A plane of weakly coupled Heisenberg chains: theoretical arguments and numerical calculations

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Abstract. The $S = \frac{1}{2}$, nearest-neighbour, quantum Heisenberg antiferromagnet on the square lattice with spatially anisotropic couplings is reconsidered, with particular attention to the following question: at $T = 0$, does Néel order develop at infinitesimal interchain coupling, or is there a non-zero critical coupling? A heuristic renormalization-group argument is presented which suggests that previous theoretical answers to this question are incorrect or at least incomplete, and that the answer is not universal but rather depends on the microscopic details of the model under consideration. Numerical investigations of the nearest-neighbour model are carried out *via* zero-temperature series expansions about Ising and dimer Hamiltonians. The results are entirely consistent with a vanishing critical interchain coupling ratio R_c; if R_c is finite, it is unlikely to substantially exceed 0.02.

1. Introduction

Lately there has been considerable interest in one- to two-dimensional crossover in Luttinger liquids. The motivation is largely the interest in possible non-Fermi liquid behaviour in two-dimensional models for high-T_c superconductors [1]. While much of this work has focused on the Hubbard or t–J model, a simpler case to understand is that of the spatially anisotropic square-lattice spin-$\frac{1}{2}$ Heisenberg antiferromagnet

$$H = \sum_{r_i - r_j = e_x} J_x S_i \cdot S_j \; + \sum_{r_i - r_j = e_y} J_y S_i \cdot S_j \tag{1.1}$$

(and see figure 1) with $0 < J_y \ll J_x$. The essential question is whether Néel order sets in for infinitesimal

$$R \equiv J_y / J_x \tag{1.2}$$

or whether there is a finite minimum coupling ratio necessary for long-range order (LRO). A subsidiary question is the nature of the magnetically disordered phase at small R, if the latter scenario holds true. While various analytical and numerical investigations of this question have appeared in the literature [2–4], it appears to be far from settled.

The purpose of this paper is twofold. In section 2 we review previous analytic arguments for or against the existence of a finite minimum ratio. We then discuss a renormalization-group framework within which previous arguments appear to be incorrect or incomplete. This approach indicates that the behaviour is not universal and that for any particular model
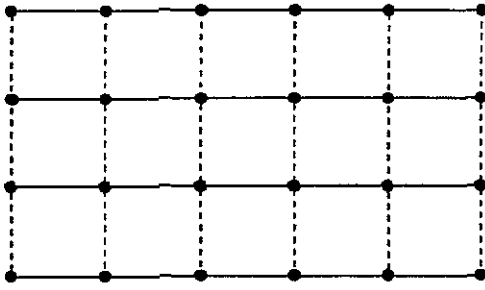
Figure 1. The spatially anisotropic Heisenberg model. The full and broken segments correspond to interactions J_x and J_y.

the question may only be answered by numerical investigation. Therefore in section 3 we present such a numerical investigation of the Hamiltonian (1.1) based on a high-order series expansion about both the Néel and dimer phases. That analysis seems to indicate that if there is a critical ratio it is rather small.

2. Theoretical arguments

2.1. Spin-wave theory

Spin-wave theory plays an important role in our understanding of antiferromagnetism. A systematic $1/S$ expansion (where S is the spin magnitude) is generally believed to give, at low orders, a fairly accurate estimate of the sublattice magnetization on various lattices. In particular, it correctly predicts the absence of long-range order at $T = 0$ for a one-dimensional antiferromagnet. This effect can be seen from the leading-order correction to the sublattice magnetization. For the anisotropic 2D model of (1.1), we have

$$\langle S_i^z \rangle = \pm \left[S - \frac{1}{2} \left(\int \frac{\mathrm{d}^2 k}{(2\pi)^2} \frac{1}{\sqrt{1 - \gamma_k^2}} - 1 \right) \right] \tag{2.1}$$

where

$$\gamma_k \equiv \frac{J_x \cos k_x + J_y \cos k_y}{J_x + J_y} \tag{2.2}$$

and the k integral runs over the Brillouin zone, $|k_i| < \pi$. For $J_y = 0$, the integrand is independent of k_y and the integral has logarithmic divergences at $k_x = 0$ and π indicating the absence of Néel order. For finite J_y the integral is finite and for small R we obtain:

$$\langle S_i^z \rangle \approx \pm \left[S + \frac{1}{2\pi} \ln R \right]. \tag{2.3}$$

If we took as a criterion for the stability of the Néel phase that the O(1) correction should be smaller than the leading O(S) term, then we would conclude that Néel order breaks down at

$$R_c \approx e^{-2\pi S}. \tag{2.4}$$

For $S = \frac{1}{2}$, numerical evaluation of the integral in (2.1) gives $R_c \approx 0.033\,67$ [2].

2.2. Chain mean-field theory

A standard method for treating dimensional crossover problems of this type is to use the known behaviour of the antiferromagnetic susceptibility for the one-dimensional system and to treat the couplings in the second dimension in mean-field theory [5]. (We refer to this as

'chain' mean-field theory to distinguish it from another mean-field theory to be discussed later.) The Hamiltonian of (1.1) is replaced by the following mean-field Hamiltonian for each chain:

$$H_{\mathrm{CMF}} \equiv \sum_i J_x S_i \cdot S_{i+1} + 2J_y \langle S^z \rangle \sum_i (-1)^i S_i^z. \qquad (2.5)$$

We now calculate $\langle S^z \rangle$ using this Hamiltonian and demand self-consistency. The mean-field critical point is then determined by

$$1 = 2R\chi_1(T_N) \qquad (2.6)$$

where χ_1 is the zero-frequency antiferromagnetic susceptibility for the one-dimensional chain with $J_x = 1$. For a half-integer spin Heisenberg antiferromagnet, $\chi_1(T)$ diverges as $1/T$, as $T \to 0$. This argument then predicts a finite Néel temperature

$$T_N \approx J_y. \qquad (2.7)$$

No matter how small J_y, the ground state is always ordered. On the other hand, for integer S, $\chi_1(0)$ has a finite value of order $1/\Delta$, the Haldane gap. Hence this argument predicts a disordered ground state for integer S and $R < R_c$ with $R_c \approx \Delta$. This result is readily generalized to d-dimensional systems. The factor of 2 in (2.6) is simply replaced by the number of nearest-neighbour chains. Indeed, it presumably becomes exact in the limit $d \to \infty$. It has an obvious problem for $d = 2$ where the Mermin–Wagner theorem tells us that Néel order should be impossible at any finite temperature. Nonetheless, we might be tempted to believe the conclusion that it does occur at $T = 0$. A more sensible application of this mean-field theory for $d = 2$ is to the case of a staggered intra-chain coupling at $T = 0$ (see section 3.2). Equation (2.6) then becomes

$$1 = 2R\lambda_{\mathrm{CMF}}^c \chi_1(\lambda_{\mathrm{CMF}}^c). \qquad (2.8)$$

Here λ is the ratio of coupling on alternate links, and λ_{CMF}^c is its critical value within the chain mean-field theory. Since a staggered interaction in one dimension has scaling dimension $\frac{1}{2}$, we conclude that $\chi_1(\lambda) \propto (1 - \lambda)^{-2/3}$ (up to log corrections). Now $1 - \lambda$ plays a role roughly analogous to a finite temperature; as $\lambda \to 1$, the mean-field theory predicts that Néel order sets in at $1 - \lambda_{\mathrm{CMF}}^c \propto R^{3/2}$.

2.3. Renormalization-group argument

Consider a system of quantum chains weakly coupled to each other at $T = 0$. They may be of XY or Heisenberg symmetry. Alternatively, consider a system of classical spins consisting of planes which are weakly coupled to each other, at finite T. In either case (ignoring topological terms, for the moment), we may represent the system at long length scales by a three-dimensional nonlinear σ-model, with action or Hamiltonian

$$S = (\Lambda/2g) \int \mathrm{d}^3x \big[(\partial_x \phi)^2 + (\partial_y \phi)^2 + R(\partial_z \phi)^2\big]. \qquad (2.9)$$

Here ϕ has unit length and either two or three components in the XY or Heisenberg case. As before, R is the ratio of inter-chain (or plane) coupling to in-chain (or plane) coupling. Λ is the ultraviolet cut-off; i.e. the field, ϕ has Fourier modes with $|k_i| < \Lambda$. (We cut off the momentum inside a cube.) The factor of Λ is inserted to make the three-dimensional coupling constant g dimensionless, as is usually done in formulating the 3D renormalization-group (RG) equations.

Note that the only trace of the quasi-two-dimensionality is the anisotropy in the $(\partial\phi)^2$ terms. We can get rid of this by a rescaling of z by a factor of $\sqrt{R}$, that is, we define a
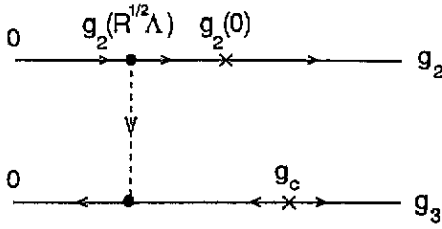
Figure 2. Renormalization-group flows for the half-integer spin quantum Heisenberg models. Here we assume $g_2(0) < g_c$ so the system orders for arbitrarily small R.

new length coordinate, $z' \equiv z/\sqrt{R}$. In momentum space, we define a new 3-component of momentum, $k_3' \equiv \sqrt{R}k_3$. The action now looks completely three-dimensional except that the cut-off is no longer a 3D cube but a squat box of area Λ^2 and height $\sqrt{R}\Lambda$. To complete the elimination of the anisotropy from the action, we reduce the length and width of the box to $\sqrt{R}\Lambda$ also, by integrating out higher momentum modes, the standard RG procedure. Because the inter-chain coupling is so weak, this may essentially be done using the 2D RG equations; in momentum space, $(k_\perp')^2$ is so small (due to the small cut-off) that we consider the planes to be essentially decoupled until we have lowered the 2D cut-off down to approximately $\sqrt{R}\Lambda$. The value of the 2D effective coupling, when the cut-off has been reduced to $\sqrt{R}\Lambda$, then acts as the initial condition for further RG calculations: as we lower the cut-off still further we should use the isotropic 3D RG equations using $g_2(\sqrt{R}\Lambda)$ as the initial value. In the limit $R \to 0$, the 2D coupling flows to its zero-cut-off fixed point, $g_2(0)$. See figure 2 for a sketch of one possible flow diagram.

In both XY and Heisenberg cases, the 3D system has ordered and disordered phases, separated by some critical coupling g_c. (For $g < g_c$ the system is ordered.) Thus, whether or not the system orders for arbitrarily small R is determined by whether or not $g_2(0) < g_c$. In the case of Heisenberg symmetry with no topological term, $g_2(0)$ is naively infinite, so the 3D system is in the disordered phase for sufficiently small R. From another point of view, the 2D system develops a finite correlation length, ξ, as we reduce the cut-off. For sufficiently small R, $\sqrt{R}\Lambda < 1/\xi$. Then further renormalization using the 3D RG equations cannot eliminate this finite correlation length. In the XY case $g_2(0)$ is basically the renormalized dimensionless temperature. It has a finite value along the Kosterlitz–Thouless (KT) critical line, $g_2(0) < g_{KT}$. The important question is whether or not $g_{KT} < g_c$. If it is, then an arbitrarily weak inter-plane coupling leads to order for all $T < T_{KT}$. In the other case, if $g_c < g_{KT}$, then there will be some special temperature, $T_c < T_{KT}$, such that below this temperature an arbitrarily weak inter-plane coupling leads to LRO but above this temperature there is a minimum inter-plane coupling necessary for LRO.

Numerical simulations of the classical layered XY model indicate that $g_{KT} < g_c$ [6]. In this case the present approach predicts a critical coupling, $g_c(R)$, for weakly coupled planes, slightly above g_{KT}. This can be estimated as the bare coupling for which the renormalized coupling at scale $\sqrt{R}\Lambda$, $g_2(\sqrt{R}\Lambda) \approx g_c$. Using the 2D Kosterlitz renormalization-group equations this gives

$$g_c(R) - g_{KT} \propto 1/(\ln R)^2 \tag{2.10}$$

in agreement with estimates based on plane mean-field theory [6] and another approach [7, 8] somewhat closer in spirit to the present one.

Now let us consider the half-integer spin quantum Heisenberg chain [9]. The two-dimensional σ-model action now has an extra topological term added to it, with topological angle π. This angle itself does not renormalize, for symmetry reasons, but it has a crucial effect on the renormalization of g_2. There is now a finite coupling critical point, $g_2(0)$, shown in figure 2. Note that the $g_2 = 0$ Néel fixed point is unstable, as required by the

quantum version of the Mermin–Wagner theorem. The $g_2(0)$ critical point exhibits quasi-long-range order, i.e. power-law decay of spin correlations. The strong coupling phase is spontaneously dimerized; it can be reached with a sufficiently strong antiferromagnetic second nearest-neighbour coupling. The three-dimensional RG flows are expected to be the same for both integer and half-integer spin. The disordered phase is expected to be different for half-integer, odd integer or even integer spin due to the presence of a Berry's phase topological term [10]. However, the value of this term (that is, whether the spin is half-integer, odd integer or even integer) is not expected to influence the existence of the order–disorder transition or, presumably, the universality class of this transition. We assume the only important effect of the topological terms is to produce a finite $g_2(0)$ critical point in two dimensions, as shown in figure 2. The situation is then similar to the classical XY case. Whether or not a disordered phase occurs for weak interchain coupling depends on whether or not $g_2(0) > g_c$.

Let us contrast this approach to either of those discussed above, in sections 2.1 and 2.2. First consider the calculation of the breakdown of the Néel state in lowest-order spin-wave theory. This can be regarded as the above calculation of the renormalization of the 2D coupling, using *only the lowest-order 2D RG equations*. For large S we begin with a very small bare coupling. However, the lowest-order RG equations always break down for small enough R. Furthermore, these equations do not distinguish integer and half-integer S. In σ-model language, the lowest-order RG is independent of the topological term. Actually the RG equations are independent of it to all orders in g; its effects are exponentially small in g. Nonetheless, for small enough R we always renormalize into the regime where these non-perturbative contributions are important. Blind use of the lowest order equations essentially leads to the conclusion that $g_2(0)$ is infinite and hence that the system is disordered at small enough R.

On the other hand consider the standard mean-field argument [5]. Because the 2D susceptibility is divergent along the whole KT critical line, or in the Heisenberg case with a topological term, it predicts LRO in all these cases. We argue that in order to go beyond a mean-field treatment one should consider not the 2D susceptibility but rather the renormalized 2D effective coupling. Naively if the 2D susceptibility is infinite, the 2D effective coupling is zero. But in fact, this is not actually the case. Since the 2D effective coupling is finite at zero cut-off we must consider whether or not it is below g_c, leading to the above conclusion.

It was suggested recently by Parola *et al* [4] that, for R less than a finite R_c, the long wavelength behaviour 'can be interpreted in terms of decoupled one-dimensional chains.' The implausibility of this proposal can be seen by considering a finite number of chains. In this case, we can analyse the scaling behaviour entirely in terms of the $(1 + 1)$-dimensional renormalization group. The inter-chain coupling, of dimension 1, is relevant. We might then naively expect from standard scaling arguments that for two chains there should be a gap, proportional to R (up to logarithms). The existence of a gap in this case has been shown numerically [11, 12]. In the case of three chains, White *et al* [12] found that the gap appears to vanish and this has been argued to be the case for any odd number of chains. However, this does not necessarily mean that the system asymptotically behaves like decoupled chains. Indeed, it seems more likely that the low-energy states would be those of a *single* $S = \frac{1}{2}$ chain. This assertion is motivated by the behaviour of a single spin S chain as a function of S. For integer S one expects a gap while for half-integer S one expects universal gapless behaviour which is independent of S (i.e. always in the free boson or $k = 1$ Wess–Zumino–Witten universality class). For half-integer S the density of low-lying excitations (after scaling out the spin-wave velocity) *does not increase* with increasing S. We may expect similar behaviour for $2S$ coupled spin-$\frac{1}{2}$ chains: inter-chain coupling is

relevant and the system scales away from decoupled chains to the single chain fixed point with fewer gapless degrees of freedom. Note that in this case, the number of low-lying degrees of freedom does not scale with the area of the system but only with the length. It is, of course, possible that, as the number of chains is increased, the gap to other excitations decreases and asymptotically approaches zero as the number of chains goes to ∞. Indeed, *this must happen if the ∞-chain system Néel orders. However, it then seems unlikely that* the low-lying excitations would be those of decoupled chains. We rather expect that, if a disordered phase exists at small R, it has a genuinely two-dimensional nature. Previous work on the isotropic $S = \frac{1}{2}$ square lattice Heisenberg antiferromagnet with next-nearest neighbour interactions suggests that a dimer-ordered ground state is the most likely to occur in a magnetically disordered phase [13]. However, other possibilities with or without a gap cannot be ruled out.

Actually, the result of our reasoning is pretty uninformative. It is simply that we cannot tell from RG arguments whether or not the system orders for arbitrarily weak inter-plane coupling, in cases where the 2D system has an infinite correlation length. We might expect that the existence or non-existence of a critical R is not universal. Different realizations of the model may have different values of g_c or $g_2(0)$, since critical temperatures (or couplings) are, in general, not universal. For instance, a different phase diagram might ensue if the chains are coupled with a first and second nearest-neighbour inter-chain coupling, both proportional to R. It would thus seem that the question of the existence of a disordered phase for finite R in a particular model must be answered by numerical work.

3. Series calculations and analyses

We now turn to numerical studies of weakly coupled, $S = \frac{1}{2}$ Heisenberg chains, and, in particular, the anisotropic two-dimensional lattice of figure 1 and (1.1). It is obviously not possible for any numerical calculation to distinguish between $J_y^c = 0$, i.e. the persistence *of Néel order for arbitrarily small interchain couplings, and a sufficiently small but positive* J_y^c. Provided that there is no strong evidence for any particular non-zero value of J_y^c, the best one can do is argue that numerical data are consistent with a vanishing J_y^c and offer reasonable upper bounds on its value.

Our numerical studies consist of a variety of zero-temperature series expansions (i.e. Rayleigh–Schrödinger perturbation theory) following the cluster-expansion techniques described in [14]. Series expansions have several advantages over finite-size calculations in two-dimensional lattice quantum many-body problems. There is no need to worry about cluster-shape effects—which should be of particular concern in anisotropic models such as the one of present interest. Given comparable computing power, series calculations can account for much further-range correlations than would be possible in an exact diagonalization calculation (see the discussion in section 5 of [14]). Finally, the fact that the *series calculations do not directly study the model of interest, but rather yields results on a* one- (or more) parameter family of models, may allow for further informative comparisons with approximate analytic calculations.

Expansions were carried out about both Ising and dimer Hamiltonians. The calculations and analyses will be described in detail below; here let us preview the results. The results of both types of expansions are consistent with $J_y^c = 0$. We believe that J_y^c is unlikely to exceed $0.02\,J_x$. This upper bound is not much smaller than the lowest-order spin-wave estimate (and hence by itself cannot be taken as very strong evidence that spin-wave theory is qualitatively wrong); however it is notably less than the value $0.1\,J_x$ suggested by Parola *et al* [4] based on exact diagonalization of clusters with up to 32 spins. In addition, the

Ising expansions yield estimates for the staggered magnetization and the correlation-length anisotropy which are in excellent agreement with spin-wave theory for J_y/J_x down to 0.1. Finally, the dimer expansions appear to be consistent with the chain mean-field theory of section 2.2 at small J_y, and thus support the proposition that $J_y^c = 0$. However, that conclusion must be tempered by comparison of the dimer expansions for a plane of chains with the corresponding calculations for a *pair* of chains.

3.1. Ising expansions

In order to discuss the Ising expansions, we consider a generalization of the coupled-chain Hamiltonian (1.1) in which Ising anisotropy is introduced, namely

$$H = \sum_{r_i - r_j = e_x} J_x\left[S_i^z S_j^z + \alpha\left(S_i^x S_j^x + S_i^y S_j^y\right)\right] + \sum_{r_i - r_j = e_y} J_y\left[S_i^z S_j^z + \alpha\left(S_i^x S_j^x + S_i^y S_j^y\right)\right]. \quad (3.1)$$

Henceforth we choose units of energy so that $J_x = 1$ (and $J_y = R$). Physical quantities are expanded in powers of α; we have calculated the ground-state energy E_g, the sublattice magnetization $M = \langle S_0^z \rangle$, and the correlation length anisotropy $(\xi_y/\xi_x)^2$ which is given explicitly by

$$\frac{\sum_i \langle S_0^z S_i^z \rangle_c y_i^2}{\sum_i \langle S_0^z S_i^z \rangle_c x_i^2} \quad (3.2)$$

where the subscript c refers to connected correlations

$$\langle S_0^z S_i^z \rangle_c = \langle S_0^z S_i^z \rangle - \langle S_0^z \rangle \langle S_i^z \rangle. \quad (3.3)$$

The energy and magnetization series were determined to order $(\alpha^2)^5$, while the $(\xi_y/\xi_x)^2$ series were only calculated to order $(\alpha^2)^4$. Note that each value of J_y requires a separate calculation of the series; since it is not possible to present the complete series expansions in a compact format they are not displayed here, but are available as supplementary material. Here we discuss the analysis.

The energy series were analysed by direct Padé approximants. The results of five different Padé approximants evaluated at $\alpha = 1$ are shown in figure 3. It is clear that they extrapolate smoothly between the one- and two-dimensional limits, that is to say between $J_y = 0$ and 1. This is consistent with the expansion being convergent up to $\alpha = 1$ for all $J_y \geqslant 0$, which is in turn consistent with $J_y^c = 0$. However, this is quite weak evidence, as we will discuss in connection with the dimer expansions. Perhaps the results for E_g could serve best as a touchstone for the quality of finite-size calculations.
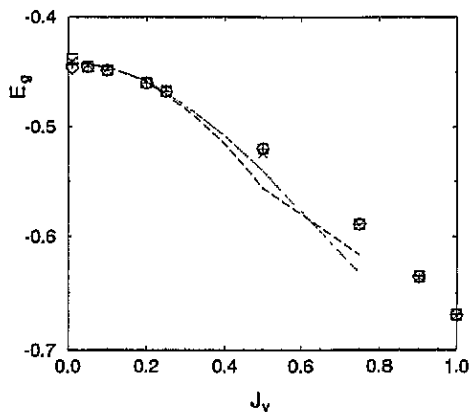

Figure 3. Padé approximants for the ground-state energy, evaluated at $\alpha = 1$. The symbols are approximants to Ising series, while the lines (which are connecting points with $J_y = 0$, 0.1, 0.2, 0.3, 0.4, 0.5, and 0.75) are approximants to dimer series.
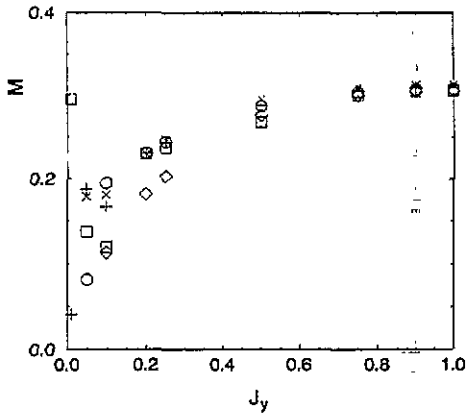
Figure 4. Padé approximants to the Ising expansion for the sublattice magnetization, evaluated at $\alpha = 1$ following the change of variables described in the text.
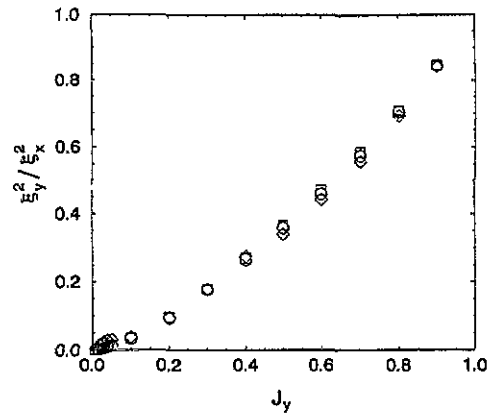
Figure 5. Padé approximants to the Ising expansion for the correlation length anisotropy, evaluated at $\alpha = 1$.

To analyse the magnetization series, we first make a change of variables originally introduced by Huse, $\delta = 1 - (1 - \alpha^2)^{1/2}$, which removes the square-root singularity at $\alpha = 1$ expected on the grounds of spin-wave theory. The results for five Padé approximants evaluated at $\alpha = 1$ are shown in figure 4. For $J_y \geqslant 0.2$ the approximants are well converged and appear to be in good agreement with spin-wave theory. For $J_y < 0.2$ the convergence is poor, but the approximants are suggestive of Néel order for all J_y and with M vanishing as a small power of J_y. Note that the chain mean-field theory implies $M \sim J_y^{1/2}$ as $J_y \to 0$. In any case, these data provide no evidence that $M \to 0$ at any particular $J_y^c > 0$.

The correlation length anisotropy series are short, however, this quantity is non-singular as $\alpha \to 1$ and the Padé approximants evaluated at $\alpha = 1$ are extremely consistent even down to very small J_y: see figure 5. For $J_y \geqslant 0.1$ there is remarkable agreement between the series estimates and the spin-wave calculation presented by Parola *et al* [4]. For smaller J_y, two of the three approximants indicate $\xi_y/\xi_x \to 0$ for J_y between 0 and 0.02, and the other approximant is ill-behaved. These data are consistent with $J_y^c = 0$, but also with a small critical interchain coupling.

3.2. Dimer expansions

The dimer expansions are in the variable λ for properties of the Hamiltonian $H = H_0 + \lambda H_1$, where for H_0 we take the columnar dimer Hamiltonian

$$H_0 = \sum_{\langle ij \rangle \in \mathcal{D}} J_x \, S_i \cdot S_j \tag{3.4}$$

with $\mathcal{D}$ the dimer covering of the square lattice shown in figure 6, and H_1 is the remainder of the couplings, so that $\lambda = 1$ corresponds to the coupled-chain model of interest, namely

$$H_1 = \sum_{r_i - r_j = e_x; \langle ij \rangle \notin \mathcal{D}} J_x \, S_i \cdot S_j + \sum_{r_i - r_j = e_y} J_y \, S_i \cdot S_j . \tag{3.5}$$

The quantities for which we have obtained series expansions, to order λ^7 (which involves evaluation of 1041 graphs), include the ground-state energy E_g, moments of the
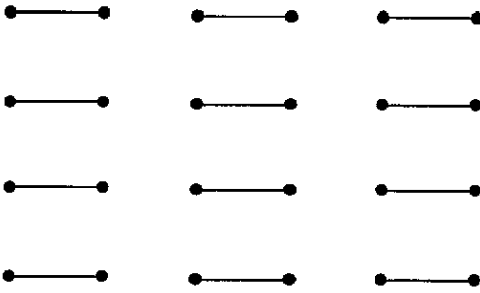
Figure 6. The columnar dimer covering $\mathcal{D}$ used for the dimer expansions; see (3.5).

antiferromagnetic equal-time structure factor

$$M_1 = \sum_i \langle S_0 \cdot S_i \rangle \pi(r_i) \tag{3.6}$$

$$M_{rr} = \sum_i \langle S_0 \cdot S_i \rangle \pi(r_i) r_i^2 \tag{3.7}$$

(where $\pi(r_i)=1$ if r_i lies on the same sublattice as r_0, and is -1 otherwise), and the antiferromagnetic susceptibility χ.

It should be clear from the form of the Hamiltonian that all these quantities possess two-variable expansions, in powers of λ and λJ_y. Hence the coefficient of λ^m in any of these series can be expressed in terms of an order-m polynomial in J_y; and calculations of the seventh-order series at eight values of J_y allows one to determine them at *any* J_y by means of polynomial interpolation.

Before considering the details of the dimer series analysis, let us look at the notions underlying this approach, and what we might expect to learn from it. Properties of the Néel-ordered phase are inaccessible to the dimer expansions (in contrast to the Ising expansions); what they can provide are estimates of $\lambda^c(J_y)$, the smallest value of λ for a given J_y at which the antiferromagnetic correlation length and susceptibility diverge. If one assumes the simplest possible phase diagrams in the J_y–λ plane, sketched in figure 7, then $\lambda^c(J_y) < 1$ implies that the uniformly coupled system ($\lambda = 1$) exhibits Néel order for that value of J_y. Furthermore, one may compare the series estimates of $\lambda^c(J_y)$ with approximate analytic calculations for the critical line.

Let us first briefly discuss the ground-state energy series. Direct Padé approximants allow for estimates of $E_g(J_y, \lambda = 1)$ which are shown in figure 3. The approximants are consistent with each other—and with the values obtained from the Ising expansions for J_y as large as 0.4. This implies that the singularity in E_g at the critical line is very weak; the alternative, that $\lambda^c > 1$ for $J_y < 0.4$, is ruled out by both the Ising expansions and the other dimer expansions.

The terms of the M_1, M_{rr}, and χ series are all positive and increasing with order in λ. Thus one may estimate $\lambda^c(J_y)$ either by ratio analyses or inhomogeneous differential approximants (of which Dlog Padé approximants are a special case) [15].

The estimates of $\lambda^c(J_y)$ which result from consideration of M_1 are poorly converged, so we will only discuss M_{rr} and χ. The results for these two sets of series are presented in figure 8. Let us address what the various curves and points signify. First, six differential approximant estimates for $\lambda^c(J_y)$ are presented for several values of J_y; these particular approximants are chosen because they utilize all the terms in the series and they yield good estimates of λ^c at both $J_y = 0$ and $J_y = 1$. The missing approximants at any J_y are either defective or (in one or two cases) off-scale. The approximants are reasonably consistent
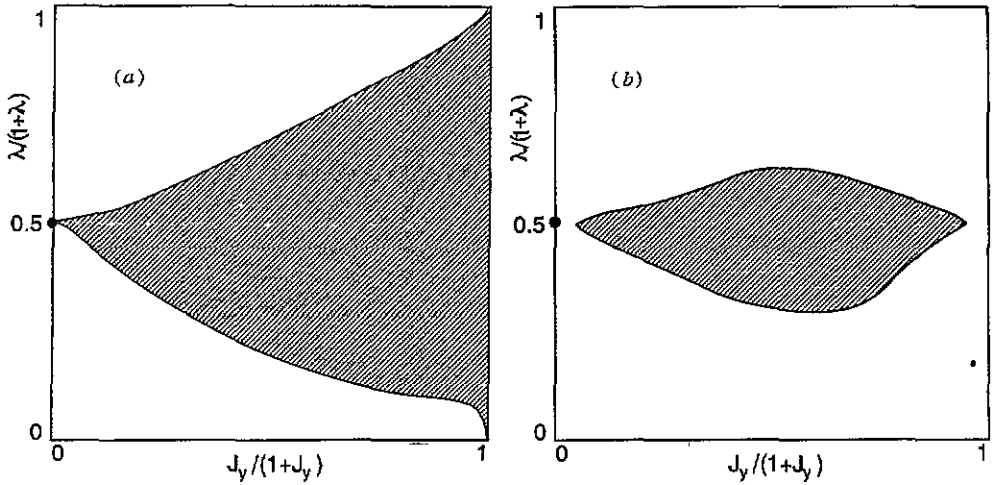
Figure 7. Sketches of the simplest plausible phase diagrams in the first quadrant of the J_y–λ plane for the Hamiltonian (3.5) assuming that (a) $J_y^c = 0$, and (b) $J_y^c > 0$. Note that units of energy are chosen so that $J_x = 1$. The phase diagrams must satisfy two contraints that follow from the invariance of correlation functions with respect to multiplication of the Hamiltonian by a constant: $(J_y, \lambda) = (a, 1)$ and $(1/a, 1)$ lie in the same phase, and so must (a, b) and $(ab, 1/b)$. In both cases the hatched regions constitute the Néel ordered phase, which are surrounded by lines of critical points. The one-dimensional Heisenberg critical point at $(J_y, \lambda) = (0, 1)$ is indicated by the large dot. The entire right boundaries of the plots, $J_y = \infty$, $0 < \lambda < \infty$, are also one-dimensional Heisenberg critical points. All other points are supposed to have only short-range correlations.
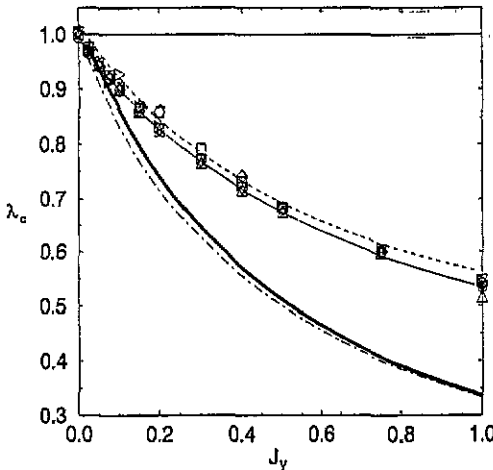

Figure 8. Estimated values of the critical λ as a function of J_y for the coupled-chain model (3.5). From the χ series, differential approximants displayed are $[2, 4; -1]$ (○), $[3, 2; 0]$ (□), and $[3, 3; -1]$ (◇); from the M_{rr} series, $[2, 4; -1]$ (△), $[3, 3; -1]$ (▽), and $[4, 2; -1]$ (▷). See the text for a discussion of the significance of the various curves.

over the entire range of J_y. Second, the thin full and broken curves are the estimates of λ^c based on ratio analysis of the three highest-order terms in the χ and M_{rr} series. For a series $\sum_n c_n \lambda^n$, the ratios c_n/c_{n-1} are plotted versus $1/n$ and pairwise linearly extrapolated to $1/n = 0$; the intercepts yield estimates of $1/\lambda^c$ based on three consecutive terms of the series. The χ ratio curve lies close to the differential approximants, which reflects the fact that the χ series are extremely well behaved. The ratio plot (corresponding to $J_y = 1$) in figure 2 of [14] provides further evidence that the antiferromagnetic susceptibility series is

better behaved than other dimer expansions. Both the ratio and differential approximant analyses suggest that $\lambda^c(J_y) < 1$ for all $J_y > 0$, and hence that there is no magnetically disordered phase along the line $\lambda = 1$.

Third, two mean-field estimates of $\lambda^c(J_y)$ are presented in the figure. The chain curve is based on 'dimer mean-field theory,' [16] that is, the zeroth- and first-order terms in $\chi(\lambda)$ are used to estimate λ_c. (This is equivalent to considering a single dimer subject to a staggered field which is determined, self-consistently, by its staggered magnetization.) That result is $\lambda_{DMF}^c = 1/(1 + 2J_y)$, and it has the remarkable (and accidental) feature that it yields the exact λ^c when $J_y = 0$. The thin full curve is based on the chain mean-field theory discussed in section 2.2. The values of $\chi_1(\lambda)$ (the antiferromagnetic susceptibility for a single chain), which are the essential input into that mean-field theory, were obtained by integrating a differential approximant to the seventh-order series presented in [14]. The thick full curve ends at $J_y \approx 0.02$ because the numerical estimates of $\chi(\lambda)$ are not reliable for λ arbitrarily close to 1. Over most of the range of J_y plotted, the dimer and chain mean-field theories give quite close values of λ^c. The agreement is somewhat better than one would expect: in both cases the leading behaviour of λ^c at large J_y is $1/2J_y$, but the next-order terms are $-3/4J_y^2$ and $-1/4J_y^2$ for the chain and dimer mean-field theories, respectively, and at $J_y = 1$ the difference is hardly negligible! At small J_y the chain mean-field theory is clearly in better agreement with the series extrapolations than the dimer mean-field theory.

To briefly recapitulate, the dimer series for the two-dimensional lattice of coupled chains are entirely consistent with $J_y^c = 0$. However, there is reason to doubt the strength of this conclusion. Since $\lambda^c(0) = 1$ and $\lambda^c(1) \approx 0.54$, it would be entirely natural to conclude from too-short series that $\lambda^c(J_y)$ interpolates smoothly between these two endpoints, even if the correct result is that λ^c does not exist for $0 < J_y < J_y^c$ as would be the case if the scenario of figure 7(b) were to hold. As a partial test of the reliability of the series estimates of $\lambda^c(J_y)$, we have considered the problem of *two* coupled chains by the dimer series expansion method. The chains were taken to lie parallel to the bonds in the columnar dimer configuration. The only differences between these calculations and those preceding are the set of connected clusters (and their lattice constants), and that we will present results for M_{xx} rather than M_{rr}. (In fact one can use M_{xx} to estimate $\lambda^c(J_y)$ for the plane of chains as well; the differences between the estimates based on M_{xx} and M_{rr} are insignificant for the J_y of interest.)

For two chains the only critical point in the λ–J_y plane is $(\lambda = 1, J_y = 0)$ [17]. Estimates of $\lambda^c(J_y)$ coming from inhomogeneous differential approximants to the χ and M_{xx} series for two chains are displayed in figure 9, on the same scale as in figure 8 for ease of comparison. The thick full and thin chain curves are the chain and dimer mean-field results, respectively, for *two* chains. (One obtains these from the mean-field results for planes of chains by the substitution $2J_y \rightarrow J_y$.) Several points are evident upon inspection. First, even at very small J_y one can distinguish between the estimates of λ^c from the differential approximants for the plane of chains and for two chains; they seem to approach zero with different slopes, on these plots. This could be taken as further evidence that, for the plane of chains, J_y^c is extremely small if not vanishing.

However, for $J_y \lesssim 0.2$, where the approximants are well converged, one might conclude that there are critical points at $\lambda \approx 1$, contrary to the known behaviour of coupled pairs of chains. We believe this line segment of 'pseudo-critical' points reflects the existence of local maxima in the correlation length at $\lambda \approx 1$ for fixed, small J_y, where the correlation length at these maxima exceeds the typical cluster length in the seventh-order calculation (which is roughly 10). That such pseudo-critical points should exist is entirely plausible: numerical studies for pairs of finite chains [4, 11] find that the gap initially *decreases* as
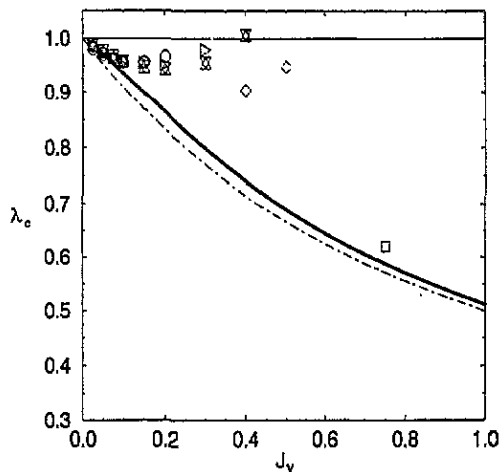
Figure 9. The symbols correspond to estimates of the critical λ for *two* chains, corresponding to the same approximants as the preceding figure (but for M_{xx} rather than M_{rr}). The curves are discussed in the text.

J_y is increased from zero. What is somewhat disturbing is that, for $J_y \lesssim 0.1$, the two-chain approximants are as consistent with chain mean-field theory (for two chains) as the plane-of-chain approximants are with chain mean-field theory (for a plane of chains). Thus it is conceivable that for the plane of chains, the values of λ^c indicated by the series at sufficiently small J_y are pseudo-critical points, rather than true critical points, as well.

To conclude, the problem of coupled chains at small J_y poses significant challenges to numerical studies. Although the series expansions are consistent with $J_y^c = 0$ they do not rule out a small but positive J_y^c. If the disordered phase exists, the correlation length along the x-direction is probably large throughout that phase, and the gap is small everywhere. A potentially fruitful avenue for future studies would be the consideration of models which include further-neighbour couplings; suitable models would have larger critical interchain couplings within spin-wave theory than the simplest coupled Heisenberg chain model studied here.

Acknowledgments

References

[1] Anderson P W 1990 *Phys. Rev. Lett.* **64** 1839
[2] Sakai T and Takahashi M 1989 *J. Phys. Soc. Japan* **58** 3131
[3] Azzouz M 1993 *Phys. Rev. B* **48** 6136
[4] Parola A, Sorella S and Zhong Q F 1993 *Phys. Rev. Lett.* **71** 4393
[5] Scalapino D J, Imry Y and Pincus P 1975 *Phys. Rev. B* **11** 2042
[6] Chui S T and Giri M R 1988 *Phys. Lett.* **128A** 49
     A summary of all numerical work to date is provided in figure 1 of
     Chattopadhyay B and Shenoy S R 1994 *Phys. Rev. Lett.* **72** 400
[7] Hikami S and Tsuneto T 1980 *Prog. Theor. Phys.* **63** 387

[8] Kosterlitz J M and Thouless D J 1978 *Progress in Low Temperature Physics* vol 7B, ed D F Brewer (Amsterdam: North-Holland)

[9] For a review see Affleck I 1990 *Fields Strings and Critical Phenomena* ed E Brezin and J Zinn-Justin (Amsterdam: Elsevier)

[10] Haldane F D M 1988 *Phys. Rev. Lett.* **61** 1029

[11] Barnes T, Dagotto E, Riera J and Swanson E S 1993 *Phys. Rev.* B **47** 3196

[12] White S R, Noack R M and Scalapino D J 1994 *Preprint* cond-mat/9403042

[13] For analytical arguments see, for example,
Read N and Sachdev S 1989 *Phys. Rev. Lett.* **62** 1694; 1991 *Phys. Rev. Lett.* **66** 1773
For numerical studies which address the issue of non-magnetic order in frustrated $S = \frac{1}{2}$ antiferromagnets see
Schulz H J and Ziman T A L 1992 *Europhys. Lett.* **18** 355
Dagotto E and Moreo A 1989 *Phys. Rev.* B **39** 4744; 1989 *Phys. Rev. Lett.* **63** 2184
Singh R R P and Narayanan R 1990 *Phys. Rev. Lett.* **65** 1072
Gelfand M P 1990 *Phys. Rev.* B **42** 8206
Gelfand M P, Singh R R P and Huse D A 1989 *Phys. Rev.* B **40** 10801

[14] Gelfand M P, Singh R R P and Huse D A 1990 *J. Stat. Phys.* **59** 1093

[15] Fisher M E and Au-Yang H 1979 *J. Phys. A: Math. Gen.* **12** 1677
Hunter D L and Baker G A Jr 1979 *Phys. Rev.* B **19** 3808

[16] Singh R R P, Gelfand M P and Huse D A 1988 *Phys. Rev. Lett.* **61** 2484

[17] Schulz H J 1986 *Phys. Rev.* B **34** 6372
Strong S P and Millis A J 1992 *Phys. Rev. Lett.* **69** 2419