Quantum spin effects and magnetic short-range order above the Curie temperature

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Using the quantum Heisenberg model calculations with the Green's function technique generalized for arbitrary spins, we found that for a system of small spins, the quantum spin effects induce the additional magnetic short-range order and strongly affect physical properties of magnets. For instance, the spin waves in the present consideration can appear as a result of short-range spin fluctuations and do not require long-range magnetic order. Our spin dynamics investigation even indicates that these quantum spin effects favor the persistence of propagating spin-wave-like excitations above the Curie temperature. These model studies are relevant to itinerant magnets and suggest the increasing influence of quantum spin effects on the magnetic short-range order with a decrease in quantum spin value. The modified expression for the Curie temperature in ferromagnets is obtained.

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A long-standing debate exists over the nature of the paramagnetic state of ferromagnetic materials, particularly in transition metals. Early inelastic neutron experiments[1–3] determined the persistence of spin-wave (SW)-like modes above the Curie temperature (T_C) in both Ni and Fe, and these modes were interpreted as evidence of considerable magnetic short-range order (MSRO) in the paramagnetic state.[4] The presence of MSRO was later supported by spin and angle-resolved photoemission studies.[5,6] This is rather unusual because the majority of magnetism theories assume an absence of SW excitations above T_C. Experimentally, the existence of SW peaks was primarily challenged by Shirane and co-workers.[7] On the theoretical side, it was pointed out that the "local band theory" of Korenman *et al.*[4] did not show how the underlying electronic structure could support strong MSRO.[8,9] Moreover, by applying the spherical model (SM) approximation to the Heisenberg model, Shastry *et al.*[10] concluded that in contrast with the experiment,[2] this model, with reasonable fairly long-ranged interactions, has little MSRO and no SW peaks above T_C in Fe. A similar conclusion was reached by a Monte Carlo spin dynamics simulation of the classical Heisenberg model for the same system.[11] Density-functional spin dynamics studies,[12] however, have found strong MSRO in the form of peaks of dynamic susceptibility above the critical temperature in itinerant system such as Ni and pose again questions about strong MSRO in paramagnetic case already from a theoretical point of view. Later results have been challenged in several theoretical papers.[13,14] Using the semiclassical spin Hamiltonian where the Heisenberg model has been modified to incorporate the amplitude of local spin fluctuations, the authors rejected the possibility of strong MSRO found in Ref. 12. This Hamiltonian, however, is applicable for very localized systems only due to the symmetry violation between longitudinal and transversal fluctuations in the weakly magnetic (itinerant) case. In addition, in Refs. 13 and 14, and in all previous simulations, the influence of quantum spin effects (QSEs) or quantum statistics has been ignored. For the itinerant magnets where the effective spin is expected to be small, such classical spin treatment is likely not appropriate. Below, we show that the inclusion of QSEs increases MSRO for small values of quantum spins and demonstrates that the requirement of SW absence at and above the Curie temperature is no longer valid if the linear spin-wave approximation is eliminated.

The Heisenberg model is widely applied to the itinerant magnet Fe. To a large extent, this approximation should be valid because bcc Fe has rather good local moments,[8,15] and there exists literature[16] showing how a system of interacting local moments can emerge from an itinerant-electron picture. In addition, the important case of small wave vector excitations (long-wavelength limit) can be described using the Heisenberg model with very little or no limitations. However, the quantum nature of spin is usually omitted in the classical Monte Carlo simulation of the Heisenberg model. In the quantum SM, the quantities T_C and susceptibility are proportional to $S(S+1)$. In the classical model, this spin coefficient is S^2. Therefore, the quantum effect contributes a factor $Q_S=1+S^{-1}$. For small S values, this Q_S can become unreasonably large. For example, in the case of nearest-neighbor (NN) coupling of the simple-cubic structure, if $S=1/2$ and $Q_S=3$, which leads to an unphysically large correlation between NN spins $\langle \boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle/S^2>1$. The same problem appeared in Ref. 10, where in the case of strong MSRO and $S=1$, $\langle \boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle/S^2=1.64$. To avoid such difficulties, a pragmatic approach is to scale the relevant quantities by $S(S+1)$, as was done in Ref. 10. As a result, the scaled quantities are independent of S in the SM, so the quantitative results for MSRO and the region of SW existence for $S=1$ and $S=\infty$ are the same.[10] While the classical Heisenberg model can describe some degree of MSRO above T_C, properly included QSE strongly increase this MSRO and affect its influence on observed physical properties, as we will demonstrate below.

For the Heisenberg hamiltonian $H=-\sum_{(ij)}J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j$ in the paramagnetic state, we use the second-order Green's function (GF) technique.[17–20] To calculate the GF $G_{ij}^{\omega}=\langle\langle S_i^-;S_j^+\rangle\rangle_\omega$, one applies the equation of motion twice and then decouples the high-order GF of forms $\langle\langle S_\rho^z S_m^z S_i^-;S_j^+\rangle\rangle_\omega$ and $\langle\langle (S_\rho^+ S_l^- - S_\rho^- S_l^+)S_i^-;S_j^+\rangle\rangle_\omega$. For $S=1/2$ in a one-dimensional system, Kondo and Yamaji[17] decoupled them by using the correction parameter α. Here, we extend their method for an arbitrary S by introducing the following decoupling scheme (for $i\neq\rho$ and $\rho\neq l$):

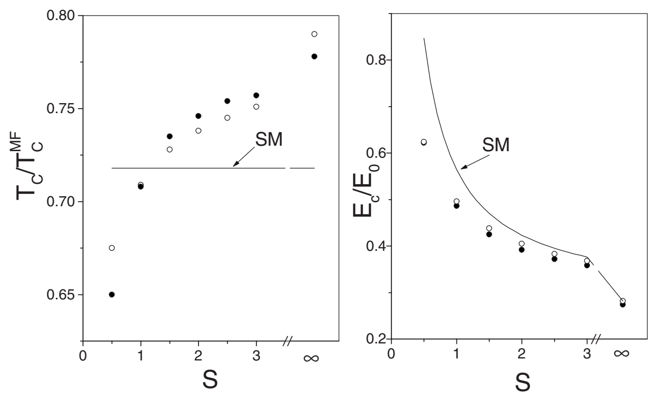

FIG. 1. T_C/T_C^{MF} and E_C/E_0 as a function of S from SM (lines), the high-temperature-expansion methods (close symbols), and our formalism (open symbols) in bcc structure in the NN coupling case.

$$\langle\langle\{S_\rho^+ S_l^- - S_\rho^- S_l^+, S_i^-\}; S_j^+\rangle\rangle_\omega \to (1-\nu_s\delta_{il})\tilde{C}_{i\rho}G_{lj}^\omega - \tilde{C}_{il}G_{\rho j}^\omega,$$

$$\langle\langle\{S_\rho^z S_m^z, S_i^-\}; S_j^+\rangle\rangle_\omega \to (1-\nu_s\delta_{im})\tilde{C}_{m\rho}^{zz}G_{ij}^\omega, \tag{1}$$

where $\tilde{C}_{m\rho}^{zz}=\alpha_{m\rho}C_{m\rho}^{zz}$ and $\tilde{C}_{i\rho}=\alpha_{i\rho}C_{i\rho}$, with $\alpha_{m\rho}=\alpha(1-\delta_{m\rho})+\delta_{m\rho}$ and $C_{m\rho}^{zz}=\langle S_\rho^z S_m^z\rangle$, $C_{li}=\langle S_l^+ S_i^-\rangle=2\langle S_l^z S_i^z\rangle$ are the spin correlations, $\{A,B\}=(AB+BA)/2$ is the symmetric product of operators, and ν_s is a S-dependent constant which will be determined later. For $S=1/2$, spin operator identities require $\nu_s=1$, and Eq. (1) is reduced to the Kondo-Yamaji decoupling.

After decoupling the high-order GF in the equation of motion using Eq. (1), we obtain the following expression for the dynamic susceptibility:

$$\chi^{+-}(\boldsymbol{q},\omega) = -\frac{2\sum_n z_n J_n C_n(1-\gamma_n^{\boldsymbol{q}})}{\omega^2-\omega_{\boldsymbol{q}}^2}, \tag{2}$$

where n is the index of shell, J_n and C_n are J_{ij} and C_{ij}, respectively. $\gamma_n^{\boldsymbol{q}}=z_n^{-1}\Sigma_{\delta_n}(1-e^{i\boldsymbol{q}\cdot\boldsymbol{\delta}_n})$, with z_n being the total number of sites on nth shell and $\boldsymbol{\delta}_n$ being sites on that shell.

The SW excitation spectrum is

$$\omega_{\boldsymbol{q}} = \left\{\sum_n z_n J_n(1-\gamma_n^{\boldsymbol{q}})[D_n - \nu_s J_n \tilde{C}_n - J^{\boldsymbol{q}}\tilde{C}_n]\right\}^{1/2}, \tag{3}$$

where $D_n=N^{-1}\Sigma_{\boldsymbol{k}}J^{\boldsymbol{k}}\gamma_n^{\boldsymbol{k}}\tilde{C}^{\boldsymbol{k}}$; $J^{\boldsymbol{k}}$ and $\tilde{C}^{\boldsymbol{k}}$ are the Fourier transforms of J_{ij} and $\tilde{C}_{ij}$, respectively. At this stage, $\nu_s=(2-S)/3S$ is obtained by comparing Eq. (3) with the well-known result $\omega_{\boldsymbol{q}}=(J^{\boldsymbol{0}}-J^{\boldsymbol{q}})S$ in the ferromagnetic spin-correlation limit $C_n=2S^2/3$.

From Eq. (2) and the spectral theorem, the spin correlation can be written as

$$C^{\boldsymbol{q}} = \sum_n z_n J_n(1-\gamma_n^{\boldsymbol{q}})\frac{C_n}{\omega_{\boldsymbol{q}}}\coth\frac{\omega_{\boldsymbol{q}}}{2T}. \tag{4}$$

With the requirements $C_n=1/N\Sigma_{\boldsymbol{q}}C^{\boldsymbol{q}}\gamma_n^{\boldsymbol{q}}$ and $C_0=1/N\Sigma_{\boldsymbol{q}}C^{\boldsymbol{q}}=2S(S+1)/3$, Eqs. (3) and (4) can be solved self-consistently. T_C is determined by $\chi^{-1}=0$ $[\chi=\chi^{+-}(0,0)/2]$. To check the validity of our method, we use Fig. 1 to compare our calculated T_C/T_C^{MF} and E_C/E_0 for the bcc structure with accurate results obtained by high-temperature expansion methods[21,22] and the SM results in the NN coupling case. Here T_C^{MF} is the mean-field Curie temperature, E_C and E_0 are the total energies at T_C and zero temperature, respectively. The parameter E_C/E_0 is a proper measure of MSRO at T_C and in the NN coupling case, E_C/E_0 is identical to the average cosine of angles between NN spins. In the mean-field approximation, there is no MSRO ($E_C/E_0=0$) at and above T_C^{MF}. The existence of MSRO suppresses T_C with respect to T_C^{MF}. Such suppression also exists in the SM and is identical for all S. In more accurate calculations, however, T_C is more suppressed at smaller S.

The MSRO parameter E_C/E_0 demonstrates an increase in MSRO for smaller S. Although in the SM, this parameter increases even faster ($E_C/E_0 \propto Q_S$), this quantity is already not well defined owing to the appearance of $E_C/E_0>1$, e.g., for the simple-cubic structure for $S=1/2$ and for $S=1$ in Ref. 10. The scaling should be introduced at this stage and it leads to the elimination of real QSE.

Our formalism allows us to obtain the following important result for T_C for $S=\infty$:

$$T_C = \alpha T_C^{\mathrm{SM}} = 3T_C^{\mathrm{MF}}/(2F+1), \tag{5}$$

where $\alpha=3F/(2F+1)$ with $F=N^{-1}\Sigma_{\boldsymbol{q}}(1-\gamma_1^{\boldsymbol{q}})^{-1}$. This new and transparent expression provides another immediate and accurate check of applicability of our generalized GF formalism. For instance, it gives $T_C/(J_1S^2)=1.49$, 2.11, and 3.25 for SC, bcc, and fcc structures, respectively. These results are very close to the respective high-temperature-expansion results 1.45, 2.06, and 3.18.[22] Equation (5) clearly indicates the importance of the correction parameter α introduced above in the GF decoupling. For $S=\infty$, the parameter $E_C/E_0=1-F^{-1}$ and is the same as the one obtained using the SM.

The similarity of our results and the high-temperature-expansion results indicates the applicability of this formalism for the case of an arbitrary S and NN interaction. We also studied a Heisenberg Hamiltonian corresponding to a realistic material: we used extended (four NN) interactions in bcc Fe: $J_2/J_1=0.5221$, $J_3/J_1=0.0056$, and $J_4/J_1=-0.0879$,[23] where $J_1S^2=2.44$ mRy. For $S=\infty$, the Monte Carlo simulation gives $T_C/T_C^{\mathrm{MF}}=0.68\sim0.70$ and $E_C/E_0=0.38\sim0.41$. In the SM, $T_C/T_C^{\mathrm{MF}}=0.59$ and $E_C/E_0=0.40Q_S$ for all S. In our formalism, for $S=1/2$, 1, and ∞, $T_C/T_C^{\mathrm{MF}}=0.51$, 0.57 and 0.67, respectively, and their $E_C/E_0=0.79$, 0.68, and 0.41. At $S=1$, $T_C^{\mathrm{MF}}=2334$ K and is more than twice larger than the experimental 1040 K of Fe, and our calculated T_C is suppressed to the much lower value 1330 K. Compared with Fig. 1, one can see the additional suppression of T_C with a considerably larger E_C/E_0. This indicates a stronger MSRO than in the corresponding NN coupling case. However, the parameters in Ref. 23 have been obtained in the long-wavelength approximation and can only describe a small MSRO in the classical case. The inset of Fig. 2 directly shows $\cos\theta_n=\langle \boldsymbol{S}_i\cdot\boldsymbol{S}_{i+\delta_n}\rangle/S^2$ and provides details of the QSE enhancement of MSRO between several neighboring spins.

The spin-correlation length ξ is often used to describe the strength of MSRO. Despite the magnitude of $\cos\theta_n$, ξ al-

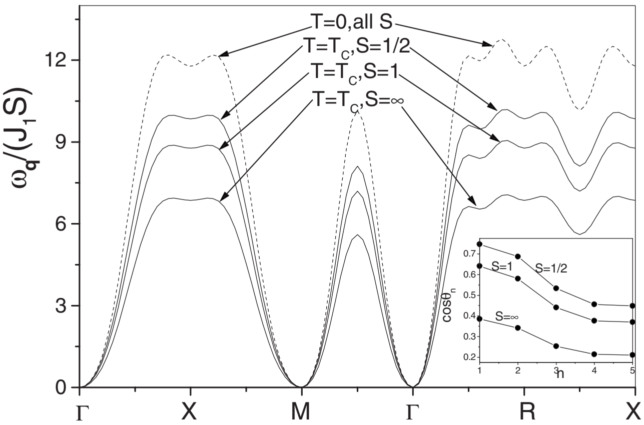

FIG. 2. The calculated SW spectrum $\omega_{\mathbf{q}}$ for different S at T_C. The dashed line is $\omega_{\mathbf{q}}$ at $T=0$ (ferromagnetic case). The inset shows $\cos\theta_n$ from the nearest to the fifth nearest neighbors.

ways tends to equal infinity when the temperature is lowered to approach T_C. In our formalism, the evaluation of ξ above T_C is straightforward from the long-wavelength behavior of the spin-correlation function $C^q \propto 1/(q^2+\xi^{-2})$. We found that at fixed T/T_C, ξ is always increasing as S becomes smaller. This is in contrast to the SM case, where ξ is independent of S. At $T=1.1T_C$, $\xi=4.1$, 3.7, and 2.8 for $S=1/2$, 1, and ∞, respectively, which again demonstrates the QSE enhancement of MSRO from another prospective.

Let us now analyze the SW excitations. In standard magnetism theories such as the random-phase approximation[24] and its various modified versions,[25] SW exist due to magnetic long-range order (LRO), so their spectrum is renormalized to zero at T_C. In our formalism, which includes non linear effects, the peaks of dynamical susceptibility can appear as a result of the short-range spin correlations, so the LRO is no longer a prerequisite for the existence of SW. The SW spectrum can therefore be finite at T_C. In Fig. 2, we plot the calculated SW spectrum obtained from Eq. (3) at T_C. To demonstrate the S dependence of the SW renormalization, the SW spectrum at $T=0$ K (the ferromagnetic case) is also plotted with all $\omega_{\mathbf{q}}$ scaled by S.

Let us estimate the renormalization factor in BCC Fe.[2] Here, SW modes have been observed above the middle of the Brillouin zone along the (110) direction, with $\mathbf{Q}=(\frac{\pi}{2}\frac{\pi}{2}0)$ (lattice constant $a=1$). The SW renormalization factors $\omega_Q(T_C)/\omega_Q^0$ (ω_Q^0 is ω_Q at $T=0$) are 0.86, 0.76, and 0.60 for $S=1/2$, 1, and ∞, respectively. Experimentally, $\omega_Q(T_C)/\omega_Q(0.3T_c)\approx 0.84$ (Ref. 2) in the bcc Fe, and the difference between ω_Q^0 and $\omega_Q(0.3T_c)$ is about 15%.[2] Therefore, the overall SW renormalization factor becomes ~ 0.71 and our result for $S=1$ is close to that. Figure 2 also indicates that $\omega_{\mathbf{q}}$ for smaller spins is less affected at elevated temperatures. This implies that QSE favors the persistence of SW modes.

Let us now estimate the influence of dynamic effects and obtain the relaxation function $F(\mathbf{q},\omega)$. Among various analytical approximations for $F(\mathbf{q},\omega)$, the three-pole approximation[26] seems to be one of the best and has been successfully applied to the typical Heisenberg system with a large spin $S=7/2$.[27,28] In this approximation, $F(\mathbf{q},\omega)$ is expressed in terms of $\delta_1^q=\langle\omega^2\rangle_{\mathbf{q}}$ and $\delta_2^q=\langle\omega^4\rangle_{\mathbf{q}}/\delta_1^q-\delta_1^q$, where $\langle\omega^n\rangle_{\mathbf{q}}$ are frequency moments of F depending on the static correlation. The evaluation of $\langle\omega^2\rangle_{\mathbf{q}}$ is straightforward.[26] $\langle\omega^4\rangle_{\mathbf{q}} \propto \langle[\ddot{S}^z_{\mathbf{q}}, i\dot{S}^z_{-\mathbf{q}}]\rangle$ (Ref. 29) contains four-spin-correlation terms which have to be properly decoupled as a product of two spin correlations. In the past, the conventional decoupling $\langle S_i^+S_l^zS_m^zS_j^-\rangle \to C_{ij}C_{lm}^{zz}$ and $\langle S_i^+S_l^+S_m^-S_j^-\rangle \to C_{im}C_{lj}+C_{ij}C_{lm}$, which is appropriate for large S, has been applied to obtain $\langle\omega^4\rangle_{\mathbf{q}}$.[26,27] For small S, the spin kernel effect, which is neglected in this decoupling, becomes important. This QSE can clearly be seen in the $S=1/2$ case, where for $i=l$ or $m=j$ the left side of the decoupled equation vanishes while the right side is finite. To take into account this QSE, we introduce the following decoupling procedure:

$$\langle\{S_i^+,S_l^z\}\{S_m^z,S_j^-\}\rangle \to f_{il}^s f_{mj}^s C_{ij}C_{lm}^{zz} \quad \text{for } R_{il}\le R_{im}, \quad R_{lj},$$

$$\langle S_i^+S_l^+S_m^-S_j^-\rangle \to f_{il}^s f_{mj}^s[f_{ij}^s f_{lm}^s C_{im}C_{lj} + f_{im}^s f_{lj}^s C_{ij}C_{lm} + (\delta_{ij}\delta_{lm}+\delta_{im}\delta_{lj})C_{il}^{zz}], \tag{6}$$

where $f_{il}^s=1-\delta_{il}/2S$. If i, l, m, and j are four different sites, then Eq. (6) is the same as the conventional decoupling. QSE occurs when two or more sites out of these four are the same. In this case, Eq. (6) at $S=1/2$ is exact and is reduced to the conventional decoupling for $S\to\infty$. With these results for two opposite limits of S and the quantum correction introduced earlier in $f_{ii}^s \sim 1/S$, one can expect that Eq. (6) will be a reasonable interpolation for an arbitrary S. By applying this decoupling procedure, one can obtain $\langle\omega^4\rangle_{\mathbf{q}}=\langle\omega^4\rangle_{\mathbf{q}}^{(0)}+\langle\omega^4\rangle_{\mathbf{q}}^{(1)}$, where $\langle\omega^4\rangle_{\mathbf{q}}^{(0)}$ corresponds to the conventional decoupling[26,27] and $\langle\omega^4\rangle_{\mathbf{q}}^{(1)}$ is the quantum correction given by

$$\langle\omega^4\rangle_{\mathbf{q}}^{(1)} = \frac{1}{4S\chi_{\mathbf{q}}}\Bigg\{\frac{1}{N}\sum_{\mathbf{k}}[J^{\mathbf{k}}(4g_{\mathbf{k}}^2-6g_{\mathbf{k}}g_{\mathbf{q}+\mathbf{k}}+2g_{\mathbf{q}+\mathbf{k}}^2) - C^{\mathbf{k}}(h_{\mathbf{k}}-h_{\mathbf{k}+\mathbf{q}})(13J^{\mathbf{k}}-7J^{\mathbf{q}+\mathbf{k}})] - (11g_{\mathbf{0}}-9g_{\mathbf{q}})(h_{\mathbf{0}}-h_{\mathbf{q}}) + S^{-1}\sum_n z_nJ_n^3C_n(1-\gamma_n^q)(5C_n+7C_0-6S)\Bigg\}, \tag{7}$$

where $\chi_{\mathbf{q}}$ is the q-dependent susceptibility, $g_{\mathbf{k}}=\Sigma_n z_n J_n C_n\gamma_n^k$, and $h_{\mathbf{k}}=\Sigma_n z_n J_n^2 C_n\gamma_n^k$.

Being a function of ω, the relaxation function $F(\mathbf{q},\omega)$ has either one maximum at $\omega=0$, if $\delta_2^q \geq 2\delta_1^q$, or three maxima at $\omega=0$ and $\omega=\pm\omega_{\mathbf{q}}^{\max}$, if $\delta_2^q<2\delta_1^q$. The latter case is often referred as the SW peak at $\omega_{\mathbf{q}}^{\max}$.[10,27,28] Using this definition, the criteria of the SW existence for a given $\mathbf{q}$ is $\delta_2^q/\delta_1^q<2$. Usually, $\omega_{\mathbf{q}}^{\max}$ is slightly larger than $\omega_{\mathbf{q}}$. In the literature, the SW peak was also defined as $\langle\omega\rangle_{\mathbf{q}}$ (Ref. 30) and is slightly smaller than $\omega_{\mathbf{q}}$. Near the critical value $\delta_2^q/\delta_1^q \lesssim 2$, the maximum of F at $\omega_{\mathbf{q}}^{\max}$ is broad. When δ_2^q/δ_1^q is decreased, the SW peak is more pronounced. In Fig. 3, we plot the magnitude of δ_2^q/δ_1^q for different S as a function of $\mathbf{q}$ at T_C. At fixed $\mathbf{q}$, δ_2^q/δ_1^q is always decreased if S becomes smaller. Along the $(qq0)$ direction, the critical values of q, when $\delta_2^q/\delta_1^q=2$, are $q_{\rm cr}\approx 0.30\pi$, 0.51π, and 0.61π for $S=1/2$, 1, and ∞, respectively. Our value of $q_{\rm cr}$ for $S=1$ agrees with the experimental

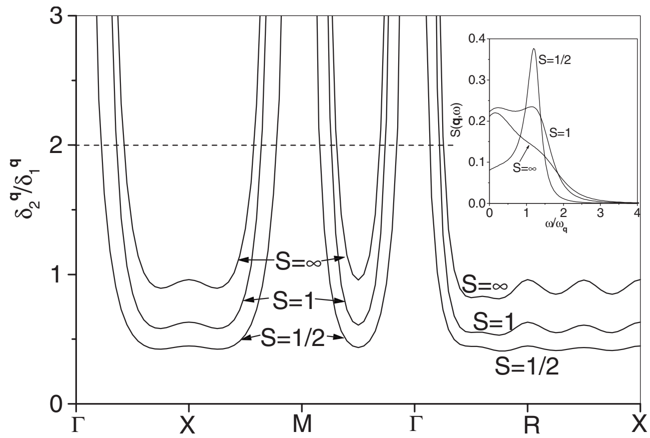

FIG. 3. The calculated δ_2^q/δ_1^q for different S at T_C as a function of $\mathbf{q}$. The criteria of SW $\delta_2^q/\delta_1^q=2$ is marked by the dashed line. The inset shows $S(\mathbf{q},\omega)$ at $\mathbf{q}=(\frac{\pi}{2}\frac{\pi}{2}0)$.

result for bcc Fe, where SW modes above T_C exist only above $q\sim\pi/2$ in the (110) direction (Fig. 2 of Ref. 2). The SW peaks were also obtained in the SM (Ref. 10) (with spin independent δ_2^q/δ_1^q) but the value of $q_{\rm cr}$ is considerably higher there. Our calculations indicate that this theory, which is equivalent to the $S=\infty$ case, will be more applicable if QSE is properly taken into account. At $\boldsymbol{q}=(\frac{\pi}{2}\frac{\pi}{2}0)$ for $S=1/2$, 1, and ∞ the ratio δ_2^q/δ_1^q is approximately 0.93, 2.2, and 3.6, respectively. These results are, respectively well below, close to, and well above the critical value $\delta_2^q/\delta_1^q=2$. The corresponding dynamic structure factor $S(\boldsymbol{q},\omega)=\omega(1-e^{-\omega/T})^{-1}\chi_{\boldsymbol{q}}F(\boldsymbol{q},\omega)$ as a function of ω is shown in the inset of Fig. 3. It is clear that at this $\boldsymbol{q}$, well-defined SW exist in the case of $S=1/2$, the tendency of SW appears for $S=1$ and there is no SW signal at all for $S=\infty$. Figure 3 shows that QSE favors the persistence of SW with the increasing impact for smaller spins. In many real magnets, "effective" S is not large ($S\approx 1.1$ in bcc Fe and $S\approx 0.3$ in fcc Ni if we assume $2S=M$, where M is an observed magnetic moment) and we believe that QSE plays an important role in the MSRO and the magnetic excitations above T_C, especially in itinerant magnets. It is also interesting to note that the quantum spin model fits the experimental Curie-Weiss constant much better [which corresponds to an atomiclike effective moment $\mu_{\rm eff}=3.13(1.62)\mu_{\rm B}$ for Fe (Ni) (Ref. 31)] than the classical spin model; the former gives $\mu_{\rm eff}\approx 3.0(1.3)\mu_{\rm B}$ for Fe (Ni) and in the latter case $\mu_{\rm eff}\approx 2.2(0.6)\mu_{\rm B}$.

While we relate our model results to real itinerant magnets, this comparison should be done with some caution. The local moment in the itinerant magnet is formed not only due to intra-atomic exchange like it is assumed in the Heisenberg model. In systems such as Ni, the local or atomic magnetic field or exchange splitting is comparable to the exchange-fluctuating fields coming from the NN atoms. While these fields can be smaller than their local analog, their contribution is crucial and the system would be nonmagnetic without them. In other words, the criteria of local moment in these systems are not fulfilled but the criteria of SRO or LRO are completely satisfied. This type of situation is realized in iron pnictides.[32] Correspondingly, systems relevant to our model, in addition to SW, will most likely have itinerant types of excitations (e.g., Landau damping). While, in general, these electron-hole excitations are destructive for the LRO existence, we expect that our theory is applicable for systems such as the recently discovered superconducting iron pnictides. In these compounds, due to the existence of an analog of the magnetic Jahn-Teller effect, the strong planar spin waves (~200 meV) already exist for small effective spins (~0.5).[33] Together with relatively low Neel temperatures (~150 K), this creates suitable conditions for the existence of SW-like propagating excitations above the Neel temperature (in the case of pnictides with completely two-dimensional nature) as well as the applicability of the presented technique. The application of the method to the frustrated nearly 2D spin systems, including high-temperature superconductors, also seems promising.

In conclusion, we analyzed analytically the possibility of MSRO presence in the Heisenberg model and identified the influence of quantum spin effects on MSRO in ferromagnets above T_C. By extending the second-order Green's function technique to an arbitrary S, we found that for a system of small spins, this quantum effect greatly contributes to MSRO and enhances its influence. The spin dynamics investigation, which was performed using the conventional method of moments, further confirms that QSE favors the persistence of spin-wave excitations. Our results demonstrate that this previously neglected QSE is directly related to the possible MSRO and SW existence above T_C. These model studies can be used for the interpretation of experimental data in paramagnetic phases of Fe, Ni, and recently discovered iron pnictides. While the complete description would require a careful analysis of both longitudinal and tranversal components of dynamic susceptibility, already our limited Heisenberg model studies indicate nontrivial connection between MSRO and quantum effects.

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