Spin-charge coupling in a band ferromagnet: Magnon-energy reduction, anomalous softening, and damping

Sudhakar Pandey* and Avinash Singh
Department of Physics, Indian Institute of Technology, Kanpur 208016, India
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The effects of correlation-induced coupling between spin and charge fluctuations on spin-wave excitations in a band ferromagnet are investigated by including self-energy and vertex corrections within a systematic inverse-degeneracy expansion scheme which explicitly preserves the Goldstone mode. Arising from the scattering of a magnon into intermediate spin-excitation states (including both magnon and Stoner excitations) accompanied with charge fluctuations in the majority-spin band, this spin-charge coupling results not only in a substantial reduction of magnon energies but also in anomalous softening and significant magnon damping for zone-boundary modes lying within the Stoner gap. Our results are in good qualitative agreement with recent spin-wave excitation measurements in colossal magnetoresistive manganites and ferromagnetic ultrathin films of transition metals.

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I. INTRODUCTION

Recent observations[1–3] of large wave-vector spin-wave (magnon) excitations in ferromagnetic ultrathin films of transition metals using spin-polarized electron energy-loss spectroscopy (SPEELS) are of crucial importance from many perspectives. For example, apart from providing insight into the microscopic mechanism of ferromagnetic ordering, which can be of direct relevance in context of recent interest in ferromagnetic nanostructures having potential technological applications for magnetoelectronic devices,[4] these observations are also of fundamental importance in understanding the electron-spin dynamics in itinerant ferromagnets.[5] This is because these large wave-vector excitations, which distinguish an itinerant ferromagnet from the relatively well understood insulating (Heisenberg) ferromagnet, have remained experimentally unexplored in the past owing to certain characteristic features such as heavy damping and large excitation energy.

Theoretical investigations of spin dynamics in these ultrathin films have been carried out mostly by considering transverse spin fluctuations at the level of random-phase approximation (RPA) in the ferromagnetic state of the Hubbard model.[6–8] However, due to neglect of the strong correlation effects in itinerant ferromagnets, RPA is well known to overestimate the spin-wave energy, spin stiffness, and Curie temperature, etc., as explicitly demonstrated in recent theoretical investigations by incorporating correlation effects beyond RPA.[9,10] Indeed, signature of inherent many-body effects have been found in recent SPEELS (Ref. 3) and angle-resolved photoemission spectroscopy[11–13] (ARPES) studies in the ferromagnetic phase of Fe. These experimental findings of the signature of strong correlation effects, for example, the much lower magnon energy in Fe film than predicted theoretically at RPA level, as observed in SPEELS,[3] and the quasiparticle mass enhancement and reduced bandwidth in comparison to that predicted within the density-functional theory, as observed in ARPES studies,[12] have provided substantial indication of the electron-magnon coupling as the possible origin.

Spin dynamics in the metallic ferromagnetic phase of colossal magnetoresistive (CMR) manganites has also attracted considerable current interest.[14] Recent spin-wave excitation measurements have revealed several anomalous features in the magnon spectrum near the Brillouin-zone boundary.[15–20] These observations are of the crucial importance for a quantitative understanding of the carrier-induced spin-spin interactions and magnon damping and have highlighted the possible limitations of various existing theoretical approaches. For example, the prediction of magnon-phonon coupling as the origin of magnon damping[16] and disorder as the origin of zone-boundary anomalous softening[21] have been ruled out in recent experiments.[18–20] Furthermore, the dramatic difference in the sensitivity of long-wavelength and zone-boundary magnon modes on the density of mobile charge carriers has emerged as one of the most puzzling feature. Observed for a finite range of carrier concentrations, while the spin stiffness remains almost constant, the softening and broadening of the zone-boundary modes show substantial enhancement with increasing hole concentration.[18,19]

Most of the theoretical investigations of spin dynamics in these ferromagnetic manganites have been carried out in the strong-coupling (double-exchange) limit ($J/W \gg 1$) of the ferromagnetic Kondo lattice model (FKLM), where mobile (e_g) electrons in a partially filled band (of bandwidth W) are coupled ferromagnetically (with exchange interaction J) to the localized core (t_{2g}) spins using a variety of approaches.[22] Although providing a good description of magnon damping, these investigations, however, could not satisfactorily account for the observed zone-boundary anomalous softening. In a recent variational investigation, anomalous softening has been demonstrated to be pronounced only in the intermediate-coupling regime ($J/W \sim 1$).[22] Furthermore, in this intermediate-coupling regime, by taking into account the Coulomb repulsion between the mobile electrons, which is the largest energy scale in manganites and often omitted in the conventional FKLM investigations, recent theoretical investigations have also demonstrated the appearance of several realistic features, such as doping-dependent asymmetry of the ferromagnetic phase and enhanced zone-boundary anomalous softening, thereby highlighting the importance of correlated motion of electrons on spin dynamics.[23,24]

It is therefore of interest to investigate theoretically the influence of correlated motion of charge carriers in a band ferromagnet on the spin-wave excitation spectrum, particularly the short-wavelength modes. The objective of the present paper is to investigate the correlation-induced renormalization of spin-wave excitation spectrum over the entire Brillouin zone in the ferromagnetic state of the Hubbard model. We will incorporate correlation effects in terms of self-energy and vertex corrections within a systematic inverse-degeneracy expansion scheme wherein the spin-rotational symmetry and hence the Goldstone mode are explicitly preserved order by order.

The inverse-degeneracy expansion scheme is a systematic expansion in powers of $1/\mathcal{N}$, where $\mathcal{N}$ is the degeneracy of the partially filled (usually d) shell, and has been discussed earlier in detail in terms of an orbitally degenerate Hubbard model,[9]

$$H=\sum_{\mathbf{k}\alpha\sigma}\epsilon_{\mathbf{k}}a^{\dagger}_{\mathbf{k}\alpha\sigma}a_{\mathbf{k}\alpha\sigma}-\frac{U}{\mathcal{N}}\mathbf{S}_i\cdot\mathbf{S}_i, \tag{1}$$

where $\mathbf{S}_i=\Sigma_\alpha\Psi^{\dagger}_{i\alpha}\frac{\boldsymbol{\sigma}}{2}\Psi_{i\alpha}$ is the total spin operator in terms of the electronic field operator $\Psi_{i\alpha}=(a_{i\alpha\uparrow}a_{i\alpha\downarrow})$, and $\alpha=1,2,\ldots,\mathcal{N}$ is the orbital index. In analogy with $1/S$ for quantum spin systems, the inverse-degeneracy parameter $1/\mathcal{N}$ plays the role of $\hbar$ in determining the magnitude of quantum corrections. The inverse-degeneracy approach systematizes the different diagrammatic contributions in powers of $1/\mathcal{N}$, such as for the irreducible particle-hole propagator $\phi(\mathbf{q},\omega)$,

$$\phi(\mathbf{q},\omega)=\phi^{(0)}+\phi^{(1)}+\phi^{(2)}+\cdots, \tag{2}$$

which yields the transverse spin-fluctuation propagator,

$$\chi^{-+}(\mathbf{q},\omega)=\frac{\phi(\mathbf{q},\omega)}{1-U\phi(\mathbf{q},\omega)}. \tag{3}$$

In the broken-symmetry state, this propagator yields both the low-energy (collective) spin-wave excitations and the high-energy (single-particle) Stoner excitations. Spin-rotation symmetry of the Hamiltonian implies a pole $(1-U\phi(0,0)=0)$ in Eq. (3) corresponding to the Goldstone mode *for arbitrary* $\mathcal{N}$. As the Goldstone-mode condition $U\phi(0,0)=1$ is already exhausted by the zeroth-order (classical) term in Eq. (2), it follows that *all* higher-order (quantum) terms must individually vanish for $q,\omega=0$. The inverse-degeneracy expansion therefore explicitly preserves the Goldstone-mode order by order.

In this paper we consider the saturated ferromagnetic state in which the Fermi energy (ϵ_F) lies in the majority-spin band owing to large exchange splitting such that magnetization m is equal to the particle density n. This is similar to the half-metallic ferromagnetic state as observed in the low-temperature ferromagnetic phase of many systems such as manganites[25] and ordered-double perovskites.[26] In Eq. (2), the bare particle-hole propagator,

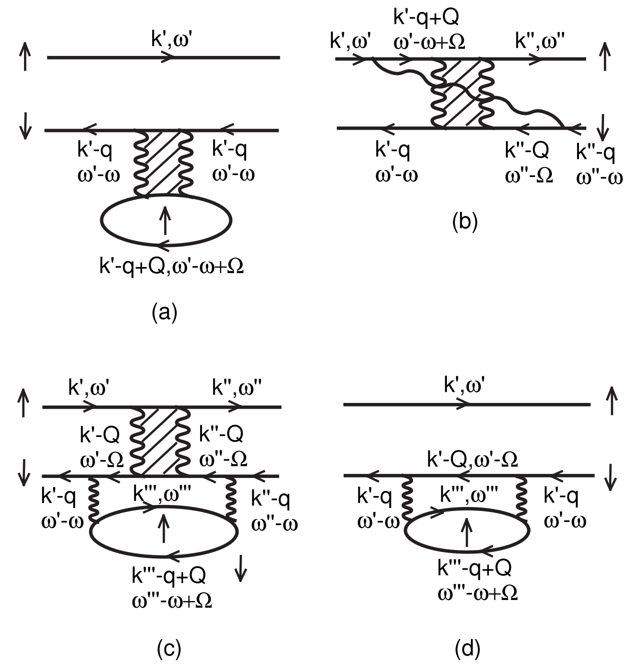

FIG. 1. First-order quantum corrections to the irreducible particle-hole propagator $\phi(\mathbf{q},\omega)$.

$$\phi^{(0)}(\mathbf{q},\omega)\equiv\chi^{0}(\mathbf{q},\omega)=\sum_{\mathbf{k}}\frac{1}{\epsilon^{\downarrow+}_{\mathbf{k}-q}-\epsilon^{\uparrow-}_{\mathbf{k}}+\omega-i\eta}, \tag{4}$$

where $\epsilon^{\sigma}_{\mathbf{k}}=\epsilon_{\mathbf{k}}-\sigma\Delta$ are the Hartree-Fock band energies, $2\Delta=mU$ is the exchange band splitting, and the superscript $+(-)$ refers to particle (hole) states above (below) the Fermi energy ϵ_F. In terms of this bare particle-hole propagator, the RPA ladder sum,

$$\chi^{-+}_{\mathrm{RPA}}(\mathbf{q},\omega)=\frac{\chi^{0}(\mathbf{q},\omega)}{1-U\chi^{0}(\mathbf{q},\omega)}\approx\frac{m_{\mathbf{q}}}{\omega+\omega^{0}_{\mathbf{q}}-i\eta}+S(\mathbf{q},\omega), \tag{5}$$

provides a classical (unrenormalized) description of noninteracting spin-fluctuation modes, which include both the low-energy magnon excitations (amplitude $m_{\mathbf{q}}\approx m$ and energy $\omega^{0}_{\mathbf{q}}$) and the high-energy Stoner excitations $S(\mathbf{q},\omega)$.

The first-order quantum corrections $\phi^{(1)}$, obtained recently for the saturated ferromagnetic state,[9] consist of four distinct processes involving self-energy and vertex corrections, as shown diagrammatically in Fig. 1. The expressions for these diagrams have been given earlier.[9] As required from the spin-rotation symmetry, the net quantum correction $\phi^{(1)}$ vanishes identically for $q,\omega=0$ due to an exact cancellation in order to explicitly preserve the Goldstone mode in the ferromagnetic state. Moreover, this cancellation holds for all ω at $q=0$, indicating no spin-wave amplitude renormalization, as expected for the saturated ferromagnet in which there are no quantum corrections to magnetization.

II. SPIN-CHARGE COUPLING

Keeping terms up to first order in ϕ, the spin-fluctuation propagator (3) can be expressed as

$$\chi^{-+}(\mathbf{q},\omega) = \frac{1}{[\chi^{-+}_{\mathrm{RPA}}(\mathbf{q},\omega)]^{-1} - \Sigma(\mathbf{q},\omega)} \tag{6}$$

in terms of the first-order magnon self-energy $\Sigma(\mathbf{q},\omega) = U^2\phi^{(1)}(\mathbf{q},\omega)$. From the expressions for the different contributions to the quantum correction $\phi^{(1)}(\mathbf{q},\omega)$, it is seen that the first-order magnon self-energy has the following approximate structure:

$$\Sigma(\mathbf{q},\omega) = \sum_{\mathbf{k},\mathbf{Q}} \int \frac{d\Omega}{2\pi i} \chi^{-+}_{\mathrm{RPA}}(\mathbf{Q},\Omega)\Gamma^2\Pi^0(\mathbf{k},\mathbf{q}-\mathbf{Q},\omega-\Omega), \tag{7}$$

highlighting the spin-charge coupling in the ferromagnetic state with the charge fluctuation term

$$\Pi^0(\mathbf{k};\mathbf{q}-\mathbf{Q},\omega-\Omega) = \frac{1}{\epsilon^{\uparrow+}_{\mathbf{k}-\mathbf{q}+\mathbf{Q}} - \epsilon^{\uparrow-}_{\mathbf{k}} + \omega - \Omega - i\eta} \tag{8}$$

in the majority-spin band. This correlation-induced coupling between the spin and charge fluctuations arises from the scattering of a magnon (with energy $-\omega=\omega^0_{\mathbf{q}}$) into intermediate spin-excitation states accompanied by charge fluctuations in the majority-spin band. These intermediate states include both the magnon excitations (with energy $-\Omega=\Omega^0_{\mathbf{q}}$) and Stoner excitations (spread over the Stoner continuum). This spin-charge coupling is similar to the three body correlations between the Fermi-sea electron-hole pair and a magnon considered in the recent variational investigation.[22]

In Eq. (7), Γ represents the interaction vertex for the spin-charge coupling and is given by

$$\Gamma(\mathbf{k};\mathbf{q},\omega;\mathbf{Q},\Omega) = U^2\left(\chi^0(\mathbf{k};\mathbf{q},\omega) - \frac{1}{2\Delta'(\mathbf{q},\omega;\mathbf{Q},\Omega)}\right), \tag{9}$$

where

$$\frac{1}{2\Delta'(\mathbf{q},\omega;\mathbf{Q},\Omega)} \equiv \frac{1}{\chi^0(\mathbf{Q},\Omega)}\sum_{\mathbf{k}'} \chi^0(\mathbf{k}';\mathbf{q},\omega)\chi^0(\mathbf{k}';\mathbf{Q},\Omega), \tag{10}$$

and

$$\chi^0(\mathbf{k};\mathbf{q},\omega) \equiv \frac{1}{\epsilon^{\downarrow+}_{\mathbf{k}-\mathbf{q}} - \epsilon^{\uparrow-}_{\mathbf{k}} + \omega - i\eta}. \tag{11}$$

This representation of the magnon self-energy, with the structure of the spin-charge interaction vertex as in Eq. (9), brings out the similarity with the corresponding result for the ferromagnetic Kondo lattice model,[27] where the term $1/2\Delta'(\mathbf{q},\omega;\mathbf{Q},\Omega)$ is simply equal to $1/(2\Delta+\omega)$. For the Hubbard model as well, the two terms in the $\mathbf{k}'$ summation in Eq. (10) decouple for $q=0$, and the term $1/2\Delta' = 1/(2\Delta+\omega)$. Generally, the term $1/2\Delta'$ has weak momentum dependence due to the averaging over momentum $\mathbf{k}'$.

For $q=0$, the spin-charge interaction vertex Γ and the magnon self-energy vanish identically, and the Goldstone mode is therefore explicitly preserved. For small q, $\Gamma^2 \sim (\mathbf{q}.\boldsymbol{\nabla}\epsilon_{\mathbf{k}})^2$, indicating short-range interaction. Also, the spin-charge coupling results in a quantum correction only to the exchange contribution to the spin stiffness as required; quantum corrections to the delocalization contribution of the type $(\mathbf{q}.\boldsymbol{\nabla})^2\epsilon_{\mathbf{k}}$ cancel exactly.[9]

The overall strength of this spin-charge interaction vertex in Eq. (9) is enhanced as $\sim(1/m)^2$ with decreasing band filling $n=m$. This results in an enhancement of the magnon self-energy as $(1/m)^2$, accounting for the two factors of m from the $\mathbf{k}$ summation and the magnon amplitude in Eq. (7). This behavior of the magnon self-energy with band filling has been investigated quantitatively with respect to both magnon damping and anomalous softening, as discussed later.

To illustrate the correlation-induced renormalization of spin-wave excitations, we have carried out quantitative investigations mostly for the square and simple-cubic (sc) lattices with band dispersion

$$\epsilon_{\mathbf{k}} = -2t\sum_{\mu}\cos(k_\mu a) + 4t'\sum_{\mu<\nu}\cos(k_\mu a)\cos(k_\nu a), \tag{12}$$

where t and t' refer to the nearest- and next-nearest-neighbor hoppings, respectively, and $\mu,\nu=x,y,z$. For the spin stiffness calculation, we have also considered the body–centered-cubic lattice with band dispersion

$$\epsilon_{\mathbf{k}} = -8t\cos(k_x a/2)\cos(k_y a/2)\cos(k_z a/2) + 2t'(\cos k_x a + \cos k_y a + \cos k_z a). \tag{13}$$

For the square and bcc lattices, the respective bandwidths are given by $W=8t$ and $W=16t$ as long as $t'<t/2$, as considered in our quantitative investigations. Similarly, for the sc lattice, the bandwidth $W=12t$ for $t'<t/4$. Our consideration for t' is motivated by its favorable role in stabilizing the ferromagnetic ordering, as predicted using a variety of approaches.[28] This has also been demonstrated recently[10] in the Goldstone-mode-preserving investigation due to reduction in correlation-induced exchange contributions to spin stiffness, which have destabilizing tendency on the ferromagnetic state. In the following we set $t=1$.

III. RENORMALIZED MAGNON SPECTRUM

The renormalized magnon energy $\omega_{\mathbf{q}}$ for mode $\mathbf{q}$ is obtained from the pole condition $[1-U\Re\phi(\mathbf{q},-\omega_{\mathbf{q}})=0]$ in Eq. (3) which also corresponds to the peak in the magnon spectral function $A_{\mathbf{q}}(\omega)=\frac{1}{\pi}\mathrm{Im}\,\chi^{-+}(\mathbf{q},-\omega)$, the broadening of which provides a quantitative measure of magnon damping, as discussed in Sec. V. The numerical evaluation of the quantum correction $\phi^{(1)}$ by integrating over the intermediate $(\mathbf{Q},\Omega)$ states has been discussed earlier.[10] We note that the evaluation of $\phi^{(1)}$ was carried out by including contributions of both the magnon and Stoner excitations.

We find that the renormalized magnon energy $\omega_{\mathbf{q}}$ for $\mathcal{N}=1$ is substantially lower in comparison to the bare (RPA) magnon energy $\omega^0_{\mathbf{q}}$ throughout the Brillouin zone, as shown in Fig. 2. This highlights the need to incorporate the strong renormalization due to spin-charge coupling in realistic comparisons. Indeed, in recent SPEELS studies,[3] the measured spin-wave energies in ultrathin films of Fe were found to be significantly smaller than the RPA-level result.

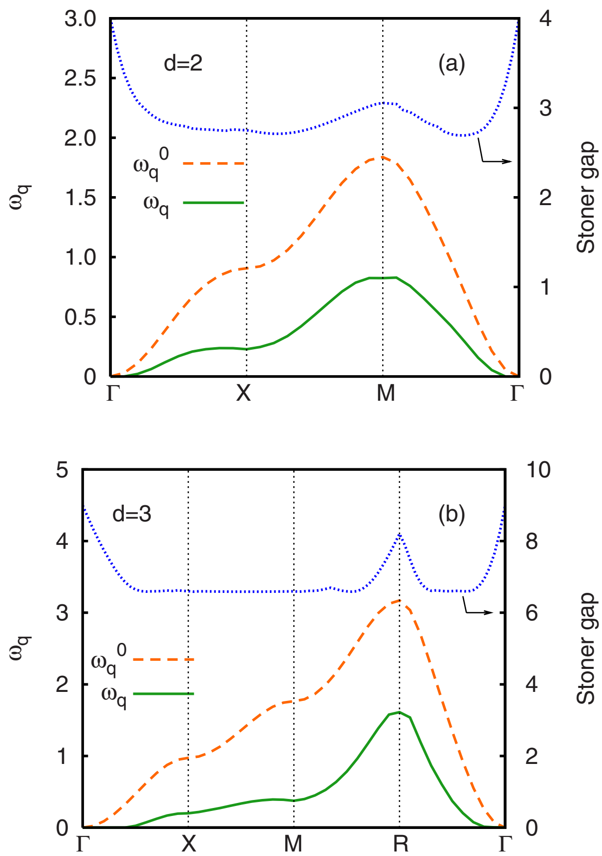

FIG. 2. (Color online) Renormalized magnon energy ($\omega_{\mathbf{q}}$) is reduced significantly in comparison to the bare (RPA) energy (ω_q^0) due to correlation-induced spin-charge coupling, as shown for (a) square and (b) simple-cubic lattices, highlighting the overestimation of RPA, as also reported in a recent spin-wave excitation measurement on the ultrathin film of Fe (Ref. 3). These results have been obtained for $n=0.5$ with $U/W=1$ and $t'=0.45$ for the square lattice and with $U/W=1.5$ and $t'=0.25$ for the cubic lattice. Magnon excitations lie well within the Stoner gap (right scale).

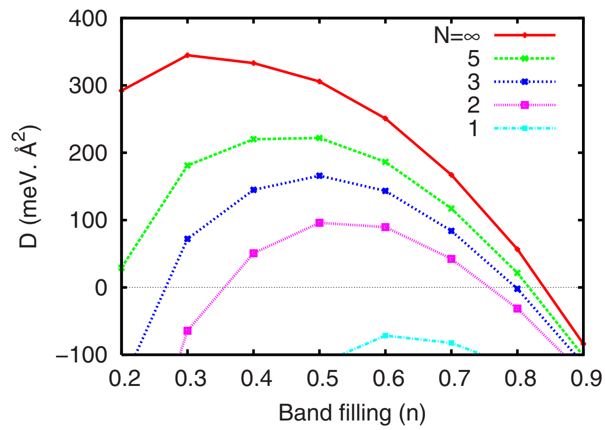

FIG. 3. (Color online) Renormalized spin stiffness for different number of orbitals $\mathcal{N}$, showing the $1/\mathcal{N}$ suppression of quantum corrections with orbital degeneracy, evaluated for the bcc lattice with bandwidth $W=16t=3.2$ eV, Coulomb interaction energy $U=W=3.2$ eV, and lattice parameter $a=2.87$ Å for Fe. The measured value for Fe is 280 meV Å^2.

For an orbitally degenerate ferromagnet (such as Fe with $\mathcal{N}=5$ $3d$ orbitals per site), the bare and renormalized magnon dispersions $\omega_{\mathbf{q}}^0$ and $\omega_{\mathbf{q}}$ shown in Fig. 2 provide, within the first-order approximation, upper and lower bounds, corresponding to $\mathcal{N}\to\infty$ and $\mathcal{N}=1$, respectively. This is because the first-order quantum correction $\phi^{(1)}$ is suppressed by the factor $1/\mathcal{N}$ for an $\mathcal{N}$-orbital-per-site system,[9] and therefore with increasing $\mathcal{N}$ the renormalized dispersion approaches the bare (RPA) dispersion $\omega_{\mathbf{q}}^0$ from below as $\mathcal{N}\to\infty$. While the RPA result ($\mathcal{N}=\infty$) provides the upper bound of the dispersion to all orders, the lower bound ($\mathcal{N}=1$) is correct only to first order as higher-order terms might yield a lower dispersion.

The above $1/\mathcal{N}$ suppression of quantum corrections was obtained for the $\mathcal{N}$-orbital Hubbard model (1) with identical intraorbital interaction $\mathbf{S}_{i\alpha}.\mathbf{S}_{i\alpha}$ and interorbital interaction (Hund's coupling) $\mathbf{S}_{i\alpha}.\mathbf{S}_{i\beta}$.[9] For arbitrary Hund's coupling J, the quantum correction factor has been obtained recently[29] and is approximately given by the expression $(U^2+(\mathcal{N}-1)J^2)/(U+(\mathcal{N}-1)J)^2$, which rapidly approaches $1/\mathcal{N}$ with increasing Hund's coupling J, particularly for large $\mathcal{N}$.

We have quantitatively examined the role of this orbital degeneracy and $1/\mathcal{N}$ suppression of quantum corrections on the spin stiffness. Figure 3 shows the renormalized spin stiffness $D=D^{(0)}-\frac{1}{\mathcal{N}}D^{(1)}$ evaluated for different numbers of orbitals $\mathcal{N}$, where $D^{(0)}$ refers to the bare spin stiffness and $D^{(1)}$ to the first-order quantum correction.[9,10] Here we have considered a bcc lattice with $t'/t=0.5$, bandwidth $W=16t=3.2$ eV, Coulomb interaction energy $U=W=3.2$ eV, and the lattice parameter $a=2.87$ Å for Fe. These parameter values are close to those considered in a recent investigation of spin-wave excitations in Fe using a realistic band-structure calculation,[30] where the interaction energy considered is $U=2.13$ eV (so that the magnetic moment evaluated per Fe atom is equal to $2.12\mu_B$) and the bandwidth from the calculated density-of-states (DOS) plot is seen to be about 4 eV. Our calculated values for the renormalized spin stiffness for $\mathcal{N}=5$ are close to the measured value 280 meV Å^2 for Fe.[31]

In an unsaturated ferromagnet, characterized by vanishing Stoner gap and spin-wave branch merging with the Stoner continuum, quantum corrections will generally involve enhanced Stoner contribution. In addition, there will be finite quantum corrections to magnetization, the O(ω) term in $\phi(\mathbf{q},\omega)$, and hence to the magnon amplitude. These additional features of spin-wave renormalization would need to be included for realistic systems such as transition metals which are not strictly saturated ferromagnets.

However, specifically with regard to bcc iron, it should be noted that the spin-resolved DOS obtained from realistic band-structure calculations show a deep minimum in the minority-spin DOS near the Fermi energy.[30] Well known as a characteristic feature of bcc-lattice transition metals,[32] this feature implies that Stoner excitations are pseudogapped. Furthermore, the majority-spin band is seen to be nearly full, implying a nearly saturated ferromagnet. A particle-hole transformation will result in a partially occupied lower band and a (nearly) empty upper band, as considered in our investigation, justifying the quantitative comparison.

IV. SELF-ENERGY CORRECTION AND ANOMALOUS SOFTENING

In addition to magnon-energy reduction due to quantum corrections (Fig. 2), the renormalized magnon spectrum also shows significant anomalous softening near the zone boundary, particularly along the Γ-X direction, highlighting the anomalous momentum dependence of the quantum correction. While the bare magnon dispersion shows nearly Heisenberg-model behavior with magnon energies at X and M (for $d=2$) in the ratio of 1:2 and at X, M, and R (for $d=3$) in the ratio of 1:2:3, the renormalized magnon dispersion clearly shows strong softening at X relative to M and R. This anomalous softening implies that additional exchange couplings J_2, J_3, J_4, etc., must be included in order to describe the magnon dispersion in terms of an effective localized-spin model. Interestingly, in addition to CMR manganites, significant anomalous softening near the zone boundary has also been reported in recent spin-wave dispersion measurement along Fe[001] for Fe film on W(110) by SPEELS.[3]

Now we investigate the effect of carrier concentration on anomalous softening in the context of CMR manganites. We find that the zone-boundary anomalous softening along the Γ-X direction is enhanced substantially with decreasing band filling, as shown in Fig. 4(a). Indeed, such behavior has been observed in recent spin-wave excitation measurements in the ferromagnetic phase of manganites.[18,19]

This zone-boundary anomalous softening is a direct consequence of the anomalous momentum dependence of the static magnon self-energy $\Sigma = U^2\phi^{(1)}$, as shown in Fig. 4(b). The large enhancement in the magnon self-energy at X yields a large reduction in the renormalized magnon energy. The substantial enhancement in the anomalous softening with decreasing band filling n is due to $\sim 1/n^2$ enhancement of spin-charge coupling as discussed below Eq. (11). These results for zone-boundary anomalous softening are in agreement with the variational calculation,[24] where a proper account of correlated electron motion was found to be necessary for the ferromagnetic manganites.

Figure 5 shows the magnon self-energy $\Sigma(\mathbf{q})$ for the sc lattice. In view of the observed anomalous softening in ferromagnetic manganites, we focus on the q dependence in the Γ-X direction and compare with the Heisenberg form $(1-\cos q)$ corresponding to nearest-neighbor coupling. We find that the bare magnon dispersion is nearly Heisenberg type and shows a weak dependence on band filling. However, the magnon self-energy shows appreciable enhancement at the zone boundary in comparison with the Heisenberg form, implying zone-boundary softening of the renormalized magnon energy $\omega_{\mathbf{q}}^0 - m\Sigma(\mathbf{q})$. Here the magnon self energy $\Sigma(\mathbf{q},\omega)$ was evaluated at the bare magnon energy $\omega = -\omega_{\mathbf{q}}^0$. In contrast, the static self-energy evaluated with $\omega=0$ shows no such zone-boundary enhancement, highlighting the role of dynamical effect. Furthermore, we find that this dynamical effect on anomalous softening becomes less pronounced with increasing band filling.

V. CORRELATION-INDUCED MAGNON DAMPING

We now turn to the role of spin-charge coupling on magnon damping. At the RPA level, magnon damping is absent

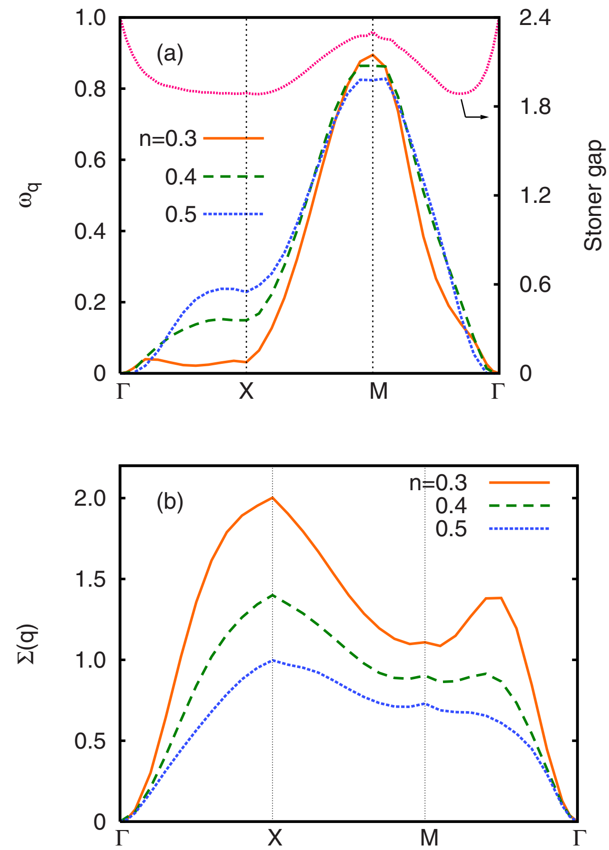

FIG. 4. (Color online) (a) Renormalized magnon spectrum for the square lattice shows anomalous softening along the Γ-X direction, which becomes more pronounced with decreasing band filling n, arising from (b) an anomalous momentum dependence of the magnon self-energy, which has a maximum at X and similar filling dependence. Here $t'=0.45$ and $U/W=1.0$. Magnon excitations lie well within the Stoner gap (right scale) even for the lowest band filling $n=0.3$.

for low-energy modes at zero temperature and arises only at energies above the Stoner gap due to decay into Stoner excitations. However, spin-charge coupling results in finite magnon damping in a band ferromagnet even for magnon modes lying within the Stoner gap. Considering in Eq. (7) only the contribution of collective excitations (5) for simplic-

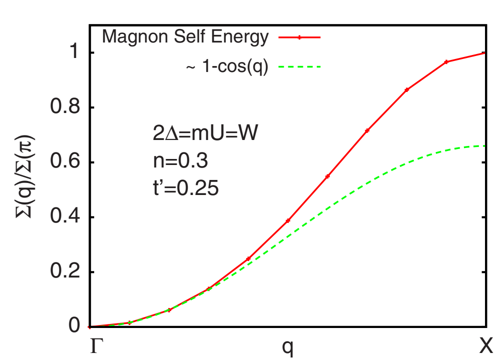

FIG. 5. (Color online) The magnon self-energy $\Sigma(\mathbf{q},\omega=-\omega_{\mathbf{q}}^0)$ for the sc lattice shows significant anomalous enhancement near the zone boundary compared to the Heisenberg form, implying anomalous softening of the renormalized magnon energy.

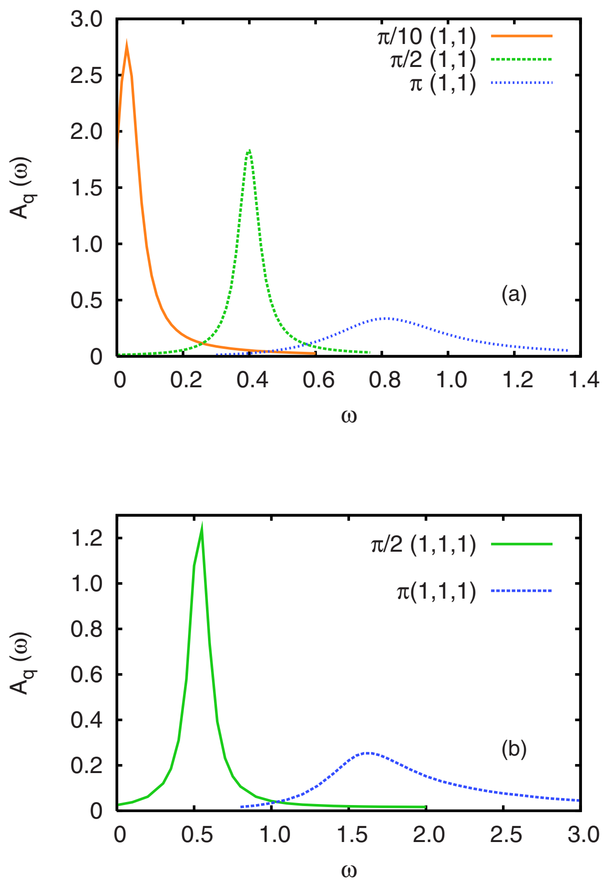

FIG. 6. (Color online) Correlation-induced spin-charge coupling results in substantial damping of magnon modes which becomes more pronounced near the zone boundary, shown here for (a) square lattice with $t'=0.45$, $n=0.4$ and $U/W=1.0$ and (b) simple-cubic lattice with $t'=0.25$, $n=0.5$, and $U/W=1.5$.

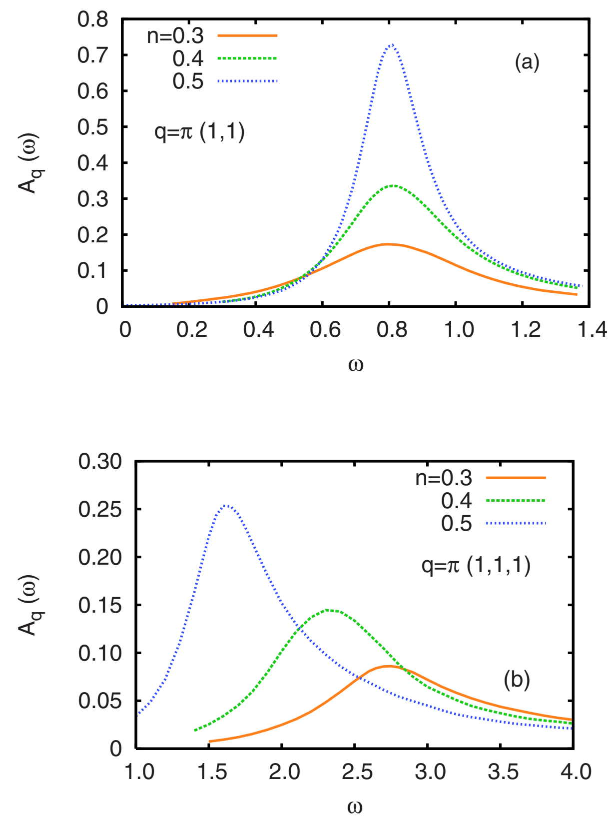

FIG. 7. (Color online) Correlation-induced magnon damping becomes more pronounced with decreasing band filling, as shown for the zone-boundary modes for (a) square lattice with $t'=0.45$ and $U/W=1.0$ and (b) simple-cubic lattice with $t'=0.25$ and $U/W=1.5$.

ity, we obtain the imaginary part of the magnon self-energy,

$$\frac{1}{\pi}\text{Im}\,\Sigma(\mathbf{q},\omega)=\sum_{\mathbf{k},\mathbf{Q}} m_{\mathbf{Q}}\Gamma^2\delta(\epsilon^{\uparrow+}_{\mathbf{k-q+Q}}-\epsilon^{\uparrow-}_{\mathbf{k}}+\omega+\Omega^0_{\mathbf{Q}}), \tag{14}$$

which yields finite magnon damping and linewidth, arising from the scattering of a magnon (energy $\omega^0_{\mathbf{q}}$) into intermediate magnon states (energy $\Omega^0_{\mathbf{Q}}$) accompanied with charge fluctuations (energy $\epsilon^{\uparrow+}_{\mathbf{k-q+Q}}-\epsilon^{\uparrow-}_{\mathbf{k}}$) in the majority-spin band. Magnon damping is further enhanced when the contribution of Stoner excitations is also included.

We have quantitatively examined magnon damping in terms of the magnon spectral function $A_{\mathbf{q}}(\omega)=\frac{1}{\pi}\text{Im}\,\chi^{-+}(\mathbf{q},-\omega)$ using Eq. (3) by including the contribution of both the magnon and Stoner excitations. In order to highlight the role of correlation-induced magnon damping, we have considered relatively large Stoner gap, as seen in Figs. 2 and 4, so that magnon damping is absent at the RPA level. Figure 6 shows the renormalized magnon spectral function $A_{\mathbf{q}}(\omega)$ which is substantially broadened near the zone boundary. This is in broad agreement with the experimental observations of magnon damping in ultrathin transition-metal films[1–3] and ferromagnetic manganites.[15–17,19]

We have also investigated the dependence of magnon damping on band filling n for the zone-boundary mode where damping is most pronounced. With decreasing band filling, damping is enhanced substantially as shown in Fig. 7, thereby highlighting the role of charge fluctuations in the magnon-damping mechanism. Similar influence of carrier concentration has also been observed recently in the ferromagnetic manganites.[19]

Several realistic features such as multilayers and interfaces (due to nonmagnetic substrate and capping layers) have also been observed to substantially influence spin-wave excitations in ferromagnetic ultrathin films of many transition metals.[33–35] These features have been investigated theoretically by taking into account their effects on electronic structure, although only at the RPA level.[7,8] Therefore an extension of our investigation with detailed electronic band structure is desirable for a more quantitative comparison.

VI. CONCLUSION

In conclusion, we have investigated the effects of correlation-induced spin-charge coupling on the spin-wave excitation spectrum in the ferromagnetic state of the Hubbard model by including self-energy and vertex corrections within a Goldstone-mode-preserving scheme. Arising from the scattering of a magnon into intermediate spin excitation states (including both magnon and Stoner excitations) accompanied with charge fluctuations in the majority-spin band, the spin-charge coupling results not only in substantial reduction of magnon energies but also in anomalous softening and damping of magnon modes near the zone boundary lying within the Stoner gap. Both the magnon damping and anomalous zone-boundary softening become more pronounced with decreasing band filling.

Even when the bare magnon dispersion showed nearly Heisenberg form, the renormalized dispersion was shown to exhibit strong softening at X relative to M (for $d=2$) and R (for $d=3$). This anomalous softening at X was shown to be a direct consequence of an anomalous enhancement of the magnon self-energy and implies that the correlated motion of electrons "generates" additional exchange couplings J_2, J_3, J_4, etc., within an equivalent localized-spin model with the same magnon dispersion.

The strong $1/\mathcal{N}$ suppression of quantum corrections due to orbital degeneracy was highlighted by an evaluation of the renormalized spin stiffness for different orbital number $\mathcal{N}$. For the $\mathcal{N}=5$ orbital case relevant for Fe and using realistic bandwidth, Coulomb interaction, and lattice-parameter values, the quantum correction to spin stiffness was found to be about 25% at optimal filling. This provides an estimate of the quantum suppression involved in the measured spin stiffness value of 280 meV Å^2 of Fe,[31] arising from the spin-charge coupling.

These results are of qualitative interest for the ferromagnetic CMR manganites and transition-metal ultrathin films in the context of the observed magnon-energy reduction, anomalous zone-boundary softening, and magnon damping, highlighting the influence of correlated electron motion on their spin dynamics. However, several realistic features need to be incorporated for a quantitative comparison with experiments. These include, for example, in the case of manganites, Hund's coupling of the e_g electrons with the core (t_{2g}) spins and their orbital degree of freedom, which was predicted to have a major influence on the anomalous softening when coupled with the lattice degree of freedom.[36] Similarly, for the ultrathin transition-metal films, a realistic electronic description of the magnetic multilayers as well as of the nonmagnetic substrates and capping layers is necessary in view of the accumulating experimental evidence for their substantial influence on the electron-spin dynamics.[33–35]

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*spandey@iitk.ac.in

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