Thermodynamics of a two-dimensional frustrated spin-$\frac{1}{2}$ Heisenberg ferromagnet

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Using the spin-rotation-invariant Green's-function method, we calculate the thermodynamic quantities (correlation functions $\langle \mathbf{S}_0 \mathbf{S}_\mathbf{R} \rangle$, uniform static spin susceptibility χ, correlation length ξ, and specific heat C_V) of the two-dimensional spin-$\frac{1}{2}$ J_1-J_2 Heisenberg ferromagnet for $J_2 < J_2^c \approx 0.44|J_1|$, where J_2^c is the critical frustrating antiferromagnetic next-nearest-neighbor coupling at which the ferromagnetic ground state gives way for a ground-state phase with zero magnetization. Examining the low-temperature behavior of χ and ξ, in the limit $T \to 0$ both quantities diverge exponentially, i.e., $\chi \propto \exp(b/T)$ and $\xi \propto \exp(b/2T)$, respectively. We find a linear decrease in the coefficient b with increasing frustration according to $b = -\frac{\pi}{2}(J_1 + 2J_2)$, i.e., the exponential divergence of χ and ξ is present up to J_2^c. Furthermore, we find an additional low-temperature maximum in the specific heat when approaching the critical point, $J_2 \to J_2^c$.

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I. INTRODUCTION

Low-dimensional quantum magnets have attracted much attention during the last decades.[1,2] They are predestined to study the influence of strong thermal and quantum fluctuations. Much attention has been paid to the theoretical investigation of the two-dimensional (2D) spin-$\frac{1}{2}$ J_1-J_2 quantum Heisenberg antiferromagnet which may serve as a canonical model to study the interplay of frustration effects and quantum fluctuations (see, e.g., Ref. 3). An additional motivation to study this model comes from the experimental side.[4] Very recently, several quasi-2D magnetic materials with a ferromagnetic nearest-neighbor (NN) coupling $J_1 < 0$ and a frustrating antiferromagnetic next-nearest-neighbor (NNN) coupling $J_2 > 0$ have been investigated experimentally, e.g., $Pb_2VO(PO_4)_2$,[5–8] $(CuCl)LaNb_2O_7$,[9] $SrZnVO(PO_4)_2$,[8,10,11] and $BaCdVO(PO_4)_2$.[7,10,12] The quite large frustrating J_2 drives these materials out of the ferromagnetic phase. The experimental findings have stimulated several theoretical studies of the ground-state and thermodynamic properties of the J_1-J_2 model with $J_1 < 0$ and frustrating $J_2 > 0$.[13–21] It was found that the ferromagnetic ground state for the spin-$\frac{1}{2}$ model breaks down at $J_2 = J_2^c \approx 0.4|J_1|$.[13–18,21,22] Note that for the classical model (spin $s \to \infty$), the corresponding transition point is at $J_2 = 0.5|J_1|$.

On the other hand, some materials considered as 2D spin-$\frac{1}{2}$ ferromagnets, such as K_2CuF_4, Cs_2CuF_4, Cs_2AgF_4, La_2BaCuO_5, and Rb_2CrCl_4,[23–27] might have also a weak frustrating NNN interaction $J_2 < J_2^c$. In contrast to the previous investigations of the 2D J_1-J_2 model with ferromagnetic J_1,[13–18,21] which have considered predominantly the case of strong frustration, in the present paper we will focus on the region of weak frustration $J_2 < J_2^c$.

Although for $J_2 < J_2^c$, the ground state remains ferromagnetic, the frustrating J_2 may influence the thermodynamics substantially, in particular, near a zero-temperature transition. This has been demonstrated for the one-dimensional (1D) frustrated ferromagnet in Ref. 28, where a change in the low-temperature behavior of the susceptibility and the correlation length as well as an additional low-temperature maximum in the specific heat have been found when approaching the zero-temperature critical point from the ferromagnetic side.

The Hamiltonian of the system considered in this paper is given by

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{[i,j]} \mathbf{S}_i \mathbf{S}_j ; \quad J_1 < 0; \quad J_2 \geq 0, \qquad (1)$$

where $(\mathbf{S}_i)^2 = 3/4$, and $\langle i,j \rangle$ denotes NN and $[i,j]$ denotes NNN bonds. The unfrustrated 2D ferromagnet ($J_2 = 0$) has been widely investigated, e.g., by the modified spin-wave theory,[29] renormalization-group approaches,[30,31] the quantum Monte Carlo method,[32–35] and by a spin-rotation-invariant second-order Green's-function method (RGM).[35–39] However, in presence of frustration ($J_2 > 0$), the choice of appropriate methods for studying temperature-dependent quantities of this system is restricted due to frustration and dimensionality. For instance, the powerful quantum Monte Carlo method is not applicable due to the minus-sign problem whereas finite-temperature density-matrix renormalization-group studies are restricted to 1D systems.

So far, only a few theoretical papers deal with the thermodynamics of the model for $J_2 > 0$, see, e.g., Refs. 13, 16, and 17, where finite lattices of $N = 16$ and $N = 20$ sites are considered. As we will see below, for these lattice sizes, the finite-size effects at low temperatures are large. Therefore, methods studying infinite systems are highly desirable. Among others, the Green's-function method is a powerful tool to study magnetic systems at finite temperatures, see, e.g., Refs. 40–42, and references therein. A specific variant appropriate for frustrated systems is the RGM. In the present paper, we use the RGM to investigate thermodynamic properties of the frustrated model (1), focusing on $J_2 \le J_2^c \approx 0.4|J_1|$. The RGM has been applied successfully to low-dimensional (frustrated) infinite quantum spin systems.[28,35–39,43–45] In particular, for the 1D spin-$\frac{1}{2}$ Heisenberg ferromagnet it was shown that the RGM reproduces Bethe-ansatz results.[28,37] Since the RGM can be formulated also for finite systems, we use full exact diagonalization (ED) of finite square lattices of $N=16$ and $N=20$ sites to compare the RGM with ED data for finite lattices.

The paper is organized as follows: in Sec. II, the RGM applied to model (1) is presented. The results for the thermodynamic quantities are discussed in Sec. III. Finally, a summary is given in Sec. IV.

II. ROTATION-INVARIANT GREEN'S-FUNCTION METHOD

To calculate the thermodynamic quantities of the model (1), we use the RGM (Refs. 28, 36, 37, 43, and 44) for determining the transverse dynamic spin susceptibility $\chi^{+-}_{\mathbf{q}}(\omega)=-\langle\langle S^+_{\mathbf{q}};S^-_{-\mathbf{q}}\rangle\rangle_\omega$, where $\langle\langle\cdots;\cdots\rangle\rangle_\omega$ denotes the two-time commutator Green's function.[40] Taking the equations of motion up to the second step and supposing spin-rotational symmetry, i.e., $\langle S_i^z\rangle=0$, we obtain

$$\omega^2\langle\langle S^+_{\mathbf{q}};S^-_{-\mathbf{q}}\rangle\rangle_\omega = M_{\mathbf{q}} + \langle\langle -\ddot{S}^+_{\mathbf{q}};S^-_{-\mathbf{q}}\rangle\rangle_\omega, \quad (2)$$

$$M_{\mathbf{q}} = \langle[[S^+_{\mathbf{q}},H],S_{-\mathbf{q}}]\rangle, \quad -\ddot{S}^+_{\mathbf{q}} = [[S^+_{\mathbf{q}},H],H]. \quad (3)$$

The moment $M_{\mathbf{q}}$ is given by the exact expression

$$M_{\mathbf{q}} = -8\sum_{k=1,2} J_k C_{1,k-1}(1-\gamma^{(k)}_{\mathbf{q}}), \quad (4)$$

where $C_{n,m}\equiv C_{\mathbf{R}}=\langle S_0^+S_{\mathbf{R}}^-\rangle = 2\langle S_0^zS_{\mathbf{R}}^z\rangle$, $\mathbf{R}=n\mathbf{e}_x+m\mathbf{e}_y$, $\gamma^{(1)}_{\mathbf{q}}=(\cos q_x+\cos q_y)/2$, and $\gamma^{(2)}_{\mathbf{q}}=\cos q_x \cos q_y$. The second derivative $-\ddot{S}^+_{\mathbf{q}}$ is approximated in the spirit of the schemes employed in Refs. 28, 35–39, and 43–45. That is, in $-\ddot{S}^+_i$ we adopt the decoupling,

$$S_i^+S_j^+S_k^- = \alpha_{i,k}\langle S_i^+S_k^-\rangle S_j^+ + \alpha_{j,k}\langle S_j^+S_k^-\rangle S_i^+. \quad (5)$$

Following the arguments of Ref. 28, we put $\alpha_{i,k}=\alpha$ in the whole temperature region. We obtain $-\ddot{S}^+_{\mathbf{q}}=\omega^2_{\mathbf{q}}S^+_{\mathbf{q}}$ and

$$\chi^{+-}_{\mathbf{q}}(\omega) = -\langle\langle S^+_{\mathbf{q}};S^-_{-\mathbf{q}}\rangle\rangle_\omega = \frac{M_{\mathbf{q}}}{\omega^2_{\mathbf{q}}-\omega^2} \quad (6)$$

with

$$\omega^2_{\mathbf{q}} = 2\sum_{k,l(=1,2)} J_kJ_l(1-\gamma^{(k)}_{\mathbf{q}})[K_{k,l}+8\alpha C_{1,k-1}(1-\gamma^{(l)}_{\mathbf{q}})], \quad (7)$$

where $K_{1,1}=1+2\alpha(2C_{1,1}+C_{2,0}-5C_{1,0})$, $K_{2,2}=1+2\alpha(2C_{2,0}+C_{2,2}-5C_{1,1})$, $K_{1,2}=4\alpha(C_{1,2}-C_{1,0})$, and $K_{2,1}=4\alpha(C_{1,0}+C_{1,2}-2C_{1,1})$. From the Green's function [Eq. (6)], the correlation functions $C_{\mathbf{R}}=\frac{1}{N}\Sigma_{\mathbf{q}}C_{\mathbf{q}}e^{i\mathbf{qR}}$ of arbitrary range $\mathbf{R}$ are determined by the spectral theorem,[40]

$$C_{\mathbf{q}} = \langle S^+_{\mathbf{q}}S^-_{\mathbf{q}}\rangle = \frac{M_{\mathbf{q}}}{2\omega_{\mathbf{q}}}[1+2n(\omega_{\mathbf{q}})], \quad (8)$$

where $n(\omega_{\mathbf{q}})=(e^{\omega_{\mathbf{q}}/T}-1)^{-1}$ is the Bose function. Taking the on-site correlator $C_{\mathbf{R}=0}$ and using the operator identity $S_i^+S_i^-=\frac{1}{2}+S_i^z$, we get the sum rule $C_0=\frac{1}{N}\Sigma_{\mathbf{q}}C_{\mathbf{q}}=\frac{1}{2}$. The uniform static spin susceptibility $\chi=\lim_{\mathbf{q}\to 0}\chi_{\mathbf{q}}$, where $\chi_{\mathbf{q}}=\chi_{\mathbf{q}}(\omega=0)$ and $\chi_{\mathbf{q}}(\omega)=\frac{1}{2}\chi^{+-}_{\mathbf{q}}(\omega)$, is given by

$$\chi = -\frac{2}{\Delta}\sum_{k=1,2} kJ_kC_{1,k-1}, \quad \Delta = \sum_{k,l=1,2} kJ_kJ_lK_{k,l}. \quad (9)$$

The correlation length may be calculated by expanding $\chi_{\mathbf{q}}$ around $\mathbf{q}=0$,[28,35,36] $\chi_{\mathbf{q}}=\chi/[1+\xi^2(q_x^2+q_y^2)]$. We find

$$\xi^2 = \frac{2\alpha(J_1^2C_{1,0}+2J_1J_2(C_{1,0}+C_{1,1})+4J_2^2C_{1,1})}{\Delta}. \quad (10)$$

The ferromagnetic long-range order (LRO), occurring at $T=0$ only, is reflected by a nonvanishing quantity C (see, e.g., Ref. 36) according to $C_{\mathbf{R}}(0)=\frac{1}{N}\Sigma_{\mathbf{q}\neq 0}C_{\mathbf{q}}(0)e^{i\mathbf{qR}}+C$, where C, typically called condensation term,[36] is connected with the magnetization m by $m^2=3C/2$. Due to the exact result $C_{\mathbf{R}\neq 0}(0)=\frac{1}{6}$, $C_{\mathbf{q}}(0)=\frac{M_{\mathbf{q}}(0)}{2\omega_{\mathbf{q}}(0)}$ must be independent of $\mathbf{q}$. Examining Eqs. (4) and (7), this requires $K_{k,l}(0)=0$ which leads to $\alpha(0)=\frac{3}{2}$ and $C_{\mathbf{q}}(0)=\frac{1}{3}$. Hence, in case of a ferromagnetic ground state, we find at zero temperature $\omega_{\mathbf{q}}=2\rho_s\mathbf{q}^2$ ($|\mathbf{q}|\ll 1$), $\rho_s=-\frac{1}{4}(J_1+2J_2)$ (where ρ_s is the spin stiffness), and $C_{\mathbf{R}}(0)=\frac{1}{3}\delta_{\mathbf{R},0}+\frac{1}{6}$. Note that the sum rule $C_0=\frac{1}{2}$ is fulfilled. In Eqs. (9) and (10), we have $\Delta(0)=0$ so that χ and ξ diverge as $T\to 0$ indicating the ferromagnetic phase transition.

To estimate the zero-temperature transition point J_2^c (see Sec. III A), we determine the ground-state correlation functions and the ground-state energy per site, $E=3(J_1C_{1,0}+J_2C_{1,1})$, for $J_2>J_2^c$. Thereby, we take into consideration the possible existence of a quantum collinear phase described by the magnetic ordering vector $\mathbf{Q}=(\pi,0)$ or $(0,\pi)$ and proceed along the lines indicated in Ref. 44.

Since we will compare the RGM data with ED data for finite lattices, see Sec. III, we have to adopt the RGM to finite N. In this case, the quantity C is not related to the magnetization and stays nonzero in the whole temperature region. In Ref. 45, it was shown that $C=2T\chi/N$.

To evaluate the thermodynamic quantities, a coupled system of six (for finite systems: seven) nonlinear algebraic self-consistency equations, including the sum rule $C_0=\frac{1}{2}$, has to be solved numerically to determine the correlators $C_{1,0}$, $C_{1,1}$, $C_{2,0}$, $C_{2,1}$, $C_{2,2}$, (C), and the vertex parameter α. To solve this system we use Broyden's method,[46] which yields the solutions with a relative error of about 10^{-8} on the average. The momentum integrals are done by Gaussian integration. To find the numerical solution of the RGM equations for $T>0$, we start at high temperatures and decrease T in small steps. Below a certain (low) temperature $T_0(J_2)$, no solutions of the RGM equations (except at $T=0$) could be found since the quantity $\Delta(T,J_2)$ in Eqs. (9) and (10) becomes exponentially small which leads to numerical instabilities. Presenting our results in the next section, we put $J_1=-1$.

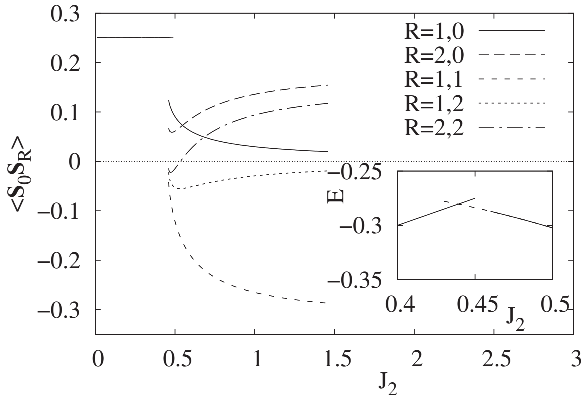

FIG. 1. Ground-state spin-spin correlation functions $\langle \mathbf{S}_0\mathbf{S}_\mathbf{R}\rangle$ in dependence on frustration J_2. (Note that for $J_2 < J_2^c \approx 0.44$ all $\langle \mathbf{S}_0\mathbf{S}_\mathbf{R}\rangle$ coincide.) Inset: ground-state energy E versus J_2 (solid line: RGM data, dashed line: extrapolated RGM data to fix the transition point, see also text).

III. RESULTS

A. Phase transition at $T=0$

In a first step, we use the RGM as described above to determine the transition point J_2^c, where the ferromagnetic ground state gives way for a ground-state phase with zero magnetization. For that we solve the RGM equations at $T=0$ (i) starting from $J_2=0$ with increasing J_2 and (ii) starting from large $J_2 \gg 1$ with decreasing J_2. In case (i), the RGM equations at $T=0$ can be solved until the classical transition at $J_2=0.5$. In case (ii), we find solutions of the RGM ground-state equations down to $J_2=0.46$. This value lies certainly above the transition point J_2^c. To fix J_2^c, we may extrapolate the ground-state energy obtained for case (ii). The crossing point of both energies at $J_2=0.44$ can be considered as the RGM estimate of J_2^c, see the inset of Fig. 1. This value is in reasonable agreement with values for J_2^c reported in other papers.[14,18,19,21,22]

The behavior of the spin-spin correlation functions at $T=0$ near the transition point J_2^c is illustrated in Fig. 1. For $J_2 \gtrsim J_2^c$, there is a noticeable variation in the correlation functions. With increasing J_2, at $J_2 \gtrsim 1$, the spin-spin correlation functions approach the corresponding values of the limiting case $J_2 \gg 1$. This behavior is in qualitative agreement with data from Lanczos ED and coupled-cluster method.[21] At the critical point, the correlation functions jump to the exact results of the ferromagnetic phase, i.e., $\langle \mathbf{S}_0\mathbf{S}_\mathbf{R}\rangle=0.25$. Together with the kink in the energy, this indicates a first-order transition. These results confirm the findings in previous papers.[14,19,22]

B. Thermodynamic properties

Now we investigate the thermodynamic properties of the model for $J_2 < J_2^c \approx 0.44$, where the ground state is ferromagnetic. First we consider the temperature dependence of the spin-spin correlation functions. The NN and NNN correlators are shown in Fig. 2 for various values of J_2. For comparison we show also ED data for $N=20$ sites. The RGM results agree qualitatively with the ED data. With increasing frustration, the correlation functions decrease more rapidly with temperature. Interestingly, for large frustration the NNN correlation function changes its sign at a certain temperature, e.g., for $J_2=0.3$, at $T \approx 1.25$ (RGM data). The faster decay of the spin-spin correlators due to frustration is related to the decrease in the correlation length ξ with increasing J_2, see the discussion below.

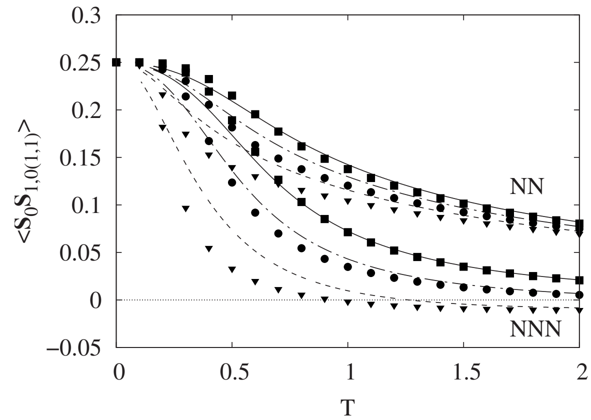

FIG. 2. NN and NNN spin-spin correlation functions for $J_2=0$, 0.15, and 0.3, from top to bottom, calculated by RGM for $N\to\infty$ (lines) and ED for $N=20$ (filled symbols).

The uniform static spin susceptibility χ and the correlation length ξ depicted in Figs. 3 and 4 show a similar behavior. Due to the ferromagnetic ground state, both quantities diverge at $T=0$ exponentially, see below. With increasing frustration J_2, the rapid increase in both quantities is shifted to lower temperatures. As shown in the insets of Figs. 3 and 4, at a certain fixed temperature both χ and ξ decrease rapidly with J_2.

Since the susceptibility (together with the correlation length) is an important quantity to analyze the critical properties for $T\to 0$, we first test the quality of our RGM approach in more detail by comparing the RGM data for $N=16$ and $N=20$ with ED data for the same system sizes, see

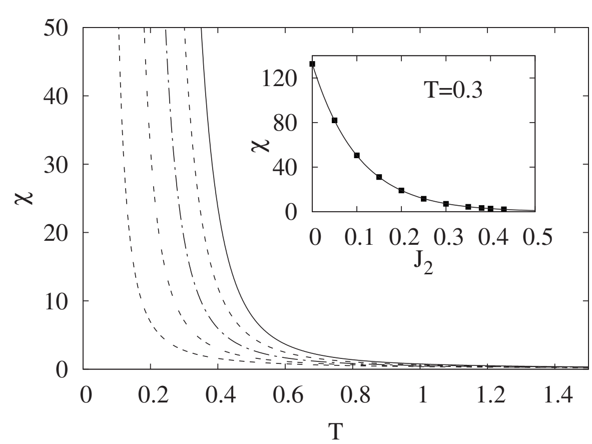

FIG. 3. Uniform static spin susceptibility χ for $J_2=0$, 0.1, 0.2, 0.3, and 0.4, from right to left. The inset shows the susceptibility for $T=0.3$ in dependence on the frustration J_2. The solid line represents an exponential fit, $\chi(T=0.3) \approx 132.8\,\exp(-9.7J_2)$, of the data points (filled squares).

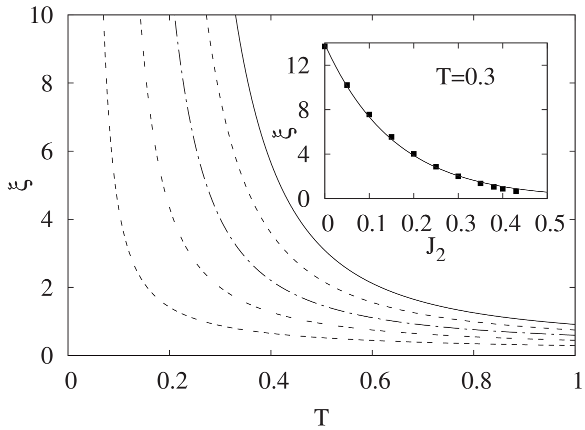

FIG. 4. Correlation length ξ for J_2=0, 0.1, 0.2, 0.3, and 0.4 from right to left. The inset shows the correlation length for T=0.3 in dependence on the frustration J_2. The solid line represents an exponential fit, $\xi(T=0.3)\approx 13.9\exp(-6.4J_2)$, of the data points (filled squares).

Fig. 5. It is obvious that the RGM and the ED data for χ are in excellent agreement. This is consistent with our previous finding[28] that for the 1D Heisenberg ferromagnet, the RGM data for $\chi(T\to 0)$ and $\xi(T\to 0)$ are in perfect agreement with exact Bethe-ansatz results. Moreover, the RGM calculations of χ for finite N allow to estimate the magnitude of the finite-size effects. As can be clearly seen in Fig. 5, the finite-size effects at $T\lesssim 0.6$ ($T\lesssim 0.4$) for J_2=0.1 (J_2=0.3) become very large. Since the correlation length ξ becomes smaller with increasing J_2 (see the inset in Fig. 4), the finite-size effects become less pronounced with growing frustration. Nevertheless, based on our data we argue that the finite systems of N=16 and N=20, accessible by exact full diagonalization, are not representative for the thermodynamic limit, see also Refs. 16 and 17. Note that for the 1D case, the ED data for N=20 are in good agreement with RGM data for $N\to\infty$.[28] Consistent to that observation, in two dimensions the system of N=400 sites with the same linear extension is already close to the thermodynamic limit, see Fig. 5.

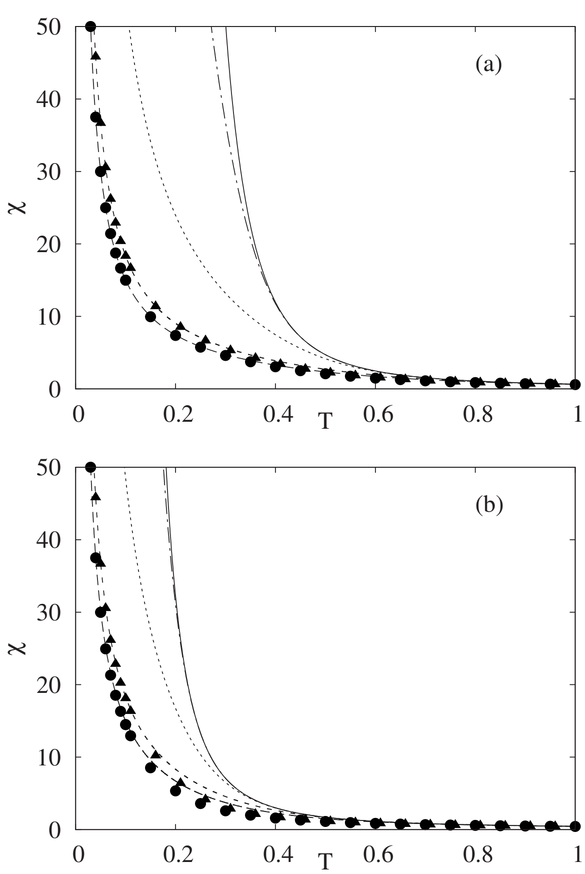

FIG. 5. Uniform static spin susceptibility χ for (a) J_2=0.1 and (b) J_2=0.3 for N=16, 20, 64, and 400, thermodynamic limit (lines, RGM) and N=16 and 20 (filled symbols, ED), from left to right. Note that for J_2=0.3, the curves for N=400 and $N\to\infty$ almost coincide.

Next we use the RGM for $N\to\infty$ to investigate the critical behavior of χ and ξ for $T\to 0$ in more detail. We start with a brief discussion of the low-temperature behavior of the unfrustrated ferromagnet. Contrary to the 1D case, where for J_2=0 exact Bethe results are available,[47] we have only approximate results for the 2D model. From low-temperature expansions of the susceptibility and the correlation length for the model with J_2=0 using renormalization-group approaches,[30,31] the modified spin-wave theory,[29] and the RGM,[37] it is known that for $T\to 0$, the susceptibility behaves as $\chi\propto T^s\exp(b/T)$ and the correlation length as $\xi\propto T^{\sigma}\exp(\beta/T)$. While different leading exponents s and σ for the (less important) pre-exponential factor were obtained by different methods, the exponential divergence is obtained by all authors.[29–31,37] However, different values for the coefficients b and β were reported, namely, $b(J_2=0)=\pi/2$ using RGM,[37] $b(J_2=0)=\pi$ using modified spin-wave theory[29] or renormalization-group approach,[30] and $b(J_2=0)=0.1327\pi$ using a different version of the renormalization-group approach.[31] In all these papers,[29–31,37] it was found that the coefficients in the exponents fulfill the relation $\beta=b/2$. We mention further that early numerical studies based on quantum Monte Carlo calculations (using, however, χ and ξ data only for quite large temperatures) give $b(J_2=0)\approx 4.5\approx 1.43\pi$ (Ref. 33) and $\beta(J_2=0)=0.254\pi$ (Ref. 32). Let us finally argue that the results for the coefficient b obtained by modified spin-wave theory[29] as well as renormalization-group approach[30] and by the RGM (Ref. 37) seem to be most reliable since these methods are well tested. Moreover, for the 1D spin-$\frac{1}{2}$ Heisenberg ferromagnet, it was shown that the RGM (Refs. 28 and 37) as well as the modified spin-wave theory[29] reproduce the exact Bethe-ansatz results for the low-temperature behavior of χ and ξ. Hence, it is to some extent surprising that there is a difference by a factor of 2 in the coefficient b between the value obtained by modified spin-wave theory[29] (as well as renormalization-group approach[30]) and the RGM for the 2D unfrustrated ferromagnet. This discrepancy is a known but unresolved problem.[35,37] However, we believe that our general conclusions concerning the exponential divergence of the frustrated model, see the discussion below, are not affected by this problem.

Next we use the RGM results to determine the coefficients b and β as functions of J_2. We assume that the general low-T behavior of these quantities is preserved for $0<J_2<J_2^c$, cf. Ref. 28, and fit our numerical RGM data for χ and

ξ at low temperatures using the ansatze's $\chi=(a_0T^{-1}+a_1+a_2T)\exp(\frac{b}{T})$ and $\xi=\sqrt{(\alpha_0T^{-1}+\alpha_1+\alpha_2T)}\exp(\frac{\beta}{T})$. Note that the leading power T^{-1} in the pre-exponential functions was derived for the unfrustrated case with the RGM in Ref. 37. We consider b, a_0, a_1, and a_2 as well as β, α_0, α_1, and α_2 as independent fit parameters. Recall that we can calculate RGM data only for temperatures down to a certain T_0, where T_0 (e.g., $T_0=0.161$ for $J_2=0$ and $T_0=0.052$ for $J_2=0.4$) is the lowest temperature where the system of RGM equations converges (see Sec. II). Thus, in addition to the leading power T^{-1} in the pre-exponential function, it is reasonable to consider higher-order terms to achieve an optimal fit of the RGM data. For the fit, we use 500 equidistant data points in the interval $T_0\ldots T_0+T_{cut}$, where T_{cut} is set to 0.05. The fit of the numerical RGM data reproduces the analytical results of Ref. 37 for $J_2=0$, i.e., $b(J_2=0)=2\beta(J_2=0)=\pi/2$, with a precision of four digits.

After having tested our fitting procedure by comparison with the analytical predictions for $J_2=0$, we now consider the frustrated model, where (to the best of our knowledge) no other results are available. From our numerical data for χ and ξ, we determine the J_2 dependence of the coefficients b and β. We find that the numerical data for b and β obtained by the fitting procedure described above are very well described by a linear decrease in both parameters with increasing frustration,

$$b=2\beta=-\frac{\pi}{2}(J_1+2J_2). \tag{11}$$

Obviously, both parameters would be zero at the classical transition point $J_2=0.5$ but they are still finite at the transition point $J_2^c\approx 0.44$ of the quantum model. Hence, the exponential divergence is present in the full parameter range $J_2\leq J_2^c$ where the ground state is ferromagnetic. We emphasize that this result is contrary to the behavior observed for the 1D frustrated spin-$\frac{1}{2}$ ferromagnet, where the critical properties change at the zero-temperature transition point.[28] We mention further that the leading coefficients a_0 and α_0 of the pre-exponential functions, see the expressions for χ and ξ given above, vanish at the transition point J_2^c whereas the next coefficients a_1 and α_1 remain finite at J_2^c. Hence, the pre-exponential temperature dependence is changed approaching the zero-temperature transition.

Let us mention that the linear decrease in the coefficients b and β, see Eq. (11), found by fitting the low-temperature behavior of χ and ξ is the same as that obtained analytically for the zero-temperature spin stiffness ρ_s, see Sec. II. This relation between ρ_s and the divergence of the correlation length and the susceptibility is in accordance with general arguments[48,49] concerning the low-temperature physics of low-dimensional Heisenberg ferromagnets.

Another interesting quantity is the specific heat C_V shown in Fig. 6. For $J_2=0$, the specific heat exhibits a typical broad maximum at about $T=0.562$. On increasing the frustration, the height of this maximum becomes smaller and it is shifted to lower temperatures. Interestingly, within our RGM approach the shape of the $C_V(T)$ curve changes for large frustration. For $J_2\gtrsim 0.34$, the specific heat shows two maxima, one at low temperatures ($T<0.193$) and another one at high temperatures ($T>0.6$). This extra low-temperature maximum signals the emergence of an additional low-energy scale when approaching the transition point J_2^c. Then many low-lying multiplets appear above the fully polarized ferromagnetic ground-state multiplet. Hence, the appearance of the additional low-temperature maximum in $C_V(T)$ can be attributed to a subtle interplay between all of these low-lying states. Note that a similar behavior was found for the 1D case.[28]

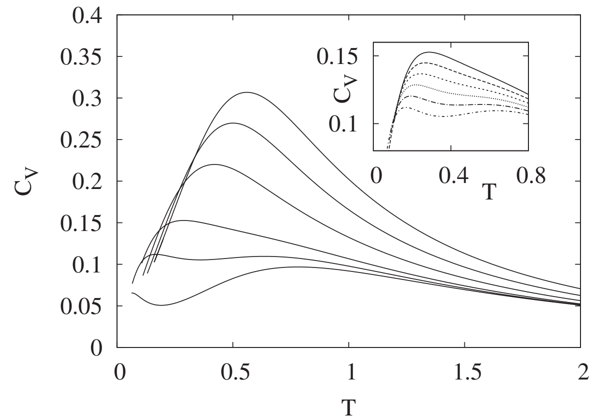

FIG. 6. Specific heat calculated by RGM for $J_2=0$, 0.1, 0.2, 0.3, 0.35, and 0.4, from top to bottom. The inset shows the specific heat for $J_2=0.3-0.35$ in steps of 0.01.

IV. SUMMARY

In this paper, we investigated the influence of the frustrating NNN coupling $J_2<J_2^c$ on the thermodynamic properties of the 2D spin-$\frac{1}{2}$ Heisenberg ferromagnet using the RGM. The RGM estimate for the critical frustration J_2^c, where the ferromagnetic ground state breaks down, is $J_2^c\approx 0.44|J_1|$.

We tested the method by comparing RGM data for the spin-spin correlation functions and the uniform susceptibility χ calculated for finite lattices of $N=16$ and $N=20$ sites with corresponding exact-diagonalization data for the same lattice sizes and found a good agreement between both methods. However, the comparison of RGM data for finite lattices and for $N\to\infty$ indicates strong finite-size effects at low temperatures. This leads to the conclusion that the finite systems of $N=16$ and $N=20$ are not representative for the low-temperature thermodynamics of large systems.

As it is known from the Mermin-Wagner theorem,[50] the thermal fluctuations are strong enough to suppress magnetic LRO for the Heisenberg ferromagnet in dimension $D<3$ at any finite temperature. Due to frustration, the fluctuations are further enhanced. Thus, frustration leads to a significant suppression of magnetic correlations at finite temperatures even if the ground state remains ferromagnetic.

The low-temperature behavior of the susceptibility χ and the correlation length ξ in the ferromagnetic ground-state region $J_2<J_2^c$ exhibits the exponential divergences $\chi\propto\exp[\frac{\pi(|J_1|-2J_2)}{2T}]$ and $\xi\propto\exp[\frac{\pi(|J_1|-2J_2)}{4T}]$. Although the numerator in the exponent decreases with growing J_2, the exponen-

tial divergence perpetuates in the whole parameter region $J_2 \leq J_2^c$. The specific heat calculated within the RGM exhibits a double-maximum structure for $J_2 \gtrsim 0.34$ analogous to the 1D model. To test our theoretical predictions, it would be interesting to reconsider experimentally quasi-2D spin-$\frac{1}{2}$ ferromagnets, such as K_2CuF_4, Cs_2CuF_4, Cs_2AgF_4, La_2BaCuO_5, and Rb_2CrCl_4 (Refs. 23–27) with respect to a possible frustration and its influence on low-temperature thermodynamics.

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