Haldane gap in the quasi-one-dimensional nonlinear σ model

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This work studies the appearance of a Haldane gap in quasi-one-dimensional antiferromagnets in the long-wavelength limit, via the nonlinear σ model. The mapping from the three-dimensional, integer-spin Heisenberg model to the nonlinear σ model is explained, taking into account two antiferromagnetic couplings: one along the chain axis (J) and one along the perpendicular planes ($J_\perp$) of a cubic lattice. An implicit equation for the Haldane gap is derived, as a function of temperature and coupling ratio $J_\perp/J$. Solutions to these equations show the existence of a critical coupling ratio beyond which a gap exists only above a transition temperature T_N. The cutoff dependence of these results is discussed.

I. INTRODUCTION

It is by now well established[1,2] that the excitation spectrum of the spin-1 antiferromagnetic Heisenberg model has a mass gap (the Haldane gap) in one dimension, whereas it is gapless in higher dimensions.[3] Experimentally, integer-spin chains are realized in quasi-one-dimensional compounds in which the antiferromagnetic coupling J along the chain direction is much higher than the transverse coupling $J_\perp$. The Haldane gap can then be observed via neutron scattering[4] or electron spin resonance.[5] It is the ratio $R = J_\perp/J$ which determines the degree of "quasi one dimensionality" of the material. For instance, R is estimated[4] to be ~ 0.02 in $CsNiCl_3$, while it is certainly much lower (~ 0.0006) in NENP $[Ni(C_2H_8N_2)_2NO_2(ClO_4)]$.[6] In $CsNiCl_3$ one-dimensional behavior (i.e., the existence of the gap) is oberved above a critical temperature (the Néel temperature T_N) of about 5 K. On the other hand, one-dimensional behavior is observed in NENP at temperatures as low as can be reached. This suggests the existence of a critical ratio R_c below which the system is one dimensional in character, whatever the temperature.

This was argued in Ref. 7, wherein corrections to the spin-wave spectrum were calculated in perturbation theory for the anisotropic Heisenberg model in two dimensions. More recently, Azzouz and Douçot[8] have performed a mean-field theory analysis on the Heisenberg model on a square lattice:

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j + J_\perp \sum_{\langle lm\rangle} \mathbf{S}_l\cdot\mathbf{S}_m, \tag{1}$$

wherein the first sum runs over nearest neighbor spins along the chains, and the second sum runs over nearest neighbors in the direction perpendicular to the chains. They found a critical ratio given, in the large s approximation, by $R_c \sim se^{-2\pi s}$, where s is the value of the integer spin.

In this work we will perform a similar analysis, but within the three-dimensional nonlinear σ model and at finite temperature. The technique used has been described in Ref. 9, wherein the temperature dependence of the gap was calculated for the purely one-dimensional case.

The value we will find for R_c is very sensitive to the cutoff prescription, but if we fix the latter with the help of the numerical result $\Delta_0 \sim 0.41J$ for the purely one-dimensional Haldane gap at zero temperature, we find the critical ratio $R_c \sim 0.026$. However, we believe that this estimate should be regarded with great caution. We also illustrate the R dependence of the Néel temperature, of the zero-temperature gap, and the temperature dependence of the gap for various values of R.

II. THE ANISOTROPIC NONLINEAR σ MODEL

The aim of this section is to show how the Heisenberg Hamiltonian (1) may be replaced, in dimension 3 and in the continuum limit, by the anisotropic nonlinear σ model, with Lagrangian density

$$\mathcal{L} = \frac{1}{2g}\left\{\frac{1}{v}(\partial_t\mathbf{m})^2 - v(\partial_z\mathbf{m})^2 - Rv(\partial_x\mathbf{m})^2 - Rv(\partial_y\mathbf{m})^2\right\}, \tag{2}$$

wherein

$$v = 2Jas\sqrt{1+2R}, \qquad g = \frac{2a^2}{s}\sqrt{1+2R}, \tag{3}$$

and where a is the lattice spacing; the field $\mathbf{m}$ is a unit vector: $\mathbf{m}^2 = 1$; this constraint alone makes the theory nontrivial. Readers willing to accept Eqs. (2) and (3) may proceed to the next section.

The mapping from the Heisenberg Hamiltonian to the nonlinear σ model has been done explicitly before in various ways,[1,10] but mostly in dimension 1. Here we wish to show explicitly how the mapping is done in dimension 3, with anisotropic couplings. We first need to write down

the action for a single site, using spin coherent states. We define a unit vector $\mathbf{n}$ such that $\mathbf{S} = s\mathbf{n}$. Then the kinetic term is well known to be the Wess-Zumino action[10]

$$S_{\rm WZ} = \int_0^T dt\ K = s\int_0^1 d\tau \int_0^T dt\ \mathbf{n}\cdot(\partial_\tau \mathbf{n}\times\partial_t\mathbf{n}). \quad (4)$$

Here the time t runs from 0 to some finite period T and τ is an auxiliary coordinate introduced in order to parametrize, along with t, the spherical cap delimited by the curve $\mathbf{n}(t)$ from $t = 0$ to $t = T$. For more details, the reader may consult Ref. 10. For our purpose, it is sufficient to know that the variation of the action upon a small change $\delta\mathbf{n}$ is

$$\delta S_{\rm WZ} = s\int_0^T dt\ \delta\mathbf{n}\cdot(\mathbf{n}\times\partial_t\mathbf{n}). \quad (5)$$

Next, we add interactions between spins on a cubic lattice Γ', with nearest neighbor vectors $(\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}})$. Anticipating short-range antiferromagnetic order, we scale the unit cell by a factor of 2 in every direction, thus obtaining a bigger lattice Γ whose points are labeled $\mathbf{r}$ (unprimed) and whose unit cell contains eight sites of Γ':

$$\mathbf{r}' = \alpha\hat{\mathbf{x}} + \beta\hat{\mathbf{y}} + \gamma\hat{\mathbf{z}}, \quad (6)$$

wherein each of α, β, and γ runs from 0 to 1. The unit cell of Γ contains eight spins which may be described by eight different vector fields, as follows:

$$\mathbf{S}(\mathbf{r}') = s(-1)^{\alpha+\beta+\gamma}\mathbf{n}(\mathbf{r}'), \quad (7a)$$

$$\mathbf{n}(\mathbf{r}') = \mathbf{m}(\mathbf{r}) + a{\sum_{i,j,k}}'(-1)^{i\alpha+j\beta+k\gamma}\mathbf{l}_{ijk}(\mathbf{r}). \quad (7b)$$

Again each of α,β,γ and i,j,k runs from 0 to 1; we have introduced seven deviation fields $\mathbf{l}_{ijk}$, the primed sum meaning that the term $i = j = k = 0$ is omitted, the latter being rather represented by the slowly varying field $\mathbf{m}$. We have included a factor of a in the definition of $\mathbf{l}_{ijk}$ in order to stress that deviations from short-range antiferromagnetic order are assumed to be small.

Now we must express the kinetic term and the Heisenberg Hamiltonian in terms of these new fields, at lowest nontrivial order in a, and then integrate out the deviation fields $\mathbf{l}_{ijk}$ to obtain an effective continuum action for $\mathbf{m}$. Let us begin with the kinetic term K, which is obtained by summing over spins the action (4). Assuming that $\mathbf{n}$ is slowly varying, we use Eq. (5) to write

$$K = s\sum_{\mathbf{r}\in\Gamma}\sum_{\alpha,\beta}(-1)^{\alpha+\beta}\delta_z\mathbf{n}(\mathbf{r}')\cdot[\mathbf{n}(\mathbf{r}')\times\partial_t\mathbf{n}(\mathbf{r}')] \quad (\mathbf{r}' = \mathbf{r} + \alpha\hat{\mathbf{x}} + \beta\hat{\mathbf{y}}), \quad (8)$$

where we defined the difference

$$\delta_z\mathbf{n}(\mathbf{r}') = \mathbf{n}(\mathbf{r}' + \hat{\mathbf{z}}) - \mathbf{n}(\mathbf{r}') \quad (9)$$

and similarly for δ_x and δ_y. The definitions (7) imply

$$\delta_z\mathbf{n}(\mathbf{r} + \alpha\hat{\mathbf{x}} + \beta\hat{\mathbf{y}}) = -2a\sum_{i,j}(-1)^{i\alpha+j\beta}\mathbf{l}_{ij1}(\mathbf{r}). \quad (10)$$

Applying the identity

$$\sum_{\alpha=0,1}(-1)^{\alpha(i+j)} = 2\delta_{ij}, \quad (11)$$

we may write the kinetic term as

$$K = 2^d as\sum_{\mathbf{r}\in\Gamma}\mathbf{l}_{111}(\mathbf{r})\cdot[\mathbf{m}(\mathbf{r})\times\partial_t\mathbf{m}(\mathbf{r})], \quad (12)$$

where d is the dimension of space, which we keep variable even though our notation is three dimensional, in order to make this derivation more general. In the continuum, this becomes

$$K = a^{1-d}s\int d\mathbf{r}\ \mathbf{l}_{111}\cdot(\mathbf{m}\times\partial_t\mathbf{m}). \quad (13)$$

The Heisenberg Hamiltonian may be expressed as $H = V_x + V_y + V_z$, where, for instance,

$$V_z = -s^2J_z\sum_{\mathbf{r}'\in\Gamma'}\mathbf{n}(\mathbf{r}')\cdot\mathbf{n}(\mathbf{r}' + \hat{\mathbf{z}}). \quad (14)$$

Up to an irrelevant constant, this is equal to

$$\tfrac{1}{2}s^2J_z\sum_{\mathbf{r}'\in\Gamma'}[\delta_z\mathbf{n}(\mathbf{r}')]^2. \quad (15)$$

We have similar expressions for $V_{x,y}$ wherein J_z and δ_z are replaced by $J_{x,y}$ and $\delta_{x,y}$. We then use Eq. (10), along with

$$\delta_z\mathbf{n}(\mathbf{r} + \alpha\hat{\mathbf{x}} + \beta\hat{\mathbf{y}} + \hat{\mathbf{z}}) = 2a\partial_z\mathbf{m}(\mathbf{r}) + 2a\sum_{i,j}(-1)^{i\alpha+j\beta}\mathbf{l}_{ij1}(\mathbf{r}), \quad (16)$$

to find

$$V_z = 2^da^2s^2J_z\sum_{\mathbf{r}\in\Gamma}\left\{2\sum_{ij}\mathbf{l}_{ij1}^2 + 2\mathbf{l}_{001}\cdot\partial_z\mathbf{m} + (\partial_z\mathbf{m})^2\right\}, \quad (17)$$

along with similar expressions for V_x and V_y.

In the continuum, we may therefore write the following Lagrangian density:

$$\mathcal{L} = a^{1-d}s\mathbf{l}_{111}\cdot(\mathbf{m}\times\partial_t\mathbf{m}) - a^{-d}s^2J_x\left\{2\sum_{i,j}\mathbf{l}_{1ij}^2 + 2\mathbf{l}_{100}\cdot\partial_x\mathbf{m} + (\partial_x\mathbf{m})^2\right\}$$
$$-a^{-d}s^2J_y\left\{2\sum_{i,j}\mathbf{l}_{i1j}^2 + 2\mathbf{l}_{010}\cdot\partial_y\mathbf{m} + (\partial_y\mathbf{m})^2\right\} - a^{-d}s^2J_z\left\{2\sum_{i,j}\mathbf{l}_{ij1}^2 + 2\mathbf{l}_{001}\cdot\partial_z\mathbf{m} + (\partial_z\mathbf{m})^2\right\}. \quad (18)$$

We now proceed to the functional integration of the fields $\mathbf{l}_{ijk}$. Since the action is quadratic in these fields, this amounts to substituting in the Lagrangian the expression of these fields obtained from the equations of motion. The latter are

$$\mathbf{l}_{111} = \frac{1}{4as}\frac{1}{J_x + J_y + J_z}\mathbf{m} \times \partial_t \mathbf{m}, \tag{19a}$$

$$\mathbf{l}_{100} = -\tfrac{1}{2}\partial_x \mathbf{m},$$

$$\mathbf{l}_{010} = -\tfrac{1}{2}\partial_y \mathbf{m},$$

$$\mathbf{l}_{001} = -\tfrac{1}{2}\partial_z \mathbf{m}, \tag{19b}$$

$$\mathbf{l}_{ijk} = 0 \qquad \text{otherwise.} \tag{19c}$$

Substitution of these equations into the above Lagrangian density yields exactly Eqs. (2) and (3), with $J_z = J$, $J_x = J_y = RJ$, and $d = 3$. Note that in the isotropic case ($J_n = J$), the Lagrangian obtained in dimension d is

$$\mathcal{L} = \frac{1}{2g}\left\{\frac{1}{v}(\partial_t \mathbf{m})^2 - v\sum_i (\partial_i \mathbf{m})^2\right\}, \tag{20}$$

with

$$v = 2Jas\sqrt{d}, \quad g = \frac{2a^{d-1}}{s}\sqrt{d}. \tag{21}$$

The above derivation is valid for any dimension greater than 1. In dimension 1 a complication occurs since there is only one deviation field $\mathbf{l}$, whose equation of motion is instead

$$\mathbf{l} = -\tfrac{1}{2}\partial_z \mathbf{m} + \frac{1}{4aJs}\mathbf{m} \times \partial_t \mathbf{m}. \tag{22}$$

Substitution into the Lagrangian yields, in addition to the action (20), a topological Hopf term, responsible for the difference in behavior between integer- and half-integer-spin chains. The above derivation shows clearly that no such term arises in dimensions $d > 1$.

So far we have eluded the question of constraints. The eight fields $\mathbf{m}$ and $\mathbf{l}_{ijk}$ are related by eight constraints coming from the relation $\mathbf{n}^2 = 1$. In the limit of small deviations ($a \to 0$) these constraints are

$$\mathbf{m}^2 = 1, \qquad \mathbf{m} \cdot \mathbf{l}_{ijk} = 0; \tag{23}$$

the second of these equations is compatible with the equations of motion (19), implying that the above substitution procedure was indeed correct. The constraint $\mathbf{m}^2 = 1$ is part of the definition of the nonlinear σ model.

III. DERIVATION OF THE GAP EQUATION

The aim of this section is to find, starting from the σ-model Lagrangian (2), an equation governing the temperature and anisotropy dependence of the Haldane gap. Before embarking upon calculations, let us simply state the results, obtained in the approximation where the cutoff Λ (proportional to the inverse lattice spacing a^{-1}) is much larger than the temperature T or the gap Δ. Let Δ_0 be the Haldane gap at zero temperature in the one-dimensional limit ($R \to 0$), and let us introduce the reduced variables and parameters

$$\delta = \frac{\Delta}{\Delta_0}, \qquad t = \frac{T}{\Delta_0}, \qquad r = \frac{R\Lambda^2}{\Delta_0^2}. \tag{24}$$

Then the reduced gap δ obeys the following equation:

$$(\delta^2 + r)\ln(\delta^2 + r) - \delta^2 \ln \delta^2 - r + 8t^2\left[G\left(\frac{\sqrt{\delta^2 + r}}{t}\right) - G\left(\frac{\delta}{t}\right)\right] = 0, \tag{25}$$

where we have defined the special function

$$G(y) = \tfrac{1}{2}y^2 \int_1^\infty dz\, \sqrt{z^2 - 1}\,[\coth(yz/2) - 1] = y\sum_{n=1}^{\infty}\frac{1}{n}K_1(ny) \tag{26}$$

(K_1 is the modified Bessel function of order 1). The remainder of this section will be devoted to the proof of Eq. (25).

A large part of this section parallels the calculations presented in Ref. 9. We start with the σ-model Lagrangian (2) expressed in terms of a rescaled variable $\varphi = \mathbf{m}/\sqrt{g}$:

$$\mathcal{L} = \frac{1}{2}\left\{(\partial_t \varphi)^2 - (\partial_z \varphi)^2 - R(\partial_\perp \varphi)^2 - \sigma(\varphi^2 - 1/g)\right\}. \tag{27}$$

Here we have set the magnon speed v to unity; it can be restored at the end by dimensional analysis; we have introduced a Lagrange multiplier $\sigma(x,t)$ whose role is to enforce the constraint $\varphi^2 = 1/g$ at every space-time point. In the path integral formalism, implementing a constraint in this way is equivalent to inserting a delta function $\delta(\varphi^2 - 1/g)$ in the path integration measure, by virtue of the representation $\delta(x) = \int (dk/2\pi)e^{ikx}$ of the delta function. The advantage of this method is to simplify the integration measure for φ, which simply becomes that of a triplet of scalar fields.

The strategy used to compute the Haldane gap is to calculate at one loop the effective potential $V(\sigma)$ for the Lagrange multiplier. This amounts to integrating the field φ, assuming σ to be constant. We then look for a minimum in $V(\sigma)$. If such a minimum exists for $\sigma \neq 0$, then the position σ of this minimum is the mass squared of the triplet field φ, namely, the square of the gap. Of course, the exact integration of φ in Eq. (27) would produce an effective action for σ containing an arbitrary number of derivatives. Assuming σ to be constant then amounts to neglecting its quantum fluctuations, driven by the derivative terms. This is the substance of the large-N limit in this problem[11] (here $N = 3$, the number of components of φ). Regarding the question of whether this approximation is justified, we may recall the exact S-matrix results of Ref. 12 for what is believed to be

the one-dimensional $O(3)$ nonlinear σ model, and which show that the only single-particle states are a triplet of massive bosons; this validates our approximation, as far as the mass gap is concerned.

At one loop, the derivative $V'(\sigma)$ of the zero-temperature effective potential in the Euclidian formalism is

$$V'(\sigma) = \frac{1}{2g} - \frac{3}{2}\int \frac{dp_0}{(2\pi)} \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{p_0^2 + p_z^2 + R\mathbf{p}_\perp^2 + \sigma}. \tag{28}$$

The gap equation is then simply $V'(\Delta^2) = 0$, where $\Delta = \sqrt{\sigma}$. The extension of this formula to a finite temperature T is obtained by replacing the integration over p_0 by a sum over Matsubara frequencies $\omega_n = 2\pi nT$: After summing over Matsubara frequencies, the gap equation becomes ($\beta = 1/T$)

$$\frac{1}{g} = \frac{3}{2}\int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{\sqrt{p_z^2 + R\mathbf{p}_\perp^2 + \Delta^2}} \times \coth\frac{\beta}{2}\sqrt{p_z^2 + R\mathbf{p}_\perp^2 + \Delta^2}. \tag{29}$$

This expression is meaningless without the introduction of a momentum cutoff Λ, which should be proportional to the inverse lattice spacing a^{-1}. We will evaluate this integral by restricting it to a cylinder of height 2Λ and radius Λ, parallel to the $\mathbf{p}_z$ axis in momentum space. Defining the integration variable $x = R\mathbf{p}_\perp^2$, we have

$$\frac{8\pi^2 R}{3g} = \int_0^\Lambda dk \int_0^{\Lambda^2 R} dx \frac{1}{\sqrt{k^2 + x + \Delta^2}} \cdot \times \coth\frac{\beta}{2}\sqrt{k^2 + x + \Delta^2}. \tag{30}$$

The integral over x can be done analytically:

$$\frac{2\pi^2 R}{3g} = T\int_0^\Lambda dk \left\{\ln\sinh\frac{\beta}{2}\sqrt{k^2 + \Delta^2 + \Lambda^2 R} - \ln\sinh\frac{\beta}{2}\sqrt{k^2 + \Delta^2}\right\}. \tag{31}$$

The remaining integral may also be done analytically, in the limit $\Lambda \gg \Delta, T$: Let us introduce the notation

$$F(\alpha, \beta, \Lambda) = \int_0^\Lambda dk \ \ln\sinh\frac{\beta}{2}\sqrt{k^2 + \alpha^2}. \tag{32}$$

After integrating by parts, this function becomes

$$F(\alpha, \beta, \Lambda) = \Lambda \ln\sinh\frac{\beta}{2}\sqrt{\Lambda^2 + \alpha^2} - \frac{\beta}{2}\int_0^\Lambda \frac{k^2 dk}{\sqrt{k^2 + \alpha^2}} \coth\frac{\beta}{2}\sqrt{k^2 + \alpha^2}. \tag{33}$$

The second term may be separated into a contribution at $T = 0$:

$$\int_0^\Lambda \frac{k^2 dk}{\sqrt{k^2 + \alpha^2}} \approx \tfrac{1}{2}\Lambda^2 + \tfrac{1}{4}\alpha^2\left(1 + \ln\frac{\alpha^2}{4\Lambda^2}\right) \qquad (\Lambda \to \infty) \tag{34}$$

plus a finite temperature correction, finite as $\Lambda \to \infty$:

$$\int_0^\infty \frac{k^2 dk}{\sqrt{k^2 + \alpha^2}} \left\{\coth\frac{\beta}{2}\sqrt{k^2 + \alpha^2} - 1\right\} = \alpha^2 \int_1^\infty dz \ \sqrt{z^2 - 1}\,[\coth(\beta\alpha z/2) - 1] = 2\alpha^2 G(\beta\alpha). \tag{35}$$

Summing up all contributions and expanding around $\Lambda = \infty$, we obtain

$$F(\alpha, \beta, \Lambda \to \infty) = \tfrac{1}{4}\beta\Lambda^2 - \Lambda\ln 2 + \tfrac{1}{8}\beta\alpha^2\left(1 - \ln\frac{\alpha^2}{4\Lambda^2}\right) - \frac{1}{\beta}G(\beta\alpha) \tag{36}$$

This result, inserted into Eq. (31), yields at last

$$\frac{16\pi^2 R}{3g} = (\Delta^2 + R\Lambda^2)\left(1 - \ln\frac{\Delta^2 + R\Lambda^2}{4\Lambda^2}\right) - \Delta^2\left(1 - \ln\frac{\Delta^2}{4\Lambda^2}\right) - 8T^2\left[G\left(\frac{\sqrt{\Delta^2 + R\Lambda^2}}{T}\right) - G\left(\frac{\Delta}{T}\right)\right]. \tag{37}$$

This is essentially the gap equation (25), except that the reduced variables (24) have not been introduced. To this end, let us consider the one-dimensional case, i.e., let us take the limit $R \to 0$. We must use the fact that

$$\frac{dG(y)}{dy} = -yH(y), \qquad H(y) = \sum_{n=1}^\infty K_0(ny). \tag{38}$$

We then obtain the one-dimensional equation

$$\frac{16\pi^2}{3g\Lambda^2} = -\ln\frac{\Delta^2}{4\Lambda^2} + 4H(\Delta/T). \tag{39}$$

Since $H(\infty) = 0$, the zero-temperature gap is $\Delta_0 = 2\Lambda\exp -(8\pi^2/3g\Lambda^2)$. In terms of the reduced variables (24) the finite-temperature gap equation in dimension 1 is then

$$\tfrac{1}{2}\ln\delta = H(\delta/t).$$

This equation also appears in Ref. 9. Finally, upon substitution of the reduced variables, the three-dimensional gap equation (37) takes the form (25).

IV. DISCUSSION

In this section we illustrate the consequences of the gap equation (25). That implicit equation may easily be solved numerically, given the expression (26) for the function G in terms of modified Bessel functions. Figure 1 shows the t dependence of δ for various values of the anisotropy parameter r.

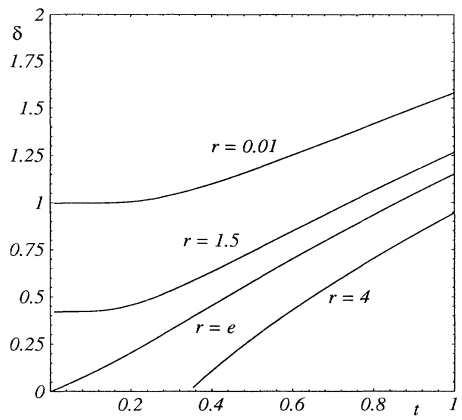

FIG. 1. Reduced Haldane gap δ as a function of the reduced temperature t for various values of the anisotropy parameter r: 0.01, 1.5, $e = 2.718\ldots$, and 4.

At zero temperature, the gap equation reduces to

$$(\delta^2 + r)\ln(\delta^2 + r) - \delta^2 \ln \delta^2 - r = 0. \tag{40}$$

This equation has the solution $\delta = 1$ in the limit $r \to 0$, and has a nonzero solution for sufficiently small r. Figure 2 illustrates the numerical solution of δ vs r. Taking the limit $\delta \to 0$ we see that the critical value of the anisotropy parameter is $r_c = e$. This in turn corresponds to a critical value R_c of the coupling ratio $R = J_\perp/J$.

Beyond this value of r, a gap will appear only above some critical temperature t_c (the Néel temperature). If we take the limit $\delta \to 0$ in Eq. (25), we obtain

$$r \ln r - r + 8t_c^2 \left[G\left(\frac{\sqrt{r}}{t_c}\right) - \pi^2/6 \right] = 0, \tag{41}$$

wherein we have substituted the special value $G(0) = \pi^2/6$. This equation may be solved numerically for t_c as a function of r, and the result is illustrated on Fig. 3.

Let us now discuss the relation existing between the critical value r_c and the microscopic parameters J and $R = J_\perp/J$. The coupling J resurfaces if the magnon

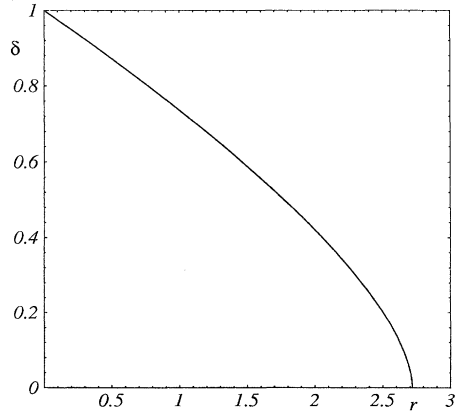

FIG. 2. Magnitude of the reduced Haldane gap $\delta = \Delta/\Delta_0$ at zero temperature as a function of the anisotropy parameter $r = R\Lambda^2/\Delta_0^2$. The critical value of r is e.

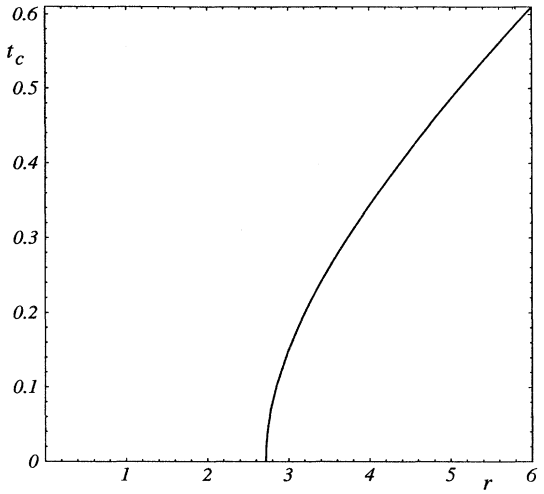

FIG. 3. Reduced Néel temperature t_c as a function of the anisotropy parameter $r = R\Lambda^2/\Delta_0^2$.

speed v is restored in the explicit value of the gap by dimensional analysis. The expression for Δ_0, the zero-temperature gap in the $R \to 0$ limit, is then

$$\begin{aligned}\Delta_0 &= 2v\Lambda \exp -(8\pi^2/3g\Lambda^2) \\ &= 4J\Lambda as \exp - \left[4\pi^2 s/3(a\Lambda)^2\right].\end{aligned} \tag{42}$$

The ratio Δ_0/J can then be related to the cutoff prescription, i.e., to the product Λa. If we accept the ratio obtained from numerical simulations,[2] namely, $\Delta_0 = 0.41J$, we are led by the above equation to the prescription $\Lambda a = 2.1$. Notice, however, that the ratio Δ_0/J is extremely dependent on the value of Λa, because of the exponential factor.

After restoration of v, the expression for the anisotropy parameter r is

$$r = \tfrac{1}{4} R \exp - \left[8\pi^2 s/3(a\Lambda)^2\right]. \tag{43}$$

The critical value $r_c = e$ then translates into a critial ratio

$$R_c = 4 \exp \left[1 - 8\pi^2 s/3(a\Lambda)^2\right]. \tag{44}$$

The choice $\Lambda a = 2.1$ then leads to $R_c = 0.026$. This value, although small, seems too high when compared to coupling ratios observed in actual materials; for instance, the ratio R has been estimated[4] to be ~ 0.02 in $CsNiCl_3$, in which a finite Néel temperature is observed. Of course, $CsNiCl_3$ and other compounds of the ABX_3 type have a hexagonal structure, not cubic.[13] It seems that trying to find the correct value of R_c from a well-chosen cutoff prescription is dangerous. However, definite predictions may be obtained from a continuum theory, up to an overall scale in all but one variable.

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