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J_1 – J_2 quantum Heisenberg antiferromagnet: improved spin-wave theories versus exact-diagonalization data

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Abstract. We reconsider the results concerning the extreme-quantum $S = 1/2$ square-lattice Heisenberg antiferromagnet with frustrating diagonal couplings (the J_1 – J_2 model) drawn from a comparison with exact-diagonalization data. A combined approach, also using some intrinsic features of the self-consistent spin-wave theory, leads to the conclusion that the theory strongly overestimates the stabilizing role of quantum fluctuations with respect to the Néel phase in the extreme-quantum case $S = 1/2$. On the other hand, the analysis implies that the Néel phase remains stable at least up to the limit $J_2/J_1 = 0.49$, which is larger than some previous estimates. In addition, it is argued that the spin-wave ansatz predicts the existence of a finite range ($J_2/J_1 < 0.323$ in linear spin-wave theory) where the Marshall–Peierls sign rule survives the frustrations.

1. Introduction

The square-lattice Heisenberg antiferromagnet with antiferromagnetic next-nearest-neighbour couplings (the J_1 – J_2 model) produces a simple and, at the same time, important example of a frustrated quantum spin system. The model is defined by the Hamiltonian

$$H = J_1 \sum_{\langle i,j \rangle} S_i S_j + J_2 \sum_{[i,j]} S_i S_j \quad J_1, J_2 > 0 \quad (1)$$

where the symbols $\langle i, j \rangle$ and $[i, j]$ mean that the summations run over the nearest-neighbour and next-nearest-neighbour (diagonal) bonds, respectively. In what follows we put $J_1 \equiv 1$, $\alpha \equiv J_2/J_1$.

At the moment, little is known about the ground-state properties of this model. In the classical limit $S = \infty$ the J_1 – J_2 model has two phases: if $\alpha < 1/2$ the ground state is a two-sublattice Néel state, whereas if $\alpha > 1/2$, the four-sublattice antiferromagnetic state is stable. At the classical transition point $\alpha = 1/2$ the model is characterized by a large degree of classical degeneracy: all states with zero elementary-plaquette spins are energetically preferable. Quantum fluctuations, however, can drastically change this picture. In general, they are determined by the microscopic structure of the model, and are expected to increase as S approaches the extreme-quantum limit $S = 1/2$, and/or the frustration becomes stronger. A simple linear spin-wave analysis already reveals such a tendency [1]. In addition, the latter theory predicts the existence of a finite range around the classical phase

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boundary $\alpha = 1/2$ where the classical long-range magnetic order is completely destroyed (for arbitrary S). However, the next-order terms in the large- S expansion show logarithmic divergences [2] connected to an additional softening of the spectrum at $\alpha = 1/2$, thus making the first-order predictions at least questionable. This situation is characteristic of most of the studied frustrated models. An open question is how to reconstruct the standard spin-wave expansion in order to avoid the mentioned difficulties. The Hartree-Fock-type theories [2-4], which could in principle serve as a starting point for a systematic expansion, predict a first-order phase transition between the magnetically ordered phases without any intermediate phase. This picture is connected with the predicted stabilizing role of quantum fluctuations with respect to the two-sublattice Néel order. Presently, however, it is not clear if these conclusions are also characteristic, at least qualitatively, for the extreme-quantum system $S = 1/2$.

Concerning the $S = 1/2$ case, at least two important issues, related to the ground-state phase diagram, remain unsettled: (i) the nature of the magnetically disordered phase, if any, in the strongly frustrated region, and (ii) the location of the phase-transition boundary. The magnetically disordered spin-Peierls dimer state is preferable in a number of studies: (a) series expansions around dimer states [5], (b) the $1/N$ expansion technique [6], (c) bond-operator techniques [7], (d) effective-action approaches leading to quantum non-linear σ -models [8], and (e) numerical exact-diagonalization data [9, 10]. However, each of the mentioned methods has its own defects, so that some other states (for example the chiral states [10-12]) seem to be possible candidates, as well.

With regard to the location of phase boundary, here the estimates are in the large interval from $\alpha_c \approx 0.15$ to $\alpha_c \approx 0.6$. The lower bound $\alpha_c \approx 0.15$ was obtained [13] by use of σ -model considerations combined with Schwinger-boson mean-field results for $S = 1/2$. On the other hand, the largest estimate $\alpha_c \approx 0.6$ is characteristic of self-consistent theories [2-4]. A series of studies give values which are near the point $\alpha_c = 0.4$ [1, 9, 10].

The outlined ambiguity signals of a lack of reliable descriptions even in the weakly frustrated region where the two-sublattice Néel phase is expected to be stable. Concerning the spin-wave theories, a way to test their quality gives the comparison with numerical exact-diagonalization data. For the J_1 - J_2 model, the first steps in this direction were made by Hirsch and Tang [14] based on Takahashi's idea [15] for a constrained spin-wave theory in low dimensions. These authors indicated that their theory systematically overestimates the effect of frustration in destroying the antiferromagnetic correlations ($N = 10, 16, 26$). Recently, Ceccatto and co-workers [16] have continued this line by use of Takahashi's self-consistent approach [17] adapted to the frustrated model [4]. A remarkable agreement with the exact results for a number of lattices ($N = 10, 20, 26$) was indicated, excluding, however, the most symmetrical lattice 4×4 .

In this paper we study the extreme-quantum system $S = 1/2$ and show that the existing exact-diagonalization results, in combination with some intrinsic properties of the self-consistent theory, lead to the following conclusions. (i) The classical Néel state is stable at least up to the limit $\alpha^* = 0.49$. Notice that the estimate is larger than the result $\alpha \approx 0.4$ mentioned above. (ii) The self-consistent spin-wave theory overestimates the role of quantum fluctuations in stabilizing the Néel state. This last conclusion also differs from previous considerations relying on a comparison with exact-diagonalization results for less symmetrical lattices $N = 10, 20, 26$ when the theory indeed gives excellent results.

2. Comparison of the theory with exact-diagonalization data

2.1. Fitting to the exact-diagonalization results: $N = 16$ lattice

In reconsidering the previous exact-diagonalization data, it is easy to see a well-pronounced tendency, i.e. the self-consistent spin-wave theory gives good correlators for a number of less-symmetrical lattices ($N = 10, 20, 26$), whereas the most symmetrical 4×4 lattice is not part of this tendency. On the other hand, the Hirsch-Tang theory overestimates the effect of frustration for all lattices (including the 4×4 lattice). In order to further check these observations, we present here new exact-diagonalization results for $N = 18$ and $N = 24$ (6×4) lattices (figures 1 and 2). The lattice $N = 18$, belonging to the class of lattices $N = 10, 20, 26$, is expected to suppress more symmetrical fluctuations, including the four-sublattice state fluctuations (because $N/2 = 9$ is odd), whereas the 6×4 lattice is rather closer to the 4×4 lattice. It is seen that the tendency is conserved: for the $N = 18$ site lattice the self-consistent theory practically reproduces the exact data up to $\alpha \approx 0.4$, whereas for the $N = 24$ lattice it evidently underestimates the role of frustrations starting from $\alpha = 0$. On the other hand, the Hirsch-Tang consideration [14], which does not take into account spin-wave interactions, predicts less sublattice magnetizations (figure 1) in both kind of lattices. Notice that the latter theory leads to completely wrong correlators (they are not presented in figure 2) for the discussed lattices. Therefore, we suggest that the symmetrical lattices $N = 16, 24$ reproduce in a more adequate way the main properties of the thermodynamic limit.

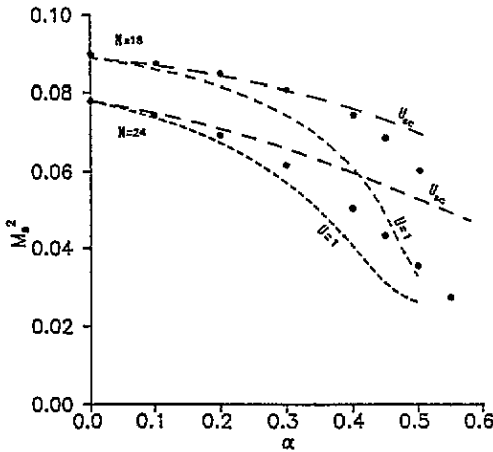


Figure 1. The square of sublattice magnetization against α for $N = 18$ and $N = 24$ lattices. The $U = 1$ (U_{sc}) curve corresponds to the Hirsch-Tang (self-consistent) theory. The points are the exact-diagonalization data.

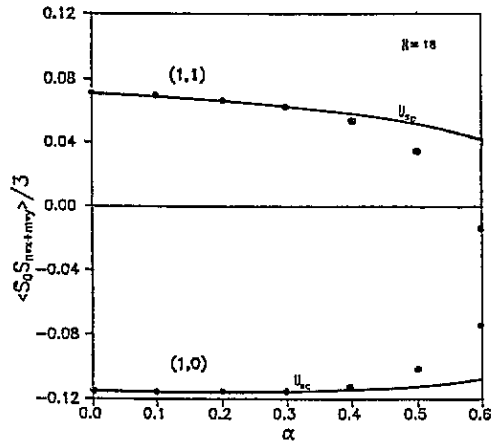


Figure 2. Spin-spin correlators ($S_0 S_R$) ($R = n\hat{x} + m\hat{y}$) for the $N = 18$ lattice in the self-consistent theory. The respective $U = 1$ curves, which are not drawn here, are very poor. The points are the exact-diagonalization data.

In what follows we address the most symmetrical 4×4 lattice. The scaling parameter $U = f/g$ (see [4]) appears in the self-consistent spin-wave theory through a Hartree-Fock decoupling of the quartic terms in the Hamiltonian. Within the theory, U is given by the self-consistent equations. In principle, one can use U as a variational parameter in the

spin-wave ansatz

$$\psi_S \sim P \exp\left(\sum_k' w_k \hat{a}_k^+ \hat{b}_{-k}^+\right) |\text{Néel}\rangle. \quad (2)$$

Here $|\text{Néel}\rangle$ is the classical Néel state. The weight factors w_k are defined by $w_k = v_k/u_k$, v_k and u_k being the well known Bogoliubov coefficients; P is a projection operator, and the prime means that the sum runs over the small Brillouin zone. This variational state is studied in [19]. Here we treat U as a fitting parameter obtained from a requirement for best fitting between the sublattice magnetization M_s^2 , as obtained from the theory, and the exact-diagonalization results. The reasoning for such a consideration comes from the following observations.

(i) From Takahashi's condition $\langle S_z \rangle = 0$, when applied in the limit $N = \infty$, one can directly deduce the following scaling relation connecting the sublattice magnetizations in the linear spin-wave approximation $m_0(\alpha)$ (when $U = 1$) and in the self-consistent theory $m(\alpha)$:

$$m(\alpha) = m_0(\alpha U) \quad N = \infty. \quad (3)$$

It is interesting to notice that the above scaling relation does not explicitly depend on the site spin S (apart from a trivial linear term). The implicit dependence is hidden in the scaling factor U , which for $\alpha = 0$ is

$$U = \frac{1 - 0.102/2S + O[(2S)^{-2}]}{1 + 0.158/2S + O[(2S)^{-2}]} \quad N = \infty. \quad (4)$$

For $S = 1/2$ one gets $U = 0.775$. The next-order term slightly diminishes the latter number. The self-consistent theory predicts a monotonic decrease of U against α in the whole range where the classical Néel state is stable ($U \approx 0.6$ at the phase transition point $\alpha_c \approx 0.62$). If one takes the self-consistent theory as a starting point for a systematic perturbation expansion, one can hardly expect any drastic qualitative change in the behaviour of U against α . The arguments are as follows. First, in this approximation the unphysical modes due to the degeneracy of the classical ground state at $\alpha = 1/2$ acquire gaps, so that some of the problems concerning the standard spin-wave approach here are resolved. Second, the denominator in (4) is just the rescaling factor of the spin-wave velocity, which is expected (from other methods as well) to be slightly α -dependent and finite at the phase boundary.

(ii) A direct calculation of the scaling factor U for $N = \infty$ and $N = 16$ gives practically the same function $U(\alpha)$. In other words, the $N = 16$ lattice is large enough in respect to this quantity, as is expected, because the factor U is a ratio of two short-ranged bosonic correlators. This observation will be used to obtain information concerning the $N = \infty$ system. The results coming from an exact fitting of the theoretical and exact-diagonalization functions M_s^2 are as follows. First, the resulting scaling factor U is approximately α -independent with a value close to the one predicted by (4). Second, one sees a remarkable fit to the exact correlators (figure 3) practically in the whole interval up to $\alpha \approx 0.45$. The misfit for $\alpha > 0.45$ is easily indicated in the ground-state energy because the small overestimates for the short-range correlators, noticed in figure 3(a), are summed. Nevertheless, we have checked that the energy is approximately unchanged by the fitting up to $\alpha \approx 0.45$.

Based on the argument (ii) and the suggestion that the $N = 16$ lattice better reflects the $N = \infty$ limit (as compared to less symmetrical lattices), one can predict the same picture

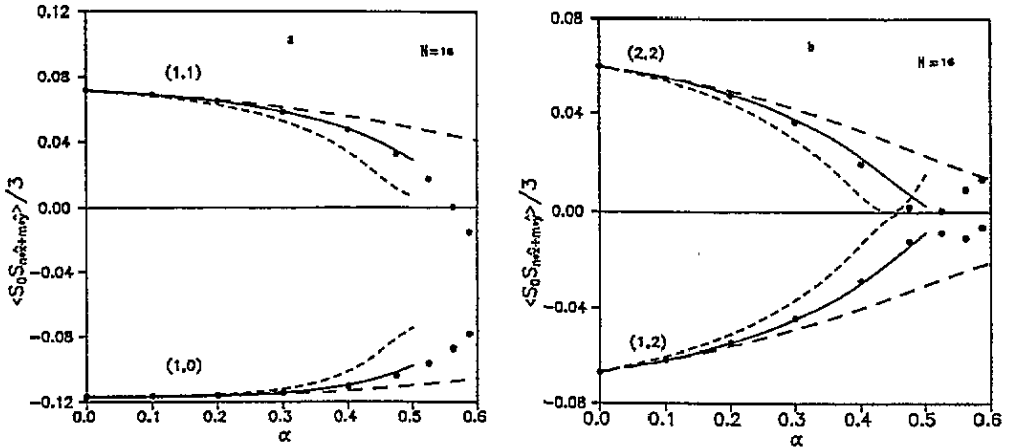


Figure 3. The correlators $\langle S_0 S_R \rangle$ ($R = n\hat{x} + m\hat{y}$) for the $N = 16$ lattice. The full curves are the results of the fitting. The other notations are the same as in figures 1 and 2.

in the thermodynamic limit: namely, the monotonic decrease in the scaling factor U against α should become smoother (as it is for $N = 16$) in a more refined approximation starting from the discussed self-consistent theory. In particular, the phase boundary $\alpha_c \approx 0.62$ should drastically move towards smaller α (because U against α is approximately constant according to the $N = 16$ fitting). The last two equations, combined with the hypothesis for a smooth decrease of the scaling factor U against α , give the following lowest limit where the Néel phase becomes unstable: $\alpha^* > 0.49$, $S = 1/2$. As a matter of fact, this estimate can be slightly increased if one takes the next-order approximation in (2).

To summarize, a combined approach relying on a comparison with exact-diagonalization data and some intrinsic features of the self-consistent spin-wave theory (the scaling relation (3), the smooth monotonic decrease of $U(\alpha)$, and the short-range character of the scaling factor U) lead to the conclusion that the theory, when applied to the extreme-quantum system $S = 1/2$, overestimates the stabilizing role of quantum fluctuations. In addition, the same analysis predicts a lowest limit $\alpha^* = 0.49$ where the Néel state is destroyed, which is larger than the previous estimate $\alpha \approx 0.4$ based on linear spin-wave theory [1, 14] and on the $N = 36$ exact-diagonalization results [10].

Further understanding of the features of the self-consistent approximation can be obtained from the spin ansatz (2). Here we address the square of the sublattice magnetization M_s^2 (figure 4). The exact M_s^2 is compared to: (i) self-consistent theory; (ii) $U = 1$, i.e. linear theory; and (iii) the ansatz $\psi_{1/2}$, equation (2) with $U = 1$. It is obvious that the function M_s^2 (calculated with the ansatz $\psi_{1/2}$, $U = 1$) strictly follows the form of the exact function $M_s^2(\alpha)$ in a large region up to $\alpha = 0.5$. The main difference between the theory and ψ_S for $U = 1$ lies in the fact that the variational function does not contain unphysical states. Therefore, the increasing misfit in M_s^2 (and in the other correlators in the Hirsch-Tang theory) is predominantly connected with the enhanced role of the unphysical bosonic states in the frustrated system (notice that already the linear spin-wave approximation in the pure $\alpha = 0$ system gives a good estimate for the reduced site spin $m_0 = 0.303$).

2.2. Violation of the Marshall–Peierls sign rule

Recent exact numerical diagonalization studies of small lattices [19] show that the ground-state wavefunction of the $S = 1/2$ J_1 - J_2 model violates the Marshall–Peierls sign rule for

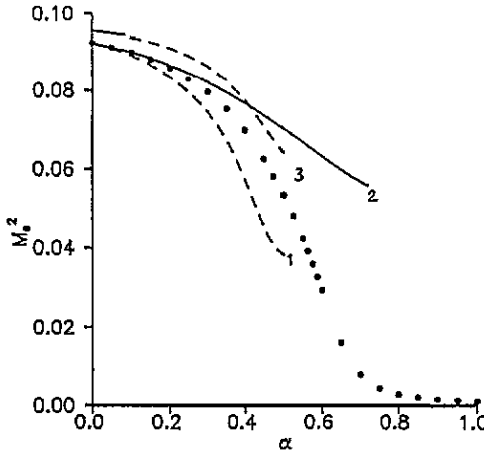


Figure 4. The square of sublattice magnetization against α for the $N = 16$ lattice. The curves 1 and 2 represent the spin-wave results for $U = 1$ and U_{sc} , respectively. The curve 3 is calculated with the spin-wave ansatz (2) for $S = 1/2$. The points are the exact-diagonalization results.

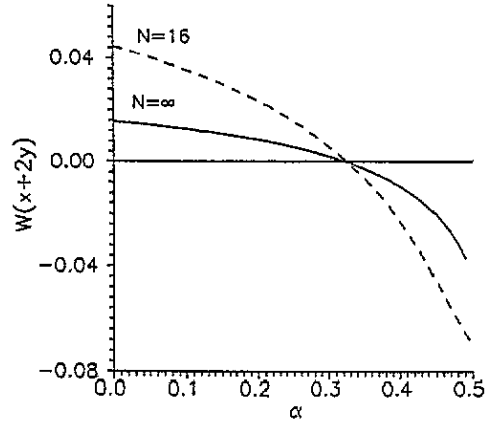


Figure 5. The pairing function $w(\hat{x} + 2\hat{y})$, as defined by (7), against α , $U = 1$; $w(\hat{x} + 2\hat{y})$ vanishes at $\alpha_M = 0.323$ for $U = 1$ in the thermodynamic limit $N = \infty$.

sufficiently large α . Here we present results which are based on the spin-wave ansatz (2). Originally, the above-mentioned rule had been proved for bipartite lattices with nearest-neighbour interactions [20]. The latter says that the ground-state wavefunction of $S = 1/2$ Heisenberg antiferromagnet is

$$\psi = \sum_n (-1)^{p_n} a_n |n\rangle \quad a_n > 0 \quad (5)$$

where $|n\rangle$ is an Ising state, p_n being the number of, say, up-spins living on, say, the A-sublattice. Notice that the proof does not work for a system with antiferromagnetic next-nearest-neighbour (diagonal) couplings. As a matter of fact, this rule is violated, as mentioned above, in the 4×4 lattice provided the frustration is strong enough.

First, let us rewrite the spin-wave ansatz (2) in the form

$$\psi_{1/2} \sim \prod_{\substack{R_r \\ \text{ReA}}} (1 - w(\mathbf{r}) S_R^+ S_{R+r}^-) |\text{Néel}\rangle \quad (6)$$

where the pairing function $w(\mathbf{r})$ is defined by

$$w(\mathbf{r}) = \frac{2}{N} \sum_k w_k \cos k\mathbf{r}. \quad (7)$$

The vector \mathbf{r} in (6) and (7) connects sites from different sublattices.

From the structure of the ansatz it is clear that the sign rule breaks if, and only if, the pairing function $w(\mathbf{r})$ changes its sign for some vector \mathbf{r} connecting two spins which live on different sublattices. For the 4×4 lattice this is just the vector $\mathbf{r} = \hat{x} + 2\hat{y}$ (and the related by symmetry vectors on the lattice). The pairing function $w(\hat{x} + 2\hat{y})$ against α is presented in figure 5. For $U = 1$, $w(\hat{x} + 2\hat{y})$ changes sign at a point practically coinciding with the

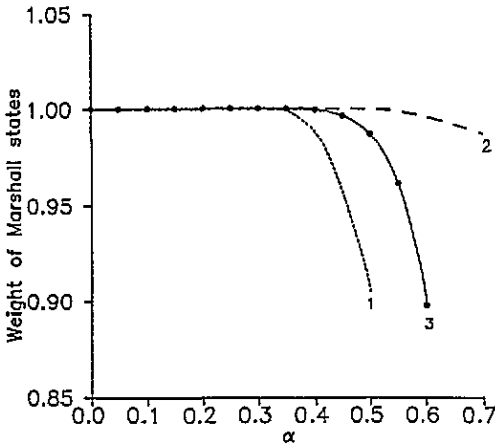


Figure 6. The weight of Marshall states against α . The curves 1 and 2 correspond to $U = 1$ and U_{sc} , and are calculated with $\psi_{1/2}$, equation (7). The curve 3 represents the exact-diagonalization results, $N = 16$.

related $N = \infty$ limit, $\alpha_M = 0.323$ (this is another indication that this symmetrical lattice covers quite well some characteristic features of the infinite system). This characteristic point precedes the instability point α^* . These observations were based on the spin-wave ansatz (2). The predicted weight of Marshall states (Ising states fulfilling the rule) against α is in agreement with the exact result presented in figure 6. Quite surprisingly, a recent study of the same problem for ground states with larger total-spin quantum numbers, $S_{total} = 1, 2$ and 3 [21] indicates a sharp increase of the weight of non-Marshall states near the point $\alpha \approx 0.52$, which is pretty close to limit 0.49 found in the present work†.

3. Concluding remarks

The analysis presented above was based on a combined approach using exact-diagonalization data for small lattices and some intrinsic features of self-consistent spin-wave theory. It was directed towards checking the predictions of the latter theory for the extreme-quantum system $S = 1/2$. It was found that the theory fits excellently to the exact data for less symmetrical clusters ($N = 10, 18, 20, 26$), whereas for $N = 16$ (and also $N = 24$) this approach evidently underestimates the effect of the frustrations. At the same time, the Hirsch-Tang theory, which does not take into account spin-wave interactions, systematically overestimates the role of the frustrations for each of the mentioned lattices. This tendency probably means that more symmetrical (e.g. 4-spin) correlations, which are suppressed in less-symmetrical lattices, are not properly taken into account in the self-consistent approach. That is why the main conclusions are drawn from a comparison with the $N = 16$ lattice, which is suggested to better reproduce the properties of the $N = \infty$ model. The comparison gives an estimate $\alpha^* > 0.49$ for the location of the instability point α^* , which is higher than some previous results [1, 8, 10]. The analysis also shows that in a more refined approximation, using as a starting point the discussed theory, α^* should move towards

† After the present paper was submitted for publication we received a preprint [22] where the same problem is analysed by an expansion for which the Takahashi approximation appears as a zeroth order. Our conclusions, drawn from the exact-diagonalization results and more intuitive considerations, seem to be in excellent agreement with the preprint mentioned above where it is found that $\alpha^* \approx 0.52$ (the collinear state is found to lose stability at $\alpha \approx 0.57$).

smaller values of α (in fact, the fitting based on the $N = 16$ lattice predicts an approximately constant rescaling factor U up to the phase boundary, which would mean, if applied to the $N = \infty$ system, that the instability of the Néel phase should be close to the estimate 0.49. Clearly, one needs some additional arguments in favour of such a suggestion (see, for example, [22]). Finally, it was shown that the spin-wave projected ansatz predicts a finite region ($\alpha < 0.323$ in linear spin-wave theory) where the Marshall–Peierls sign rule is fulfilled in the frustrated $N = \infty$ model. For $N = 16$, this result was shown to be in accord with the exact-diagonalization data.

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References

- [1] Chandra P and Doucot B 1988 *Phys. Rev.* **B38** 9335
Oguchi T and Kitatani H 1990 *J. Phys. Soc. Japan* **59** 3322
- [2] Chubukov A 1991 *Phys. Rev. B* **44** 392
Bruder C and Mila F 1992 *Europhys. Lett.* **17** 463
- [3] Nishimori H and Saika Y 1990 *J. Phys. Soc. Japan* **59** 4454
Barabanov A F and Stary'h O A 1990 *Pis'ma Zh. Eksp. Teor. Fiz.* **51** 271 (Engl. transl. 1990 *JETP Lett.* **51** 311)
Mila F, Poilblanc D and Bruder C 1991 *Phys. Rev. B* **43** 7891
Bergomi L and Jolicœur Th 1992 *J. Physique* **2** 371
- [4] Xu J H and Ting C S 1990 *Phys. Rev. B* **42** 6861
Ivanov N B and Ivanov P Ch 1992 *Phys. Rev. B* **46** 8206
- [5] Gelfand M P, Singh R R P and Huse D A 1989 *Phys. Rev. B* **40** 10801
- [6] Read N and Sachdev S 1989 *Phys. Rev. Lett.* **62** 1694
Read N and Sachdev S 1989 *Nucl. Phys. B* **316** 609
- [7] Sachdev S and Bhatt R N 1990 *Phys. Rev. B* **41** 9323
Chubukov A V and Jolicœur Th 1991 *Phys. Rev. B* **44** 12050
- [8] Einarsson T and Johannesson H 1991 *Phys. Rev. B* **43** 5867
- [9] Dagotto E and Moreo A 1989 *Phys. Rev. Lett.* **63** 2148
Singh R R and Narayanan R 1990 *Phys. Rev. Lett.* **65** 1072
- [10] Schulz J and Ziman T A L 1992 *Europhys. Lett.* **18** 355
- [11] Wen X G, Wilczek F and Zee A 1989 *Phys. Rev. B* **39** 11413
- [12] Richter J, Gros C and Weber W 1991 *Phys. Rev. B* **44** 906
Richter J 1993 *Phys. Rev. B* **47** 5794
- [13] Einarsson T, Fröjdh P and Johannesson H 1992 *Phys. Rev. B* **45** 13121
- [14] Hirsch J E and Tang S 1989 *Phys. Rev. B* **39** 2887
- [15] Takahashi M 1987 *Phys. Rev. Lett.* **58** 168
- [16] Ceccatto H A, Gazza C J and Trumper A E 1992 *Phys. Rev. B* **45** 7832
- [17] Takahashi M 1989 *Phys. Rev. B* **40** 2494
- [18] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **22** 1133
- [19] Retzlaff K, Richter J and Ivanov N B 1993 *Z. Phys. B* **93** 21
- [20] Marshall W 1955 *Proc. R. Soc. A* **232** 48
- [21] Richter J, Ivanov N B and Retzlaff K 1994 *Europhys. Lett.* at press
- [22] Gochev I 1994 *Phys. Rev. B* to be published