon_k + \omega + \Omega - i\eta}\right)^2
\times \sum_{k'} \left(\frac{1}{\epsilon_{k'-q} + \epsilon_{k'}^- + \omega - \Omega - i\eta}\right),
\]
\[
\phi^{(d)}(q, \omega) = \sum_{Q} \int \frac{d\Omega}{2\pi i} \left[U^2 + (N - 1)J^2\right]
\times \sum_{k} \left(\frac{1}{\epsilon_{k^-} - \epsilon_k + \omega + \Omega - i\eta}\right)^2
\times \left(\frac{1}{\epsilon_{k^-} - \epsilon_k + \omega - \Omega - i\eta}\right),
\]
where the kernels \(\Gamma_{\alpha\alpha}^+\) and \(\Gamma_{\alpha\beta}^+\) for the spin-wave propagators are defined in terms of \(\chi_{\alpha\alpha}^-\) and \(\chi_{\alpha\beta}^+\), and from equations (11) and (12) are obtained as:
\[
[\Gamma_{\alpha\alpha}^+]_{\text{RPA}} = \frac{[\chi_{\alpha\alpha}^-]_{\text{RPA}} - \chi_0}{\chi_0} = \frac{1}{N}
\times \left[U^+ \frac{1}{1 - U^+ \chi_0} + (N - 1)U^- \frac{1}{1 - U^- \chi_0}\right],
\]
\[
[\Gamma_{\alpha\beta}^+]_{\text{RPA}} = \frac{[\chi_{\alpha\beta}^+]_{\text{RPA}}}{\chi_0} = \frac{1}{N}
\times \left[U^+ \frac{1}{1 - U^+ \chi_0} - \frac{U^-}{1 - U^- \chi_0}\right].
\]

It should be noted that the quantum corrections (13)–(16) are all well defined as \(U \to \infty\), highlighting the non-perturbative nature of the present expansion scheme. Also, the terms with coefficient \((N - 2)\) in equations (13)–(16), which result from orbital-index summation with the condition \(\mu \neq v \neq \alpha\) in figure 1 diagrams, are completely absent in the two-orbital case. The presence of several such terms with coefficient \((N - 2)\) in the exact Goldstone-mode cancelation shown below highlights the non-trivial nature of the extension from two orbitals to \(N\) orbitals.

To demonstrate the exact cancelation and hence the Goldstone mode for \(q = 0\), we note that the boson term (quantity in braces) in equation (14) for \(\phi^{(b)}\) can be expressed as:
\[
U\Gamma_{\alpha\alpha}^+ + (N - 1)J\Gamma_{\alpha\beta}^+ = \left\{U^2 + (N - 1)J^2\right\}\chi_{\alpha\alpha}^+ + \left[2(N - 1)U^2 + (N - 1)(N - 2)J^2\right]\chi_{\alpha\beta}^+ / \chi_0.
\]
which is identical to the boson term in equation (13) for \(\phi^{(a)}\).

The above identity is shown in the appendix. Similarly, using equations (17) and (18), the kernels in the boson term of equation (15) for \(\phi^{(c)}\) can be written in terms of \(\chi^+\) and \(\chi_0\). Using the above substitutions in equations (13)–(16), and with \(\epsilon_{k^-}^+ - \epsilon_k^- = 2\Delta\) for \(q = 0\), we obtain:
\[
\phi^{(1)}(q = 0, \omega) = \phi^{(a)} + \phi^{(b)} + \phi^{(c)} + \phi^{(d)}
= \sum_{Q} \int \frac{d\Omega}{2\pi i} \left(\frac{1}{2\Delta + \omega - i\eta}\right)^2
\times \sum_{k} \left(\frac{1}{\epsilon_{k^-}^+ - \epsilon_k^- + \omega - \Omega - i\eta}\right)
\times \left[(U^2 + (N - 1)J^2)\chi_{\alpha\alpha}^+ + (N - 1)UJ + (N - 1)(N - 2)J^2\chi_{\alpha\beta}^+\right]
\times \left[(U^2 + (N - 1)J^2)\chi_{\alpha\alpha}^+ + (N - 1)UJ + (N - 1)(N - 2)J^2\right]
\times \chi_{\beta\alpha}^+ + \left[U^2 + (N - 1)J^2\right] \chi_0],
\]

which yields identically vanishing contributions for each spin-fluctuation mode \(Q\). We note that this mode-by-mode exact cancelation is quite independent of the spectral distribution of the spin-fluctuation spectrum between collective spin-wave and particle–hole Stoner excitations. Furthermore, the cancelation holds for all \(\omega\), indicating no spin-wave amplitude renormalization, as expected for the saturated ferromagnet in which there are no quantum corrections to magnetization.

We shall now obtain an effective quantum parameter which approximately determines the strength of the quantum corrections obtained above. Due to the uncorrelated nature of the inter-orbital spin fluctuations \((S_{\alpha\alpha}^z S_{\beta\beta}^z) = 0\), the contribution of the inter-orbital propagator \(\chi_{\alpha\beta}^+\) in equation (13) is much smaller than the contribution of the intra-orbital propagator \(\chi_{\alpha\alpha}^+\), and hence only the contribution from the orbital-diagonal term \([U^2 + (N - 1)J^2]\chi_{\alpha\alpha}^+\) essentially survives, leaving an overall factor \([U^2 + (N - 1)J^2]\) on carrying out the \(Q, \Omega\) integration. Comparing with the corresponding factor \([U + (N - 1)J^2]/[U + (N - 1)J^2]\) obtained for the equivalent single-orbital case (with identical exchange splitting) yields an overall relative factor of \([U^2 + (N - 1)J^2]/[U + (N - 1)J^2]\). Similarly, the quantum corrections \(\phi^{(b)}, \phi^{(c)}\) and \(\phi^{(d)}\) also yield the same overall factor.

Thus, the total first-order quantum correction approximately bears an overall relative factor of \([U^2 + (N - 1)J^2]/[U + (N - 1)J^2]\) compared to the equivalent single-orbital case. This relative factor thus plays the role of an effective quantum parameter which determines the strength of the correlation-induced quantum corrections in a realistic multi-band metallic ferromagnet with arbitrary intra- and inter-orbital Coulomb interactions. This quantum parameter is exact in the orbitally independent limit \(J/U \to 0\) where it approaches 1, and in the orbitally symmetric limit \(J/U \to 1\) where it approaches 1. Also, the quantum parameter falls rapidly with Hund’s coupling \(J\), especially for large \(N\), highlighting the important role of orbital degeneracy and Hund’s coupling in stabilizing metallic ferromagnetism by suppressing the quantum corrections.
5. Quantum corrections to spin stiffness

As the Goldstone mode is explicitly preserved in our approach, it allows investigation of correlation effects on spin stiffness and hence on the ferromagnetic stability with respect to long wavelength fluctuations. Here, we will evaluate the first-order quantum correction to spin stiffness exactly and then compare its $J$ dependence with that of the effective quantum parameter obtained above. This quantitative comparison will highlight the usefulness of the effective quantum parameter.

The first-order quantum correction to spin stiffness is obtained by expanding $\phi^{(1)}(q)$ for small $q$ as in the two-orbital case [25]. There is no quantum correction to the delocalization contribution ($\nabla^2 \epsilon_k$) in the spin stiffness constant; only the exchange contribution in the spin stiffness is renormalized by the surviving second-order terms in $\delta \equiv \epsilon_k - \epsilon_{k-q}$, and we obtain for the first-order quantum correction to spin stiffness:

$$
D^{(1)} = 2 \Delta U^+ \phi^{(1)}/q^2 = \frac{1}{d} \left( \frac{U}{(2\Delta)^3} \right) \sum_Q \int \frac{d\Omega}{2\pi i} \left[ \sum_{k,k'} \frac{\nabla \epsilon_{k'}}{\epsilon_{k'} - \epsilon_{k+Q} - \Omega - i\eta} \right.
$$

$$
\times \left( \sum_{k,k'} \frac{\nabla \epsilon_{k'}}{\epsilon_{k'} - \epsilon_{k+Q} - \Omega - i\eta} \right)
$$

$$
\times \left( \sum_{k,k'} \frac{1}{\epsilon_{k+Q} - \epsilon_{k'} - \Omega - i\eta} \right)
$$

$$
\times \left( \sum_{k,k'} \frac{\nabla \epsilon_{k'}}{\epsilon_{k'} - \epsilon_{k+Q} - \Omega - i\eta} \right)
$$

$$
\times \left( \sum_{k,k'} \frac{1}{\epsilon_{k+Q} - \epsilon_{k'} - \Omega - i\eta} \right)
$$

$$
\times [U^2 + (N-1)J^2] + \left( \sum_{k,k'} \frac{1}{\epsilon_{k+Q} - \epsilon_{k'} - \Omega - i\eta} \right)
$$

$$
\times \left( \frac{\nabla \epsilon_{k'}}{\epsilon_{k'} - \epsilon_{k+Q} - \Omega - i\eta} \right)
$$

(21)

where the effective interactions:

$$
U^\text{e.f.} = U^2 + (N-1)J^2 \chi_{\sigma\sigma} + 2(N-1)UJ
$$

$$
+ (N-1)(N-2)J^2 \chi_{\sigma\sigma},
$$

$$
U^\text{eff} = U_0^\text{eff} - (U^2 + (N-1)J^2) \chi_0.
$$

Evaluation of quantum corrections for the two-orbital case has been discussed earlier [25]. The calculated quantum correction to spin stiffness, normalized so that it equals 1 for $J/U = 0$, is plotted in figure 2 as a function of $J/U$ for $N = 5$ orbitals. Here we have considered the sc lattice, band filling $n = 0.3$, $t' = 0.25$, and fixed $U + (N-1)J = 1.5$ W. Also shown for comparison is the quantum parameter obtained above, which is seen to be exact in the orbital independent ($J/U \rightarrow 0$) and the orbital symmetric ($J/U \rightarrow 1$) limits, and it remains quite close to the calculated corrections even in the intermediate range, as expected from the uncorrelated nature of inter-orbital spin fluctuations [31].

Including the quantum correction to spin stiffness as obtained above, the renormalized spin stiffness is then obtained as:

$$
D = D^{(0)} - D^{(1)},
$$

(23)

where the bare-level (RPA) spin stiffness:

$$
D^{(0)} = \frac{1}{d} \left[ \frac{1}{2} \left( \nabla^2 \epsilon_k \right) - \frac{\langle (\nabla \epsilon_k)^2 \rangle}{2\Delta} \right]
$$

(24)

involves the two characteristic terms representing delocalization energy loss and exchange energy gain upon spin twisting.

6. Effective orbital degeneracy

In section 5 we obtained an effective quantum parameter $[U^2 + (N-1)J^2] \chi_{\sigma\sigma}$ in terms of the physically important parameters $U^2 + (N-1)J^2$, $\chi_{\sigma\sigma}$ for a multi-orbital band ferromagnet. This quantum parameter determines, in analogy with $1/N$ for the orbitally symmetric $N$-orbital Hubbard model and $1/S$ for quantum spin systems, the strength of quantum corrections to magnetic excitation energies. The quantum parameter is strongly suppressed by Hund’s coupling $J$, and rapidly approaches the limiting value of $1/N$, especially for large $N$.

This suggests that quantum corrections in a realistic multi-band ferromagnet with arbitrary $N$, $U$, $J$ can be approximately investigated in terms of the orbitally symmetric Hubbard model (having identical intra- and inter-orbital local spin interactions):
We have taken the lattice parameter $t_0 \approx 5$ within the bcc lattice with realistic bandwidth $W = 16t = 3.2$ eV and $J / U \approx 1 / 4$, and the interaction strength $U$ of the order of bandwidth $W$ as appropriate for a strongly correlated system. This yields $U \approx W = 16t = 3.2$ eV and $J = 0.8$ eV, which are close to the parameter values considered in the band structure [14] and constrained LDA [9] studies for iron. With these parameters, and $N = 5$ corresponding to the five 3d orbitals in iron, the effective quantum parameter $[U^2 + (N - 1)J^2] / [U + (N - 1)J] \approx \frac{1}{2}$, which corresponds to $N_{\text{eff}} \approx 3$ within the $N$-orbital Hubbard model. An appreciable magnitude of second-neighbor hopping as considered here is reasonable as second neighbors on a bcc lattice are only about $15\%$ more distant than the nearest neighbors.

In the following, we will obtain first-order quantum corrections using realistic multi-band Hamiltonian parameters as above, and determine characteristic magnetic properties such as spin stiffness, magnon energies, electron self-energy and density of states, and finite-temperature spin dynamics.

### 6.1. Spin stiffness

Figure 3 shows the renormalized spin stiffness for the bcc lattice for different effective number of orbitals $N_{\text{eff}}$. The spin stiffness at low band filling is negative for $N_{\text{eff}} = 1$ and rapidly becomes positive with increasing $N_{\text{eff}}$, indicating the strong role of orbital degeneracy in stabilizing ferromagnetism. The optimum filling occurs near $n = 0.5$ for finite $N_{\text{eff}}$. With realistic parameters taken as above, the calculated values of the renormalized spin stiffness (290 meV Å$^2$ at $n = 0.51$) are close to the measured value of 280 meV Å$^2$ for iron obtained from neutron scattering studies [32].

Figure 3. The renormalized spin stiffness as a function of band filling for different effective number of orbitals $N_{\text{eff}}$, evaluated for the bcc lattice with realistic bandwidth $W = 16t = 3.2$ eV, $t'/t = 0.5$, interaction term $U_{\text{eff}} = 6.4$ eV $\approx 2W$, and lattice parameter $2a = 2.87$ Å for Fe. The measured value for Fe is 280 meV Å$^2$.

### 6.2. Renormalized magnon dispersion

The renormalized magnon energy $\omega_q$ for mode $q$ was obtained from the pole condition $[1 - U \text{ Re} \phi(q, -\omega_q) = 0]$ in the total spin-fluctuation propagator:

$$\chi^{+}(q, \omega) = \frac{\phi(q, \omega)}{1 - U \phi(q, \omega)}$$

(28)

where the irreducible particle–hole propagator:

$$\phi = \phi^{(0)} + \frac{1}{N_{\text{eff}}} \phi^{(1)}$$

(29)

up to first order in $1/N_{\text{eff}}$. The numerical evaluation of the quantum correction $\phi^{(1)}$ by integrating over the intermediate $(Q, \Omega)$ states has been discussed earlier [24]. Both collective and Stoner excitations are included. While the bare particle–hole propagator $\phi^{(0)}(q, \omega)$ remains real in the relevant $\omega$ range, the quantum correction $\phi^{(1)}(q, \omega)$ is complex for any finite $\omega$ due to the coupling with charge fluctuations, resulting in finite zero-temperature magnon damping [22].

Figure 4 shows the renormalized magnon dispersion for the bcc lattice for different $N_{\text{eff}}$. The magnon energy exhibits a Goldstone mode at both $\Gamma$ and M, as they are equivalent points in our extended Brillouin zone which extends from $-\pi/a$ to $\pi/a$ in each direction, whereas the bcc lattice parameter is $2a$. We find that for $N_{\text{eff}} = 3$ and 5, the magnon energy renormalization is nearly momentum independent in the $\Gamma$–X, X–M, and M–R directions. However, near $(\pi/2, \pi/2, \pi/2)$ between $\Gamma$–R, the magnon energy is softened relatively more strongly.

### 6.3. Finite-temperature spin dynamics

For a spin-$S$ Heisenberg ferromagnet, the temperature dependence of magnetization can be obtained by self-
constantly solving the set of three coupled equations [33]:

\[ \langle S_z \rangle_T = \frac{(S - \Phi) (1 + \Phi)^{2S+1} + (S + 1) \Phi^{2S+1}}{(1 + \Phi)^{2S+1} - \Phi^{2S+1}} \]  

\[ \Phi = \sum Q \frac{1}{e^{\beta \Omega_Q} - 1} \]  

\[ \Omega_Q = \frac{\Omega_Q(S_z)_T/(S_z)_0}{(32)} \]

where \( \Phi \) is the magnon amplitude in terms of the thermally renormalized magnon energies \( \Omega_Q \).

For our itinerant model, an equivalent Heisenberg model description will therefore allow for an approximate analysis of the finite-temperature spin dynamics as above. An approximate equivalence to an effective Heisenberg ferromagnet is discussed below in terms of the renormalized magnon energies \( \Omega_Q \) as evaluated in subsection 6.2 and with \( 2S = mN_{\text{eff}} \) for the effective spin quantum number, where \( m \) is the magnetization for each orbital. While the dominant finite-temperature renormalizations in an itinerant ferromagnet involving the electronic density, magnetization, and magnon energies (all related to the thermal renormalization of the \( \omega \) term in the magnon propagator) are self-consistently incorporated in this picture, it neglects the finite-temperature correction of the induced spin couplings.

In an itinerant model, it is the exchange of the particle–hole propagator which mediates the effective spin couplings. In our \( N_{\text{eff}} \)-orbital model, with local Coulomb interaction \( U_{\text{eff}}/N_{\text{eff}} \) as in equation (25), the effective spin couplings between the total spins at sites \( i \) and \( j \) will be given by \( J_{ij} = N_{\text{eff}} (U_{\text{eff}}/N_{\text{eff}})^2 \phi_{ij} \), where the factor \( N_{\text{eff}} \) results from the sum of the (orbitally diagonal) spin couplings. Now, for a spin-\( S \) Heisenberg ferromagnet with couplings \( J_{ij} \), the magnon dispersion \( \Omega_Q = 2S \sum (J_{ij}/2)[1 - \exp(iQ \cdot r_{ij})] \) has an explicit \( 2S \) factor. Comparing with the magnon dispersion \( \Omega_Q \) obtained for the \( N_{\text{eff}} \)-orbital itinerant model, which is explicitly independent of \( N_{\text{eff}} \) and has an \( m \) factor, implies that \( 2S = mN_{\text{eff}} \).

Another indicator of this equivalence is provided by the low-temperature magnetization reduction due to thermal magnon excitations. From equation (30) for the spin model, the low-temperature \( (\Phi \ll 1) \) reduction in magnetization is given by \( \langle S_z \rangle_T \approx S - \Phi \), which yields a relative factor of \( (1/S) \) in the thermal reduction term. Similarly for the itinerant model, the low-temperature magnetization reduction resulting from the spectral-weight transfer due to the electron–magnon coupling self-energy yields an explicit factor of \( 1/mN_{\text{eff}} \), as in equation (37), again pointing to the equivalence \( 2S = mN_{\text{eff}} \). We will therefore calculate the finite-temperature magnetization from the self-consistent Callen equations for an equivalent spin-\( S \) Heisenberg model [33], with \( 2S = mN_{\text{eff}} \) and the renormalized magnon energies \( \Omega_Q \) as obtained above including the correlation-induced quantum corrections incorporated in terms of self-energy and vertex corrections.

Instead of performing the \( Q \) summation in equation (31) exactly, it is instructive to separately consider the long- and short wavelength contributions:

\[ \Phi = \sum Q \frac{1}{e^{\beta \Omega_Q} - 1} = \sum_{Q>\Lambda} \frac{1}{e^{\beta \Omega_Q} - 1} + \sum_{Q<\Lambda} \frac{1}{e^{\beta \Omega_Q} - 1} \]  

\[ (33) \]

where \( \Lambda \) represents an appropriate momentum cut-off. The small-\( Q \) contribution can be evaluated explicitly by integration, whereas the large-\( Q \) contribution can be approximated by a single term corresponding to the ‘dominant mode energy’, since the magnon density of states (DOS) exhibits a pronounced peak at this energy corresponding to short wavelength modes, as shown in figure 5. Thus, \( \Phi = \Phi_{LW} + \Phi_{DMA} \), corresponding to the long wavelength contribution and the dominant mode approximation. The evaluation of \( \Phi_{LW} \) is discussed below.

For small-\( Q \) modes, the magnon energy \( \tilde{\Omega}_Q = \tilde{D}Q^2 \) in terms of the thermally renormalized spin stiffness at temperature \( T \):

\[ \tilde{D} = D \langle S_z \rangle_T / \langle S_z \rangle_0 \]  

\[ (34) \]
The renormalized electronic DOS is evaluated by incorporating the self-energy correction due to electron–magnon coupling. A spin-down particle (energy $\epsilon_{k}^{\downarrow} > \epsilon_{F}$) can decay into a magnon and a spin-up particle, resulting in considerable spin-down spectral-weight transfer to just above the Fermi energy. Since we are considering a saturated ferromagnet with no spin-down density, a spin-up particle cannot decay into a spin-down particle due to spin conservation, and hence there are no quantum corrections at $T=0$ to the spin-up DOS. As the results of this subsection are qualitative in nature, they refer to the $N$-orbital Hubbard model parameters $U$ and $N$ rather than $U_{\text{eff}}$ and $N_{\text{eff}}$.

The spin-down self-energy is calculated within an approximate resummation procedure [11] which incorporates particle–particle correlations:

$$\Sigma_{\downarrow}(k, \omega) = \frac{\Sigma_{\downarrow}^{(0)}}{1 - \Sigma_{\downarrow}^{(1)}(k, \omega)/\Sigma_{\downarrow}^{(0)}},$$

where $\Sigma_{\downarrow}^{(0)} = 2\Delta = mU$ is the HF-level self-energy, and the first-order self-energy:

$$\Sigma_{\downarrow}^{(1)}(k, \omega) = \frac{1}{N} U^{2} \sum_{Q} \int \frac{d\Omega}{2\pi i} \rho_{\text{RPA}}^{\pm}(Q, \Omega) \left( \frac{1}{\omega - \Omega - \epsilon_{k}^{\downarrow} + i\eta} \right)$$

$$= \frac{1}{mN} \sum_{Q} \omega - \Omega - \epsilon_{Q}^{\uparrow} - \epsilon_{k-Q}^{\downarrow} + i\eta$$

(where $2\Delta = mU$).

Figure 7 shows the renormalized DOS for $N=3$ and 5 orbitals. The spin-down band HF DOS is also shown for comparison. The spin-down DOS is seen to be renormalized considerably with significant band narrowing, band shift, as well as spectral-weight transfer from the bare band to just above the Fermi energy.

Figure 8 shows the energy momentum dispersion of spin-down electrons in terms of an intensity plot of the renormalized spectral function $A_{k}^{\downarrow}(\omega)$ obtained from the Green’s function:

$$G_{\downarrow}(k, \omega) = \frac{1}{G^{\downarrow}(k, \omega) - \Sigma_{\downarrow}(k, \omega)}.$$  

The bare (HF) dispersion for the minority spin is also plotted for comparison. The renormalization is seen to be especially strong near the X and R points, indicating significant band flattening and mass renormalization, and also the strong non-quasiparticle character of the low-energy minority-spin states near the Fermi energy, as further discussed below.
Figure 7. The spin-resolved DOS for the bcc lattice at band filling \( n = 0.5 \), showing the transfer of spin-\( \downarrow \) spectral weight due to correlation effects and the emergence of non-quasiparticle (NQP) states just above the Fermi energy.

An important aspect in figure 7 is the emergence of new non-quasiparticle (NQP) states just above the Fermi energy at 0 K, corresponding to strongly incoherent spectral function near the X and R points in figure 8. These NQP states are important in view of recent tunneling conductance measurements on Heusler alloy-based magnetic tunneling junctions, where a strong suppression of spin polarization is observed with temperature [4]. This suppression has been attributed to the emergence of NQP states at and below the Fermi energy due to correlation effects arising from the electron–magnon coupling.

7. Conclusions

The correlated motion of electrons in metallic ferromagnets was investigated in terms of a multi-orbital model with \( \mathcal{N} \)-fold orbital degeneracy and arbitrary intra-orbital Coulomb interaction \( U \) and inter-orbital Hund’s coupling \( J \). A spin rotationally symmetric and non-perturbative scheme was developed to study correlation-induced quantum corrections beyond the RPA, wherein self-energy and vertex corrections were incorporated systematically so that the Goldstone mode is explicitly preserved order by order.

An effective quantum parameter \( \frac{U^2+(\mathcal{N}-1)J^2}{(U+(\mathcal{N}-1)J)} \) was obtained which determines, in analogy with \( 1/S \) for quantum spin systems and the inverse-degeneracy parameter \( 1/N \) for the \( \mathcal{N} \)-orbital Hubbard model, the strength of quantum corrections to spin stiffness and magnon energies. The rapid suppression of this quantum parameter with Hund’s coupling \( J \), especially for large \( \mathcal{N} \), provides fundamental insight into the phenomenon of strong stabilization of metallic ferromagnetism by orbital degeneracy and Hund’s coupling. For \( J/U \sim 1/4 \) and \( \mathcal{N} = 5 \), this effective quantum expansion parameter is approximately \( 1/3 \), and hence the error due to neglect of second- and higher-order quantum corrections in our systematic expansion in powers of this quantum parameter was estimated at about 10%.

With realistic bandwidth, interaction, and lattice parameters corresponding to ferromagnetic iron, both the calculated spin stiffness and Curie temperature values obtained were in close agreement with measurements. The correlation-induced quantum corrections to magnon energies were found to reduce the Curie temperature in the dominant mode approximation to nearly half of the RPA result. On including the contribution of long wavelength spin-fluctuation modes, a further nearly 25% reduction was obtained in the calculated Curie temperature, which is an important feature of our Goldstone-mode-preserving approach, especially in view of the overestimation of the Curie temperature in approaches where only local spin-fluctuation modes are included. While the dominant thermal renormalizations in terms of the renormalized magnon amplitude and energies were included in our approach for finite-temperature spin dynamics, it neglected the finite-temperature correction of the induced spin couplings. The strong electronic spectral function renormalization near the X and R points, indicating significant band flattening and mass renormalization, and also the strong non-quasiparticle character of the minority-spin states near the Fermi energy highlight the important role of electron–magnon coupling on electronic spectral properties.

Appendix

The identity used in equation (19) is derived here. From equations (17) and (18), and with \( U = [U^+ + (\mathcal{N}-1)U^-]/\mathcal{N} \) and \( J = [U^+ - U^-]/\mathcal{N} \), we obtain:

\[ \text{(19)} \]
\[ UT_{aa}^{-} + (N - 1)\Gamma_{af}^{-} = \frac{1}{N} \left[ (U^2)^2 + \frac{(N - 1)(U^-)^2}{1 - U^- \chi_0} \right], \]  
\[ \text{which can be written in terms of a superposition:} \]

\[ \frac{1}{N} \left[ (U^2)^2 + \frac{(N - 1)(U^-)^2}{1 - U^- \chi_0} \right] = \frac{A}{N} \left[ 1 - U^- \chi_0 + \frac{N - 1}{1 - U^- \chi_0} \right] + \frac{B}{N} \left[ 1 - U^- \chi_0 + \frac{1}{1 - U^- \chi_0} \right], \]

of the two functions in equations (11) and (12). Solving for \( A \) and \( B \) yields:

\[ A = U^2 + (N - 1)J^2, \]
\[ B = 2(N - 1)(U + (N - 1)(N - 2))J^2, \]

so that in terms of \( \chi_{aa}^{-} \) and \( \chi_{af}^{-} \) from equations (11) and (12), we obtain:

\[ UT_{aa}^{-} + (N - 1)\Gamma_{af}^{-} = \{|U^2 + (N - 1)J^2\} \chi_{aa}^{-} + [2(N - 1)U + (N - 1)(N - 2)J^2] \chi_{af}^{-} \}/\chi_0. \]

References

[1] Schäfer J, Hsingis M, Rotenberg E, Blaha P and Claessen R 2005 Phys. Rev. B 72 155115
[2] Tang W X, Zhang Y, Tudos I, Prokop J, Etzkorn M and Kirschen J 2007 Phys. Rev. Lett. 99 087202
[3] Zhang Y, Buczek P, Sandratskii L, Tang H, Plihal M and Mills D L 2009 Phys. Rev. Lett. 102 177206
[4] Chioncel L, Sakuraba Y, Arrigoni E, Katsnelson M I, Oogane M, Ando Y, Miyazaki T, Burzo E and Lichtenstein A I 2008 Phys. Rev. Lett. 100 086402
[5] For a recent review see for example Vollhardt D, Blümer N, Held K, Kollar M, Schlüpf J, Ulmke M and Wahle J 1999 Adv. Solid State Phys. 38 383
[6] Wolters W, Potthoff M, Hermann T and Wegner T 2001 Paper No. LNP580 Band Ferromagnetism ed K Baberschke, M Donath and W Wolters (Berlin: Springer)
[7] Sánchez-Barriga J et al 2009 Phys. Rev. Lett. 103 267203
[8] Lichtenstein A I and Katsnelson M I 1998 Phys. Rev. B 57 6884
[9] Lichtenstein A I, Katsnelson M I and Kotliar G 2001 Phys. Rev. Lett. 87 067205
[10] Hertz J A and Edwards D M 1973 J. Phys. F: Met. Phys. 3 2174
[11] Hertz J A and Edwards D M 1973 J. Phys. F: Met. Phys. 3 2191
[12] Cooke J F, Lynn J W and Davis H L 1980 Phys. Rev. B 21 4118
[13] Costa A T, Muniz R B and Mills D L 2006 Phys. Rev. B 73 054426
[14] Naito M and Hiroshima D S 2007 J. Phys. Soc. Japan 76 044703
[15] Pajda M, Kudrnovsky J, Turek I, Drchal V and Brun P 2001 Phys. Rev. B 64 174402
[16] Lichtenstein M I and Katsnelson M I 2000 Phys. Rev. B 61 8906
[17] Thoene J, Chadov S, Fecher G, Felser C and Kühler J 2009 J. Phys. D: Appl. Phys. 42 084013
[18] Zhang J, Ye F, Sha H, Dai P, Fernandez-Baca J A and Plummer E W 2007 J. Phys.: Condens. Matter 19 315204
[19] Savrasov S Y 1998 Phys. Rev. Lett. 81 2570
[20] Buczek P, Ernst A, Sandratskii L and Bruno P 2010 J. Magn. Mater. 322 1396
[21] Buczek P, Ernst A and Sandratskii L M 2010 J. Phys.: Conf. Ser. 200 042006
[22] Kamble B and Singh A 2009 Phys. Rev. B 79 064410
[23] Irkhin V Yu and Katsnelson M I 2003 Phys. Rev. B 68 104436
[24] Thoene J, Chadov S, Fecher G, Felser C and Kühler J 2009 J. Phys.: Condens. Matter 19 315204
[25] Savrasov S Y 1998 Phys. Rev. Lett. 81 2570
[26] Buczek P, Ernst A, Sandratskii L and Bruno P 2010 J. Magn. Mater. 322 1396
[27] Irkhin V Yu and Katsnelson M I 2000 Phys. Rev. B 64 174402
[28] Lichtenstein M I and Katsnelson M I 2000 Phys. Rev. B 61 8906
[29] Thoene J, Chadov S, Fecher G, Felser C and Kühler J 2009 J. Phys. D: Appl. Phys. 42 084013
[30] Zhang J, Ye F, Sha H, Dai P, Fernandez-Baca J A and Plummer E W 2007 J. Phys.: Condens. Matter 19 315204
[31] Savrasov S Y 1998 Phys. Rev. Lett. 81 2570
[32] Singh A 2006 Phys. Rev. B 75 224437
[33] Pandey S and Singh A 2008 Phys. Rev. B 78 014414
[34] Singh A 2006 Phys. Rev. B 75 064412
[35] Kamble B and Singh A 2009 Phys. Rev. B 79 064410
[36] Irkhin V Yu and Katsnelson M I 1999 J. Phys.: Condens. Matter 2 7151
[37] Irkhin V Yu and Katsnelson M I 2005 Phys. Rev. B 72 054421
[38] Katsnelson M I, Irkhin V Yu, Chioncel L, Lichtenstein A I and de Groot R A 2008 Rev. Mod. Phys. 80 315
[39] Singh D K, Kamble B and Singh A 2010 Phys. Rev. B 81 064433
[40] Singh D K, Kamble B and Singh A 2010 J. Phys.: Condens. Matter 22 396001
[41] Kamble B 2010 An effective quantum parameter for metallic ferromagnets: role of orbital degeneracy, Hund’s coupling, and quantum corrections PhD Thesis Indian Institute of Technology, Kanpur
[42] Collins M F, Minkiewicz V J, Nathans R, Passell L and Shirane G 1969 Phys. Rev. 179 417
[43] Callen H B 1963 Phys. Rev. 130 890

B Kamble and A Singh