Thermodynamics of the frustrated $J_1$-$J_2$ Heisenberg ferromagnet on the body-centered cubic lattice with arbitrary spin

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Abstract

We use the spin-rotation-invariant Green’s function method as well as the high-temperature expansion to discuss the thermodynamic properties of the frustrated spin-$S$ $J_1$-$J_2$ Heisenberg magnet on the body-centered cubic lattice. We consider ferromagnetic nearest-neighbor bonds $J_1 < 0$ and antiferromagnetic next-nearest-neighbor bonds $J_2 \geq 0$ and arbitrary spin $S$. We find that the transition point $J_2^c$ between the ferromagnetic ground state and the antiferromagnetic one is nearly independent of the spin $S$, i.e., it is very close to the classical transition point $J_{1,\text{clas}}^c = \frac{2}{3} |J_1|$. At finite temperatures we focus on the parameter regime $J_2 < J_2^c$ with a ferromagnetic ground state. We calculate the Curie temperature $T_C(S, J_2)$ and derive an empirical formula describing the influence of the frustration parameter $J_2$ and spin $S$ on $T_C$. We find that the Curie temperature monotonically decreases with increasing frustration $J_2$, where very close to $J_2^c$ the $T_C(J_2)$-curve exhibits a fast decay which is well described by a logarithmic term $\frac{1}{\log(\frac{2}{3}|J_1| - J_2)}$. To characterize the magnetic ordering below and above $T_C$, we calculate the spin-spin correlation functions $\langle S_0 S_R \rangle$, the spontaneous magnetization, the uniform static susceptibility $\chi_0$ as well as the correlation length $\xi$. Moreover, we discuss the specific heat $C_V$ and the temperature dependence of the excitation spectrum. As approaching the transition point $J_2^c$ some unusual features were found, such as negative spin-spin correlations at temperatures above $T_C$ even though the ground state is ferromagnetic or an increase of the spin stiffness with growing temperature.

1 Introduction

Heisenberg models with competition between nearest-neighbor (NN) bonds $J_1$ and next-nearest-neighbor (NNN) bonds $J_2$ ($J_1$-$J_2$ models) can serve as canonical models to study frustration effects in magnetic systems. In case of ferromagnetic NN exchange, $J_1 < 0$, and antiferromagnetic NNN exchange, $J_2 > 0$, the ferromagnetic ground state gives way for an antiferromagnetic state with zero net magnetization at a critical value $J_2^c$ that depends on the dimension $D$ of the system [1][4]. In lower dimension $D < 3$ and for low spin quantum number $S$ the ground state for $J_2 > J_2^c$ may have unconventional properties, see e.g. Refs. [3][1][6][7]. Although, in the ferromagnetic regime,
where \( J_2 < J_2^\text{c} \), the ground state is the simple fully polarized ferromagnetic state, the influence of the frustrating coupling \( J_2 \) on the thermodynamic properties can be strong, as it has been recently discussed for systems with dimension \( D = 1 \) and \( D = 2 \) \cite{8,14}.

In the present study we extend our previous studies of the frustrated \( J_1-J_2 \) Heisenberg ferromagnet in dimensions \( D = 1 \) (Refs. \cite{10,13,14}) and \( D = 2 \) (Ref. \cite{11}) to the three-dimensional case. In \( D = 3 \) the body-centered cubic (BCC) lattice is appropriate to compare with \( D = 1 \) and \( D = 2 \), since the antiferromagnetic \( J_2 \) bonds are in competition with \( J_1 \), but do not frustrate each other \cite{15,18,49}.

The Hamiltonian of the spin-\( S \) \( J_1-J_2 \) Heisenberg model on the BCC lattice considered in this paper is given by

\[
H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{[i,j]} S_i \cdot S_j ,
\]

where \( S_i^2 = S(S+1) \), and \( \langle i,j \rangle \) runs over NN bonds and \([i,j]\) over all NNN bonds. We consider \( J_1 < 0 \) and \( J_2 \geq 0 \). In what follows we define the energy scale by setting \( J_1 = -1 \). In the classical limit \( S \to \infty \), the ground state is ferromagnetic for \( J_2 < J_2^\text{c,clas} = \frac{2}{3} |J_1| \), and it is a collinear antiferromagnetic state with the magnetic wave-vector \( Q = (\pi, \pi, \pi) \) for \( J_2 > J_2^\text{c,clas} \) \cite{15,18}. In what follows we want to discuss the thermodynamics of the model (1) for arbitrary spin quantum number \( S \) and focus on the parameter regime \( J_2 < J_2^\text{c} \), where the ferromagnetic ground state is realized.

As in our previous papers on frustrated ferromagnets, \cite{10,11,13} we use the rotationally invariant Green’s function method (RGM) to study the influence of the frustrating NNN bond \( J_2 \) and of the spin quantum number \( S \) on the thermodynamic properties of the model (1). This Green’s function approach has been applied successfully to several quantum spin systems \cite{10,11,13,19,39}. We complement the Green’s function study by using the high-temperature expansion (HTE) technique \cite{40,41,43,44}.

The paper is organized as follows: In Sec. 2 the RGM is developed for the model (1) and a brief instruction of the HTE approach is given. Some relevant features of the zero-temperature transition between the ferromagnetic ground-state and the collinear antiferromagnetic state are discussed in Sec. 3. Finite-temperature properties are then analyzed in Sec. 4. We summarize our findings in Sec. 5.

2 Methods

2.1 Rotation-invariant Green’s function method (RGM)

As already mentioned above, the RGM is a well established method in the field of magnetic systems including strongly frustrated quantum spin systems. It was initially introduced by Kondo and Yamaji for spin-1/2 systems \cite{19}. Later on, an extension to arbitrary spin \( S \) was developed, see, e.g., Refs. \cite{13,20,22,31,36}.

To determine the spin-spin correlation functions and the thermodynamic quantities, we calculate the transverse dynamic spin susceptibility \( \chi^+_{q} (\omega) = -\langle \langle S^+_q ; S^-_{-q} \rangle \rangle_{\omega} \) (here, \( \langle \ldots ; \ldots \rangle_{\omega} \) denotes the two-time commutator Green’s function \cite{45,47}). Taking the equation of motion up to the second step (the decoupling of the higher order Green’s function is performed in the second-order equation of motion, i.e., one order beyond standard random-phase approximation) and supposing spin rotational symmetry, i.e., \( \langle S^z_i \rangle = 0 \), we obtain \( \omega^2 \langle \langle S^+_q ; S^-_{-q} \rangle \rangle_{\omega} = M_q + \langle \langle \tilde{S}^+_q ; S^-_{-q} \rangle \rangle_{\omega} \) with \( M_q = \langle \langle [S^+_q , H] , S^-_{-q} \rangle \rangle \) and \( \tilde{S}^+_q = \langle [S^+_q , H] , H \rangle \). For the model (1) the moment \( M_q \) is given by
the exact expression
\[ M_q = -2J_1 z_1 c_{001}(1 - \gamma_q^{(1)}) - 2J_2 z_2 c_{101}(1 - \gamma_q^{(2)}), \]
where \( c_{hkl} \equiv c_R = \langle S_0^+ S_R^- \rangle = 2(\langle S_0 S_R \rangle / 3, R = h\mathbf{a}_1 + k\mathbf{a}_2 + l\mathbf{a}_3, \mathbf{a}_i = \frac{1}{2} \sum_j [(1 - 2\delta_{j,i}) \mathbf{e}_j] (\mathbf{e}_j \text{ are the Cartesian unit vectors}), \gamma_q^{(1)} = \cos \frac{q_x}{2} \cos \frac{q_y}{2} \cos \frac{q_z}{2} \text{ and } \gamma_q^{(2)} = \frac{1}{3}(\cos q_x + \cos q_y + \cos q_z). \) The quantities \( z_1 = 8 \) and \( z_2 = 6 \) are the NN and NNN coordination numbers of the BCC lattice, respectively. For the second derivative \( -\ddot{S}_q^+ \) we use the standard decoupling of the RGM, see, e.g., Refs. \[10, 11, 13, 19–27, 35–37\]. To be specific, in \( -\ddot{S}_q^+ \) we apply the decoupling in real space
\[ S_i^+ S_j^+ S_k^- = \alpha_{i,k} \langle S_i^+ S_k^- \rangle S_j^+ + \alpha_{j,k} \langle S_j^+ S_k^- \rangle S_i^+, \]
\[ S_i^+ S_j^- S_k^+ = \langle S_j^+ S_k^- \rangle S_i^+ + \lambda_{i,j} \langle S_i^+ S_j^- \rangle S_k^+, \]
where \( i \neq j \neq k \neq i \). The quantities \( \alpha_{i,j} \) and \( \lambda_{i,j} \) are vertex parameters introduced to improve the decoupling approximation. Note that products of three spin operators with two coinciding sites, see Eq. (4), appear only for \( S \geq 1 \), i.e., the vertex parameter \( \lambda_{i,j} \) is irrelevant for \( S = 1/2 \) \[13, 22, 36\]. By using the operator identity \( S_i^2 = S_i^+ S_i^- - S_i^2 + (S_i^2)^2 \), the expectation value \( \langle S_j^+ S_j^- \rangle \) entering Eq. (1) is given by
\[ \langle S_j^+ S_j^- \rangle = \langle S_j^+ S_j^- \rangle = \frac{2}{3} S(S + 1), \]
where \( \langle S_j^+ \rangle = 0 \) was used. For systems with a ferromagnetic ground state it is known from Refs. \[11, 30, 35, 37\] that we may set \( \alpha_{i,k} = \alpha \) and \( \lambda_{i,j} = \lambda \), i.e., we approximate the various multispin correlation functions appearing in the equation of motion on an equal footing. We obtain \( -\ddot{S}_q^+ = \omega_q^2 S_q^+ \) and
\[ \lambda_q^+ - \omega_q \langle \langle S_q^+, S_q^- \rangle \rangle = \frac{M_q}{\omega_q^2 - \omega^2}, \]
with the spin-wave excitation dispersion relation
\[ \omega_q^2 = J_1^2 z_1 (\gamma_q^{(1)} - 1) \alpha (c_{001} - c_{002} - 3(c_{101} + c_{121}) + z_1 c_{001} \gamma_q^{(1)}) - (J_2^2 z_2 (\gamma_q^{(1)} - 1) + J_2^2 z_2 (\gamma_q^{(2)} - 1)) \left( \lambda c_{001} + \frac{2}{3} S(S + 1) \right) + J_2^2 z_2 (\gamma_q^{(2)} - 1) \alpha (c_{101} - c_{202} - 4c_{121} + z_1 c_{001} \gamma_q^{(1)}) + J_1 J_2 z_2 (\gamma_q^{(2)} - 1) \alpha (-3c_{120} - 3c_{001} + z_2 c_{101} \gamma_q^{(1)}) + J_1 J_2 z_2 (\gamma_q^{(1)} - 1) \alpha (z_2 c_{101} \gamma_q^{(1)}) + J_1 J_2 z_2 z_2 c_{001} (\gamma_q^{(1)} - 1) (\gamma_q^{(2)} - 1), \]
where we have used, on grounds of symmetry, \( c_{01-1} = c_{121} \) and \( c_{11-1} = c_{221} = c_{120}. \)

The correlation functions \( c_R = \frac{1}{N} \sum_q c_q e^{i q R} \) are determined by the spectral theorem, \[45\]
\[ c_q = \langle S_q^+ S_q^- \rangle = \frac{M_q}{2 \omega_q} \left[ 1 + 2n(\omega_q) \right], \]
where \( n(\omega) = (e^{\omega/T} - 1)^{-1} \) is the Bose-Einstein function. Taking the on-site correlator \( c_{R=0} \) and using the operator identity \[3\], we get the sum rule
\[ \frac{1}{N} \sum_q c_q = \frac{2}{3} S(S + 1). \]
To calculate the uniform static spin susceptibility \( \chi_0 = \chi_{q=0}(\omega = 0) \), we use the relation \( \chi_q(\omega) \equiv \chi_{zz}(\omega) = \frac{1}{2} \chi_{r}^{\mp}(\omega) \). In the limit \( \omega = 0 \) and \( q = 0 \) we get from Eq. (6)

\[
\chi_0 = \frac{c_{001}J_1 + c_{101}J_2}{\Delta_{\chi_0}},
\]

where

\[
\Delta_{\chi_0} = J_1^2 \alpha (9c_{001} - c_{002} - 3(c_{101} + c_{121})) - J_1J_2\alpha (c_{001} - 8c_{101} + 7c_{120}) + J_2^2\alpha (7c_{101} - 4c_{121} - c_{220}) - \lambda (J_1^2c_{001} + J_2^2c_{011}) - \frac{2}{3}S(S + 1)(J_1^2 + J_2^2).
\]  

(11)

The phase with magnetic long-range order at \( T \leq T_C \) is described by the divergence of the static susceptibility at the ferromagnetic ordering vector \( Q_0 = 0 \), i.e., by \( \chi_0^{-1} = 0 \). In the long-range ordered phase the correlation function \( c_R \) is written as [21, 24, 36, 39]

\[
c_R = \frac{1}{N} \sum_{q(\neq 0)} c_q e^{iqR} + C,
\]

(12)

where \( c_q \) is given by Eq. (8). The condensation term \( C \) determines the magnetization \( M \) which is given in the spin-rotationally invariant form by

\[
M^2 = \frac{3}{2N} \sum_R c_R = \frac{3}{2} C.
\]

(13)

According to Eq. (10) the condition for ferromagnetic long-range order is finally given by \( \Delta_{\chi_0} = 0 \), where \( \Delta_{\chi_0} \) is defined in Eq. (11). The magnetic correlation length above \( T_C \) is obtained by expanding \( \chi_q \) in the neighborhood of the vector \( Q_0 \) [19, 24, 39]. For the ferromagnet we have \( Q_0 = 0 \), and we find

\[
\xi^2 = \frac{A + B - 16\alpha (c_{001}^2J_1^3 + c_{101}^2J_2^3)}{16 (c_{001}J_1 + c_{101}J_2) \Delta_{\chi_0}},
\]

(14)

\[
A = -J_1^2J_2\alpha \left( 12c_{001}^2 + c_{001}(31c_{101} - 4c_{120}) + c_{101}(c_{002} + 3(c_{101} + c_{121}) \right)
\]

\[
- c_{101} \left( \lambda c_{001} + \frac{2}{3}S(S + 1) \right),
\]

(15)

\[
B = -3J_1J_2^2\alpha \left( c_{001}(36c_{101} - 4c_{121} - c_{220}) + c_{101}(16c_{101} + 3c_{120}) \right)
\]

\[
+ c_{001} \left( \lambda c_{011} + \frac{2}{3}S(S + 1) \right),
\]

(16)

To evaluate the thermodynamic properties, we have to determine the correlation functions \( c_R \), the vertex parameters \( \alpha \) and \( \lambda \), and, for \( T < T_C \), the condensation term \( C \). For the correlation functions we use Eq. (12) in combination with Eq. (8). Further we use the sum rule (9) and the condition for long-range order, \( \Delta_{\chi_0} = 0 \), relevant for \( T \leq T_C \). That is sufficient for \( S = 1/2 \), where the vertex parameter \( \lambda \) is not present. For \( S > 1/2 \) we need one more equation. For \( T = 0 \) we use the known correlation functions of the ferromagnetic ground state, \( c_R(T = 0) = \frac{3}{2}S \delta_{R,0} + \frac{2}{3}S^2 \), to obtain \( \alpha(T = 0) = 3/2 \) and \( \lambda(T = 0) = 2 - 1/S \). To find the missing equation for \( S > 1/2 \) and \( T > 0 \), we follow Refs. 31, 35, 36 and consider the ratio

\[
r(T) \equiv \frac{\lambda(T) - \lambda_\infty}{\alpha(T) - \alpha_\infty} = r(0)
\]

(17)
as independent of temperature. Here $\lambda_\infty$ and $\alpha_\infty$ are the vertex parameters for $T \to \infty$ which can be easily determined as $\lambda_\infty = 1 - 3[4S(S+1)]^{-1}$ and $\alpha_\infty = 1$. To solve the set of RGM equations numerically we use Broyden’s method,\textsuperscript{48} which yields the solutions with a relative error of about $10^{-8}$ on the average. The momentum integrals are done by Gaussian integration.

In the low-temperature limit, several analytical expressions can be found from the RGM equations which are identical to those obtained by the linear spin-wave theory (cf., e.g., Ref. \textsuperscript{47}): The dispersion relation at zero temperature and $\omega_q(T = 0) = \rho_s(0)q^2$, where $\rho_s(0) = \rho_s(T = 0) = S|J_1 + J_2|$ is the spin stiffness. Note that, by contrast to the one- and two-dimensional frustrated models, the stiffness remains finite at the classical transition point $J_2^c = 2|J_1|$. The spin stiffness also determines the low-temperature regime of the magnetization and the specific heat,

\[ \frac{M}{S} \sim 1 - \frac{\zeta(\frac{3}{2})}{2S} \left( \frac{T}{4\pi\rho_s(0)} \right)^{\frac{3}{2}}, \]

\[ C_V \sim \frac{15\zeta(\frac{5}{2})}{8} \left( \frac{T}{4\pi\rho_s(0)} \right)^{\frac{3}{2}}, \]

where $\zeta(s)$ denotes the Riemann zeta function.

Some remarks are in order here with respect to the comparison between the RGM and the standard random-phase approximation (RPA), see, e.g., Refs. \textsuperscript{35,45,49,51}. The spin-wave excitation energies calculated within the RGM, see Eq. (7), exhibit a temperature renormalization that is wavelength dependent and proportional to the correlation functions, so that the existence of spin-wave excitations does not imply a finite magnetization. That is in contrast to the RPA, where the temperature renormalization of the spin-wave excitations is independent of wavelength and proportional to the magnetization, see, e.g., Refs. \textsuperscript{45,46}. Correspondingly, in our theory the stiffness becomes temperature dependent $\rho_s(T) = \sqrt{\alpha(J_1 + J_2)(c_{001}J_1 + c_{101}J_2)}$ due to the temperature dependences of $\alpha$, $c_{001}$, and $c_{101}$. Moreover, it is known \textsuperscript{35,45,46} that the RPA fails in describing magnetic excitations and magnetic short-range order for $T > T_C$, reflected, e.g., in the specific heat. On the other hand, the magnetization for $T \leq T_C$ is typically well described within RPA.

### 2.2 High-temperature series expansion

A very general approach to calculate thermodynamic quantities at high and moderate temperatures is the high-temperature expansion (HTE) technique \textsuperscript{40,44}. Here we use a recently developed tool \textsuperscript{52} to calculate the HTE series of the specific heat and the uniform static susceptibility of model \textsuperscript{11} up to order ten. The region of validity of the HTE series can be extended by Padé approximants \textsuperscript{40,44,53}. The Padé approximants $[m,n]$ are ratios of two polynomials $[m,n] = P_m(x)/R_n(x)$ of degree $m$ and $n$ and they provide an analytic continuation of a function $g(x)$ given by a power series. As a rule, Padé approximants with $m \sim n$ provide the best results.

We can use the HTE series for the susceptibility $\chi_0 = \sum_n c_n T^{-n}$ to calculate the Curie temperature. Here we use two variants to extract $T_C$ from the HTE series.

(i) We analyze the quotient $q_n = c_n/c_{n-1}$, see, e.g., Refs. \textsuperscript{44,54,56}. For a three-dimensional ferromagnet the critical behavior of $\chi_0$ is given by $\chi_0(T) \propto (T - T_C)^{-\gamma}$. The expansion of $(T - T_C)^{-\gamma}$ in powers of $1/T$ yields for the quotient $q_n = T_C + (\gamma - 1)\frac{T_C}{n}$. For higher orders $n$ the HTE series of the model \textsuperscript{11} obeys this relation, supposed that a finite critical temperature exists. We made a fit of our HTE data for $q_n$ linearly in $1/n$ including data points for $n = 5, \ldots, 10$ to
get approximate values for $T_C$ and the critical index $\gamma$. The mean square deviation of the linear fit provides information on the reliability of this estimate.

(ii) A more sophisticated and more powerful approach to determine $T_C$ and $\gamma$ is based on the so-called differential approximants (DA) \cite{57,61}. Within this method one considers differential equations of the form $\sum_{\nu=0}^{K} S_{\nu}(\beta) \chi_0^{(\nu)}(\beta) + Y(\beta) = 0$, where $S_{\nu}(\beta)$ and $Y(\beta)$ are polynomials in $\beta = 1/T$ and $\chi_0^{(\nu)}$ denotes the $\nu$-th derivative of the susceptibility $\chi_0$. (Note that the usual Padé approximants follow from $K = 0$.) The polynomials $S_{\nu}(\beta)$ and $Y(\beta)$ can be chosen arbitrarily with the constraint that the total number of free coefficients of all polynomials is equal to the highest order $n$ of the HTE series (here $n = 10$). The coefficients of the polynomials can be determined by inserting the derivatives of the HTE series of $\chi_0$ in the equation given above which yields a simple linear system of equations for the coefficients. Assuming critical behavior for the susceptibility $\chi_0$, we can determine the Curie temperature $T_C = 1/\beta_C$ from $S_K(\beta_C) = 0$ and the critical exponent $\gamma$ is given by $\gamma = K - 1 - \frac{S_{K-1}(\beta_C)}{S_K(\beta_C)}$. By varying the degree of the polynomials $S_{\nu}(\beta)$ and $Y(\beta)$ a set of 21 different differential equations was obtained which yields a corresponding set of values for $T_C$ and $\gamma$. However, some of the differential equations lead to unphysical results (negative or even complex solutions for $T_C$) and have to be discarded. The average of the data for $T_C$ and $\gamma$ obtained from the remaining differential equations yields typically precise estimates of $T_C$ and $\gamma$, where the mean square deviation provides a measure of the accuracy (for more details see Refs. \cite{57,61}). It is in order to mention here that the HTE naturally works well only if the Curie temperature is not too small. In particular, for increasing frustration $J_2$ towards the critical value $J^c_2$ one may expect that the critical temperature becomes small, and then the determination of $T_C$ and $\gamma$ from the HTE series fails.

We mention that in Ref. \cite{13} the HTE series for the staggered susceptibility was used to determine the Néel temperature $T_N$ as a function of $J_2/J_1$ for the model \cite{11} with antiferromagnetic $J_1$. Moreover, the Curie temperature of the unfrustrated BCC ferromagnet (i.e., $J_2 = 0$) for spin quantum numbers $S = 1/2, 1$ and $3/2$ was calculated from the HTE series in Ref. \cite{62}.

### 3 Zero-temperature properties

First we use the RGM formalism to study the zero-temperature properties. For $J_2 < J^c_2$ the ground state is the simple ferromagnetic eigenstate with $\langle S_0 S_R \rangle = S^2 (R \neq 0)$. The excitation spectrum $\omega_q(T = 0)$ depends on $J_2$, see Fig. 4. Since the spin stiffness is given by $\rho_s(0) = S|J_1 + J_2|$, see Sec. 2.1, the excitation energy in the long-wavelength limit is reduced by frustration, but the leading $q^2$-term in $\omega_q$ remains finite even at $J_2 = J^c_2$. In the classical model the transition to the collinear antiferromagnetic ground state with magnetic wave vector $Q = (\pi, \pi, \pi)$ is related by the emergence of a soft mode at $q = Q$, i.e., $\omega_Q = 0$ at $J_2 = J^c_{2,\text{clas}}$, for ferro- as well as for antiferromagnetic $J_1$. We mention here the difference to the $J_1$-$J_2$ ferromagnet in dimension $D = 1$ (Refs. \cite{10,13,14}) and $D = 2$ (Ref. \cite{11}). In $D = 1$ there is no soft mode, the spin stiffness $\rho_s$ vanishes at $J_2 = J^c_2 = |J_1|/4$ (i.e., the leading term in $\omega_q$ is proportional to $q^4$ at $J_2 = J^c_2$), the transition point $J^c_2$ is independent of $S$, and the magnetic wave vector $Q$ changes smoothly from $Q = 0$ to $Q \neq 0$ when crossing the transition point $J^c_2$, see also Refs. \cite{11,12,17}. In $D = 2$ the behavior is again different. At the classical transition point $J^c_{2,\text{clas}} = |J_1|/2$ all excitation energies $\omega_q$ with $q = (q, 0)$ and $q = (0, q)$, $0 \leq q \leq \pi$, become soft (i.e., there is a flat part in $\omega_q$). However, this flat soft part is irrelevant for the quantum model, since $J^c_{2,\text{quant}} < J^c_{2,\text{clas}}$, i.e., the transition between the ferromagnetic and the antiferromagnetic ground states is shifted to smaller frustration strength ($J^c_{2,\text{quant}} \sim 0.4|J_1|$ for $S = 1/2$, see Refs. \cite{3,5}).
Figure 1: Dispersion relation of the spin-waves at $T = 0$ and for different values of $J_2$ and fixed $J_1 = -1$. The points in the Brillouin zone are defined as $\Gamma = (0, 0, 0), P = (\pi, \pi, \pi), H = (0, 0, 2\pi), N = (\pi, \pi, 0)$. Note that for $T = 0$ the dispersion $\omega_q/S$ is independent of $S$.

In view of these results for $D = 1$ and $D = 2$ the question arises, whether for $D = 3$ the transition point $J_c^2$ of the quantum model is different from that of the classical model. Let us first mention that for the model with antiferromagnetic NN bond, $J_1 > 0$, there is a slight shift of $J_c^2$ to $J_c^2 \sim 0.7J_1 > J_c^{2, \text{clas}}$ for the $S = 1/2$ model [15, 17, 49]. To find $J_c^2$ for our model with ferromagnetic $J_1$ we extend our RGM approach to the antiferromagnetic region, i.e., to $J_2 > J_c^2$, see Fig. 2. We follow Ref. [5] and use the intersection of the ferromagnetic ground-state energy $E_{FM}/N = -4|J_1|S^2 + 3J_2S^2$ and the RGM energy of the collinear antiferromagnetic state to estimate $J_c^2$, see Fig. 2. For $S = 1/2$ we get $J_c^2 \approx 0.63|J_1|$. Since the RGM description of the collinear antiferromagnetic state with only one vertex parameter $\alpha$ is a poor approximation, [21, 23, 39] a more accurate value for $J_c^2$ can be obtained using an improved description of the collinear antiferromagnetic ground state with two vertex parameters $\alpha_1$ and $\alpha_2$, see, e.g., Refs. [24, 27, 33, 39]. The RGM with two vertex parameters yields $J_c^2 \approx 0.68|J_1|$ for $S = 1/2$ and reproduces the classical value $J_c^{2, \text{clas}} = 2|J_1|/3$ in the large-$S$ limit [63]. Note that the RPA value for $J_c^2$, estimated by the vanishing of $T_C(J_2)$, see the next section, is $J_c^2 = 0.6799|J_1| [64].$

4 Finite-temperature properties

4.1 Spin-spin correlation functions, magnetization and Curie temperature

The spin-spin correlation functions $\langle S_0 S_R \rangle$, the magnetization $M$ and the Curie temperature $T_C$ represent the basic quantities to characterize the ferromagnetic phase. First we discuss the Curie temperature $T_C$ as a function of the frustration parameter $J_2$ as shown in Fig. 3 for $S = 1/2$. 


Figure 2: Various ground-state spin-spin correlation functions $\langle S_0 S_R \rangle$ as a function of $J_2$ for the spin-1/2 model in the ferromagnetic ($Q_{FM} = 0$) and the antiferromagnetic regime ($Q_{AFM} = P = (\pi, \pi, \pi)$). The inset shows the intersection of the energies per site of the ferromagnetic state and the collinear antiferromagnetic phase that is used to estimate $J_2^c$. For comparison the GS energy of the classical model is also shown (labeled by 'AFM cl').

(Note that HTE results for the Curie temperature for $S = 1/2, 1, \ldots, 5/2$ and selected values of $J_2$ are also given in Table 2 in Sec. 4.2.) We compare the RGM data with the HTE results, variants (i) and (ii), see Sec. 2.2, and the RPA results of Ref. 64. Moreover, for the unfrustrated BCC ferromagnet ($J_2 = 0$) we can compare with HTE data of Ref. 62 for $S = 1/2, 1$ and 3/2. Note that our HTE data for $J_2 = 0$ within the accuracy of drawing in Fig. 3 coincide with those of Ref. 62, where HTE data up to orders 14 ($S = 1/2$), 12 ($S = 1$), and 9 ($S = 3/2$) were used. For $J_2 = 0$ and $S = 1/2$ the RGM (RPA) value is about 7% (13%) larger than the HTE value. The general dependence on $J_2$ is very similar for all methods. As expected, the error bars of the HTE estimates of $T_C$ become larger with increasing $J_2$, and the HTE fails as approaching $J_2^c$, since the relevant temperatures are too small. Obviously, the more powerful approach using DA (i.e., HTE variant (ii)) works more reliable until large values of $J_2$. By contrast to the HTE approach, the RGM and RPA provide $T_C$ data until the classical transition point $J_2^{c, clas}$. As approaching $J_2^{c, clas}$, the Curie temperature remains quite large up to about $J_2 = 0.65$ and finally drops down quickly at the transition point. The fast decay very close to $J_2^{c, clas}$ is well described by a logarithmic term $1/\log(\frac{3}{2}|J_1 - J_2|)$ (cf. also Refs. 36 and 65). The inset in Fig. 3 demonstrates that the RGM data for the Curie temperature scaled by $S(S + 1)$ are only weakly dependent on $S$. The $S$-dependence of the HTE estimate of $T_C/S(S + 1)$ is more pronounced, but it remains also weak (e.g., for $J_2 = 0.3$ the difference between the extreme quantum case $S = 1/2$ and the classical limit $S \to \infty$ is about 20%). Hence, the curves for $S = 1/2$ shown in the main panel of Fig. 3 may be more or less considered as representative for arbitrary $S$. A good description of the RGM
Figure 3: Main panel: Curie temperatures $T_C/S(S+1)$ as a function of the frustration parameter $J_2$ and $J_1 = -1$ for spin quantum number $S = 1/2$ obtained by the RGM, RPA (data from Ref. [64]), and by the HTE, variants (i) and (ii). Inset: Curie temperatures $T_C/S(S+1)$ as a function of $1/S$ for various frustration parameters $J_2$. Note that within the RPA approach $T_C/S(S+1)$ is independent of $S$.

Table 1: Coefficients $A$ and $B$ of the empirical fit function of the Curie temperature $T_C/S(S+1)$, see Eq. (20), for various spin quantum numbers $S$.

| $S$  | $1/2$ | $1$  | $3/2$ | $2$  | $5/2$ | $100$ |
|------|-------|------|-------|------|-------|-------|
| $A$  | 3.29  | 3.42 | 3.34  | 3.27 | 3.22  | 3.04  |
| $B$  | 1.41  | 1.41 | 1.35  | 1.31 | 1.28  | 1.18  |

data for $T_C/S(S+1)$ in the entire range $0 \leq J_2 \leq \frac{2}{3}|J_1|$ is provided by the fit function

$$\frac{T_C}{S(S+1)} = \frac{A(S)}{B(S) - \log(\frac{2}{3}|J_1| - J_2)}.$$  \quad (20)

The fit parameters $A$ and $B$ as a function $S$ are given in Table 1. Obviously, the $S$-dependence of $A$ and $B$ is weak.

Next we consider the spin-spin correlation functions $\langle S_0 S_R \rangle$. In Fig. 4 we compare the temperature dependence of the correlation functions between nearest neighbors ($R = (1, 0, 0)$), next-nearest neighbors ($R = (1, 1, 0)$), and between spins separated by $R = (2, 2, 0)$ for $J_2 = 0$ and $J_2 = 0.6$. For $T < T_C$ the behavior of the correlation functions for $J_2 = 0$ and $J_2 = 0.6$ is quite similar, although their decay with increasing $T$ is faster for larger $S$. Interestingly, above $T_C$ the correlation functions for particular separations $R$ for larger values of frustration become negative irrespective of the fact that the ground state is still ferromagnetic. These negative correlators are precursors of the collinear antiferomagnetic Néel order present for $J_2 > J_c^2$, since they belong to separations $R$, e.g. $R = (1, 1, 0)$, connecting spins on different sublattices of the large-$J_2$ collinear...
antiferromagnetic phase, cf. also Fig. 2. The general behavior of $\langle S_0 S_R \rangle$ for $T \geq T_C$ at large separation $|R|$ is given by $\langle S_0 S_R \rangle \sim e^{-\frac{|R|}{\xi(T)} (|R|^{D+2-\eta})}$, where $D = 3$ and the critical exponent $\eta$ is close to zero, see, e.g., Refs. [66–68]. The long-distance behavior of RGM correlation functions at $T = T_C$ turns out to fit well to a power law with $\eta \approx 0$ for arbitrary $S$ and $J_2$.

In Fig. 5 we show the temperature dependence of the magnetization for three values of $S$ and for two values of the frustration parameter, $J_2 = 0$ and $J_2 = 0.6$. The influence of $J_2$ on the $M/S$ vs. $T/T_C$ curve is rather small, an increase of the spin quantum numbers $S$ leads to a flattening of the $M/S$ vs. $T/T_C$ curve.

According to Refs. [69] and [70] the spontaneous magnetization of a ferromagnet can be described by the formula

$$\frac{M}{S} = \left[ 1 - \phi \left( \frac{T}{T_C} \right)^{1.5} - (1 - \phi) \left( \frac{T}{T_C} \right)^{2.5} \right]^\beta,$$

(21)

where $\phi$ is the so-called shape parameter and $\beta$ is the critical index of the order parameter, which is $\beta = 1/2$ within our RGM approach, cf., e.g., Ref. [30]. This formula yields the correct low-temperature behavior and a critical behavior for $T \to T_C$ with the exponent $\beta$. Indeed, a corresponding fit of our RGM data for $M$ using the shape parameter $\phi$ as a single fit parameter yields a very good description of $M(T)$ in the entire temperature region $0 \leq T \leq T_C$. We show the shape parameter $\phi$ in the inset of Fig. 5. Based on the low-$T$ properties known from spin-wave theories and on early estimates of $T_C$, [71] Kuz'min et al. [69] argued that the dependence of $\phi$ on $S$ and $J_2$ should be weak. Moreover, they found a relation $0 < \phi < 5/2$. Our results for $\phi$ support these statements.
Figure 5: Main panel: Magnetization $M/S$ as a function of the normalized temperature $T/T_C$ for spin quantum numbers $S = 1/2, 2$ and 100 and for two values of the frustration strength $J_2 = 0$ (solid lines) and $J_2 = 0.6$ (dashed lines). Inset: Shape parameter $\phi$ of the fitting function $[21]$ in dependence on $1/S$ for various values of frustration $J_2$.

Figure 6: Inverse scaled susceptibility $1/(|J_2 + J_1|)\chi$ as a function of the normalized temperature $T/T_C$. Main panel: RGM results for $S = 1/2$ (solid lines) and $S = 5/2$ (dashed lines) for frustration parameters $J_2 = 0$ (blue lines) and $J_2 = 0.5$ (red lines). Inset: Comparison of RGM data (lines) with Padé approximants [6, 4] of the 10th order HTE data (symbols).
Table 2: Critical exponent $\gamma$ of the susceptibility and Curie temperature $T_C/S(S+1)$ obtained from HTE (i) and HTE (ii), cf. Sec. 2.2 for different spins $S$ and frustration parameters $J_2$ and fixed $J_1 = -1$.

| $S$ | $J_2 = 0$ | $J_2 = 0.1$ | $J_2 = 0.3$ |
|-----|-----------|-------------|-------------|
|     | HTE (i)   | HTE (ii)    | HTE (i)     | HTE (ii)    | HTE (i)     | HTE (ii)    |
| 1/2 | 1.53 ± 0.05 | 1.34 ± 0.04 | 1.51 ± 0.10 | 1.33 ± 0.08 | 0.26 ± 2.07 | 1.38 ± 0.40 |
| 1   | 1.49 ± 0.04 | 1.44 ± 0.20 | 1.42 ± 0.10 | 1.42 ± 0.08 | 0.46 ± 1.30 | 1.39 ± 0.10 |
| 3/2 | 1.46 ± 0.04 | 1.40 ± 0.10 | 1.41 ± 0.09 | 1.41 ± 0.07 | 0.57 ± 1.18 | 1.36 ± 0.03 |
| 2   | 1.45 ± 0.04 | 1.39 ± 0.10 | 1.39 ± 0.09 | 1.43 ± 0.10 | 0.61 ± 1.13 | 1.40 ± 0.10 |
| 5/2 | 1.44 ± 0.04 | 1.45 ± 0.20 | 1.39 ± 0.09 | 1.40 ± 0.07 | 0.64 ± 1.09 | 1.39 ± 0.07 |

4.2 Susceptibility and correlation length

Next we discuss the uniform susceptibility $\chi_0$ and the correlation length $\xi$. In addition to the spin-spin correlation functions, see Sec. 4.1, both quantities characterize the paramagnetic phase above $T_C$. We show the inverse susceptibility in Fig. 6. The susceptibility multiplied by $(|J_2 + J_1|)$ shows an almost universal behavior as a function of the normalized temperature $T/T_C$, i.e., the dependence on $S$ and $J_2$ is small. The RGM results agree well with the HTE data (see the inset in Fig. 6). While the RGM critical exponents deviate from the correct values, the HTE approach provides more accurate exponents. We present HTE data for $\gamma$ in Table 2. As expected, $\gamma$ is almost independent of $S$ and $J_2$ and it is close to the correct value $\gamma \sim 1.39$ of the three-dimensional Heisenberg ferromagnet, see, e.g., Ref. [68]. As already noticed in Sec. 4.1, the HTE approach (ii) to determine $T_C$ and $\gamma$ using differential approximants is more accurate and works well until large values of $J_2$. Thus, the analysis of the quotient of the HTE series for $\chi_0$, i.e., HTE (i), starts to fail already at $J_2 \sim 0.3$, see the large least-square deviations in Table 2.

The RGM results for the correlation length are shown in Fig. 7. Again the influence of the spin quantum number $S$ and the frustration $J_2$ on the $\xi(T/T_C)$-curve is weak. The decay of $\xi$ with temperature is fast, already at $T \sim 1.3T_C$ the correlation length is of the order of the lattice constant.
Figure 7: Correlation length $\xi$ as a function of the normalized temperature $T/T_C$ for $S = 1/2$ (solid lines) and $S = 5/2$ (dashed lines) for frustration parameters $J_2 = 0$ (blue lines) and $J_2 = 0.5$ (red lines).

Figure 8: Temperature dependence of the dispersion relation $\omega_q/S$ of the spin excitations for different values of $J_2$ and fixed $J_1 = -1$. The points in the Brillouin zone are defined as $\Gamma = (0,0,0), P = (\pi,\pi,\pi), H = (0,0,2\pi), N = (\pi,\pi,0)$. 
4.3 Excitation spectrum and specific heat

Let us now consider energetic quantities. By contrast to the RPA, the RGM provides a reasonable description of the excitation spectrum $\omega_q$ for arbitrary temperatures. We show the dispersion relation for various temperatures, spin quantum numbers and frustration parameters in Fig. 8. First we notice that for finite temperatures $\omega_q/S$ becomes dependent on $S$, see Figs. 8a and b. It is also evident that for a wide range of temperatures up to about 50% of the Curie temperature the changes in $\omega_q$ are quite small, see also Fig. 9. The main aspects of the influence of the temperature on $\omega_q$ are the following: For small values of $J_2 \lesssim 0.3$ the excitation energies for all $q$-vectors are reduced by increasing $T$. Around the maximum at $H = (0, 0, 2\pi)$ this reduction is present for all values of $J_2$. However, the temperature dependence of $\omega_q$ around the dip/minimum at the soft-mode wave vector $q = P = (\pi, \pi, \pi)$ as well as for $q \to 0$ differs for smaller $J_2$ from that for larger $J_2$. (Note that the second dip/minimum between the H- and N-points at about $q = 0.66(\pi, \pi, \pi)$ is related to that at $q = P$, i.e. it appears only due to the choice of path $H \to N$ in the Brillouin zone.) At $q = P$ the excitation energy $\omega_P$ decreases with growing $T$ for smaller $J_2$, but it increases for larger $J_2$, see Fig. 9b. The influence of $T$ on $\omega_q$ near the $\Gamma$-point, i.e., at small $|q|$, is more subtle: For $T < T_C$ the temperature dependence of the excitation energies is given by the temperature dependence of the spin stiffness $\rho_s$ describing the quadratic term in $\omega_q$ for small $|q|$, while for $T > T_C$ a linear term in $\omega_q$ determines the behavior near the $\Gamma$-point. We show $\rho_s(T)$ for $S = 1/2$ for various values of $J_2$ in Fig. 9a. As expected for ferromagnets, the stiffness becomes smaller with increasing of $T$ for $J_2 \lesssim 0.6$. Interestingly, for $J_2 \gtrsim 0.6 \rho_s(T)$ is growing with $T$. This unusual behavior of $\rho_s(T)$ near the zero-temperature transition point to an antiferromagnetic state has recently been discussed in Ref. [74] using non-linear and self-consistent spin-wave theories. Note, however, that in Ref. [74] the frustrated FCC ferromagnet is considered, whereas for our BCC model $\rho_s(T = 0) > 0$ at $J_2^c$. For small and moderate frustration, the spin-wave approach of Ref. [74] yields a decrease of $\rho_s$ with $T$ according to $\rho_s(T) = \rho_s(0) - BT^\mu$, $\mu = 5/2$ and $B > 0$. As approaching the zero-temperature transition point to the antiferromagnetic ground state, the exponent $\mu$ changes to $\mu = 5/4$ and the prefactor $B$ becomes negative, i.e. the stiffness can grow with increasing $T$. Our RGM data for $\rho_s(T)$ confirm these predictions: We find that $\rho_s(T)$ is well described by the power law given above with $B > 0$ and $\mu \approx 2.5$ for $J_2 \lesssim 0.5$, whereas for $J_2 = 0.6$ we have $B \approx -0.05$ and $\mu \approx 1.5$.  


Figure 9: Temperature dependence of the spin stiffness $\rho_s$ (left) and excitation energy $\omega_P$ at the soft-mode $\mathbf{q}$-vector $\mathbf{P} = (\pi, \pi, \pi)$ (right) for spin $S = 1/2$.

Figure 10: Specific heat $C_V$ as a function of the normalized temperature $T/T_c$. Main panel: RGM data for $S = 1/2, 1, 3/2$ and $5/2$ for frustration parameters $J_2 = 0$ (solid lines) and $J_2 = 0.5$ (dashed lines). Inset: Comparison of RGM data (dotted lines) with Padé approximants [6, 4] of the 10th order HTE data (symbols).

The specific heat $C_V$ is shown in Fig. 10. By contrast to the susceptibility and the correlation length the influence of the spin $S$ and the frustration $J_2$ is noticeable. The $C_V(T)$ curves show the
characteristic cusplike behavior at the transition temperature around $T_C$ for small spin quantum numbers $S$ indicating the second-order phase transition. With increasing $S$ in the long-range ordered phase the slope of the $C_V$ curves near $T_C$ decreases, and the cusplike shape develops to a kinklike one. This behavior for larger $S$ may be considered as a shortcoming of the RGM, cf. Ref. [36]. For $T > T_C$ we can compare the RGM data with HTE results, see the inset in Fig. 10. As for the susceptibility, the agreement is very good. The low-temperature behavior is given by Eq. (19), i.e., $C_V(T)$ increases with increasing $J_2$. Note, however, that the specific heat as a function of the normalized temperature $T/T_C$ shows the opposite trend, see Fig. 10.

5 Summary

In this paper we use the rotation-invariant Green’s function method (RGM) to calculate thermodynamic quantities, such as the Curie temperature $T_C$, the spontaneous magnetization $M$, the spin-spin correlation functions $\langle S_0 S_R \rangle$, the uniform susceptibility $\chi_0$, the correlation length $\xi$, the specific heat $C_V$ and the spin stiffness $\rho_s$ of a frustrated spin-S Heisenberg magnet on the BCC lattice with ferromagnetic NN exchange $J_1$ and antiferromagnetic NNN exchange $J_2$. We focus on the ferromagnetic regime, i.e., $J_2 \leq 2|J_1|/3$, such that the ground state is ferromagnetic. For $T > T_C$ our Green’s function approach is complemented by 10th order high-temperature expansion for the susceptibility and the specific heat.

The RGM goes one step beyond the random-phase approximation (RPA). As a result, several shortcomings of the RPA, see, e.g., Refs. [45, 46, 49–51], such as the artificial equality of the critical temperatures $T_N = T_C$ for ferro- and antiferromagnets or the failure in describing the paramagnetic phase at $T > T_C$, can be overcome. For the Curie temperature and the spontaneous magnetization $M$ we derive simple fit formulas describing $T_C$ as a function of $S$ and $J_2$ and the temperature dependence of $M(S, J_2)$. As approaching the ground-state transition point to the antiferromagnetic phase at $J_2^c \approx 2|J_1|/3$, the thermodynamic properties deviate from the ordinary ferromagnetic behavior. Thus, the spin-spin correlators may become negative at $T > T_C$ indicating the collinear antiferromagnetic Néel order present for $J_2 > J_2^c$, and the temperature profile of the spin stiffness $\rho_s$ for $T < T_C$ exhibits an increase with $T$ instead of the ordinary decrease.

The present investigations are focussed on theoretical aspects, in particular, with respect to previous discussions of one- and two-dimensional frustrated ferromagnets. There might be some relevance for ferromagnetic compounds [75–77] especially near a quantum phase transition, e.g., driven by doping.

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