Finite size and temperature effects in the J_1-J_2 model on a strip

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Within Takahashi's spin-wave theory we study finite size and temperature effects near the quantum critical point in the J_1-J_2 Heisenberg antiferromagnet defined on a strip ($L\times\infty$). In the continuum limit, the theory predicts universal finite size and temperature corrections and describes the dimensional crossover in magnetic properties from $2+1$ to $1+1$ space-time dimensions.

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Takahashi's spin-wave theory is a useful tool for qualitative study of thermodynamic properties in low-dimensional spin systems.[1] For instance, the theory is capable to reproduce the universal low-temperature behavior in two-dimensional (2D) Heisenberg antiferromagnets[2] (HAFM) originally predicted on the basis of the $2+1$ nonlinear σ model[3] in the limit $\rho_s \ll T$ (ρ_s is the spin-wave stiffness constant). Near the quantum critical point 2D HAFM is expected to possess universal magnetic properties for arbitrary T/ρ_s provided $\rho_s, T\ll J$, J being a characteristic exchange energy.[4] Finite size and temperature effects in 2D HAFM in the limit $\rho_s \ll T$ have previously been analyzed in the geometry $L\times L$.[5]

In the present work we apply Takahashi's approach to a frustrated J_1-J_2 Heisenberg antiferromagnet defined on a strip with linear dimensions $L\times\infty$. In this geometry the coupled self-consistent equations for the spectral gap Δ, the current field $g=-\langle a_{\mathbf{0}}^\dagger b_{\hat{x}}^\dagger\rangle$, and the density field $f=\langle a_{\mathbf{0}}^\dagger a_{\hat{x}+\hat{y}}\rangle$ can be represented in the form[6]

$$S+\frac{1}{2}=\frac{1}{2L}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\frac{1}{\sqrt{1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2}}\coth\left(\frac{\epsilon_{\mathbf{k}}}{2T}\right),$$

$$g=S+\frac{1}{2}-\frac{1}{2L}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\frac{1-\gamma_{\mathbf{k}}^2\eta_{\mathbf{k}}}{\sqrt{1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2}}\coth\left(\frac{\epsilon_{\mathbf{k}}}{2T}\right),$$

$$f=S+\frac{1}{2}-\frac{1}{2L}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\frac{1-\kappa_{\mathbf{k}}}{\sqrt{1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2}}\coth\left(\frac{\epsilon_{\mathbf{k}}}{2T}\right), \quad (1)$$

where $\epsilon_{\mathbf{k}}=4J_1 g\,\eta_{\mathbf{k}}^{-1}\sqrt{1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2}$ is the magnon dispersion relation [$\eta_{\mathbf{k}}^{-1}=1-(\alpha f/g)(1-\kappa_{\mathbf{k}})+\mu$, $\kappa_{\mathbf{k}}=\cos k_1\cos k_2$, $\gamma_{\mathbf{k}}=(\cos k_1+\cos k_2)/2$], $\alpha=J_2/J_1$ is the frustration parameter, and S is the value of the lattice spin. The components of the wave vector $\mathbf{k}=k_1\hat{\mathbf{x}}+k_2\hat{\mathbf{y}}$ take the values $k_1=2\pi n_1/L$ [$n_1=0,\pm1,\ldots,\pm(L-1)/2$] and $k_2\in[-\pi,\pi]$, where L is an odd integer. We use a system of units where $\hbar=k_B=a=1$, a is the lattice spacing. The chemical potential μ is connected to the spectral gap by the relation $\Delta=4J_1 g\sqrt{2\mu}$.

At $T=0$ and in an infinite geometry ($L=\infty$) the system is in the magnetic Néel state, characterized by the on-site magnetization

$$m_0=S+\frac{1}{2}-\frac{1}{2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dk_1dk_2}{(2\pi)^2}\frac{1}{\sqrt{1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2}}, \quad (2)$$

up to the quantum critical point α_c. Recent studies predict that the system is magnetically disordered from $\alpha_c=0.38$ up to $\alpha\approx0.6$, and support the hypothesis that α_c is a second-order phase-transition point described by the $O(3)$ nonlinear σ model.[7] Equations (1) are supposed to describe the magnetically disordered phase at finite temperatures both in the infinite $\infty\times\infty$ and in the strip $L\times\infty$ geometries. In addition, the theory can also be applied to the magnetically disordered ground state of the strip system. In both cases the excitation gap $\Delta\neq0$ appears as a result of the constraint that implies zero total staggered magnetization [the first of Eqs. (1)], and the theory is restricted to strip systems with integer rung spins (LS). An equivalent spin-wave description of the ground state of finite size systems has originally been proposed by Hirsch and Tang.[8]

Leading corrections in T and $1/L$ near the quantum critical point $(T,\alpha)=(0,\alpha_c)$ can be obtained in the low-energy long-wavelength limit of the theory when the magnon dispersion relation takes the form

$$\epsilon_{\mathbf{k}}=c\sqrt{M^2+k^2}. \quad (3)$$

Here $c=4J_1 g\beta$ is the spin-wave velocity ($\beta=\sqrt{1/2-\alpha f/g}$) and $M=\sqrt{2\mu}/\beta$ is the magnon "mass," which is connected to the spectral gap by the relation $\Delta=cM$. In the framework of the discussed theory, the spin-wave stiffness constant is defined by the relation $\rho_s=2J_1 g\beta^2 m_0$. In the long-wavelength limit, Eqs. (1) are simplified to

$$S+\frac{1}{2}-f+g=\frac{1}{\beta}W(L,T),$$

$$S+\frac{1}{2}-g=\frac{2\beta^2+1}{4\beta}U(L,T)+\frac{\beta}{2}M^2W(L,T),$$

$$S+\frac{1}{2}-f=\frac{1}{2\beta}U(L,T), \quad (4)$$

where

$$W(L,T)=\frac{2T}{cL}\sum_{n=-\infty}^{\infty}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\frac{1}{\omega_n^2/c^2+M^2+k^2},$$

$$U(L,T)=\frac{2T}{cL}\sum_{n=-\infty}^{\infty}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\frac{k^2}{\omega_n^2/c^2+M^2+k^2}. \quad (5)$$

In the last equations $\omega_n=2\pi nT$ and $k=\sqrt{k_1^2+k_2^2}$.

Finite size effects at $T=0$

In the ground state, the functions $W_0(L)\equiv W(L,0)$ and $U_0(L)\equiv U(L,0)$ take the forms

$$W_0(L)=\frac{1}{L}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\frac{1}{\sqrt{M^2+k^2}}$$

and

$$U_0(L)=\frac{1}{L}\sum_{k_1}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\sqrt{M^2+k^2}-M^2W_0(L).$$

To extract the finite size corrections we follow the method suggested in Ref. 9 (see also Ref. 10). Using integral representations for the integrands (see Ref. 11), the above two equations are, respectively, transformed to

$$W_0(L)=\int_0^{\infty}\frac{dt}{2\pi}\frac{e^{-M^2t}}{t}\mathrm{erf}(\pi\sqrt{t})Q_L(t)$$

and

$$U_0(L)=M+\int_0^{\infty}\frac{dt}{2\sqrt{\pi}}\frac{e^{-M^2t}}{t^{3/2}}\left[1-\frac{\mathrm{erf}(\pi\sqrt{t})}{\sqrt{4\pi t}}Q_L(t)\right]-M^2W_0(L),$$

where $\mathrm{erf}(z)$ is the error function and $Q_L(t)=(1/L)\Sigma_{n=-L/2+1/2}^{L/2-1/2}\exp[-(2\pi n/L)^2t]$. Note that $\lim_{L\to\infty}Q_L(t)=\mathrm{erf}(\pi\sqrt{t})/\sqrt{4\pi t}$.

The finite size contributions in $W_0(L)=W_0(\infty)+\delta W_0(L)$ and $U_0(L)=U_0(\infty)+\delta U_0(L)$ can be separated by using the asymptotic formula ($L\gg 1$) (see Ref. 10, p. 148)[12]

$$Q_L(t)\cong\frac{1}{\sqrt{4\pi t}}\left[\mathrm{erf}(\pi t^{1/2})+2\sum_{l=1}^{\infty}\exp(-l^2L^2/4t)\right]. \quad (6)$$

The result reads

$$\delta W_0(L)=\frac{M}{\sqrt{\pi}}\sum_{l=1}^{\infty}\int_0^{\infty}\frac{dt}{2\pi}t^{-3/2}\times\exp\left(-t-\frac{l^2L^2M^2}{4t}\right)\mathrm{erf}\left(\frac{\pi\sqrt{t}}{M}\right),$$

$$\delta U_0(L)=-\frac{M^3}{\sqrt{\pi}}\sum_{l=1}^{\infty}\int_0^{\infty}\frac{dt}{4\pi}t^{-5/2}\times\exp\left(-t-\frac{l^2L^2M^2}{4t}\right)\mathrm{erf}\left(\frac{\pi\sqrt{t}}{M}\right)-M^2\delta W_0(L).$$

For $M\ll 1$ the error function in the above equations can be replaced by unity and after some algebra one gets

$$\delta W_0(L)=\frac{1}{\pi L}\mathrm{Li}_1(e^{-LM}) \quad (7)$$

and

$$\delta U_0(L)=-\frac{1}{\pi L^3}F(LM). \quad (8)$$

Here $\mathrm{Li}_s(z)=\Sigma_{n=1}^{\infty}z^n/n^s$ is the polylogarithmic function of s kind and

$$F(y)\equiv y^2\mathrm{Li}_1(e^{-y})+y\mathrm{Li}_2(e^{-y})+\mathrm{Li}_3(e^{-y}). \quad (9)$$

Using Eq. (2), near the quantum critical point $(T,\alpha)=(0,\alpha_c)$, the first of Eqs. (4) takes the form

$$cM=\frac{2c}{L}\mathrm{arcsinh}\left[\frac{1}{2}\exp\left(-\frac{2\pi\rho_sL}{c}\right)\right]. \quad (10)$$

Finally, a subtraction of the $L=\infty$ contributions in the last two of Eqs. (4) leads to the expressions

$$g=g_c+\frac{(2\beta_c^2+1)}{4\pi\beta_c}\frac{1}{L^3}F(LM)-\frac{(2\beta_c^2-1)}{4\beta_c^2}U_0(\infty)(\beta-\beta_c)-\frac{\beta_c}{2}M^2\delta U_0(L) \quad (11)$$

and

$$f=f_c+\frac{1}{2\pi\beta_c}\frac{1}{L^3}F(LM)+\frac{U_0(\infty)}{2\beta_c^2}(\beta-\beta_c). \quad (12)$$

Here g_c, f_c, and β_c are the values of the respective functions at the quantum critical point. The above expressions are valid near the quantum critical point.

Equation (10) exactly reproduces the saddle-point equation (with an appropriate regularization) in the $1/N$ expansion of the $O(N)$ nonlinear σ model in 2+1 space-time dimensions.[13] As can be expected from the relativistic dispersion relation (3), the ratio c/L plays the role of an effective temperature. It is well known that the gap equation (10) describes three different regimes, i.e., (i) the renormalized classical, (ii) the quantum critical, and (iii) the quantum disordered regimes (see, e.g., Ref. 10).

(i) For $\rho_sL/c\gg 1$ (large linear-size behavior) the approximate solution reads $\Delta\equiv Mc=(c/L)\exp(-2\pi\rho_sL/c)$. Using the mentioned symmetry and the refined result[14] for the correlation length ξ at low temperatures, the expression for Δ can be improved to

$$\frac{\Delta(L)}{c}=A\exp\left(-\frac{2\pi\rho_sL}{c}\right)\left(1-\frac{c}{4\pi\rho_sL}\right), \quad (13)$$

where A is some dimensionless parameter. The last equation may be interpreted as the spectral gap of a 1D HAFM defined on a ladder characterized by the integral "rung" spin $S_{eff}=\rho_s L/c$.[15]

(ii) Exactly at the quantum critical point, Eq. (10) gives

$$\Delta = y_0 \frac{c}{L}, \tag{14}$$

where $y_0 = 2\ln(1/2+\sqrt{5}/2)$ is a universal constant.

Equations (11) and (12) lead to the universal finite size contribution for the internal energy per spin $[e(L)=-2J_1(g^2-\alpha f^2)]$,

$$e(L) = e_c(\infty) - \frac{c}{\pi L^3}\tilde{F}(LM), \tag{15}$$

where $\tilde{F}(y)=F(y)-(y^2/2)\mathrm{Li}_1(e^{-y})$.

It can be shown that for $\alpha<\alpha_c$ and in the limit $LM \ll 1$ the function $\tilde{F}(LM)$ reduces to $\tilde{F}=\zeta(3)$, whereas exactly at the critical point we have $\tilde{F}=4\zeta(3)/5+y_0^3/12$: the last result is obtained by using Sachdev's identity (Ref. 16). Here $\zeta(x)$ is the Riemann zeta function.

(iii) Finally, in the quantum disordered regime $(\alpha>\alpha_c)$ we get

$$e(L) = e_c(\infty) - \frac{cM^2}{2\pi L}\exp(-LM). \tag{16}$$

The exponential form of the finite size corrections reflects the existence of an excitation gap in the quantum disordered phase. Notice, however, that in this regime the system is known to possess gapped triplet excitations,[3] whereas Takahashi's theory is entirely based on transverse spin-wave excitations.

Finite size effects at low temperatures

Using the Jacobi identity

$$\sum_{m=-\infty}^{\infty} \exp(-um^2) = \sqrt{\frac{\pi}{u}} \sum_{m=-\infty}^{\infty} \exp\left(-\frac{\pi^2 m^2}{u}\right)$$

and the Poisson summation formula, one can transform Eqs. (5) into the forms $W(L,T)=W(\infty,0)+\delta W(L,T)$ and $U(L,T)=U(\infty,0)+\delta U(L,T)$. In what follows we will consider only finite size and temperature corrections to the internal energy. Since at low temperatures the magnon mass M is exponentially small, it is enough to calculate the function $\delta U(L,T)$ for $M=0$. The result reads

$$\delta U(L,T)_{M=0} = \frac{2\Gamma(3/2)}{\pi^{3/2}c^3} T^3 \sum_{m,n=-\infty}^{\infty} (m^2+n^2L^2T^2/c^2)^{-3/2}, \tag{17}$$

where the term $m=n=0$ must be omitted.

(i) In the regime $T \gg c/L$ it is convenient to transform Eq. (17) to the form

$$\delta U(L,T)_{M=0} = \frac{2\zeta(3)T^3}{\pi c^3} + \frac{4\zeta(2)T}{\pi c L^2} + \frac{16T^2}{c^2 L}\sum_{l,m=1}^{\infty}\frac{l}{m}K_1\left(\frac{2\pi l m L T}{c}\right), \tag{18}$$

$[K_1(x)$ is the McDonald function$]$ which yields the following expression for the internal energy per spin:

$$e(L,T) = e_c(\infty,0) + \frac{2\zeta(3)}{\pi c^2}\{1+O[(TL/c)^{-3/2}e^{-2\pi(TL/c)}]\} \times T^3 + \frac{4\zeta(2)}{\pi L^2}T. \tag{19}$$

In the considered long-wavelength approximation the expansion parameter $(TL/c)^{-1}$ gives exponentially small contributions in the T^3 prefactor. In the bulk limit the T^3 term in Eq. (19) exactly reproduces the expected contribution to the internal energy of the 2D HAFM from the Goldstone modes at $\mathbf{k}=(0,0)$ and $\mathbf{k}=(\pi,\pi)$ (see, e.g., Ref. 5).

(ii) In the regime $T \ll c/L$ it is convenient to use instead of Eq. (18) the expression

$$\delta U(L,T)_{M=0} = \frac{2\zeta(3)}{\pi L^3} + \frac{4\zeta(2)T^2}{\pi c^2 L} + \frac{16T}{cL^2}\sum_{l,m=1}^{\infty}\frac{l}{m}K_1\left(\frac{2\pi l m c}{LT}\right), \tag{20}$$

which leads to the formula

$$e(L,T) = e_c(\infty,0) + \frac{2c\zeta(3)}{\pi}\{1+O[(TL/c)^{3/2}e^{-2\pi(c/TL)}]\} \times \frac{1}{L^3} + \frac{4\zeta(2)}{\pi c L}T^2. \tag{21}$$

In conclusion, based on Takahashi's spin-wave theory we have obtained expressions for the spectral gap and the internal energy per spin of a frustrated Heisenberg antiferromagnet defined on a strip. The expressions are valid in the continuum limit and close to the quantum critical point and have a universal form depending only on the macroscopic magnetic parameters ρ_s and c.

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