Phase diagram of the frustrated quantum-XY model on the honeycomb lattice studied by series expansions: Evidence for proximity to a bicritical point

J. Oitmaa
School of Physics, The University of New South Wales, Sydney 2052, Australia

R. R. P. Singh
Department of Physics, University of California Davis, California 95616, USA
(Received 18 February 2014; revised manuscript received 17 March 2014; published 27 March 2014)

We study the nearest-neighbor exchange (J_1) and second-nearest-neighbor exchange (J_2) XY antiferromagnet on the honeycomb lattice using ground state series expansions around Néel, columnar, and dimer phases. The conventional two-sublattice XY Néel order at small J_2 vanishes at $J_2/J_1 = 0.22 \pm 0.01$ in agreement with results from density matrix renormalization group (DMRG) studies. Near the transition, we find evidence for an *approximate* emergent symmetry between XY and Ising degrees of freedom, namely the nearest-neighbor Ising and XY spin correlations become nearly equal. This suggests that the system is close to a bicritical point separating XY and Ising orders. At still larger J_2/J_1 the columnar and dimer energies are found to be nearly degenerate. At even larger J_2 the columnar phase is obtained. The ground state energies in all three phases are in good agreement with the values found in the DMRG studies.

DOI: 10.1103/PhysRevB.89.104423 PACS number(s): 75.10.Jm, 73.43.Nq, 75.10.Kt

Frustrated quantum spin models continue to interest and surprise us [1,2]. While the physics of unfrustrated models is dominated by a single classical order, frustrated models can have a variety of magnetic and nonmagnetic order parameters, as well as quantum spin-liquid phases with topological order or no order whatsoever [3]. In many cases, phases ordered in vastly different ways compete with each other with very small energy differences [4]. While much of the studies in recent years have focused on Heisenberg models with full $SU(2)$ symmetry, frustrated quantum XY models provide a slightly different variety, opening an avenue to explore new physics, an example being order by disorder in the pyrochlore antiferromagnets [5]. Long-range order is usually more robust in XY models than in Heisenberg models as quantum fluctuations are weaker, but they also allow for emergent phenomena that may be unique to XY models such as Bose metals [6].

We consider here the antiferromagnetic spin-1/2 XY model on the honeycomb lattice, a subject of much recent interest [7–9], with Hamiltonian

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + \lambda S_i^y S_j^y \right) + J_2 \sum_{\langle\langle i,k \rangle\rangle} \left(S_i^x S_k^x + \lambda S_i^y S_k^y \right), \tag{1}$$

where the first sum runs over nearest neighbors and the second over the second nearest neighbors of the honeycomb lattice. The exchange constants J_1 and J_2 are both positive, providing a frustrated antiferromagnetic model. This model, with XY symmetry ($\lambda = 1$) was recently studied by exact diagonalization [7], and variational wave functions [8] by Varney *et al.*, and by density matrix renormalization group (DMRG) [9] methods by Zhu *et al.* The two groups have proposed very different phases at intermediate J_2/J_1, once the conventional XY Néel order is lost. Varney *et al.* proposed a quantum spin-liquid or Bose-metal phase with a "clearly identifiable Bose surface" [7], a phase with no long-range order but a surface of low energy excitations in momentum space [6]. In contrast, the DMRG study [9] found an emergent Ising antiferromagnetic phase, with spins weakly ordered along the Z axis. The latter is a surprising result as there are no $S_i^z S_j^z$ interaction terms in the bare Hamiltonian. Thus the entire stabilization energy for this phase must come from higher order quantum fluctuations. At still larger J_2/J_1, columnar and dimer phases were found to have very close energies. At even larger J_2/J_1 the columnar XY phase is stabilized. At still larger J_2/J_1 noncollinear phases may be realized [7], but we will not study them in this paper.

The purpose of this paper is to study the phase diagram of this model using series expansion methods [10,11]. Our work confirms various findings of the DMRG study. We find that the XY Néel phase is stable until a critical value of $J_2/J_1 = 0.22 \pm 0.01$. Near this point there is an approximate emergent Heisenberg symmetry in the system, where nearest-neighbor XY and Ising correlations become equal. This suggests that the system is close to a point where XY and Ising orders interchange dominance [12]. However, we are not able to study the Ising ordered phase by series expansion methods due to lack of convergence. On the other hand, we can investigate the columnar and dimer phases, such as calculating their respective energies (see fig. 1) using series expansions at still larger J_2/J_1 values. In all three phases, XY-Néel, dimer, and columnar, our ground state energies are in very good agreement with the values from the DMRG calculations. In the region just beyond the XY Néel phase the DMRG study finds an Ising ordered antiferromagnet, whose energy is clearly lower than the dimer and columnar state energies we calculate. This lends further support to this emergent phase in the model [9].

To study the XY Néel phase (or the XY columnar phase), we consider the model in Eq. (1) as a function of λ. At $\lambda = 0$, it has simple classical ground states. Properties such as ground state energy, on-site magnetization, and nearest-neighbor XX, YY, and ZZ correlations are calculated as power-series expansions in the variable λ [10,11]. Note that choosing X as the ordering direction breaks the symmetry of rotation in

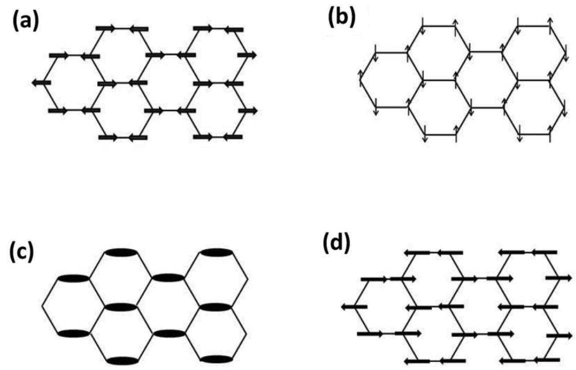

FIG. 1. Four possible ground state phases of the model are (a) XY-Néel, (b) Ising-(ZZ)-Néel, (c) dimer, and (d) XY-columnar.

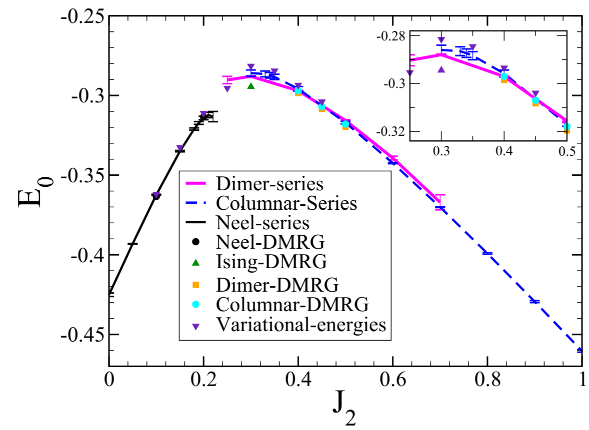

FIG. 2. (Color online) Ground state energy as a function of J_2. Series expansion results are presented for Néel, columnar, and dimer expansions. Results from density matrix renormalization group (DMRG) in Néel, Ising, Dimer, and columnar phases from Ref. [9], and variational energies from Ref. [8] are also presented. The inset shows the same data on a more magnified scale in the region $0.25 < J_2 < 0.5$.

the XY plane and hence the XX and YY correlations need not be equal.

To carry out the dimer series expansions, we consider all the nearest-neighbor exchanges that point along one axis of the honeycomb lattice (as shown in the dimer phase of Fig. 1) to have a strength of unity and all other exchanges are multiplied by a factor of α. Then series expansions can be calculated for ground state properties in powers of α [10,11].

Series for ground state energies and nearest-neighbor correlation functions are analyzed using simple Padé approximants. However, to analyze the order-parameter series, we first apply a transformation of variables that removes the strong square-root singularity known to arise for the order parameter due to long wavelength spin waves [13,14], and then carry out the Padé approximants. Details of series generation and analysis methods can be found in the literature [10,11].

For all the calculations, we set the exchange constant $J_1 = 1$. Ground state energies obtained from the various series expansions are shown in Fig. 2. DMRG energies are shown by symbols and have error bars much smaller than the symbols. Given the closeness of various energies, a list of selected energies and comparison with other studies is shown in Table I. Series for the XY-Néel and XY-columnar phases converge well, and these are clearly the ground states at small J_2 and at $J_2 = 1$, respectively. The intermediate region is more interesting and discussed below. The order parameters for the Néel and columnar XY phases are shown in Fig. 3 . The error bars reflect the spread in Padé approximant values [10,11]. While the Néel order parameter at small J_2 goes smoothly to zero at $J_2 = 0.22 \pm 0.01$, the order parameter for the columnar phase remains nearly constant from large values of J_2 down to about $J_2 \approx 0.4$, and only for J_2 around 0.35 it begins to go down to zero.

At intermediate J_2, there is a range of parameter values where XY-columnar and dimer state energies are nearly degenerate and are also in agreement with the DMRG energies. The DMRG study finds [9] that the model has a phase transition from the columnar phase to a dimer phase around $J_2 \approx 0.5$ and then another transition to an Ising ordered antiferromagnet around $J_2 \approx 0.35$ [9]. Looking closely at the data in Table I, we also find supporting evidence for this. At $J_2 = 0.6$, we find the energy of the columnar phase to be -0.3425 ± 0.0004, which is clearly lower than the dimer phase energy $-0.3393 \pm 0.0.0011$. At $J_2 = 0.5$, the energy of the columnar phase is -0.3171 ± 0.0008. It is marginally lower than the energy of the dimer phase -0.3157 ± 0.0005 and is consistent with the DMRG energy -0.318. On the other hand, at $J_2 = 0.4$ the energy of the dimer phase is -0.2971 ± 0.0002. It is marginally lower than the energy of the columnar phase -0.2958 ± 0.0014 and is consistent with the DMRG energy -0.297.

The only parameter region, where series expansions do not give accurate ground state energies compared to DMRG is in the region immediately next to the XY-Néel phase boundary at $J_2/J_1 = 0.22$. This is where the exotic emergent Ising phase was found in DMRG and a Bose-metal phase [6] was proposed

TABLE I. Ground state energies (with $J_1 = 1$) for different values of J_2 calculated by series expansions for Néel (N), Dimer (D) and Columnar (C) phases. Results from DMRG [9] and Variational (VAR) [8] studies are also shown.

J_2	0.1	0.2	0.3	0.4	0.5	0.6
Series N	-0.3624 ± 0.0004	-0.314 ± 0.001				
Series D			-0.2880 ± 0.0003	-0.2971 ± 0.0002	0.3157 ± 0.0005	-0.3393 ± 0.0011
Series C			-0.2860 ± 0.002	-0.2958 ± 0.0014	-0.3171 ± 0.0008	-0.3425 ± 0.0004
DMRG	-0.3634	-0.3135	-0.2945	-0.297	-0.318	
VAR	$-0.361\,88$	$-0.311\,07$	$-0.281\,54$	$-0.293\,47$		

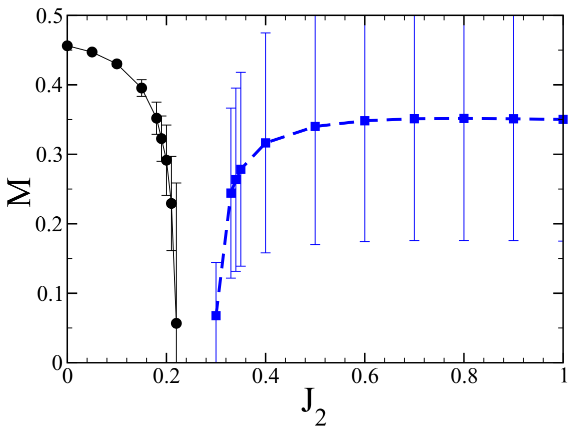

FIG. 3. (Color online) Local XY magnetization in the Néel (solid circles) and columnar (solid squares) phases obtained by series expansions.

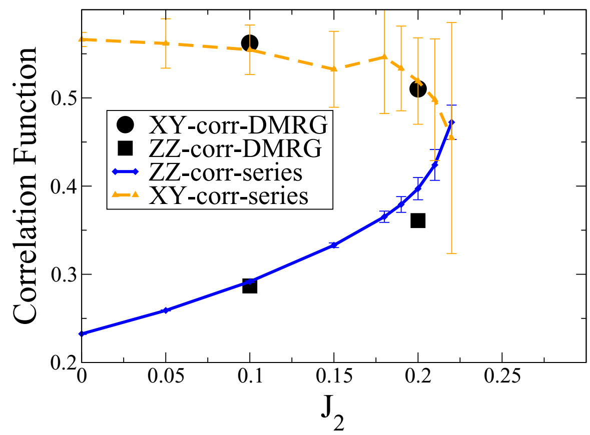

FIG. 5. (Color online) Averaged nearest-neighbor correlations in the XY plane versus nearest-neighbor correlations along the Z axis from Fig. 4. Absolute values for the correlations are shown. Results from DMRG calculations from Ref. [9] are also shown.

in the exact diagonalization study [7]. From Table I, one can see that at $J_2 = 0.3$, the DMRG energy -0.2945 is clearly lower than either dimer (-0.2880 ± 0.0003) or the columnar energy (-0.2860 ± 0.002) well beyond the estimated uncertainties.

In Figs. 4 and 5 we show the nearest-neighbor correlation functions in the XY Néel phase. All correlations are antiferromagnetic. Only the absolute values of the correlation functions are plotted. When J_2 is small, the XY order is very robust, and the correlation along the ordering direction (X from our choice) is completely dominant. As the transition point $J_2 \approx 0.22$ is approached, the XX correlation strongly decreases, while the correlations along the Y and Z directions grow. As one would approach the transition away from that phase, the symmetry in the XY plane would be restored. Hence, it makes sense to average the XX and YY correlations to obtain the average XY correlations between neighboring spins for a comparison at the transition point. In Fig. 5, the averaged XY correlations are compared with the ZZ correlations. Data from DMRG are also shown. It is clear that the average correlation in the XY plane approaches the ZZ correlation near the transition. Note that the DMRG data show a somewhat slower growth in ZZ correlations, implying that the two would cross at a slightly larger J_2 value. This near crossing, at the transition, is evidence that the system is close to a bicritical point, separating XY and Ising ordered phases [12]. On general grounds, one expects either a first-order transition between the two ordered phases, or an intermediate phase where neither order survives. Only when the system is fine tuned with a second parameter, one should be able to realize a continuous bicritical transition between the phases [12]. In the present case, an additional coupling that may allow one to tune the system to the bicritical point is a nearest-neighbor Ising coupling. An antiferromagnetic Ising coupling would favor the Ising ordered phase, whereas a ferromagnetic Ising coupling would disfavor such a phase. Our study suggests that the J_1-J_2 honeycomb-lattice XY model, with zero Ising coupling, is close to such a bicritical point. In principle, this bicritical point can be studied in the future by DMRG.

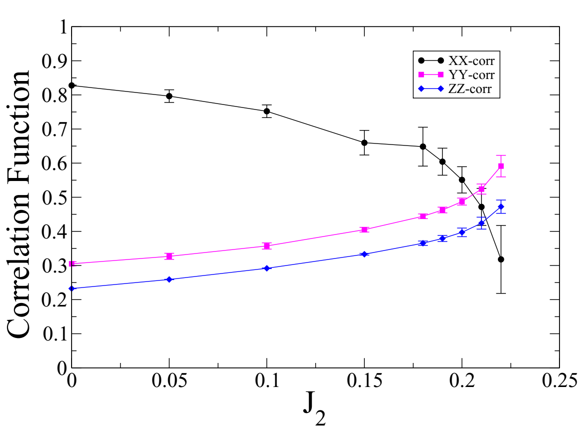

FIG. 4. (Color online) Components of nearest neighbor correlations in the Néel phase obtained by series expansions. Absolute values for the correlation functions are shown. Also, the correlation functions are for the σ-variables, which are four times the usual spin-spin correlation functions.

However, we have been unable to carry out a convergent ground state series expansion for the Ising phase, which suggests that this phase is quite fragile. The way one approaches such a problem in series expansions [10,11] is by considering a different Hamiltonian, which is a sum of the original XY Hamiltonian multiplied by η plus a nearest-neighbor Ising Hamiltonian multiplied by $(1 - \eta)$. Thus, at $\eta = 0$ the model has ground states with complete Ising order, whereas at $\eta \to 1$, the original Hamiltonian is recovered. One then carries out a series expansion for ground state properties in powers of η to study the possibility of Ising order remaining in the system even as the Ising interactions are turned off and the XY Hamiltonian is realized. Unfortunately, in our case, such a series expansion shows very poor convergence as $\eta \to 1$, and we are unable to get any useful information about this phase. A comparison of the energy of this Ising phase found in DMRG with dimer and columnar state energies, calculated in our study, shows that it is indeed stabilized by very small energy differences relative to these other phases. It should be noted that just based on series expansions alone, we cannot rule out an even more exotic phase such as the Bose liquid proposed in the study of Varney *et al.* in this intermediate J_2/J_1 region [7].

In conclusion, in this paper we have studied the frustrated quantum XY model by series expansion methods. Our main goal was to shed further light on the remarkable finding in the recent DMRG study of an emergent Ising phase in the model with the ordered spins pointing along the Z axis. Although we have not directly been able to study this phase, our study provides indirect support for its existence. Firstly, we find that the XY Néel order vanishes at $J_2/J_1 = 0.22 \pm 0.01$ in agreement with the DMRG study. Secondly, we find that as this transition is approached from the XY-Néel side, the nearest-neighbor ZZ correlations rise to become equal to the nearest-neighbor XY correlations consistent with the development of stronger ZZ correlations or Ising order along the Z axis at larger J_2. Ground state energies for the XY-Néel, XY-columnar, and dimer phases are in excellent agreement with the DMRG calculations. In the region of the emergent Ising phase, the energy of other competing phases are clearly higher, further supporting such a phase.

This work is supported in part by NSF Grant No. DMR-1004231, and by the computing resources provided by the Australian (APAC) National facility. We thank Michel Gingras for interesting us in this problem and a critical reading of the manuscript and Zhenyue Zhu and Steve White for making available their detailed DMRG data.

[1] L. Balents, Nature (London) **464**, 199 (2010).
[2] R. K. Kaul, R. G. Melko, and A. W. Sandvik, Ann. Rev. of Cond. Math Phys. **4**, 179 (2013).
[3] X. G. Wen, Phys. Rev. B **65**, 165113 (2002); **44**, 2664 (1991).
[4] S. Yan, D. A. Huse, and S. R. White, Science **332**, 1173 (2011); S. Depenbrock, I. P. McCulloch, and U. Schollwock, Phys. Rev. Lett. **109**, 067201 (2012); H. C. Jiang, Z. H. Wang, and L. Balents, Nat. Phys. **8**, 902 (2012).
[5] L. Savary, K. A. Ross, B. D. Gaulin, J. P. C. Ruff, and L. Balents, Phys. Rev. Lett. **109**, 167201 (2012); M. E. Zhitomirsky, M. V. Gvozdikova, P. C. W. Holdsworth, and R. Moessner, *ibid.* **109**, 077204 (2012); J. Oitmaa, R. R. P. Singh, B. Javanparast, A. G. R. Day, B. V. Bagheri, and M. J. P. Gingras, Phys. Rev. B **88**, 220404(R) (2013); A. W. C. Wong, Z. Hao, and M. J. P. Gingras, *ibid.* **88**, 144402 (2013); P. A. McClarty, P. Stasiak, and M. J. P. Gingras, *ibid.* **89**, 024425 (2014).
[6] M. S. Block, D. N. Sheng, O. I. Motrunich, and M. P. A. Fisher, Phys. Rev. Lett. **106**, 157202 (2011).
[7] C. N. Varney, K. Sun, V. Galitski, and M. Rigol, Phys. Rev. Lett. **107**, 077201 (2011).
[8] J. Carrasquilla, A. Di Ciolo, F. Becca, V. Galitski, and M. Rigol, Phys. Rev. B **88**, 241109(R) (2013).
[9] Z. Zhu, D. A. Huse, and S. R. White, Phys. Rev. Lett. **111**, 257201 (2013).
[10] J. Oitmaa, C. Hamer, and W. Zheng, *Series Expansion Methods for Strongly Interacting Lattice Models* (Cambridge University Press, Cambridge, UK, 2006).
[11] M. P. Gelfand and R. R. P. Singh, Adv. Phys. **49**, 93 (2000); M. P. Gelfand, R. R. P. Singh, and D. A. Huse, J. Stat. Phys. **59**, 1093 (1990).
[12] J. M. Kosterlitz, D. R. Nelson, and M. E. Fisher, Phys. Rev. B **13**, 412 (1976).
[13] D. A. Huse, Phys. Rev. B **37**, 2380 (1988).
[14] R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989); R. R. P. Singh and D. A. Huse, *ibid.* **40**, 7247 (1989).