CONDENSED MATTER THEORIES
VOLUME 17

M. P. DAS AND F. GREEN
(EDITORS)

Nova Science Publishers, Inc.
New York

Senior Editors: Susan Boriotti and Donna Dennis
Editorial Coordinator: Tatiana Shohov
Office Manager: Annette Hellinger
Graphics: Wanda Serrano
Editorial Production: Vladimir Klestov, Matthew Kozlowski, Tom Moceri and Maya Columbus
Circulation: Ave Maria Gonzalez, Vera Popovic, Luis Aviles, Raymond Davis, Melissa Diaz, Marlene Nunez, Magdalene Nunez, and Jeannie Pappas
Communications and Acquisitions: Serge P. Shohov
Marketing: Cathy DeGregory

Library of Congress Cataloging-in-Publication Data
Available upon request

ISBN 1-59033-632-1

400 Oser Ave, Suite 1600
Hauppauge, New York 11788-3619
Tele. 631-231-7269 Fax 631-231-8175
e-mail: Novascience@earthlink.net
Web Site: http://www.novapubishers.com

Printed in the United States of America

Condensed Matter Theories
Volume 17

QUANTUM PHASE TRANSITIONS IN SPIN-LATTICE SYSTEMS WITH AND WITHOUT FRUSTRATION

Raymond F. Bishop

Department of Physics,
University of Manchester Institute of Science & Technology (UMIST),
P.O. Box 88, Manchester M60 1QD, United Kingdom

Sven E. Krüger

Department of Electrical Engineering,
IESK, Cognitive Systems, Universität Magdeburg,
PF 4120, 39016 Magdeburg, Germany

1. INTRODUCTION

The coupled cluster method (CCM) [1] has become one of the most pervasive and most powerful of all *ab initio* formulations of quantum many-body theory. It has yielded numerical results which are among the most accurate available for a wide range of both finite and extended, physical and chemical systems defined on a spatial continuum [2]. This widespread success has spurred recent applications to similar quantum-mechanical systems defined on an extended regular spatial lattice.

Such lattice systems have become the subject of intense theoretical study. They include many examples of systems characterised by novel ground states which display *quantum order* in some region of the Hamiltonian parameter space, delimited by critical values which mark the position of the corresponding *quantum phase transitions.* The critical phenomena in these quantum-mechanical models often differ profoundly from those of their classical counterparts. Furthermore, the subtle correlation present usually cannot sensibly be treated by such standard many-body approaches as mean-field theory or perturbation theory. One of the key challenges for modern quantum many-body theory is to develop and exploit microscopic techniques capable of handling both these novel and the more traditional systems. Our recent work [3,4] shows that the CCM is capable of bridging this divide.

In particular, we have shown how the systematic inclusion of multispin correlations for a wide variety of quantum spin-lattice problems can be very efficiently

implemented with the CCM [3-12]. It is important to note that the method is not restricted to bipartite lattices or to non-frustrated systems, and can thus deal with problems where the quantum Monte Carlo (QMC) simulation techniques would be faced with the infamous "minus sign problem". The method is also easily extended to models of strongly interacting electrons on lattices, such as the Hubbard model [13-16], as well as to various Hamiltonian lattice field theories, such as the gauge theories U(1) [17] and SU(2) [18], and lattice chiral meson-field theory via the nonlinear O(4) sigma model [19].

In all of the above cases the CCM may readily be implemented to high orders (e.g., in a localised LSUBn scheme) by the use of computer-algebraic techniques. Values for ground- and excited-state properties are thereby obtained which are fully competitive with those from other state-of-the-art methods, including the much more computationally intensive QMC techniques in cases where the latter can be applied. The raw LSUBn results themselves are generally excellent. They converge rapidly and can also provide valuable information on the *quantum order* and *quantum criticality*. In this paper we illustrate these points by an application to a model with two types of nearest-neighbour Heisenberg interactions [10,12] on a two-dimensional square lattice. For certain values of the interaction strengths the method exhibits the very interesting phenomenon of competition between magnetic order and dimerization.

2. A TYPICAL MODEL EXHIBITING COMPETITION

We consider a spin-half Heisenberg model on a square lattice with two kinds of nearest-neighbour bonds J and J', as shown in Fig. 1,

$$H = J \sum_{\langle ij \rangle_1} \mathbf{s}_i \cdot \mathbf{s}_j + J' \sum_{\langle ij \rangle_2} \mathbf{s}_i \cdot \mathbf{s}_j . \tag{1}$$

The expressions $\langle ij \rangle_1$ and $\langle ij \rangle_2$ indicate nearest-neighbour bonds arranged in a regular zigzag pattern, as shown in Fig. 1 by the dotted and solid lines, respectively. Each square-lattice plaquette consists of three J bonds and one J' bond. If J' and J have different signs then the plaquettes are frustrated, whereas competition without frustration is realized for antiferromagnetic bonds $J' > J > 0$. A model with such a zigzag pattern of bonds has been treated previously by a variety of methods [10,12,20,21].

The case of antiferromagnetic J' bonds with $J' > J > 0$ resembles the situation in bilayer systems and in the depleted square-lattice antiferromagnet CaV_4O_9, in which the competition between two different antiferromagnetic bonds leads to a phase transition from antiferromagnetic long-range order to quantum disorder with a finite gap. We see in this article that the transition point obtained for the model of Eq. (1) is quite close to that obtained for the bilayer model [22].

For special values of J, J' the model represents: (i) the spin-half Heisenberg antiferromagnet (ferromagnet) on the square lattice for $J = J' = 1$ ($J = J' = -1$), (ii) the spin-half Heisenberg antiferromagnet (ferromagnet) on the honeycomb lattice for $J = 1$, $J' = 0$ ($J = -1$, $J' = 0$), and (iii) the spin-one Heisenberg antiferromagnet on the triangular lattice for $J = 1$, $J' = -\infty$.

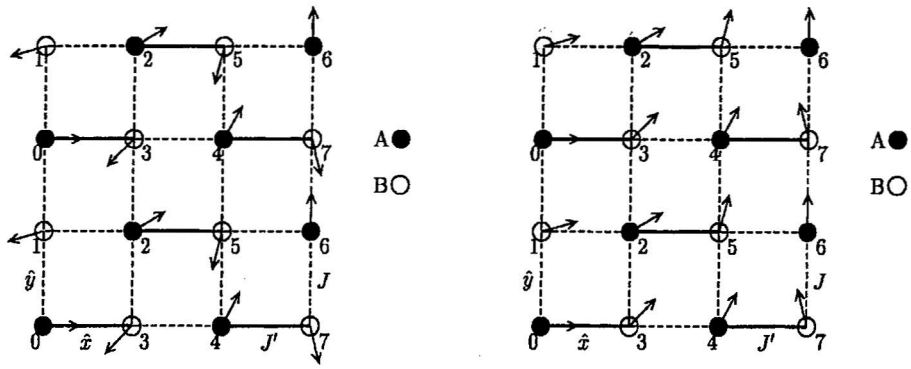

Figure 1. Illustration of the model (J-bonds correspond to dotted lines and J'-bonds to solid lines) and of the classical spiral state for antiferromagnetic $J = +1$ and ferromagnetic $J' < -1/3$ (left graph), and vice versa ($J = -1$, $J' > 1/3$) (right graph). As discussed in the text, both spiral states can be transformed into each other by reversing all of the spins on the B sublattice.

2.1. The classical ground state

For $J = +1$ and $J' > -1/3$ the Néel state is the classical ground state of the Hamiltonian of Eq. (1). At $J'_c = -1/3$ there is classically a second-order phase transition to a ground state of helical nature (see Fig. 1), with a characteristic pitch angle $\Phi = \pm|\Phi_{\rm cl}|$ given by

$$\begin{aligned} |\Phi_{\rm cl}| &= 0 \qquad\qquad\qquad ; \quad J' > -\frac{1}{3} \\ |\Phi_{\rm cl}| &= \arccos\left(\frac{1}{2}\sqrt{1-\frac{1}{J'}}\right) ; \quad J' \le -\frac{1}{3}, \end{aligned} \tag{2}$$

where the different signs correspond to the two chiralities [23] of this helical state. Note that for $\Phi = 0$ this is just the Néel state. More generally, the pitch angle varies with J' from $|\Phi_{\rm cl}| = 0$ for $J' > -1/3$ to $|\Phi_{\rm cl}| = \pi/3$ for $J' = -\infty$. Note that $|\Phi_{\rm cl}| = \pi/3$ (realized at $J' = -\infty$) corresponds to the ground state of the spin-1 triangular lattice. For the $J = +1$ case we describe the directions of the spins $\mathbf{s}_A$ and $\mathbf{s}_B$, belonging to the A and B sublattices respectively, for the classical helical state with a characteristic angle Φ as follows [10] (and see Fig. 1),

$$\begin{aligned} \mathbf{s}_A(\mathbf{R}) &= \hat{\mathbf{u}}\cos\mathbf{Q}\cdot\mathbf{R} + \hat{\mathbf{v}}\sin\mathbf{Q}\cdot\mathbf{R}, \\ \mathbf{s}_B(\mathbf{R}+\hat{x}) &= \hat{\mathbf{u}}\cos(\mathbf{Q}\cdot\mathbf{R}+\pi+3\Phi) + \hat{\mathbf{v}}\sin(\mathbf{Q}\cdot\mathbf{R}+\pi+3\Phi), \end{aligned} \tag{3}$$

where $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ are perpendicular unit vectors in the spin space, $\mathbf{R}$ runs over the sites of the sublattice A, and we have $\mathbf{Q} = (2\Phi, 0)$ for the pitch vector $\mathbf{Q}$. We note that this general helical state does not have a periodicity in the x-direction because Φ is in general not of the form $m\pi/n$ with m and n integral. We also note that we have only three different angles between nearest-neighbour spins, namely $\pm(\pi - \Phi)$ for the $J = 1$ couplings and $(\pi - 3\Phi)$ for the coupling with J'.

The maximum frustration for $J = +1$ is in the region around $J' \approx -1$. Bearing in mind the situation for the J_1–J_2 model, one might expect that for the extreme quantum case (spin-half) quantum fluctuations might be able to open a window to a spin-liquid phase for a finite range of parameters around this region of maximum frustration. On the other hand, for strong antiferromagnetic bonds ($J' \gg 1$) there is, of course, no indication in the classical model for the breakdown of the Néel order.

By contrast to the quantum case, the classical model with $J = -1$ can be simply transformed into its counterpart with $J = +1$ considered above by the simultaneous substitutions $J \to -J$, $J' \to -J'$, $\mathbf{s}_{i\in B} \to -\mathbf{s}_{i\in B}$. Hence, the physics for the $J = -1$ sector of the classical model is essentially the same as for the $J = +1$ sector (and see Fig. 1).

3. THE CCM FOR LATTICE HAMILTONIANS

The starting point for any CCM calculation (and see overview in Ref. [1]) is the choice of a normalized model or reference state $|\Phi\rangle$, together with a set of mutually commuting multispin creation operators C_I^+ which are defined over a complete set of many-body configurations I. The operators C_I are the multispin destruction operators and are defined to be the Hermitian adjoints of the C_I^+. We choose $\{|\Phi\rangle; C_I^+\}$ in such a way that we have $\langle\Phi|C_I^+ = 0 = C_I|\Phi\rangle$, $\forall I \neq 0$, with $C_0^+ \equiv 1$.

For spin systems an appropriate choice for the CCM model state $|\Phi\rangle$ is often a classical spin state [3], in which the most general situation is one in which each spin can point in an arbitrary direction. After a local canonical transformation on each site to rotate each spin to the down $(-z)$ direction, we have

$$|\Phi\rangle = |\cdots\downarrow\downarrow\downarrow\cdots\rangle; \quad C_I^+ = s_r^+,\ s_r^+ s_{r'}^+,\ s_r^+ s_{r'}^+ s_{r''}^+, \cdots, \tag{4}$$

(where the indices $r, r', r'', \ldots$ denote any lattice site) respectively, for the model state and the multispin creation operators which consist of spin-raising operators only.

The CCM parameterizations of the ket and bra ground states are given by

$$|\Psi\rangle = e^S|\Phi\rangle, \quad S = \sum_{I\neq 0} \mathcal{S}_I C_I^+, \qquad \langle\tilde{\Psi}| = \langle\Phi|\tilde{S}e^{-S}, \quad \tilde{S} = 1 + \sum_{I\neq 0} \tilde{\mathcal{S}}_I C_I. \tag{5}$$

To find the ket-state and bra-state correlation coefficients we require that the expectation value $\bar{H} = \langle\tilde{\Psi}|H|\Psi\rangle$ be stationary with respect to all variations in the bra-state and ket-state correlation coefficients. Thus, the CCM ket-state equations, for example, are given by

$$\langle\Phi|C_I e^{-S} H e^S|\Phi\rangle = 0, \quad \forall I \neq 0. \tag{6}$$

The problem of determining the CCM equations now becomes a *pattern-matching exercise* of the $\{C_I\}$ to the terms in $e^{-S}He^S$ in Eq. (6). The excited states may also be parameterized in an analogous fashion (and see Refs. [1-4] for details).

We now use the lattice symmetries in order to find all *different* possible configurations with respect to the point and space group symmetries (of both the lattice and

Table 1

Number of fundamental ground-state configurations of the LSUBn approximation for the Hamiltonian of Eq. (1), using a Néel state ($\Phi = 0$) and a helical state ($\Phi \neq 0$) for the CCM model state, and the number of fundamental excited-state configurations using the Néel model state only, for n=2, 4, 6, 8.

LSUBn	ground state: $\Phi = 0$	$\Phi \neq 0$	excited state: $\Phi = 0$
2	3	5	1
4	22	76	16
6	267	1638	331
8	4986	42160	7863

Hamiltonian) with up to n spins flips spanning a range of no more than n adjacent lattice sites (LSUBn approximation), and these are referred to as the ***fundamental*** configurations or clusters. Details of the CCM computational algorithm for spin quantum number $s = 1/2$ are given in Refs. [3,9] and for general s in Ref. [4]. The resulting numbers of CCM LSUBn configurations for the present model for $n \leq 8$ are given in Table 1, using both the Néel and the spiral states as model states.

4. RESULTS

4.1 $J = +1$; $J' > 0$: Competition without frustration (Néel versus dimer)

Let us consider first the regime where $J = +1$, $J' > 0$. The two terms in the Hamiltonian are not "frustrating" each other, but they do compete since the first (J) term favours Néel longe-range order on the honeycomb lattice on which it acts in the absence of the other term ($J' = 0$), while the second (J') term by itself favours an uncorrelated product state of local pair singlets (as discussed more fully below). We recall that no such competition exists in this regime in the classical model.

Mean Field Approach: We start with a simple mean-field (MF) like description of the order-disorder transition. The corresponding uncorrelated MF state for Néel long-range order (LRO) is the Néel state $|\phi_{\mathrm{MF}_1}\rangle = |\uparrow\downarrow\uparrow\ldots\rangle$, and for the dimerized singlet state it is the rotationally-invariant product state of local pair singlets $|\phi_{\mathrm{MF}_2}\rangle = \prod_{i\in A}[|\uparrow_i\downarrow_{i+\hat{x}}\rangle - |\downarrow_i\uparrow_{i+\hat{x}}\rangle]/\sqrt{2}$ where i and $i+\hat{x}$ correspond to those sites which cover the J' bonds. In order to describe the transition between both states, we consider an uncorrelated product state interpolating between $|\phi_{\mathrm{MF}_1}\rangle$ and $|\phi_{\mathrm{MF}_2}\rangle$ of the form [24,10]

$$|\Psi_{\mathrm{MF}}(t)\rangle = \prod_{i\in A} \frac{1}{\sqrt{1+t^2}} [|\uparrow_i\downarrow_{i+\hat{x}}\rangle - t|\downarrow_i\uparrow_{i+\hat{x}}\rangle] . \qquad (7)$$

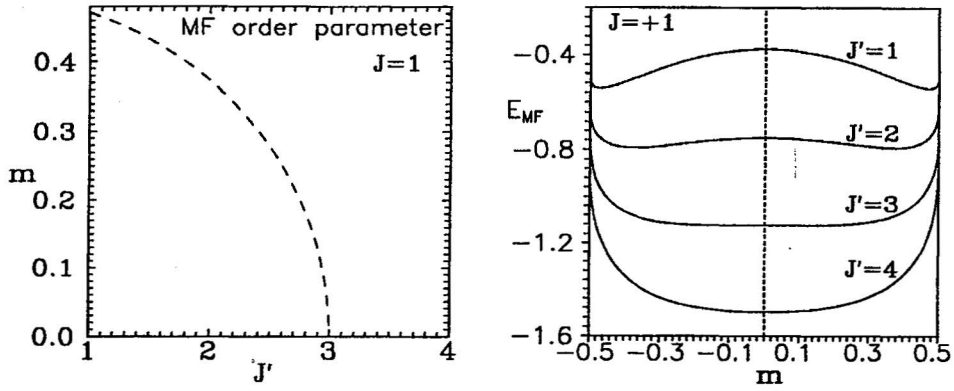

Figure 2. Sublattice magnetization versus J' (for $J = 1$) (left graph), and the corresponding energy versus sublattice magnetization (right graph), using the mean-field approach of Eq. (7).

We have $|\Psi_{\rm MF}(t=0)\rangle = |\phi_{\rm MF_1}\rangle$, and $|\Psi_{\rm MF}(t=1)\rangle = |\phi_{\rm MF_2}\rangle$. We minimize $E = \langle\Psi_{\rm MF}|H|\Psi_{\rm MF}\rangle$ with respect to t and obtain

$$E_{\rm MF}/N = -\frac{3J'}{8} - \frac{1}{24J}(3J - J')^2; \quad J' \leq 3J$$
$$E_{\rm MF}/N = -\frac{3J'}{8} \qquad ; \quad J' > 3J, \tag{8}$$

for the energy per site. For the sublattice magnetization $m \equiv \langle\Psi_{\rm MF}|s^z_{i\in A}|\Psi_{\rm MF}\rangle$ we get $m = \sqrt{(3J - J')(3J + J')}/(6J)$ for $J' \leq 3J$ and $m = 0$ otherwise. Note that m vanishes at a critical point $J'_c = 3J$, and that the critical index is the MF index 1/2. Equation (8) may be rewritten in terms of m as $E_{\rm MF}/N = -\frac{1}{8}J' - \frac{1}{4}J'\sqrt{1-4m^2} - \frac{3}{2}Jm^2$, and Fig. 2 illustrates that the dependence of $E_{\rm MF}$ on m corresponds to the typical scenario of a second-order transition. We can expand $E_{\rm MF}$ up to the fourth order in m near the critical point and find a Landau-type expression, given by $E_{\rm MF}/N = -\frac{3}{8}J' + \frac{1}{2}(J' - 3J)m^2 + \frac{1}{2}J'm^4$. However, as discussed elsewhere for a similar magnetic model for CaV_4O_9 [25], MF theory probably does not describe the critical behaviour correctly.

CCM: Let us therefore now apply a high-order CCM approach (and for details see Refs. [3,10]) to this model. We set the classical collinear Néel state to be the reference state $|\Phi\rangle$. We calculate the ground-state (GS) wave function, $|\Psi\rangle = e^S|\Phi\rangle$, within the LSUB$n$ approximation scheme up to $n = 8$, and extrapolate to $n \to \infty$. The CCM results for the order parameter are shown in the left graph of Fig. 3 and they are compared to results of linear spin wave theory (SWT), exact diagonalization (ED) of N=16, 18, 20, 26, 32 sites, and the MF theory. The CCM is able to describe correctly the order-disorder transition, whereas conventional SWT cannot (and for more details concerning the SWT and ED results see Ref. [10]). The critical value predicted by extrapolation of the LSUBn results is, however, found to be slightly too large. We may also consider the inflection points of m versus J' for the LSUBn approximations. It is assumed that the true $m(J')$-curve will have a negative curvature up to the critical point. Thus we might expect that (for increasing n) the inflection point

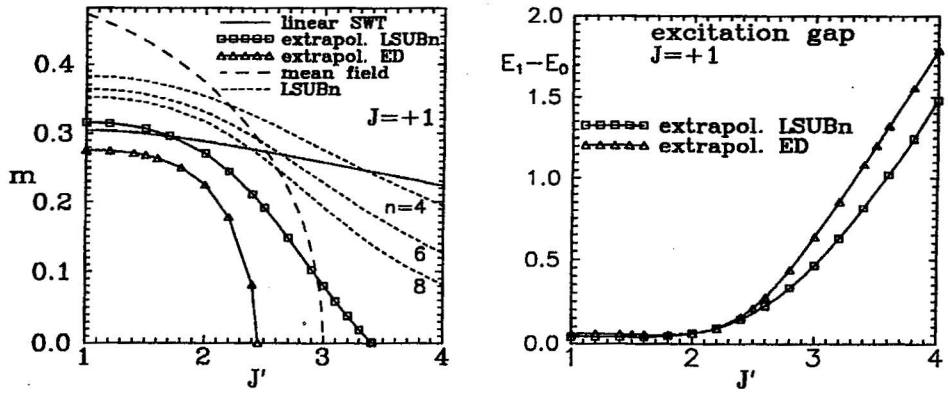

Figure 3. Sublattice magnetization (left graph) and excitation gap (right graph) versus J', for the case $J = +1$.

approaches the critical point. We find the corresponding inflection points at $J' = 3.1$ (n=2), $J' = 3.0$ (n=4), $J' = 2.9$ (n=6) and $J' = 2.85$ (n=8), indicating a critical value J'_c somewhere between $2.5J$ and $3J$. Notice that the estimation of $2.5 \lesssim J'_c/J \lesssim 3$ is consistent with results of series expansions and exact diagonalizations [20,10]. The breakdown of Néel long-range order (LRO) due to singlet formation is also accompanied by the opening of an excitation gap between the singlet GS and the first triplet excitation. This behaviour is well described by the CCM (right graph of Fig. 3) which predicts that the gap opens in the range $2J < J' < 3J$ (and notice that the non-zero gap below $2J$ is a result of the limited accuracy of the extrapolation).

4.2 $J = +1$; $J' < 0$: Competition with frustration (Néel versus spiral)

In this and the following subsection we now consider the frustrated regimes of the model where J and J' have opposite signs. We first consider the case $J = +1$, $J' < 0$ where the Néel and spiral phases compete, and in Sec. 4.3 consider the case $J = -1$, $J' > 0$ where the ferromagnetic and spiral phases compete. In both cases the ED technique for finite-size lattices is expected to be less useful because of the incommensurate nature of the classical spiral states. By contrast, the CCM considers the limit $N \to \infty$ from the outset and should have no such problem dealing with incommensurate states. In both cases we use the corresponding classical state of Sec. 3.1 as the CCM model state. However, since quantum fluctuations can clearly change the spiral pitch angle from its classical value, we determine the "quantum pitch angle" Φ by minimizing $E_{\mathrm{LSUB}n}(\Phi)$ with respect to Φ in each order n.

Results for $E(\Phi)$ and $\Phi(J')$ are shown in Fig. 4 for the case $J = +1, J' < 0$. A number of key points emerge. Firstly, it is clear that the CCM continues to yield a consistent description of the system in both these collinear and spiral phases. Secondly, the quantum Néel state remains the ground state up to much stronger frustration than in the classical case. This is in keeping with the general observation that quantum fluctuations in spin systems tend to favour collinear spin structures over non-collinear ones. Thirdly, and very strikingly, we observe that in this case the

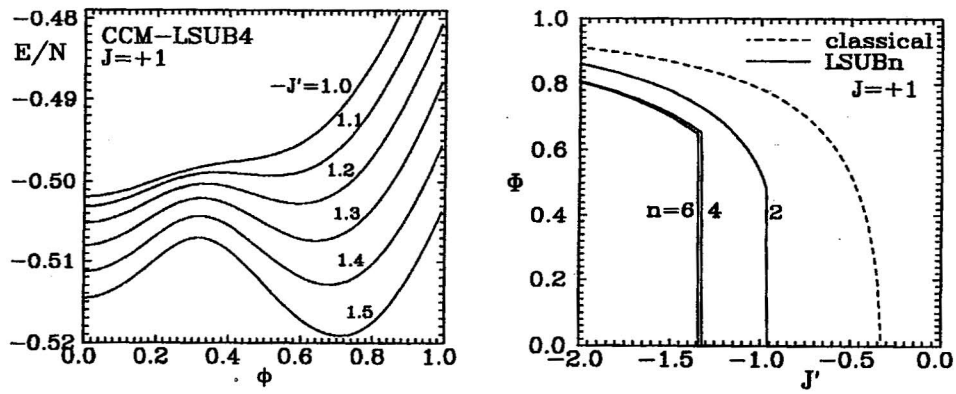

Figure 4. Energy versus quantum pitch angle for LSUB4 (left graph) and quantum pitch angle versus J' (right graph) for the case $J = +1$. Note that $\Phi = 0$ corresponds to the Néel state.

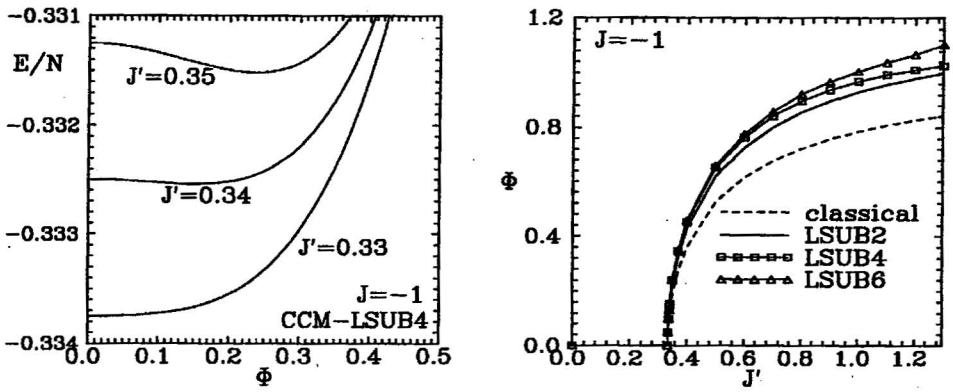

Figure 5. Energy versus quantum pitch angle for LSUB4 (left graph) and quantum pitch angle versus J' (right graph) for the case $J = -1$. Note that $\Phi = 0$ corresponds to the fully polarized ferromagnetic state.

quantum fluctuations also change the order of the phase transition from second order in the classical case to first order in the quantum case.

4.3 $J = -1$; $J' > 0$: Competition with frustration (ferro versus spiral)

We now contrast the case considered in Sec. 4.2 with the case where $J = -1$, $J' > 0$. Whereas in the classical model we again have a second-order transition between collinear and spiral phases, the quantum model in these two regimes behaves quite differently. Although the collinear antiferromagnetic phase contains strong quantum fluctuations as we saw above, the fully polarized, collinear ferromagnet contains no such fluctuations. The corresponding results for $E(\Phi)$ and $\Phi(J')$ are displayed in Fig. 5. In this case the order of the transition from the collinear (ferromagnetic) to the noncollinear (spiral) phase remains second-order, as in the classical

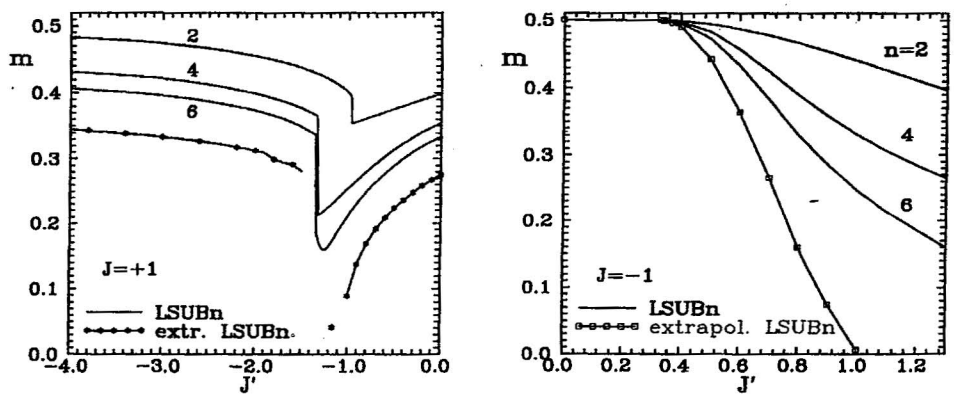

Figure 6. On-site magnetic moment versus J' for $J = +1$ (left graph) and $J = -1$ (right graph).

case. Furthermore, the quantum critical point remains exactly at the classical value, $J'/J = -1/3$.

4.4 Comparison of the various cases

The difference between the two cases considered in Secs. 4.2 and 4.3 is particularly illustrated by Fig. 6 which contrasts the behaviour of the order parameter, namely the on-site magnetic moment m, in the two regimes. For $J = +1$ there exists a discontinuity in m at every level of LSUBn approximation. This is a reflection of the behaviour observed in $E(\Phi)$ in Fig. 4, where a *local* minimum at $\Phi \neq 0$ appears for $J' \lesssim -1.1$, which for values $J' \lesssim -1.35$ becomes a *global* minimum. The extrapolation of m to the exact $n \to \infty$ limit does, however, become imprecise close to the phase transition point, and we cannot decide with certainty whether the order parameter does vanish at the transition point or, indeed, over a small finite regime around it. Figure 6 displays a minimum extrapolated value of $m \approx 0.05$ at $J'_c \approx -1.2$. We cannot exclude entirely a disordered quantum *spin-liquid phase* with $m = 0$ caused by quantum fluctuations plus frustration, but if it does exist it can clearly occur only over a very narrow regime in J' around $-1.5 \lesssim J' \lesssim -1.1$. The most likely scenario however is a single phase boundary at a value $J'_c \approx -1.35$ between spiral and Néel phases, with no intervening separate spin-liquid phase.

By contrast, Fig. 6 shows a smooth change in m at the critical point $J'_c = 1/3$ for $J = -1$. For increasing $J' > J'_c$ the spiral magnetic order becomes weaker and finally vanishes at $J' \approx 1$. The underlying reason for this is again local singlet formation (i.e., dimerization), as discussed in Sec. 4.1. On the other hand, a much smaller critical strength J'_c is needed for dimerization than in the case $J = +1$ (where $2.5 \lesssim J'_c \lesssim 3$), due to the effects of frustration which now assist in the formation of local singlets [24].

Finally, in Fig. 7 we show both the ground-state energy $E(J')$ and the order parameter $m(J')$ in the case $J = +1$ over the regimes spanning the spiral, Néel, and dimer-like phases. We observe excellent agreement between the CCM results

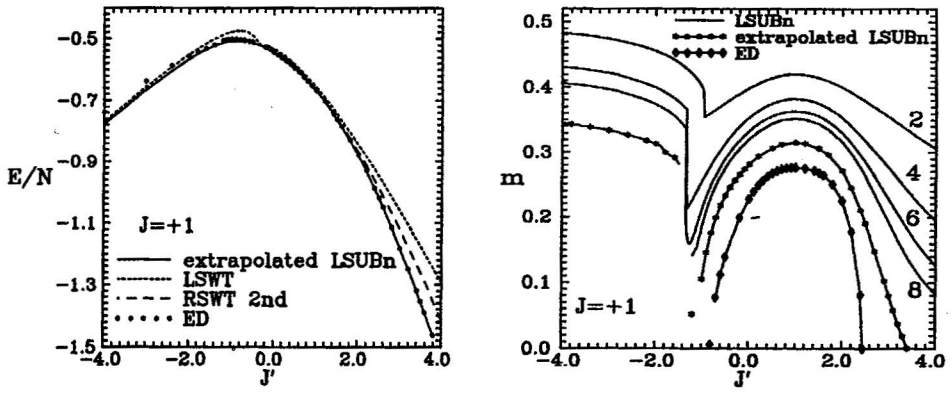

Figure 7. Left: Ground-state energy versus J', for the case $J = +1$, for the extrapolated CCM-LSUBn approximations, in comparison with results of spin-wave theory (SWT) (linear and second-order renormalized) [21], and with the extrapolated results of exact diagonalization (ED) data. Right: Ground-state magnetic order parameter versus J', for the case $J = +1$, for the CCM-LSUBn approximation. The results are compared (for the Néel region only) with the extrapolated results of exact diagonalization (ED) data. Note that both extrapolated results fit poorly in a region around $J' \approx -1$, and we therefore plot them here as isolated points, omitting the solid lines.

and the results from exact diagonalization (ED) for $J' > 0$. By contrast, spin-wave theory (SWT) calculations [21] show a significant deviation for larger $J' \gg 1$. These latter are obviously poor since they lie *above* the simple variational upper bound of Eq. (8). The CCM and ED results, by comparison, lie slightly below the mean-field variational result.

We note that although the Néel state is the starting reference state for both CCM and SWT calculations, the CCM is much better able than SWT to describe the transition to the rotationally-invariant disordered state and hence to its limiting form, namely the fully dimerized state of Eq. (7) with $t = 1$. For example, even the simplest LSUB2 CCM approximation gives the correct asymptotic behaviour for the ground-state energy, $E/N \to -3J'/8$ as $J' \to \infty$, whereas SWT does not.

5. DISCUSSION AND CONCLUSIONS

In this article we have investigated the zero-temperature phase transitions of a spin-half Heisenberg system on the square lattice. The main results of our treatment are:

- Quantum fluctuations plus competition without frustration are able to destroy Néel long-range order by local singlet formation. This is a pure quantum effect and has no classical counterpart. The control parameter is the strength of the competition and the breakdown of Néel ordering is accompanied by the opening of a spin gap. Standard SWT (even to higher orders) fails to describe this transition, whereas the CCM describes both the order parameter and the gap satisfactorily. Since we have no frustration, most standard techniques (e.g.,

QMC) are applicable and a quantitative description is possible. As was discussed in Ref. [25], the critical properties seem to correspond to the 3D classical Heisenberg model.

- Competition due to frustration was found to give more complex magnetic properties. In the model considered we have a second-order transition between collinear (antiferro- or ferro-magnetic) and noncollinear (spiral) states driven by frustration in the classical case. In the quantum spin-half model, standard techniques (e.g., QMC) are not applicable due to the violation of Marshall's sign rule. By contrast, the CCM provides a consistent description of collinear, noncollinear, and disordered phases. Furthermore, we find a strong influence of quantum fluctuations on the nature of the collinear-noncollinear transition, and quantum fluctuations (which favour collinear ordering) may change the second-order classical transition to a first-order quantum transition. If quantum fluctuations are suppressed in the collinear phase, the transition to the spiral phase is similar for the quantum and classical models.

Based on the success of the CCM to describe the model considered here and other complex magnetic lattice models, it is of interest to enquire about possible extensions. One particularly important such extension would be to nonzero temperatures, in order to investigate quantitatively, and in a fully *ab initio* microscopic framework, the competing effects of quantum and thermal fluctuations on the full phase diagram of a given model system.

REFERENCES

[1] R.F. Bishop, in *Microscopic Quantum Many-Body Theories and Their Applications*, edited by J. Navarro and A. Polls, Lecture Notes in Physics Vol. **510** (Springer-Verlag, Berlin, 1998), p. 1.

[2] R.F. Bishop, Theor. Chim. Acta **80**, 95 (1991); R.J. Bartlett, J. Phys. Chem. **93**, 1697 (1989).

[3] C. Zeng, D.J.J. Farnell, and R.F. Bishop, J. Stat. Phys. **90**, 327 (1998).

[4] D.J.J. Farnell, R.F. Bishop, and K.A. Gernoth, J. Stat. Phys. **108**, 401 (2002).

[5] R.F. Bishop, R.G. Hale, and Y. Xian, Phys. Rev. Lett. **73**, 3157 (1994).

[6] D.J.J. Farnell, S.E. Krüger, and J.B. Parkinson, J. Phys.: Condens. Matter **9** 7601 (1997).

[7] R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, Phys. Rev. B **58**, 6394 (1998).

[8] R.F. Bishop, D.J.J. Farnell, and C. Zeng, Phys. Rev. B **59**, 1000 (1999).

[9] R.F. Bishop, D.J.J. Farnell, S.E. Krüger, J.B. Parkinson, J. Richter, and C. Zeng, J. Phys.: Condens. Matter **12**, 6887 (2000).

[10] S.E. Krüger, J. Richter, J. Schulenburg, D.J.J. Farnell, and R.F. Bishop, Phys. Rev. B **61**, 14607 (2000).

[11] D.J.J. Farnell, R.F. Bishop, and K.A. Gernoth, Phys. Rev. B **63**, 220402(R) (2001).

[12] S.E. Krüger and J. Richter, Phys. Rev. B **64**, 024433 (2001).

[13] M. Roger and J.H. Hetherington, Europhys. Lett. **11**, 255 (1990).

[14] C.F. Lo, E. Manousakis, and Y.L. Wang, Phys. Lett. **A156**, 42 (1991).

[15] F. Petit and M. Roger, Phys. Rev. B **49**, 3453 (1994).

[16] R.F. Bishop, Y. Xian, and C. Zeng, Int. J. Quantum Chem. **55**, 181 (1995).

[17] S.J. Baker, R.F. Bishop, and N.J. Davidson, Phys. Rev. D **53**, 2610 (1996).

[18] C.H. Llewellyn Smith and N.J. Watson, Phys. Lett. **B302**, 463 (1993); D. Schütte, Zheng Weihong, and C.J. Hamer, Phys. Rev. D **55**, 2974 (1997); A. Wichmann, D. Schütte, B.C. Metsch, and V. Wethkamp, Phys. Rev. D **65**, 094511 (2002).

[19] N.E. Ligterink, N.R. Walet, and R.F. Bishop, Ann. Phys. (NY) **267**, 97 (1998); *ibid.*, Phys. Rev. E **63**, 037103 (2001).

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

[21] N.B. Ivanov, S.E. Krüger, and J. Richter, Phys. Rev. B **53**, 2633 (1996).

[22] A.W. Sandvik and D.J. Scalapino, Phys. Rev. Lett. **72**, 2777 (1994).

[23] J. Villain, J. Phys. C: Solid State **10**, 4793 (1977).

[24] C. Gros, W. Wenzel, and J. Richter, Europhys. Lett. **32**, 747 (1995).

[25] M. Troyer, M. Imada, and K. Ueda, J. Phys. Soc. Jpn. **66**, 2957 (1997).