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Conformal invariance and the phase diagram of the anisotropic Heisenberg spin-$\frac{1}{2}$ ladder

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Abstract. The phase diagram of two coupled anisotropic spin-1/2 Heisenberg chains forming a ladder is studied via the finite-size machinery arising from conformal invariance. Our results show that this system has similar behaviour to the anisotropic spin-1 Heisenberg chain. Both models for low values of anisotropies have a massless phase of Gaussian type, governed by a $c = 1$ conformal field theory. The operator that destroys the massless phase in these models is the same as in the Gaussian picture. We also verify that the massive phase in the anisotropic Heisenberg ladder has the same type of nonlocal order as that in the spin-1 Heisenberg chain.

The experimental study of materials such as $(VO)_2P_2O_7$ [1] and $Sr_2Cu_4O_6$ [2] suggested that the magnetic properties of such compounds are described by two coupled antiferromagnetic spin-1/2 Heisenberg chains. This observation motivated several studies of the spectral properties of spin-1/2 antiferromagnetic ladders [3–13]. These studies indicate that for an even number of legs the isotropic model has a gap, while for an odd number the model remains gapless as in the isotropic Heisenberg chain. A similar behaviour happens in the spin-S antiferromagnetic chain. According to the Haldane conjecture [14–16], for integral spin the chain has a gap and for half-odd-integer spin the chain is gapless. These facts lead to the conjecture that the antiferromagnetic Heisenberg ladders with an even number of legs are described by an effective antiferromagnetic Heisenberg chain with integer spin.

Recently, by introducing additional interactions in the isotropic Heisenberg ladder with two legs, White [12] showed numerically that the isotropic spin-1 Heisenberg chain and the ladder belong to the same phase in an extended phase diagram. Motivated by these results we decided to study such models by using the machinery arising from conformal field theory in two dimensions.

As is well known [17–19], the conformal anomaly and dimensions of operators governing the underlying field theory can be calculated by exploiting a set of important relations between these quantities and the energy spectrum of the Hamiltonian with a finite number, L, of sites. These relations are consequences (see Cardy [17] for a review) of the conformal invariance of the infinite system at a critical point. The relevant relations, for our purposes, may be stated as follows. For each primary operator [17] O_α, with anomalous dimension x_α and spin s_α, in the operator algebra of the massless infinite chain, there exists an infinite tower of states in the quantum Hamiltonian, in a periodic chain of L sites, whose energy and momentum as $L \to \infty$ are given by

$$E^{\alpha}_{j,j'}(L) = E_0(L) + \frac{2\pi v}{L}(x_\alpha + j + j') + o(L^{-1}) \qquad (1)$$

and

$$P^{\alpha}_{j,j'}(L) = \frac{2\pi}{L}(s_\alpha + j - j') \tag{2}$$

where $j, j' = 0, 1, 2, \ldots$. The ground-state energy of the finite chain is denoted by $E_0(L)$ and the constant v (model dependent) is the velocity of sound. In addition to these relations, conformal invariance also predicts [18, 19] that, at criticality, the L-site ground-state energy $E_0(L)$, in a periodic chain, behaves asymptotically as

$$\frac{E_0(L)}{L} = e_\infty - \frac{\pi c v}{6L^2} + \mathrm{o}(L^{-2}). \tag{3}$$

Here c is the central charge of the conformal class governing the critical behaviour and e_∞ is the bulk limit ($L \to \infty$) of the ground-state energy per particle.

The isotropic spin-1/2 Heisenberg ladder is expected to be massive (gapped) [5, 9, 10, 12, 13]. In order to better understand the underlying physics, previous experience [20–22] in conformal invariance studies of finite Heisenberg chains indicates that it should be better to consider an anisotropic version of the model with the Hamiltonian given by

$$H = H_\parallel + H_\perp \tag{4}$$

where

$$H_\parallel = J_\parallel \sum_{i=1}^{L} \sum_{j=1}^{2} (S^x_{i,j} S^x_{i+1,j} + S^y_{i,j} S^y_{i+1,j} + \Delta S^z_{i,j} S^z_{i+1,j}) \tag{5}$$

$$H_\perp = J_\perp \sum_{i=1}^{L} (S^x_{i,1} S^x_{i,2} + S^y_{i,1} S^y_{i,2} + \Delta S^z_{i,1} S^z_{i,2}). \tag{6}$$

The horizontal and vertical exchange constants are given by $J_\parallel$ and $J_\perp$ respectively, Δ is the anisotropy and (S^x, S^y, S^z) are the SU(2) spin-1/2 matrices. In the following we consider periodic lattices with $J_\parallel = 1$.

Let us consider initially the case where $J_\perp = 0$, where we have two decoupled anisotropic Heisenberg $S = 1/2$ chains. These single chains are massive for $|\Delta| > 1$ with antiferromagnetic or ferromagnetic order depending on whether $\Delta > 1$ or $\Delta < 1$, respectively. For $-1 \leqslant \Delta \leqslant 1$ they are in a disordered critical phase (gapless), with critical fluctuations governed by a U(1) conformal field theory with central charge $c = 1$ (see, e.g., references [23–27]). The anomalous dimensions of the operators (related to the critical exponents) ruling the massless phase are given by integers or by the Gaussian-like dimensions [28]

$$x_{n,m} = n^2 x_p + \frac{m^2}{4x_p} \qquad n, m = 0, \pm 1, \pm 2, \ldots \tag{7}$$

where $x_p = (\pi - \cos^{-1}(\Delta))/2\pi$. These correspond, in the Gaussian model [29, 30], to the dimensions of the operators $O_{n,m}$ composed of a spin-wave excitation with index n and a 'vortex' excitation of vorticity m.

At $J_\perp = 0$ the eigenspectra of (4) are obtained by adding the energies of two decoupled Heisenberg chains, which have $c = 1$ and dimensions given by (7). The relations (1), (2) and (3) imply that the underlying conformal field theory has conformal charge $c = 2$ and operators with dimensions given either by integers, $x_{n,m}$, or $x_{n,m} + x_{n',m'}$ ($n, m, n', m' = 0, \pm 1, \pm 2, \ldots$).

When we now perturb the decoupled chains by turning on $J_\perp > 0$, the problem is to know which among the above dimensions will be associated with the operator responsible for such perturbation. Since this perturbation does not destroy the whole U(1) symmetry of the decoupled chain,

$$[H_{\|}, S^z] = [H_{\|} + H_{\perp}, S^z] = 0 \qquad S^z = \sum_{i=1}^{L}\sum_{j=1}^{2} S^z_{i,j} \tag{8}$$

we expect, from the Gaussian model analogue, that such an operator should have zero spin-wave number index ($n = 0$). Moreover, from the previous work [5, 9, 10, 12], at $\Delta = 1$, the ladder is expected to be massive for small values of $J_{\perp}$, which implies that the perturbing operator should become relevant at some point in the interval $-1 \leqslant \Delta \leqslant 1$ since at $\Delta = 1$ the perturbation destroys the massless phase. The possible dimensions satisfying such requirements are $x_{0,1}$, which is relevant for $\Delta > -\sqrt{2}/2$, and $2x_{0,1}$, which is relevant for $\Delta > 0$. A possible way to test such possibilities comes from the analysis of the underlying field theory in the massive phase at around $J_{\perp} = 0$.

The mass spectrum can be inferred by applying the scheme followed by Sagdeev and Zamolodchikov [31] in the study of the Ising model in an external magnetic field. To do such calculations we should initially find the finite-size corrections of the zero-momenta eigenenergies $E_k(J_{\perp}, \Delta, L)$ ($k = 0, 1, 2, \ldots$) (E_0 being the ground-state energy), at the conformal invariant line $J_{\perp} = 0$. In the case of the decoupled chains the results of references [23, 24] tell us that such corrections, for arbitrary values of Δ ($-1 \leqslant \Delta \leqslant 1$), are governed mainly by the irrelevant operator with dimension $\bar{x} = x_{0,2} = 1/x_p$ and the descendant of the identity operator with dimension 4. From references [23, 24] we have

$$\begin{aligned} E_k(J_{\perp} = 0, \Delta, L) = e_{\infty}L + \frac{2\pi v}{L}\left(x_k - \frac{c}{12}\right) + a_1\left(\frac{1}{L}\right)^3 \\ + a_2\left(\frac{1}{L}\right)^{\bar{x}-1} + a_3\left(\frac{1}{L}\right)^{2\bar{x}-3} + a_4\left(\frac{1}{L}\right)^{3\bar{x}-5} + \cdots \end{aligned} \tag{9}$$

where x_k is one of the dimensions (7) associated with E_k, and $a_1, a_2, \ldots$ are L-independent factors; also $v = \pi \sin(\gamma)/\gamma$, where $\gamma = \cos^{-1}(\Delta)$. According to the scheme of reference [31], if the perturbed operator which produces the massive behaviour has dimension y, we should calculate the eigenspectra in the asymptotic regime $J_{\perp} \to 0$, $L \to \infty$, with

$$X = J_{\perp}^{1/(2-y)}L \tag{10}$$

kept fixed. In this regime (9) is replaced by

$$\begin{aligned} E_k(J_{\perp}, L) = e_{\infty}L + J_{\perp}^{1/(2-y)}F_k(X) + J_{\perp}^{(\bar{x}-1)/(2-y)}G_k(X) \\ + J_{\perp}^{(2\bar{x}-3)/(2-y)}V_k(X) + J_{\perp}^{(3\bar{x}-5)/(2-y)}H_k(X) + \cdots. \end{aligned} \tag{11}$$

The masses of the continuum field theory are obtained from the large-X behaviour of the function [31] $F_k(X)$, i.e.,

$$m_k \sim F_k(X) - F_0(X). \tag{12}$$

Diagonalizing the ladder Hamiltonian (4) for lattice sizes up to $L = 12$ (24 sites), and using in (11) $y = 2x_{0,1}$, our numerical analysis indicates a massive phase for $\Delta > 0$. In table 1 we show, for the sake of illustration, for two values of Δ, the finite-size estimates for the mass ratios. If we repeat this analysis using $y = x_{0,1}$ in (11), we obtain meaningless finite-size estimates, with even negative mass ratios.

The expected values appearing in table 1 would be obtained by taking the limit $X \to \infty$. However, for just $X = 14$ the worst finite-size estimate of these ratios deviates by only 9% from the conjectured value. The massive phase appearing at $\Delta = 0$ is also in agreement

Table 1. Finite-size estimates for the lowest mass ratios obtained from (12). The masses are obtained in the limit $X \to \infty$.

	$\Delta = \frac{1}{2}$		$\Delta = \frac{\sqrt{2}}{2}$	
X	m_2/m_1	m_3/m_1	m_2/m_1	m_3/m_1
6	2.832	2.503	3.828	3.102
10	2.260	2.190	2.548	2.429
14	2.117	2.094	2.183	2.170
Conjectured	2	2	2	2

with the results of Strong and Millis [4] based on the bosonization approach in a slightly different model where $\Delta = 1$ in (6).

Our results indicate a twofold-degenerate single mass M, plus a continuum starting at $2M$.

In the case of a single chain, the relevant perturbations, that do not destroy the U(1) symmetry, depending on the value of Δ, also produce beyond these masses bound states as in the sine–Gordon theory.

The phase diagram for arbitrary values of $J_\perp$ and Δ could be estimated from a direct calculation of the gap. However, our results would be very poor since such calculations require much larger lattice sizes. An alternative approach via exploring the conformal invariance in the massless phase of the phase diagram is possible. Our finite-size studies, based on conformal invariance [20–22], show that the massless phase exhibited by the model, when $J_\perp \neq 0$, is ruled by a Gaussian-like field theory with $c = 1$ and dimensions $x_{n,m}$ ($n, m \in \mathbb{Z}$) as in (7), but with x_p depending continuously on Δ and $J_\perp$. As an example, the dimensions $x_{n,0}$ are obtained from the bulk limit of the sequence

$$x_{n,0}(L) = \frac{E_n^{(0)}(L) - E_0^{(0)}(L)}{E_0^{(1)}(L) - E_0^{(0)}(L)} \tag{13}$$

where $E_n^{(k)}(L)$ is the lowest eigenenergy in the sector with U(1) charge $n = \sum_{ij} S_{i,j}^z$ and momentum $(2\pi/L)k$ $(k = 0, 1, \ldots)$.

A possible way to estimate the boundary of the Gaussian phase, which proved to be very effective in earlier applications [20, 32], is obtained by exploring the fact that due to (7) we must have $x_{2,0}/x_{1,0} = 4$ over the whole massless Gaussian phase. Even for small lattices, if we are inside the massless phase this quotient is very close to 4 and shows large variations once we leave the massless phase. If we assume as a finite-size estimate of the massless phase the points where $4 \geqslant x_{2,0}(L)/x_{1,0}(L) \geqslant 3.98$, then the estimates for the phase diagram in the plane $(J_\perp, \Delta)$ are as shown in figure 1, for lattices sizes $L = 6$–12. On considering instead of 3.98 the value 3.985, only a small change in the finite-size curves occurs. The points on the left of these curves satisfy the above inequality and are in the massless phase. Apart from finite-size effects which are large near $J_\perp \approx 0$, since there is a crossover to the two decoupled chains, we see from this figure that, as $L \to \infty$, the lower part of the asymptotic curve tends to stick on the $J_\perp = 0$ axis. This is in qualitative agreement with our earlier analysis, which indicates a massless phase for $\Delta \leqslant 0$. In the Gaussian phase, for $J_\perp \neq 0$, our results show that as Δ increases the exponent $\eta = 2x_{1,0}$ governing the correlation function $\langle S^x(r)S^x(0)\rangle \sim r^{-\eta}$ increases up to 1/4. In figure 2 we show, for lattice sizes $L = 6$–12, the points in the plane $(\Delta, J_\perp)$ where our finite-size estimates reach the value $2x_{1,0} = \eta = 1/4$. The points on the left of these curves satisfy

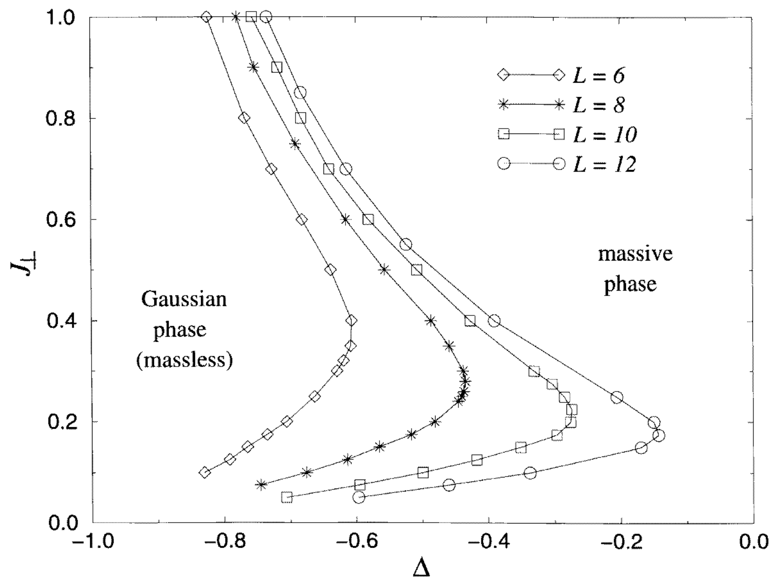

Figure 1. Finite-size estimates for the phase diagram of (4) for lattice sizes $L = 6$–12. The points on the left of these curves satisfy the inequality $4 \geqslant x_{2,0}/x_{1,0} \geqslant 3.98$.

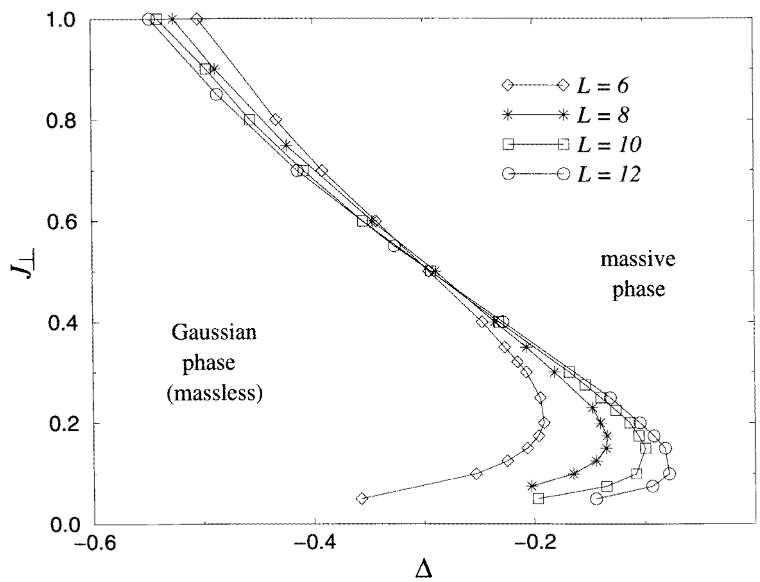

Figure 2. Finite-size estimates for the phase diagram of (4). The curves, for lattice sizes $L = 6$–12, are the points where $2x_{1,0}(L)$ reaches the value 1/4.

the above inequality and are in the massless phase. The resemblance of figures 1 and 2 indicates that over the whole massless phase the operator associated with the Δ perturbation has dimension $x_{0,1} = 1/4x_{1,0}$. When this operator becomes relevant the massless phase is destroyed. When $J_\perp \to 0$ the dimension $x_{0,1}$ tends toward the value $\pi/(\pi - \cos^{-1}\Delta)$ used in (11). This is similar to the anisotropic spin-1 Heisenberg model [21, 22], where the operator that destroys the Gaussian-like phase, producing the massive Haldane phase, also has dimension $x_{0,1}$.

The massive Haldane phase in the spin-1 Heisenberg chain, although not having a long-range order of Néel type, exhibits a hidden order characterized by alternating signs in the successive nonzero spins (take for example, the S^z-basis). This nonlocal order produces a nonzero value of the string correlation function [33–36]:

$$\mathcal{O}^z(j) = \left\langle S_1^z \exp\left(\mathrm{i}\pi \sum_{k=1}^{j-1} S_k^z\right) S_j^z \right\rangle \tag{14}$$

where the S^z are spin-1 Pauli matrices. Following [12] we can try to interpret the ladder Hamiltonian (4) as an effective spin-1 chain. In this case we should consider in (14) the combination $S_k^z = S_{k,1}^z + S_{k+1,2}^z$ $(k = 1, 2, \ldots)$.

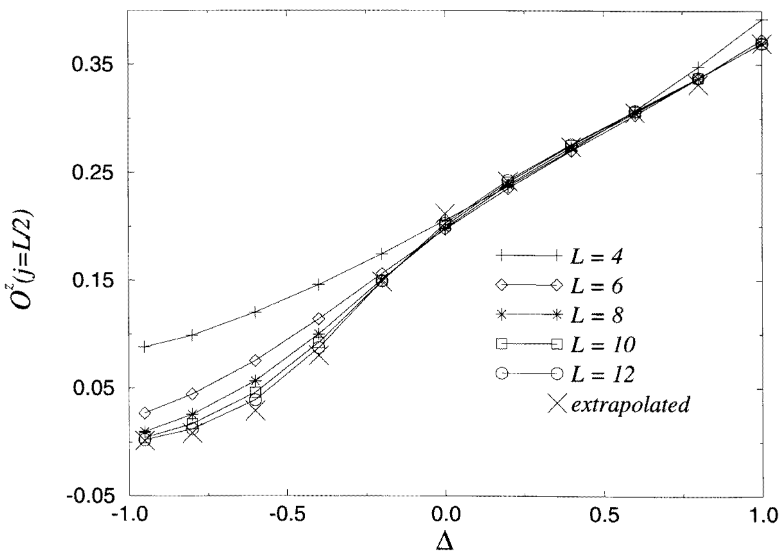

Figure 3. The string correlation function $\mathcal{O}^z(L/2)$, given in (14), as a function of Δ for several lattice sizes, together with the extrapolated values. These values are calculating by taking $J_\perp = 1$ in (4).

In figure 3 we show for $J_\perp = 1.0$ the finite-size estimates of (14) at $j = L/2$, together with the extrapolated results. The extrapolation was done by using the alternating-ϵ algorithm [37] which is a variant of of the VBS method [38], and the error bars are of the same size as the symbol $\times$ used in the figure. We clearly see that for $\Delta \gtrsim -0.8$ the string correlation function is nonzero like in the Haldane phase of the spin-1 single chain. In figure 4 we show for the ladder Hamiltonian (4) with $L = 10$ the values of $\mathcal{O}^z(L/2)$ for several values of $J_\perp$. Apart from finite-size effects this figure indicates the same type of nonlocal order in the massive phase of (4) as in the Haldane phase of the spin-1 Heisenberg chain.

For completeness we also considered the anisotropic version of the extended ladder model introduced by White [12]. In this Hamiltonian (see figure 5) we include in (4) a ferromagnetic interaction along the diagonal:

$$H = H_\parallel + H_\perp + H_/ \tag{15}$$

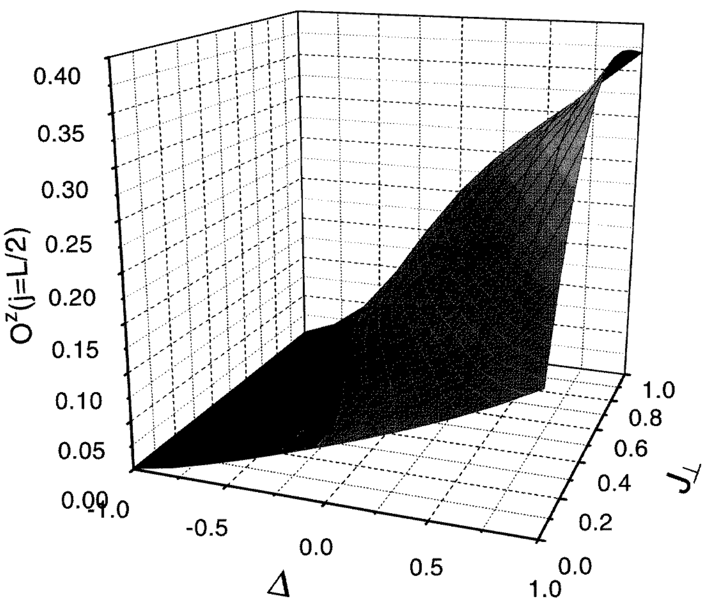

Figure 4. The string correlation function $\mathcal{O}^z(L/2)$ for the Hamiltonian (4) with lattice size $L = 10$, as a function of Δ and $J_\perp$.

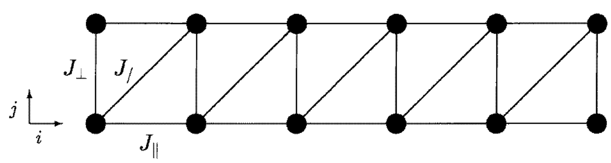

Figure 5. Schematic interactions of the Hamiltonian given in (15).

where

$$H_/ = -J_/ \sum_{i=1}^{L} (S^x_{i,1} S^x_{i+1,2} + S^y_{i,1} S^y_{i+1,2} + S^z_{i,1} S^z_{i+1,2}). \tag{16}$$

This Hamiltonian when $J_/ \to \infty$ is precisely the spin-1 anisotropic Heisenberg chain, since the singlet states of the spins coupled by $J_/$ have infinite energy. White showed [12] numerically that the isotropic chain ($J_\perp = 1$, $\Delta = 1$) does not undergo any phase transition as $J_/$ is varied from $J_/ = \infty$ to $J_/ = 0$, which implies that the massive Haldane phase of the spin-1 chain and the massive phase of the isotropic ladder are identical.

Our results show again a Gaussian-like phase for the Hamiltonian (15), which is destroyed once the operator with dimension $x_{0,1}$ becomes relevant. In figure 6 we also show for $J_\perp = 1$ the finite-size estimates of the phase diagram obtained by imposing $2x_{1,0}(L) = 1/4$, like in figure 2. This figure shows that at $J_/ = 0$ the massive phase starts at $\Delta \approx -0.55$, in agreement with figure 2, but for $J_/ \to \infty$ the massive phase starts at $\Delta \approx 0$, in agreement with the anisotropic spin-1 chain [20–22, 39].

In conclusion, our results show that like the spin-1 Heisenberg chain the anisotropic spin-1/2 Heisenberg ladder has massless phases governed by a Gaussian-like $c = 1$ conformal

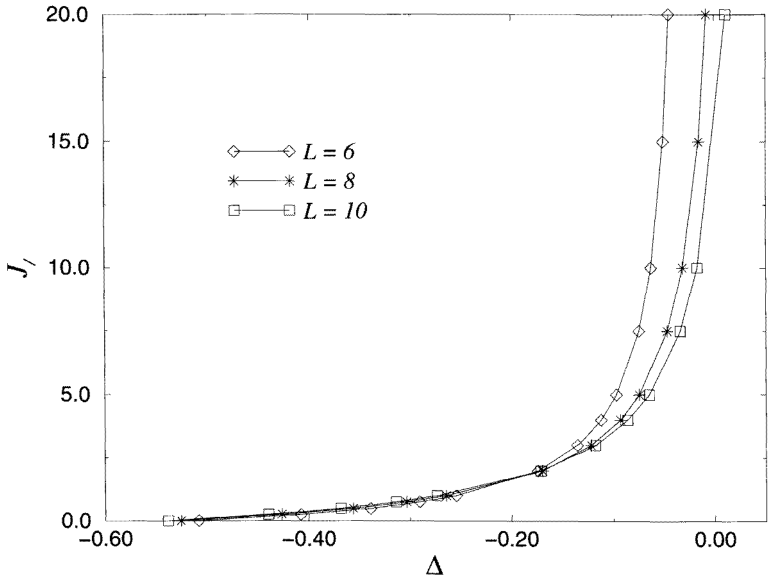

Figure 6. Finite-size estimates for the phase diagram of (15). The curves, for lattice sizes $L = 6$–12, are the points where $2x_{1,0}(L) = 1/4$.

field theory. In all of these models the operator with zero vorticity and spin-wave number 1 yields the massive phase once it becomes relevant.

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