Phase diagram of the XXZ chain with next-nearest-neighbor interactions

R. D. Somma and A. A. Aligia

Comisión Nacional de Energía Atómica, Centro Atómico Bariloche and Instituto Balseiro, 8400 San Carlos de Bariloche, Argentina (Received 2 November 2000; revised manuscript received 15 February 2001; published 19 June 2001)

We calculate the quantum phase diagram of an XXZ chain with nearest-neighbor (NN) J_1 and next-NN exchange J_2 with anisotropies Δ_1 and Δ_2 , respectively. In particular we consider the case $\Delta_1 = -\Delta_2$, to interpolate between the XX chain ($\Delta_i = 0$) and the isotropic model with ferromagnetic phase J_2 . For $\Delta_1 < -1$, a ferromagnetic phase and two antiferromagnetic phases exist. For $|\Delta_i| < 1$, the boundary between the dimer and spin fluid phases is determined by the method of crossing of excitation spectra. For large J_2/J_1 , this method seems to indicate the existence of a second spin fluid critical phase. However, an analysis of the spin stiffness and magnetic susceptibility for $\Delta_1 = \Delta_2 = 1$ suggests that a small gap is present.

DOI: 10.1103/PhysRevB.64.024410

PACS number(s): 75.10.Jm, 75.30.Kz

I. INTRODUCTION

In recent years, several interesting quasi-one-dimensional magnetic systems have been studied experimentally.¹⁻⁴ Among them, some compounds containing CuO chains with edge-sharing CuO₄ plaquettes were expected to be described by the XXZ model with an important next-nearest-neighbor exchange J_2 in comparison with the nearest-neighbor (NN) exchange J_1 , and the latter can also be negative if the Cu-O-Cu angle is near 90° ⁴. In addition, there has recently been a renewed interest in this XXZ model (which is equivalent to a zigzag ladder).⁵⁻¹⁶ In particular, for the XX chain (Δ_1 $=\Delta_2=0$), field-theoretical methods predicted a critical (gapless) phase with incommensurate correlations for J_2 $\gg J_1 > 0$. This seems to be confirmed by recent numerical work.¹⁰ The effects of magnetic field and magnetization jumps (metamagnetism) were also studied recently.¹¹⁻¹⁴ Metamagnetism is more likely to occur in nature for ferromagnetic J_1 , because smaller anisotropies are required¹³. Interestingly, for ferromagnetic small J_1 a very small gap with an astronomically large associated correlation length was found by field theory calculations, and seems consistent with density-matrix renormalization group calculations.¹⁶

The phase diagram of the model for $\Delta_1 = \Delta_2 > 0$ was accurately determined by Nomura and Okamoto using the method of level crossings of the excitation spectra, supported by results of conformal field theory and the renormalization group.¹⁷ This method was also used successfully to determine phase diagrams of electronic models,¹⁸ and is related in some cases to jumps in topological numbers determined by Berry phases.^{19,20} Using the method of level crossings, the phase diagram was recently extended to the region $\Delta_1 = \Delta_2$ $<0.^{15}$ However, to assume that $\Delta_2 < 0$ implies a different sign of the z component of J_2 with respect to those of the x, y plane. This is an unrealistic anisotropy (this inconvenience is not present for J_1 because the sign of its x, y components can be changed by rotating every second spin in the chain by π around the z axis). In addition, the above-mentioned systems, containing CuO chains with edge-sharing plaquettes and Cu-O-Cu angle near 90°, are expected to lie near the isotropic cases $\Delta_1 = -1$ and $\Delta_2 = 1$.

In this work we calculate the phase diagram of the system

for $\Delta_2 = |\Delta_1|$ and $-1.2 < \Delta_1 < 1.2$, using the method of level crossings. This includes interpolations between the *XX* chain and the isotropic cases with ferromagnetic or antiferromagnetic J_1 .

II. MODEL AND METHOD OF LEVEL CROSSINGS

The model is

$$H = \sum_{i} \left[J_1(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta_1 S_i^z S_{i+1}^z) + J_2(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta_2 S_i^z S_{i+2}^z) \right],$$
(1)

where S_i^{β} is the β component of the spin-1/2 operator at site *i*.

The basic idea of the method of level crossings is that the properties of a critical phase at low energies and large distances are ultimately determined by a scale-invariant fixed point.¹⁷ Then, using conformal field theory, one can relate the excitation energy which corresponds to some operator A_i at site *i* (for example a spin flip S_i^+ or S_i^-), to the dependence of the correlation functions of this operator with distance:

$$E_A(L) - E_g(L) = \frac{2\pi v x_A}{L}, \quad \langle A_{i+d} A_i \rangle \sim \frac{1}{d^{2x_A}}.$$
 (2)

Here *L* is the length of the system, *v* the spin-wave velocity, $E_g(L)$ the ground-state energy, and x_A the critical dimension for the excitation *A*. For example, if $J_2=0$, the XXZ model was exactly solved and its properties are well known.^{21,22} The long distance dependence of the main correlation functions is

$$\langle S_{i+d}^+ S_i^- \rangle \sim (-1)^d r^{-1/K}, \quad \langle S_{i+d}^z S_i^z \rangle \sim (-1)^d r^{-K}$$
 (3)

with

$$K = \frac{\pi}{\pi - \arccos(\Delta_1)} \tag{4}$$

if $|\Delta_1| \le 1$. For $|\Delta_1| < 1$, the minimum excitation corresponds to a spin flip with a wave vector π . The ground state has a total spin projection $S^z = \pm 1$; its wave vector differs



FIG. 1. Phase diagram of the model [Eq. (1)] in the Δ_1 , $\alpha = J_2/J_1$ plane, keeping $\Delta_2 = |\Delta_1|$. *F* denotes the fully magnetized ferromagnetic phase, and AF2 a phase with long-range order $\uparrow \uparrow \downarrow \downarrow \ldots$.

from that of the ground state in π , and its parity under inversion *P* is opposite to that of the ground state.¹⁷ The matrix element of $S_i^{+(-)}$ between the ground state and the first excited doublet is different from zero. Then the correlation functions $\langle S_{i+d}^+ S_i^- \rangle$ are the dominant ones at large distances.

At $\Delta_1 = 1$, the above-mentioned doublet crosses the excited state with $S^z = 0$, (with a wave vector differing from the ground state in π , and P and T opposite to those of the ground state, where T is the parity under a spin reversal). Then, for $\Delta_1 > 1$, $\langle S_{i+d}^z S_i^z \rangle$ are the dominant correlations at large distances. At $\Delta_1 = 1$, a gap opens, and conformal invariance ceases to be valid. However, for a sufficiently small gap, so that the correlation length is much larger than the size of the system, Eqs. (2) are still expected to hold.

In summary, inside a critical phase or near its boundaries, the quantum numbers of the first excited state determine the dominant correlations at large distances, and therefore the crossings of the excited states determine the boundaries. For small J_2/J_1 , the use of a renormalization group allows one to determine the size dependence of the crossings, and to extrapolate them very accurately to the thermodynamic limit.¹⁷

III. RESULTS

The phase diagram we obtain in the plane $\alpha = J_2/J_1$, as a function of Δ_1 , with $\Delta_2 = |\Delta_1|$, is represented in Fig. 1. The transition between dimer and spin fluid I phases for $\Delta_1 \ge 0$ was obtained previously by Nomura and Okamoto.¹⁷ The spin fluid I phase is the well-known ground state of the model for $\alpha = 0$ and $|\Delta_1| < 1$. The dimer or spin Peierls phase has a spin gap and a broken translational symmetry (the unit cell is doubled) in the thermodynamic limit. The first excited state in finite systems has the same quantum numbers *P* and *T* as the ground state, but its wave vector differs by π .¹⁷ The new results for the spin-fluid-I-dimer transition are displayed in Fig. 2. The transition points (open squares) were accurately determined by extrapolating the



FIG. 2. Details of the boundary of the "spin fluid I" phase of Fig. 1 for negative Δ_1 .

crossing of the first excited state using data for chain lengths L=12, 16, and 20. As explained earlier,¹⁷ the crossing point has a $1/L^2$ size dependence. We have also verified this for negative Δ_1 (see Fig. 3). However, in the region denoted by ? in Fig. 3 (constructed with data for L=16), the first excited state has values of P and T opposite to those of the ground state. This is unexpected for the dimer phase. This might be a finite-size effect related to the high degeneracy at the point $\Delta_1 = -\Delta_2 = -1$, $\alpha = 0.25$.^{13,23} The other possibility is that a new phase exists there, but this seems unlikely.

After a transition to a dimer phase, if α is increased further, the crossing of excitation spectra indicates another transition to a phase in which the first excited state has $S^{z} = \pm 1$ and a wave vector $k_c = \pi/2$. We denote this phase as "spin fluid II," because, as we discuss below, its nature is not established for all values of Δ_i . For $\Delta_i = 0$, from field



FIG. 3. Size dependence of the crossing between dimer and "spin fluid I" excitations.



FIG. 4. Size dependence of the crossing between dimer and "spin fluid II" excitations.

theory results one might expect a spin fluid phase for large α .⁸ One also expects that k_c is actually incommensurate and slightly different from $\pi/2$.^{5,6,8,9} However, we are not able to detect this difference using periodic boundary conditions. While the use of twisted boundary conditions has given interesting results concerning this incommensurability,⁹ to implement them in the level-crossing method is time consuming and present technical complications, which we avoid in this work.

As shown in Fig. 4, the level crossing for the dimer-spin fluid II transition does not follow a $1/L^2$ dependence, and the extrapolation to the thermodynamic limit is not so accurate as for the dimer-spin fluid I transition. We have used a quadratic extrapolation in $1/L^2$, using the data for L=8, 12, 16, and 20. Field-theoretical results suggest that there is a small gap, and therefore no spin fluid phase for $\Delta_1 = \Delta_2 = 1$, and $J_2 \gg J_1$.^{6,7,14} For $\Delta_1 = -1$ and $\Delta_2 = 1$, a tiny gap is predicted, with an associated astronomically large length scale.¹⁶ A direct extrapolation of the gap from our finite-size results has an error larger than or of the order of the gap itself, and therefore is not able to establish if the gap is open or not. However, in principle we can check if a given phase is a spin fluid phase by other methods. For example, the energy per site should vary with system size as

$$e(L) = e(\infty) - \frac{\pi}{6L^2} v_s, \qquad (5)$$

where v_s is the spin velocity (or the sum of spin velocities if there were several types of low-energy excitations). We have

checked that Eq. (5) is not satisfied inside the dimer phase. A fit of the energies for L=12, 16, 20, and 24, with Eq. (5), gives an error of v_s which is of the order of v_s itself. Instead, inside both "spin fluid" phases the fit is good. The error in v_s is of order of 0.1% inside spin fluid I, and of order of 1% inside spin fluid II. Within spin fluid I, we also find that several relations derived from conformal field theory hold, and are consistent within them within ~5%. The spin velocity can be calculated as

$$v_1 = \frac{E(2\pi/L) - E(0)}{2\pi/L},\tag{6}$$

where E(q) is the lowest energy in the $S^z=0$ sector. The extrapolation of v_1 to the thermodynamic limit using a quadratic polynomial in 1/L is only slightly less than the value of v_s obtained by fitting Eq. (5). Also, from a numerical calculation of the susceptibility χ and spin stiffness D_s ,

$$\chi_{s} = \frac{1}{\frac{\partial^{2} e}{\partial m^{2}}} = \frac{1}{L[E(1) + E(-1) - 2E(0)]}$$
(7)

$$D_s = \frac{L}{2} \frac{\partial^2 E}{\partial \phi^2},\tag{8}$$

where here $E(S^z)$ is the lowest energy for total spin S^z , and ϕ is a flux opposite for spin-up and -down,⁹ we can obtain *K* in two independent ways from the relations²²

$$\chi_1 = \frac{K}{2\pi v_1}, \quad D_1 = \frac{K v_1}{4\pi} \tag{9}$$

The correlation exponents obtained from these two equations and Eqs. (6)–(8), with $\chi_1 = \chi_s$ and $D_1 = D_s$, also agree within 2–10% in the spin fluid phase I. The agreement improves with increasing Δ_1 .

A simple analysis based on Eqs. (7)-(9) is not possible in the "spin fluid II" phase. Equations (5) and (6) suggest that the low-energy properties of this phase are given by *two* free bosonic theories (this is of course true if $J_1=0$): $v_s=v_1$ $+v_2$, with v_2 slightly larger than v_1 . This is reasonable in principle, since if there are two branches of low-energy excitations, Eq. (6) should give the smallest velocity. Also one expects that Eq. (8) gives the sum of both spin stiffnesses:

$$D_s = \frac{K_1 v_1 + K_2 v_2}{4 \pi} \tag{10}$$

The case of the susceptibility is more delicate. From thermodynamics, the total susceptibility should be the sum of those of both branches. However, our numerical study suggests that when one flips only the spin, it goes to the branch of lowest velocity.

The results of field theory in the case $J_2 \gg J_1$ (Refs. 7 and 8) (and also those of the Hubbard ladder for small interchain hopping^{24,25}) suggest that the effective low-energy theory splits in two sectors, symmetric φ_+ and antisymmetric φ_- ; in general, at least the latter is gapped. For $\Delta_1 = \Delta_2 = 0$, φ_+

is massless and φ_{-} has a gap which depends on J_2/J_1 as a power law.^{8,9} In the isotropic case $\Delta_1 = \Delta_2 = 1$, both sectors have an exponentially small gap.⁷ These field theory results are inconsistent with the hypothesis, of two branches of massless excitations in the "spin fluid II" phase. To check this hypothesis we investigated the consistency of Eqs. (5) with $v_s = v_1 + v_2$, [Eqs. (6) and (10)], and an expression for the total susceptibility for some values of K_1 and K_2 in the above-mentioned cases ($\Delta_1 = \Delta_2 = 0$, and $\Delta_1 = \Delta_2 = 1$). We do not find reasonable results. For example, eliminating K_i from these equations, sometimes one negative result arises. The most plausible explanation is that at least one of the modes is gapped, but the system is not large enough to detect it in the size dependence of the energy [Eq. (5) is only valid for sufficiently large L]. In fact, some of our fittings suggest that the magnitude of the slope of e vs $1/L^2$ is decreasing with system size.

To end this section, we discuss the observed phases for $1.2 > |\Delta_i| > 1$. For $\Delta_1 < -1$, the ground state changes from a fully polarized ferromagnet ($S^z = L/2$) to $S^z = 0$ at the solid squares of Fig. 1. Actually, there is a small region of intermediate S^z between both phases, but it decreases with system size and seems to disappear in the thermodynamic limit. In the phase with $S^z = 0$, the first excited state has a wave vector $\pi/2$. This fact, a study of correlation functions,²⁶ and a trivial analysis of energies in the classical limit $-\Delta_1 = \Delta_2 \rightarrow \infty$, suggests that the phase has long-range AF order of the type $\uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \ldots$ (denoted as AFII). The same features denoting the presence of the AFII phase, are also found for $\Delta_i > 1$ and large α . We expect that for $|\Delta_i| > 1$, a spin-wave approximation can qualitatively describe the essential physics.

- ¹M. Hase, I. Terasaki, and K. Uchinokura, Phys. Rev. Lett. **70**, 3651 (1993).
- ²N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. 76, 3212 (1996).
- ³R. Coldea, D. A. Tennant, R. A. Cowley, D. F. McMorrow, B. Dorner, and Z. Tylczynski, Phys. Rev. Lett. **79**, 151 (1997).
- ⁴Y. Mizuno, T. Tohyama, S. Maekawa, T. Osafune, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. B 57, 5326 (1998).
- ⁵R. Bursill, G. A. Gehring, D. J. J. Farnell, J. B. Parkinson, T. Xiang, and C. Zeng, J. Phys.: Condens. Matter 7, 8605 (1995).
- ⁶S. R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996).
- ⁷D. Allen and D. Sénéchal, Phys. Rev. B 55, 299 (1997).
- ⁸A. A. Nersesyan, A. O. Gogolin, and F. H. L. Essler, Phys. Rev. Lett. **81**, 910 (1998).
- ⁹A. A. Aligia, C. D. Batista, and F. H. L. Essler, Phys. Rev. B 62, 3259 (2000).
- ¹⁰T. Hikihara, M. Kaburagi, and H. Kawamura, cond-mat/0007095 (unpublished).
- ¹¹C. Gerhardt, K.-H. Mütter, and H. Kröger, Phys. Rev. B 57, 11 504 (1998).
- ¹²S. Hirata, cond-mat/9912066 (unpublished).
- ¹³A. A. Aligia, Phys. Rev. B **63**, 014402 (2001).
- ¹⁴D. Cabra, A. Honecker, and P. Pujol, Eur. Phys. J. B 13, 55

IV. DISCUSSION

Using the method of level crossings, we have calculated the phase diagram of the XXZ model with next-NN exchange [Eq. (1)] for $\Delta_2 = |\Delta_1|$. For the dimer–spin-fluid-I transition our results are quite robust, and extend previous results^{17,15} to the case $1 \leq \Delta_1 = -\Delta_2 < 0$. In this region, the transition takes place near $\alpha \sim 0.3$. For larger values of α the method predicts a transition from the dimer phase to a second spin fluid phase. The transition is at $\alpha_c = 1.42$ for $\Delta_1 = \Delta_2 = 0$, in qualitative agreement with $\alpha_c \sim 1.26$ obtained in Ref. 10. For these values of Δ_i , field theoretical results predict the existence of this phase.⁸

For $\Delta_1 = -1$, a tiny gap with an astronomically large length scale is predicted in Ref. 16. Such a length is of course much larger than the system sizes we use, and our finite-size results are consistent with those of Ref. 16.

For $\Delta_1 = \Delta_2 = 1$, we have tried to interpret the thermodynamic properties of the "spin fluid II" phase as a sum of two independent fluids, but the results are not consistent. We then conclude that at this point, the extrapolation of the level crossings is not reliable; in agreement with other calculations,^{6,7,14} the gap persists for large J_2 .

From the parameters estimated for several compounds near the isotropic limit $\Delta_1 = -\Delta_2 = -1$ —La₆Ca₈Cu₂₄O₄₁ ($\alpha \sim 0.36$), Li₂CuO₂ ($\alpha \sim 0.62$), and Ca₂Y₂Cu₅O₁₀ ($\alpha \sim 2.2$) (Ref. 4)–our results indicate that these compounds lie outside the usual spin fluid I phase. They are in the AF2 phase if $\Delta_1 < -1$. If $\Delta_1 \ge -1$, La₆Ca₈Cu₂₄O₄₁ is clearly in the dimer phase. One expects a very small, perhaps unobservable gap for Ca₂Y₂Cu₅O₁₀ and spin-spin correlations with a wave vector near $\pi/2$. Li₂CuO₂ lies in between. The interchain interactions might affect this scenario.

(2000).

- ¹⁵S. Hirata and K. Nomura, Phys. Rev. B **61**, 9453 (2000).
- ¹⁶C. Itoi and S. Qin, Phys. Rev. B **63**, 224423 (2001).
- ¹⁷K. Nomura and K. Okamoto, J. Phys. A 27, 5773 (1994).
- ¹⁸M. Nakamura, Phys. Rev. B **61**, 16 377 (2000).
- ¹⁹A. A. Aligia, K. Hallberg, C. D. Batista, and G. Ortiz, Phys. Rev. B **61**, 7883 (2000).
- ²⁰ M. E. Torio, A. A. Aligia, K. Hallberg, and H. A. Ceccatto, Phys. Rev. B **62**, 6991 (2000).
- ²¹J. D. Johnson, S. Krinsky, and B. M. Mc Coy, Phys. Rev. A 8, 2526 (1973).
- ²²A. Gogolin, A. A. Nersesyan and A. M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, New York, 1998).
- ²³T. Hamada, J. Kane, S. Nakagawa, and Y. Natsume, J. Phys. Soc. Jpn. 57, 1891 (1988).
- ²⁴L. Balents and M. P. A. Fisher, Phys. Rev. B 53, 12 133 (1996);
 M. Fabrizio, Phys. Rev. B 54, 10 054 (1996).
- ²⁵The Hubbard zigzag ladder at half-filling in the limit of large on-site Coulomb repulsion reduces to the isotropic case $\Delta_1 = \Delta_2$ of the present model.
- ²⁶R. D. Somma and A. A. Aligia, Solid State Commun. **117**, 273 (2001).