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LETTER TO THE EDITOR

Phase transitions in a highly anisotropic Heisenberg chain with staggered interaction

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Abstract. The behaviour of the antiferromagnetic nearest-neighbour spin-$\frac{1}{2}$ Heisenberg chain is studied in a space of interactions that include exchange anisotropy (α), bond alternation (λ), and spin–lattice interaction (γ). Using the coherent state method for spin, we analyse magnetically driven lattice instabilities and find that phase transitions occur under the condition of large bond alternation or strong spin–lattice coupling, which means that more staggered interactions make it easy for phase transitions to take place. The three-phase diagram and the tri-critical point are obtained.

The interest in models that deal with many-body problems in low-dimensional systems has been recently revived because of the discovery of high-T_c superconductivity [1]. The anisotropic Heisenberg chain with antiferromagnetic coupling is one of them. For a strictly one-dimensional system, there can be no phase transition at a finite temperature because of fluctuations. But a one-dimensional system can undergo a phase transition when coupled to phonons [2]. In this Letter we consider a lattice of a spin-$\frac{1}{2}$ linear highly anisotropic antiferromagnetic Heisenberg chain with a phenomenological spin–lattice coupling to investigate the lattice instabilities and phase transitions.

It is physically evident that the antiferromagnetic order, which has a periodicity of twice the lattice parameter, will couple predominantly with the lattice mode of the same wavelength. Thus, since we are primarily interested in qualitative trends, we can drop all the other modes and write for the Hamiltonian of the system

$$H = N\left(\frac{P^2}{2M} + \tfrac{1}{2}M\omega_0^2 Q^2\right) + \sum_l \varepsilon_l (J + \gamma(-1)^l Q) \times \left(S_z(l+1)S_z(l) + \frac{\alpha}{2}[S_x(l+1)S_x(l) + S_y(l+1)S_y(l)]\right) \tag{1}$$

where $P^2/2M$ is the kinetic energy of an ion, $l = 1, 2, \ldots, N$ characterises the chain sites, $(-1)^l Q$ represents the ionic displacement at site l associated to a lattice wave having wavelength of twice the lattice parameter, $S_i(l)$ are the i-components of the spin at site l, γ is a spin–lattice coupling constant, M is the mass of magnetic ion, ω_0 is the one type of mode and α is the exchange anisotropic parameter. Bond alternation is

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controlled by λ via

$$\varepsilon(l) = \begin{cases} 1 & \text{even } l \\ \lambda & \text{odd } l \end{cases} \qquad (0 < \lambda \leqslant 1). \tag{2}$$

Technically, we generalise an analytical non-perturbative solution for the anisotropic antiferromagnetic Heisenberg model, which is valid for strong antiferromagnetic order [3, 4]. In the spirit of the adiabatic approximation (the spins respond rapidly to change in the ionic configuration) we can drop $P^2/2M$ in a first step. The Hamiltonian then reads

$$H = \sum_l \varepsilon_l (J + \gamma(-1)^l Q)\left(S_z(l+1)S_z(l) + \frac{\alpha}{2}[S_+(l+1)S_-(l) + S_+(l)S_-(l+1)] \right) \tag{3}$$

where Q now plays the role of a parameter, J is the spin–spin coupling constant and $S_\pm = S_x \pm iS_y$. The boson-like operators [3, 4] that reverse spin pairs are defined through

$$\varphi_e^+(k) = \left(\frac{2}{N}\right)^{1/2} \sum_{l=\text{even}} e^{ikl} S_+(l+1)S_-(l) + \alpha\left(\frac{N}{8}\right)^{1/2} \frac{(J+\gamma Q)}{\lambda(J-\gamma Q)} \delta_{k,0} \tag{4a}$$

$$\varphi_o^+(k) = \left(\frac{2}{N}\right)^{1/2} \sum_{l=\text{odd}} e^{ikl} S_+(l)S_-(l+1) + \alpha\left(\frac{N}{8}\right)^{1/2} \frac{\lambda(J-\gamma Q)}{(J+\gamma Q)} \delta_{k,0} \tag{4b}$$

where N is the total number of sites in the chain, and k is in the Brillouin zone of one of the two sublattices determined by the antiferromagnetic spin alignment. The commutator algebra for φ_e and φ_o can be straightforwardly calculated [3, 4]. It yields a rather complicated relation that may be simplified to a boson algebra if one assumes the quasi-Ising limit ($0 \leqslant \alpha \ll 1$) and makes the replacement

$$S_z(l) \to \tfrac{1}{2}(-1)^l. \tag{5}$$

For this regime, we obtain the following commutation relations:

$$[\varphi_e(k), \varphi_e^+(k')] = [\varphi_o(k), \varphi_o^+(k')] = \delta_{k,k'} \tag{6}$$

$$[\varphi_e(k), \varphi_o(k')] = [\varphi_e(k), \varphi_o^+(k')] = 0. \tag{7}$$

With these boson-like operators, the Hamiltonian of (3) becomes

$$H = \sum_k \lambda(J-\gamma Q)\varphi_e^+(k)\varphi_e(k) + (J+\gamma Q)\varphi_o^+(k)\varphi_o(k) + E_0(Q) \tag{8}$$

where $E_0(Q)$ is the ground-state energy.

The ground state $|G(Q)\rangle$ is determined by the set of equation

$$\varphi_e(k)|G(Q)\rangle = \varphi_o(k)|G(Q)\rangle = 0 \tag{9}$$

whose solution [3, 4] is

$$|G(Q)\rangle = \exp\left[-\frac{\alpha}{2}\left(\frac{N}{2}\right)^{1/2} \frac{(J+\gamma Q)}{\lambda(J-\gamma Q)} (\varphi_e^+(0) - \varphi_e(0)) \right.$$
$$\left. - \frac{\alpha}{2}\left(\frac{N}{2}\right)^{1/2} \frac{\lambda(J-\gamma Q)}{(J+\gamma Q)} (\varphi_o^+(0) - \varphi_o(0)) \right] |\mathcal{N}\rangle \tag{10}$$

where $|\mathcal{N}\rangle$ is the Néel state, which assigns the spins up to the sites of even l. The ground-state energy $E_0(Q)$ obtained by $\hat{H}|G(Q)\rangle = E_0(Q)|G(Q)\rangle$ is

$$\frac{E_0(Q)}{N} = -\frac{\alpha^2}{8}\left(\frac{\lambda^2(J-\gamma Q)^2}{J+\gamma Q} + \frac{(J+\gamma Q)^2}{\lambda(J-\gamma Q)}\right) - \tfrac{1}{8}(J+\gamma Q) - \tfrac{1}{8}\lambda(J-\gamma Q). \tag{11}$$

Thus when $J > \gamma Q$, the contribution of the spin–lattice coupling to the ground-state energy has a maximum at $Q = Q_m$. Retaining terms only up to second order in Q, equation (11) becomes

$$\frac{E_0(Q)}{N} = -\frac{\alpha^2}{8}\left(\lambda + \frac{1}{\lambda}\right)J - \tfrac{1}{8}(1+\lambda)J + \frac{1}{2}\left[M\omega_0^2 - \alpha^2\left(\frac{1}{\lambda}\right)\frac{\gamma^2}{J}\right](Q-Q_m)^2$$

$$-\frac{1}{2}\left[M\omega_0^2 - \alpha^2\left(\lambda+\frac{1}{\lambda}\right)\frac{\gamma^2}{J}\right]Q_m^2 \tag{12}$$

where

$$Q_m = [\tfrac{3}{8}\alpha^2(1/\lambda - \lambda) + \tfrac{1}{8}(1-\lambda)]\gamma/[M\omega_0^2 - \alpha^2(\lambda + 1/\lambda)\gamma^2/J] \tag{13}$$

and the dimerised energy

$$E_{dim} = \tfrac{1}{2}[\tfrac{3}{8}\alpha^2(1/\lambda - \lambda) + \tfrac{1}{8}(1-\lambda)]^2 J/[M\omega_0^2 J/\gamma^2 - \alpha^2(\lambda + 1/\lambda)]. \tag{14}$$

Hence, the spin–lattice interaction softens the lattice mode which has wavelength of twice the interatomic distance and the lattice configuration has a spontaneously dimerised structure under the condition $\lambda \neq 1$. The ground state is unstable in the extreme case when $M\omega_0^2 < \alpha^2(\lambda + 1/\lambda)\gamma^2/J$.

Let us now concentrate on the more likely situation, in which the elastic energy is larger than the magnetic energy gained from dimerising the system ($M\omega_0^2 > \alpha^2(\lambda + 1/\lambda)\gamma^2/J$) and investigate the influence of the system temperature T. The energy of an excited state of the Hamiltonian (3) reads

$$\frac{E(Q)}{N} = -\tfrac{1}{8}\alpha^2(\lambda + 1/\lambda)J + \tfrac{1}{2}Q^2[M\omega_0^2 - \alpha^2(\lambda + 1/\lambda)\gamma^2/J] - [\tfrac{3}{8}\alpha^2(1/\lambda - \lambda)$$

$$+ \tfrac{1}{8}(1-\lambda)]\gamma Q + \frac{1}{N}\sum_k \lambda(J-\gamma Q)n_e + \frac{1}{N}\sum_k (J+\gamma Q)n_o \tag{15}$$

where $n_e(k)$ and $n_o(k)$ are the occupation numbers of the bosonic excitations as given by the following equations:

$$n_e(k) = \langle \varphi_e^+(k)\, \varphi_l(k)\rangle = 1/e^{\beta\lambda(J-\gamma Q)} - 1 \tag{16a}$$

$$n_o(k) = \langle \varphi_o^+(k)\, \varphi_o(k)\rangle = 1/e^{\beta(J+\gamma Q)} - 1. \tag{16b}$$

When $\beta\gamma Q \ll 1$, retaining terms only up to second order in Q, we find the dispersion relation from (15)

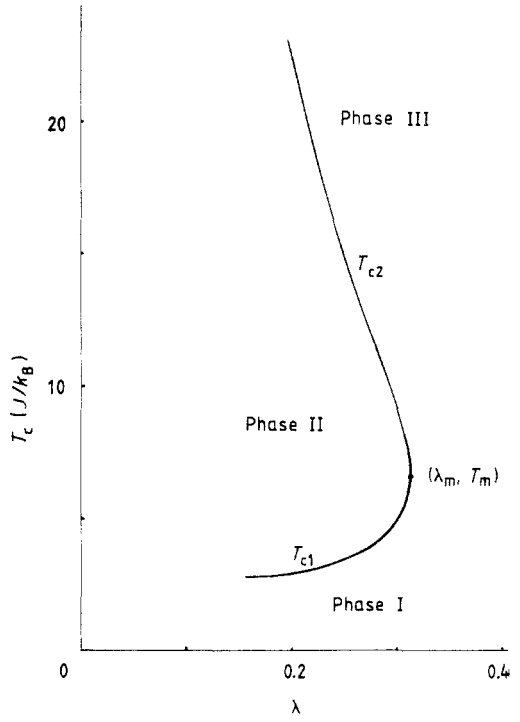

Figure 1. Three-phase diagram. Reduced critical temperature T_c (J/k_B) as a function of the bond alternation parameter λ at a fixed value of $b = 0.4$ and an anisotropic parameter $\alpha = 0.1$. Reduced tri-critical point $T_m = 6.630$ at $\lambda_m = 0.313$. Phase I is the spontaneously dimerised phase. Phase II is the spin–Peierls dimerised phase. Phase III is the dimerised disordered phase.

$$M\omega^2 = M\omega_0^2 - \alpha^2(\lambda + 1/\lambda)\gamma^2/J + J(A_1/B_1)(A_3/A_1 - B_3/B_1 - A_2B_2/A_1B_1 + B_2^2/2B_1^2)\beta^2\gamma^2 - (C_1/D_1)(C_2/C_1 - D_2/D_1)\beta\gamma^2 \tag{17}$$

where

$$A_1 = \lambda\, e^{\beta J} + e^{\beta\gamma J} - (1+\lambda)$$
$$A_2 = \lambda(e^{\beta J} - e^{\lambda\beta J})$$
$$A_3 = \tfrac{1}{2}\lambda(e^{\beta J} + \lambda e^{\beta\lambda J})$$
$$B_1 = e^{\beta(1+\lambda)J} - e^{\beta J} - e^{\beta\lambda J} + 1$$
$$B_2 = e^{\beta(1+\lambda)J}(1-\lambda) - e^{\beta J} + \lambda\, e^{\beta\lambda J}$$
$$B_3 = \tfrac{1}{2}[(1-\lambda)^2\, e^{\beta(1+\lambda)J} - e^{\beta J} - \lambda^2\, e^{\beta\gamma J}]$$
$$C_1 = \lambda\, e^{\beta J} - e^{\beta\lambda J} + (1-\lambda)$$
$$C_2 = \lambda(e^{\beta J} + e^{\lambda\beta J})$$
$$D_1 = e^{\beta(1+\lambda)J} - e^{\beta J} - e^{\lambda\beta J} + 1$$
$$D_2 = e^{\beta(1+\lambda)J}(1-\lambda) - e^{\beta J} + \lambda\, e^{\lambda\beta J}. \tag{18}$$

The lattice stability limit is determined by setting $\beta = \beta_c = 1/k_B T_c$, $\omega = 0$ in the expression for the lowest-lying renormalised phonon. Let $x = J/k_B T$; the critical temperature T_c from (17) is then given by

$$f(x_c, \lambda) = g(b, \alpha, \lambda) \tag{19}$$

where

$$f(x, \lambda) = (C_1/D_1)(C_2/C_1 - D_2/D_1)x - x^2(A_1/B_1)(A_3/A_1 - B_3/B_1 - A_2B_2/A_1B_1 + B_2^2/2B_1^2) \tag{20a}$$

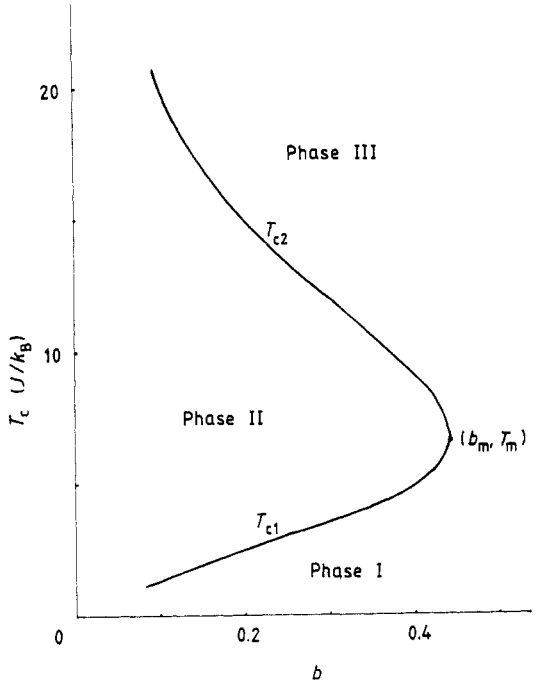

Figure 2. Three-phase diagram. Reduced critical temperature T_c (J/k_B) as a function of relative intensity of the spin–lattice coupling b at a fixed value of $\lambda = 0.3$ and an anisotropic parameter $\alpha = 0.1$. Reduced tri-critical point $T_m = 6.813$ at $b_m = 0.4415$. Phase I is the spontaneously dimerised phase. Phase II is the spin–Peierls dimerised phase. Phase III is the dimerised disordered phase.

$$g(b, \alpha, \lambda) = b - \alpha^2(\lambda + 1/\lambda) \tag{20b}$$

$$b = M\omega_0^2 J/\gamma^2. \tag{20c}$$

Here, b is called the relative intensity of spin–lattice coupling. b decreases with increasing spin–lattice coupling γ and satisfies the relation $b \geqslant \alpha^2(\lambda + 1/\lambda)$ under the condition $M\omega_0^2 \geqslant \alpha^2(\lambda + 1/\lambda)\gamma^2/J$, and thus the function $g(b, \alpha, \lambda)$ is always positive.

Equation (19) is studied numerically. In the case where $\lambda = 1$, there is no spontaneous dimerisation in the ground state because $Q_m = 0$. The function $f(x, \lambda = 1)$ is negative for an arbitrary value of x and there is no solution of (19) because the function $g(b, \alpha, \lambda)$ is positive. It shows that there is no spin–Peierls phase transition at finite temperature [2]. This result was not demonstrated in [3]. We now reduce the value of λ and study (19) at an anisotropic parameter $\alpha = 0.1$ and find that the phase transitions take place only under the condition of relative small values of λ and b. For example, phase transitions occur only at $0 \leqslant \lambda \leqslant \lambda_m = 0.313$ at a fixed value of $b = 0.4$, or for $0.0363 \leqslant b \leqslant b_m = 0.4415$ at a fixed value of $\lambda = 0.3$, which is illustrated in figure 1 and figure 2. In the phase diagrams (see figure 1 and figure 2), when the temperature T of the system increases to the critical temperature T_c, a spin–Peierls phase transition [2] takes place, and phase II is the so-called spin–Peierls dimerised phase. As the temperature continues to increase, at the critical temperature T_{c2} another phase transition takes place, and phase III may be a dimerised disorder phase [5]. Phase I is a spontaneously dimerised phase. As $\lambda > \lambda_m$ at fixed $b = 0.4$ or $b > b_m$ at fixed $\lambda = 0.3$, there is no spin–Peierls phase transition at finite temperature and the critical points (λ_m, T_m) and (b_m, T_m) are the so-called tri-critical points. The interaction difference between nearest bonds (degree of staggered interaction) is

$$\Delta J = (1 - \lambda)J + (1 + \lambda)\gamma Q \tag{21}$$

where ΔJ increases with decreasing λ (large bond alternation) and increases with increasing γ (strong spin–lattice coupling). We can see that phase transitions take place when ΔJ becomes large. That is to say, more staggered interaction make the system easily able to undergo phase transitions, and the bond alternation is a necessary factor.

The three-phase diagram is meaningful when the approximation method used to diagonalise the anisotropic Heisenberg Hamiltonian with coupling coefficient depending on the lattice configuration is extended to two- and three-dimensional systems. It is well known that, for small enough δ, $La_2CuO_{4-\delta}$ exhibits three-dimensional antiferromagnetic order [6]. The Néel temperature T_N may be as high as $T_N = 240$ K, but decreases rapidly with oxygen deficiency δ. However, long-ranged two-dimensional antiferromagnetic correlations in CuO_2 planes characteristic of these layered perovskites do survive for temperatures well above T_N [7]. It is not yet clear how the two-dimensional antiferromagnetic order is affected by δ, but indirect evidence has been provided concerning its connection with the tetragonal-to-orthorhomic-structure phase transition [8]. Neutron scattering experiments on the closely related compound $La_2NiO_{4+\delta}$, also a layered perovskite, show that for $\delta \simeq 0.05$ the three-dimensional antiferromagnetic order sets in at $T_N \simeq 70$ K and the tetragonal-to-orthorhombic-structure phase transition takes place at $T_s = 240$ K. Strong two-dimensional antiferromagnetic correlations are observed for $T_N \leqslant T \leqslant T_s$, but the correlation length is drastically reduced [8] when the temperature exceeds T_s. If one thinks the bond alternation parameter λ and spin–lattice coupling γ in our model might depend strongly on the oxygen deficiency δ (or the dopant concentration), our physical picture might provide some enlightenment on the high-T_c superconductivity.

In conclusion, we have studied the highly anisotropic spin-Heisenberg chain using the coherent-state method for spin. The three-phase diagram and the tri-critical point are obtained under the condition of strong spin–lattice coupling and large bond alternation, namely the large staggered-interaction condition. This is our main physical result. The detailed properties of the three phases are open problems and need to be further investigated.

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References

[1] Bednorz J G and Müller K A 1986 *Z. Phys.* B **64** 189
[2] Pytte E 1974 *Phys. Rev.* B **10** 2039, 4637
[3] Gottlieb D and Lagos M *Magnetically Driven Lattice Instability* IC/88/304 (Miramare-Trieste)
[4] Lagos M and Cabrera C G 1988 *Solid State Commun* **67** 221; 1988 *Phys. Rev.* B **38** 659
[5] Singh R R P and Gelfand M P 1988 *Phys. Rev. Lett.* **61** 2133
[6] Vaknin D *et al* 1987 *Phys. Rev. Lett.* **58** 2802
[7] Shirane G *et al* 1987 *Phys. Rev. Lett.* **59** 1613
[8] Aeppli G and Buttrey D J 1987 *Phys. Rev. Lett.* **61** 203