Effect of anisotropy on the ground-state magnetic ordering of the spin-half quantum J_1^{XXZ}–J_2^{XXZ} model on the square lattice

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We study the zero-temperature phase diagram of the two-dimensional quantum J_1^{XXZ}–J_2^{XXZ} spin-1/2 anisotropic Heisenberg model on the square lattice. In particular, the effects of the anisotropy Δ on the z-aligned Néel and (collinear) stripe states, as well as on the xy-planar-aligned Néel and collinear stripe states, are examined. All four of these quasiclassical states are chosen in turn as model states, on top of which we systematically include the quantum correlations using a coupled cluster method analysis carried out to very high orders. We find strong evidence for two *quantum triple points* (QTPs) at ($\Delta^c=-0.10\pm0.15$, $J_2^c/J_1=0.505\pm0.015$) and ($\Delta^c=2.05\pm0.15$, $J_2^c/J_1=0.530\pm0.015$), between which an intermediate magnetically disordered phase emerges to separate the quasiclassical Néel and stripe collinear phases. Above the upper QTP ($\Delta\gtrsim2.0$) we find a direct first-order phase transition between the Néel and stripe phases, exactly as for the classical case. The z-aligned and xy-planar-aligned phases meet precisely at $\Delta=1$, also as for the classical case. For all values of the anisotropy parameter between those of the two QTPs there exists a narrow range of values of J_2/J_1, $\alpha^{c1}(\Delta)<J_2/J_1<\alpha^{c2}(\Delta)$, centered near the point of maximum classical frustration, $J_2/J_1=\frac{1}{2}$, for which the intermediate phase exists. This range is widest precisely at the isotropic point, $\Delta=1$, where $\alpha^{c1}(1)=0.44\pm0.01$ and $\alpha^{c2}(1)=0.59\pm0.01$. The two QTPs are characterized by values $\Delta=\Delta^c$ at which $\alpha^{c1}(\Delta^c)=\alpha^{c2}(\Delta^c)$.

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I. INTRODUCTION

The exchange interactions that lead to collective magnetic behavior are clearly of purely quantum-mechanical origin. Nevertheless, the underlying quantum nature has often safely been ignored in describing, at least at the qualitative level, many magnetic phenomena of interest in the past. On the other hand, the investigation of magnetic systems and magnetic phenomena, where the intrinsically quantal effects play a *dominant* role, and hence have to be accounted for in detail, has evolved in recent years to become a burgeoning area at the forefront of condensed matter theory. Thus, the investigation of quantum magnets and their phase transitions, both quantum and thermal, has developed into an extremely active area of research.

From the experimental viewpoint major impetus has come both from the discovery of high-temperature superconductors and, since then, from the ever-increasing ability of materials scientists to fabricate a by-now bewildering array of novel magnetic systems of reduced dimensionality, which display interesting quantum phenomena.[1] While high-temperature superconductivity has raised the question of the link between the mechanism of superconductivity in the cuprates, for example, and spin fluctuations and magnetic order in one-dimensional (1D) and two-dimensional (2D) spin-half antiferromagnets, the new magnetic materials exhibit a wealth of new quantum phenomena of enormous interest in their own right.

For example, in 1D systems, the universal paradigm of Tomonaga-Luttinger liquid[2,3] behavior has occupied a key position of interest since Fermi liquid theory breaks down in 1D. More generally, in *all* restricted geometries the interplay between reduced dimensionality, competing interactions, and strong quantum fluctuations generates a plethora of new states of condensed matter beyond the usual states of quasiclassical long-range order (LRO). Thus, for high-temperature superconductivity, for example, it is suggested[4] that quantum-spin fluctuation and frustration due to doping could lead to the collapse of the 2D Néel-ordered antiferromagnetic phase present at zero doping, and that this could be the clue for the superconducting behavior. This, and many similar experimental observations for other magnetic materials of reduced dimensionality, has intensified the study of order-disorder quantum phase transitions. Thus, low-dimensional quantum antiferromagnets have attracted much recent attention as model systems, in which strong quantum fluctuations might be able to destroy magnetic LRO in the ground state (GS). In the present paper we consider a system of $N\to\infty$ spin-1/2 particles on a spatially isotropic 2D square lattice.

The spin-1/2 Heisenberg antiferromagnet with only nearest-neighbor (NN) bonds, all of equal strength, exhibits magnetic LRO at zero temperature on such bipartite lattices as the square lattice considered here. A key mechanism that can then destroy the LRO for such systems, with a given lattice and spins of a given spin quantum number s, is the introduction of competing or frustrating bonds on top of the NN bonds. The interested reader is referred to Refs. 1 and 5 for a more detailed discussion of 2D spin systems in general.

An archetypal model of the above type that has attracted much theoretical attention in recent years (see, e.g., Refs. 6–19) is the 2D spin-1/2 J_1–J_2 model on a square lattice with both NN and next-nearest-neighbor (NNN) antiferro-

magnetic interactions, with strength $J_1>0$ and $J_2>0$, respectively. The NN bonds $J_1>0$ promote Néel antiferromagnetic order, while the NNN bonds $J_2>0$ act to frustrate or compete with this order. All such frustrated quantum magnets continue to be of great theoretical interest because of the possible spin-liquid and other such novel magnetically disordered phases that they can exhibit (and see, e.g., Ref. 20). The recent syntheses of magnetic materials that can be well described by the spin-1/2 J_1–J_2 model on the 2D square lattice—such as the undoped precursors to the high-temperature superconducting cuprates for small J_2/J_1 values, $VOMoO_4$ for intermediate J_2/J_1 values,[21] and Li_2VOSiO_4 for large J_2/J_1 values[22,23]—has fuelled further theoretical interest in the model.

The properties of the spin-1/2 J_1–J_2 model on the 2D square lattice are well understood in the limits when $J_2=0$ or $J_1=0$. For the case when $J_2=0$, and the classical GS is perfectly Néel ordered, the quantum fluctuations are not sufficiently strong enough to destroy the Néel LRO, although the staggered magnetization is reduced to about 61% of its classical value. Indeed, the best estimates for this order parameter are $61.4\pm0.1\%$ from quantum Monte Carlo studies,[24] 63.5% from exact diagonalizations of small clusters,[25] $61.4\pm0.2\%$ from series expansions,[26] $61.5\pm0.5\%$ from the coupled cluster method (CCM) employed here,[27–29] and 61.4% from third-order spin-wave theory.[30] Clearly, they all agree remarkably well in this $J_2=0$ limit. The opposite limit of large J_2 is a classic example[8] of the phenomenon of order by disorder.[31,32] Thus, in the case where $J_1\rightarrow0$ with $J_2\neq0$ and fixed, the two sublattices each order antiferromagnetically at the classical level, but in directions which are independent of each other. This degeneracy is lifted by quantum fluctuations and the GS becomes magnetically ordered collinearly as a stripe phase consisting of successive alternating rows (or columns) of parallel spins.

For intermediate values of J_2/J_1 it is now widely accepted that the quantum spin-1/2 J_1–J_2 model on the 2D square lattice has a ground-state (gs) phase diagram showing the above two phases with quasiclassical LRO [viz., a Néel-ordered (π,π) phase at smaller values of J_2/J_1, and a collinear stripe-ordered phase of the columnar $(\pi,0)$ or row $(0,\pi)$ type at larger values of J_2/J_1], separated by an intermediate quantum paramagnetic phase without magnetic LRO in the parameter regime $\alpha^{c1}<J_2/J_1<\alpha^{c2}$, where $\alpha^{c1}\approx0.4$ and $\alpha^{c2}\approx0.6$. The precise nature of the intermediate magnetically disordered phase is still not fully resolved. Suggested candidates include a homogeneous spin-liquid state of various types with no broken symmetry (see, e.g., Ref. 19), or a valence-bond solid (VBS) phase with some broken symmetry. Possible spin-liquid states include a resonating-valence-bond (RVB) state proposed by Anderson,[4] which has been supported more recently by variational quantum Monte Carlo studies.[14] Other studies[7,33–36] have supported a spontaneously dimerized state for the intermediate phase with both translational and rotational symmetry broken, and thus representing a columnar VBS phase. Yet other studies[13,37] have supported instead a plaquette VBS state for the intermediate phase, with translational symmetry broken but with rotational symmetry preserved.

There has also been considerable discussion in recent years as to whether the quantum phase transition between the quasiclassical Néel phase and the magnetically disordered (intermediate paramagnetic) phase in the spin-1/2 J_1–J_2 model on the 2D square lattice is first-order or of continuous second-order type. A particularly intriguing suggestion by Senthil *et al.*[38] is that there is a second-order phase transition in the model between the Néel state and the intermediate disordered state (which these authors argue is a VBS state), which is not described by a Ginzburg-Landau-type critical theory, but is rather described in terms of a deconfined quantum critical point. Such direct second-order quantum phase transitions between two states with different broken symmetries, and which are hence characterized by two seemingly independent order parameters, are difficult to understand within the standard critical theory approach of Ginzburg and Landau, as we indicate below.

Thus, the competition between two such distinct kinds of quantum order associated with different broken symmetries would lead generically in the Ginzburg-Landau scenario to one of only three possibilities: (i) a first-order transition between the two states, (ii) an intermediate region of coexistence between both phases with both kinds of order present, or (iii) a region of intermediate phase with neither of the orders of these two phases present. A direct second-order transition between states of different broken symmetries is only permissible within the standard Ginzburg-Landau critical theory if it arises by an accidental fine tuning of the disparate order parameters to a multicritical point. Thus, for the spin-1/2 J_1–J_2 model on the 2D square lattice and its quantum phase transition suggested by Senthil *et al.*,[38] it would require the completely accidental coincidence (or near coincidence) of the point where the magnetic order parameter (i.e., the staggered magnetization) vanishes for the Néel phase, with the point where the dimer order parameter vanishes for the VBS phase. Since each of these phases has a different broken symmetry (viz., spin-rotation symmetry for the Néel phase and the lattice symmetry for the VBS phase), one would naively expect that each transition is described by its own independent order parameter (i.e., the staggered magnetization for the Néel phase and the dimer order parameter for the VBS phase) and that the two transitions should hence be mutually independent.

By contrast, the "deconfined" type of quantum phase transition postulated by Senthil *et al.*[38] permits direct second-order quantum phase transitions between such states with different forms of broken symmetry. In their scenario the quantum critical points still separate phases characterized by order parameters of the conventional (i.e., in their language, "confining") kind, but their proposed new critical theory involves fractional degrees of freedom (viz., spinons for the spin-1/2 J_1–J_2 model on the 2D square lattice) that interact via an emergent gauge field. For our specific example the order parameters of both the Néel and VBS phases discussed above are represented in terms of the spinons, which themselves become "deconfined" exactly at the critical point. The postulate that the spinons are the fundamental constituents of both order parameters then affords a natural explanation for the direct second-order phase transition between two states of the system that otherwise seem very different on the basis of their broken symmetries.

We note, however, that the deconfined phase transition theory of Senthil *et al.*[38] is still the subject of controversy.

Other authors believe that the phase transition in the spin-1/2 J_1–J_2 model on the 2D square lattice from the Neél phase to the intermediate magnetically disordered phase need not be due to a deconfinement of spinons. For example, Sirker *et al.*[36] have argued on the basis of both spin-wave theory and numerical results from series expansion analyses that this transition is more likely to be a (weakly) first-order transition between the Neél phase and a VBS phase with columnar dimerization. Other authors have also proposed other, perhaps less radical, mechanisms to explain such second-order phase transitions (if they exist) and their seeming disagreement (except by accidental fine tuning) with Ginzburg-Landau theory. What seems clearly to be a minimal requirement is that the order parameters of the two phases with different broken symmetry should be related in some way. Thus, a Ginzburg-Landau-type theory can only be preserved if it contains additional terms in the effective theory that represent interactions between the two order parameters. For example, just such an effective theory has been proposed for the 2D spin-1/2 J_1–J_2 model on the square lattice by Sushkov *et al.*,[39] and further discussed by Sirker *et al.*[36]

From the classical viewpoint frustrated models often exhibit "accidental" degeneracy, and the degree of such degeneracy, which can vary enormously, has become widely viewed as a measure of the frustration. Among the effects that can act to lift any such degeneracy are thermal fluctuations, quantum fluctuations, and such "perturbations" as spin-orbit interactions, spin-lattice couplings, further neglected exchange terms, and impurities, all of which might be present in actual materials. In the present paper we focus particular attention on the role of quantum fluctuations. From the quantum viewpoint such frustrated quantum magnets as the spin-1/2 J_1–J_2 model on the 2D square lattice often have ground states that are macroscopically degenerate. This feature leads naturally to an increased sensitivity of the underlying Hamiltonian to the presence of small perturbations. In particular, the presence in real systems that are well characterized by the J_1–J_2 model, of anisotropies, either in spin space or in real space, naturally raises the issue of how robust the properties of the model are against any such perturbations.

Combining the above two viewpoints, it is clear that it is of particular interest in the study of frustrated quantum magnets to focus special attention on the mechanisms or parameters that are available to us to "tune" or vary the quantum fluctuations that play such a key role in determining their gs phase structures. Apart from changing the spin quantum number or the dimensionality and lattice type of the system, or tuning the relative strengths of the competing exchange interactions, another key mechanism is the introduction of anisotropy into the existing exchange bonds. Such anisotropy can be either in real space[40–45] or in spin space.[46–49]

In order to investigate the effect in real space an interesting generalization of the pure J_1–J_2 model has been introduced recently by Nersesyan and Tsvelik[40] and further studied by other groups including ourselves.[41–45] This generalization, the so-called J_1–J_1'–J_2 model, introduces a spatial anisotropy into the 2D J_1–J_2 model on the square lattice by allowing the NN bonds to have different strengths J_1 and J_1' in the two orthogonal spatial lattice dimensions, while keeping all of the NNN bonds across the diagonals to have the same strength J_2. In previous work of our own[44,45] on this J_1–J_1'–J_2 model we studied the effect of the coupling J_1' on the quasiclassical Néel-ordered and stripe-ordered phases for both the spin-1/2 and spin-1 cases. For the spin-1/2 case,[44] we found the surprising result that there exists a quantum triple point (QTP), below which there is a second-order phase transition between the quasiclassical Néel and columnar stripe-ordered phases with magnetic LRO, whereas only above this point are these two phases separated by the intermediate magnetically disordered phase seen in the pure spin-1/2 J_1–J_2 model on the 2D square lattice (i.e., at $J_1'=J_1$). We found that the quantum critical points for both of the quasiclassical phases with magnetic LRO increase as the coupling ratio J_1'/J_1 is increased, and an intermediate phase with no magnetic LRO emerges only when $J_1'/J_1 \gtrsim 0.6$, with strong indications of a quantum triple point at $J_1'/J_1=0.60\pm0.03$, $J_2/J_1=0.33\pm0.02$. For $J_1'/J_1=1$, the results agree with the previously known results of the J_1–J_2 model described above.

In the present paper we generalize the spin-1/2 J_1–J_2 model on the 2D square lattice in a different direction by allowing the bonds to become anisotropic in spin space rather than in real space. Such spin anisotropy is relevant experimentally, as well as theoretically, since it is likely to be present, if only weakly, in any real material. Furthermore, the intermediate magnetically disordered phase is likely to be particularly sensitive to *any* tuning of the quantum fluctuations, as we have seen above in the case of spatial anisotropy. Indeed, other evidence indicates that the intermediate phase might even disappear altogether in certain situations, such as increasing the dimensionality or the spin quantum number.

Thus, for example, the influence of frustration and quantum fluctuations on the magnetic ordering in the GS of the spin-1/2 J_1–J_2 model on the body-centered cubic (bcc) lattice has been studied using exact diagonalization of small lattices and linear spin-wave theory,[50] and also by using linked-cluster series expansions.[51] Contrary to the results for the corresponding model on the square lattice, it was found for the bcc lattice that frustration and quantum fluctuations do not lead to a quantum disordered phase for strong frustration. Rather, the results of all approaches suggest a first-order quantum phase transition at a value $J_2/J_1 \approx 0.70$ from the quasiclassical Néel phase at low J_2 to a quasiclassical collinear phase at large J_2. Similarly, the intermediate phase can also disappear when the spin quantum number s is increased for the J_1–J_2 model on the 2D square lattice. Thus, we[45] found no evidence for a magnetically disordered state (for larger values of J_2/J_1) for the $s=1$ case, in contrast with the $s=1/2$ case.[44] Instead, we found a quantum tricritical point in the $s=1$ case of the J_1–J_1'–J_2 model on the 2D square lattice at $J_1'/J_1=0.66\pm0.03$, $J_2/J_1=0.35\pm0.02$, where a line of second-order phase transitions between the quasiclassical Néel and columnar stripe-ordered phases (for $J_1'/J_1 \lesssim 0.66$) meets a line of first-order phase transitions between the same two phases (for $J_1'/J_1 \gtrsim 0.66$).

As in our previous work[44,45] involving the effect of spatial anisotropy on the spin-1/2 and spin-1 J_1–J_2 models on the 2D square lattice, we again employ the CCM to investigate now the effect on the same model of spin anisotropy. The

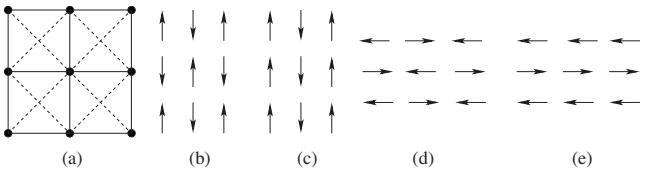

FIG. 1. (a) The J_1^{XXZ}–J_2^{XXZ} Heisenberg model; —J_1; - - - J_2; (b) and (c) z-aligned states for the Néel and stripe columnar phases, respectively; (d) and (e) planar x-aligned states for the Néel and stripe columnar phases, respectively. Arrows in (b), (c), (d), and (e) represent spins situated on the sites of the square lattice [symbolized by ● in (a)].

CCM is one of the most powerful techniques in microscopic quantum many-body theory.[52,53] It has been applied successfully to many quantum magnets.[27,54–59] It is capable of calculating with high accuracy the ground- and excited-state properties of spin systems. In particular, it is an effective tool for studying highly frustrated quantum magnets, where such other numerical methods as the quantum Monte Carlo method and the exact diagonalization method are often severely limited in practice, e.g., by the "minus-sign problem" and the very small sizes of the spin systems that can be handled in practice with available computing resources, respectively.

II. THE MODEL

The usual 2D spin-1/2 J_1–J_2 model is an isotropic Heisenberg model on a square lattice with two kinds of exchange bonds, with strength J_1 for the NN bonds along both the row and the column directions, and with strength J_2 for the NNN bonds along the diagonals, as shown in Fig. 1(a).

Here we generalize the model by including an anisotropy in spin space in both the NN and NNN bonds. We are aware of only a very few earlier investigations with a similar goal.[46–48] The two most detailed have studied the extreme limits, where either the frustrating NNN interaction becomes anisotropic but the NN interaction remains isotropic[46] (viz., the J_1–J_2^{XXZ} model) and the opposite case where the NN interaction becomes anisotropic but the NNN interaction remains isotropic[47] (viz., the J_1^{XXZ}–J_2 model). In real materials one might expect both exchange interactions to become anisotropic. To our knowledge the only study of this case[48] (viz., the J_1^{XXZ}–J_2^{XXZ} model) has been done using the rather crude tool of (linear or) lowest-order spin-wave theory (LSWT), from which it is notoriously difficult to draw any firm quantitative conclusions about the positions of the gs phase boundaries of a system. It is equally difficult to use LSWT to predict with confidence either the number of phases present in the gs phase diagram or the nature of the quantum phase transitions between them. We comment further on the application of spin-wave theory to the J_1–J_2 model and its generalizations in Sec. V. The aim of the present paper is to use the CCM, as a much more accurate many-body tool, to investigate the spin-1/2 J_1^{XXZ}–J_2^{XXZ} model on the 2D square lattice.

In order to keep the size of the parameter space manageable the anisotropy parameter Δ is assumed to be the same in both exchange terms, thus yielding the so-called J_1^{XXZ}–J_2^{XXZ} model, whose Hamiltonian is described by

$$H = J_1 \sum_{\langle i,j \rangle} (s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z) + J_2 \sum_{\langle\langle i,k \rangle\rangle} (s_i^x s_k^x + s_i^y s_k^y + \Delta s_i^z s_k^z), \tag{1}$$

where the sums over $\langle i,j \rangle$ and $\langle\langle i,k \rangle\rangle$ run over all NN and NNN pairs, respectively, counting each bond once and once only. We are interested only in the case of competing antiferromagnetic bonds, $J_1 > 0$ and $J_2 > 0$, and henceforth, for all of the results shown in Sec. IV, we set $J_1 = 1$. Similarly, we shall be interested essentially only in the region $\Delta > 0$ (although for reasons discussed below in Sec. IV we shall show results also for small negative values of Δ).

This model has two types of classical antiferromagnetic ground states, namely a z-aligned state for $\Delta > 1$ and an xy-planar-aligned state for $0 < \Delta < 1$. Since all directions in the xy plane in spin space are equivalent, we may choose the direction arbitrarily to be the x direction, say. Both of these z-aligned and x-aligned states further divide into a Néel (π, π) state and stripe states [columnar stripe $(\pi, 0)$ and row stripe $(0, \pi)$], the spin orientations of which are shown in Figs. 1(b)–1(e), accordingly. There is clearly a symmetry under the interchange of rows and columns, which implies that we need only consider the columnar stripe states. The (first-order) classical phase transition occurs at $J_2^c = \frac{1}{2} J_1$, with the Néel states being the classical GS for $J_2 < \frac{1}{2} J_1$, and the columnar stripe states being the classical GS for $J_2 > \frac{1}{2} J_1$.

III. THE COUPLED CLUSTER METHOD

We briefly outline the CCM formalism (and see Refs. 27 and 52–59 for further details). The first step of any CCM calculation is to choose a normalized model (or reference) state $|\Phi\rangle$, which can act as a cyclic vector with respect to a complete set of mutually commuting multiconfigurational creation operators, $C_I^+ \equiv (C_I^-)^\dagger$. The index I here is a set-index that labels the many-particle configuration created in the state $C_I^+ |\Phi\rangle$. The requirements are that any many-particle state can be written exactly and uniquely as a linear combination of the states $\{C_I^+ |\Phi\rangle\}$, together with the conditions,

$$\langle \Phi | C_I^+ = 0 = C_I^- | \Phi \rangle \quad \forall\, I \neq 0; \quad C_0^+ \equiv 1, \tag{2}$$

$$[C_I^+, C_J^+] = 0 = [C_I^-, C_J^-]. \tag{3}$$

The Schrödinger equations for the many-body gs ket and bra states are

$$H|\Psi\rangle = E|\Psi\rangle, \tag{4a}$$

$$\langle \tilde{\Psi} | H = E \langle \tilde{\Psi} |, \tag{4b}$$

respectively, with normalization chosen such that $\langle \tilde{\Psi} | \Psi \rangle = 1$ [i.e., with $\langle \tilde{\Psi} | = (\langle \Psi | \Psi \rangle)^{-1} \langle \Psi |$], and with $|\Psi\rangle$ itself satisfying the intermediate normalization condition $\langle \Phi | \Psi \rangle = 1 = \langle \Phi | \Phi \rangle$. In terms of the set $\{|\Phi\rangle; C_I^+\}$, the CCM employs the exponential parametrization

$$|\Psi\rangle = e^S|\Phi\rangle, \quad S = \sum_{I\neq 0} \mathcal{S}_I C_I^+ \tag{5a}$$

for the exact gs ket energy eigenstate. Its counterpart for the exact gs bra energy eigenstate is chosen as

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

It is important to note that while the parametrizations of Eqs. (5a) and (5b) are not manifestly Hermitian conjugate, they do preserve the important Hellmann-Feynman theorem at all levels of approximation (viz., when the complete set of many-particle configurations $\{I\}$ is truncated).[53] Furthermore the amplitudes $(\mathcal{S}_I, \tilde{\mathcal{S}}_I)$ form canonically conjugate pairs in a time-dependent version of the CCM, in contrast with the pairs $(\mathcal{S}_I, \mathcal{S}_I^*)$, coming from a manifestly Hermitian-conjugate representation for $\langle\tilde{\Psi}| = (\langle\Phi|e^{S^\dagger}e^S|\Phi\rangle)^{-1}\langle\Phi|e^{S^\dagger}$, that are *not* canonically conjugate to one another.[53]

The static gs CCM correlation operators, S and $\tilde{S}$, contain the real c-number correlation coefficients, $\mathcal{S}_I$ and $\tilde{\mathcal{S}}_I$, that need to be calculated. Clearly, once the coefficients $\{\mathcal{S}_I, \tilde{\mathcal{S}}_I\}$ are known, all other gs properties of the many-body system can be derived from them. To find the gs correlation coefficients we simply insert the parametrizations of Eqs. (5a) and (5b) into the Schrödinger Eqs. (4a) and (4b) and project onto the complete sets of states $\langle\Phi|C_I^-$ and $C_I^+|\Phi\rangle$, respectively. Completely equivalently, we may simply demand that the gs energy expectation value, $\bar{H} \equiv \langle\tilde{\Psi}|H|\Psi\rangle$, is minimized with respect to the entire set $\{\mathcal{S}_I, \tilde{\mathcal{S}}_I\}$. In either case we are easily led to the equations

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

$$\langle\Phi|\tilde{S}e^{-S}[H, C_I^+]e^S|\Phi\rangle = 0; \quad \forall\, I \neq 0, \tag{6b}$$

which we then solve for the set $\{\mathcal{S}_I, \tilde{\mathcal{S}}_I\}$. Equation (6a) shows that the gs energy at the stationary point has the simple form

$$E = E(\{\mathcal{S}_I\}) = \langle\Phi|e^{-S}He^S|\Phi\rangle. \tag{7}$$

It is important to realize that this (bi-)variational formulation does not necessarily lead to an upper bound for E when the summations for S and $\tilde{S}$ in Eqs. (5a) and (5b) are truncated, due to the lack of manifest Hermiticity when such approximations are made. Nonetheless, one can prove[53] that the important Hellmann-Feynman theorem *is* preserved in all such approximations.

We note that Eq. (6a) represents a coupled set of nonlinear multinomial equations for the c-number correlation coefficients $\{\mathcal{S}_I\}$. The nested commutator expansion of the similarity-transformed Hamiltonian,

$$e^{-S}He^S = H + [H,S] + \frac{1}{2!}[[H,S],S] + \cdots, \tag{8}$$

and the fact that all of the individual components of S in the expansion of Eq. (5a) commute with one another by construction [and see Eq. (3)] together imply that each element of S in Eq. (5a) is linked directly to the Hamiltonian in each of the terms in Eq. (8). Thus, each of the coupled Eq. (6a) is of Goldstone *linked-cluster* type. In turn, this guarantees that all extensive variables, such as the energy, scale linearly with particle number, N. Thus, at any level of approximation obtained by truncation in the summations on the index I in Eqs. (5a) and (5b), we may (and do) always work from the outset in the limit $N \to \infty$ of an infinite system.

Furthermore, each of the linked-cluster Eq. (6a) is of finite length when expanded, since the otherwise infinite series of Eq. (8) will always terminate at a finite order, provided only (as is usually the case, including that of the Hamiltonian considered here) that each term in the Hamiltonian, H, contains a finite number of single-particle destruction operators defined with respect to the reference (vacuum) state $|\Phi\rangle$. Hence the CCM parametrization naturally leads to a workable scheme that can be computationally implemented in a very efficient manner.

Before discussing the possible CCM truncation schemes, we note that it is very convenient to treat the spins on each lattice site in a chosen model state $|\Phi\rangle$ as equivalent. In order to do so we introduce a different local quantization axis and a correspondingly different set of spin coordinates on each site, so that all spins, whatever their original orientations in $|\Phi\rangle$ in a global spin-coordinate system, align along the negative z direction, say, in these local spin coordinates. This can always be done by defining a suitable rotation in spin space of the global spin coordinates at each lattice site. Such rotations are canonical transformations that leave the spin commutation relations unchanged. In these local spin axes where the configuration indices I simply become a set of lattice site indices, $I \to \{k_1, k_2, \cdots k_m\}$, the generalized multiconfigurational creation operators C_I^+ are simple products of single spin-raising operators, $C_I^+ \to s_{k_1}^+ s_{k_2}^+ \cdots s_{k_m}^+$, where $s_k^\pm \equiv s_k^x \pm i s_k^y$, and (s_k^x, s_k^y, s_k^z) are the usual SU(2) spin operators on lattice site k. For the quasiclassical magnetically ordered states that we calculate here, the order parameter is the sublattice magnetization, M, which is given within our local spin coordinates defined above as

$$M \equiv -\frac{1}{N}\langle\tilde{\Psi}|\sum_{k=1}^{N} s_k^z|\Psi\rangle. \tag{9}$$

It is usually convenient to take the classical ground states as our (initial) choices for the model state $|\Phi\rangle$. Hence, we may choose here either a Néel state or a (columnar) stripe state for $|\Phi\rangle$. Each of these can be further subdivided into a z-aligned choice or a planar (say, x-aligned) choice, which we expect to be appropriate for $\Delta > 1$ and $|\Delta| < 1$, respectively, on purely classical grounds. We present results below in Sec. IV based on all four of these classical ground states as choices for $|\Phi\rangle$.

Clearly the CCM formalism is exact when one includes all possible multispin configurations I in the sums in Eqs. (5a) and (5b) for the cluster correlation operators S and $\tilde{S}$. In practice, however, truncations are needed. As in much of our previous work for spin-half models we employ here the so-called LSUBn scheme,[27,52–59] in which all possible multispin-flip correlations over different locales on the lattice defined by n or fewer contiguous lattice sites are retained.

TABLE I. Numbers of fundamental configurations (# f.c.) retained in the CCM LSUBn approximation for the z-aligned states and the planar x-aligned states of the $s=1/2$ $J_1^{XXZ}-J_2^{XXZ}$ model.

	z-aligned states # f.c.		Planar x-aligned states # f.c.	
Scheme	Néel	stripe	Néel	stripe
LSUB2	1	1	1	2
LSUB4	7	9	10	18
LSUB6	75	106	131	252
LSUB8	1287	1922	2793	5532
LSUB10	29605	45825	74206	148127

(Two sites are defined to be contiguous here if they are NN sites on the lattice.) The numbers of such fundamental configurations (viz., those that are distinct under the symmetries of the Hamiltonian and of the model state $|\Phi\rangle$) that are retained for the z-aligned and planar x-aligned states of the current model in their Néel and stripe phases in the various LSUBn approximations are shown in Table I.

Parallel computing is employed to solve the corresponding coupled sets of CCM bra- and ket-state Eqs. (6a) and (6b).[60] Our computing power is such that we can obtain LSUBn results for $n=\{2,4,6,8,10\}$ for both the z-aligned model states and the x-aligned model states, as shown in Table I. However the very large numbers of fundamental configurations retained in the latter case at the LSUB10 level is only possible with supercomputing resources. For example, the solution of the equations involving the nearly 150 000 fundamental configurations for the stripe phase of the planar x-aligned state required the simultaneous use of 600 processors running for approximately 6 h, for each value of the anisotropy parameter Δ in the Hamiltonian of Eq. (1).

The final step in any CCM calculation is then to extrapolate the approximate LSUBn results to the exact, $n\to\infty$, limit. Although no fundamental theory is known on how the LSUBn data for such physical quantities as the gs energy per spin, E/N, and the gs staggered magnetization, M, scale with n in the $n\to\infty$, limit, we have a great deal of experience in doing so from previous calculations.[27,28,44,45,54,55,58,59,61] Thus, we employ here the same well-tested LSUBn scaling laws as we have used, for example, for the $J_1-J_1'-J_2$ model,[44,45] namely

$$E/N = a_0 + a_1 n^{-2} + a_2 n^{-4} \tag{10}$$

for the gs energy per spin, and

$$M = b_0 + n^{-0.5}(b_1 + b_2 n^{-1}) \tag{11}$$

for the gs staggered magnetization, both of which have been successfully used previously for systems showing an order-disorder quantum phase transition. An alternative leading power-law extrapolation scheme for the order parameter,

$$M = c_0 + c_1 n^{-c_2}, \tag{12}$$

has also been successfully used previously to determine the phase transition points. For most systems with order-disorder transitions the two extrapolation schemes of Eqs. (11) and (12) give remarkably similar results almost everywhere, as demonstrated explicitly, for example, for the case of quasi-one-dimensional quantum Heisenberg antiferromagnets with a weak interchain coupling.[61] However, in regions very near quantum triple points the form of Eq. (11) is more robust than that of Eq. (12) due to the addition of the next-to-leading correction term, as has been explained in detail elsewhere.[44] Hence, in this work we use the extrapolation schemes of Eqs. (10) and (11).

Obviously, better results are obtained from the LSUBn extrapolation schemes if the data with the lowest n values are not used in the fits. However, a robust and stable fit to any fitting formula with m unknown parameters is generally only obtained by using at least $(m+1)$ data points. In particular, a fit to only m data points should be avoided whenever possible. In our case both fitting schemes in Eqs. (10) and (11) have $m=3$ unknown parameters to be determined. For all four model states we have LSUBn data with $n=\{2,4,6,8,10\}$, and it is clear that the optimal fits should be obtained using the sets $n=\{4,6,8,10\}$. All the extrapolated results that we present below in Sec. IV are obtained in precisely this way. However, we have also extrapolated E/N and M using the sets $n=\{2,4,6,8,10\}$, $n=\{2,4,6,8\}$, and $n=\{4,6,8\}$. In almost all cases they lead to very similar results, which adds credence to the stability of our numerical results and to the validity of our conclusions presented below.

IV. RESULTS

Figure 2 shows the extrapolated results for the gs energy per spin as a function of J_2 (with $J_1=1$) for various values of Δ, for the z-aligned and planar x-aligned model states. For each model state, two sets of curves are shown, one (for smaller values of J_2) using the Néel state, and the other (for larger values of J_2) using the stripe state. As we have discussed in detail elsewhere,[53,54,57] the coupled sets of LSUBn [Eqs. (6a) and (6b)] have natural termination points (at least for values $n>2$) for some critical value of a control parameter (here the anisotropy, Δ), beyond which no real solutions to the equations exist. The extrapolation of such LSUBn termination points for fixed values of Δ to the $n\to\infty$ limit can sometimes be used as a method to calculate the physical phase boundary for the phase with ordering described by the coupled cluster method (CCM) model state being used. However, since other methods exist to define the phase transition points, which are usually more precise and more robust for extrapolation (as we discuss below), we have not attempted such an analysis here.

Instead, in Fig. 2, the $E_{\max}$ points shown, for each set of calculations based on one of the four CCM model states used, are either those natural termination points described above for the highest (LSUB10) level of approximation we have implemented, or the points where the ground-state (gs) energy becomes a maximum should the latter occur first (i.e., as one approaches the termination point). The advantage of this usage of the $E_{\max}$ points is that we do not then display gs energy data in any appreciable regimes where LSUBn calcu-

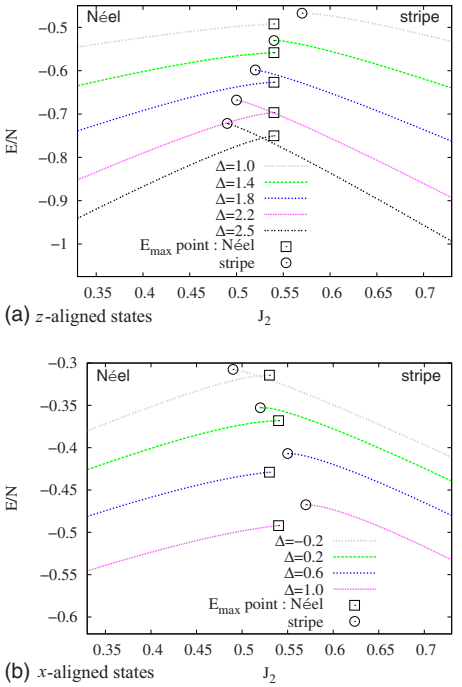

FIG. 2. (Color online) Extrapolated CCM LSUBn results using (a) the z-aligned and (b) the planar x-aligned states for the gs energy per spin, E/N, for the Néel and stripe phases of the $s=1/2$ $J_1^{XXZ}-J_2^{XXZ}$ model. The LSUBn results are extrapolated in the limit $n\to\infty$ using the sets $n=\{4,6,8,10\}$ for both the z-aligned states and the planar x-aligned states. The NN exchange coupling $J_1=1$. The meaning of the $E_{\max}$ points shown is described in the text.

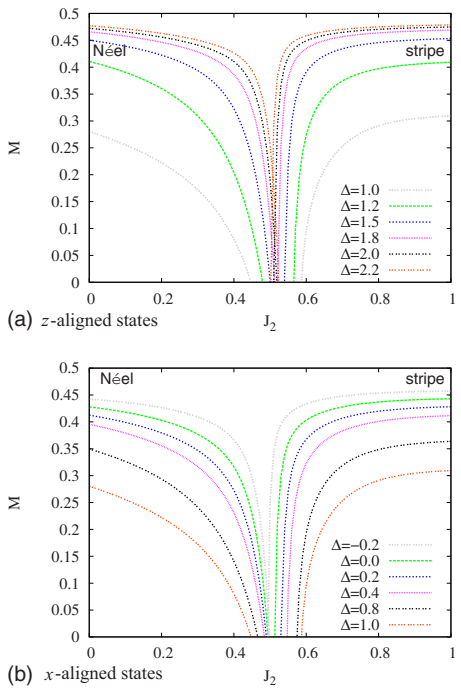

FIG. 3. (Color online) Extrapolated CCM LSUBn results using (a) the z-aligned and (b) the planar x-aligned states for the gs staggered magnetization, M, for the Néel and stripe phases of the $s=1/2$ $J_1^{XXZ}-J_2^{XXZ}$ model. The LSUBn results are extrapolated in the limit $n\to\infty$ using the sets $n=\{4,6,8,10\}$ for both the z-aligned states and the planar x-aligned states. The NN exchange coupling $J_1=1$.

lations with very large values of n (higher than can feasibly be implemented) would not have solutions, by dint of having terminated already.

Curves such as those shown in Fig. 2(a) illustrate very clearly that the corresponding pairs of gs energy curves for the z-aligned Néel and stripe phases cross one another for all values of Δ above some critical value, $\Delta\gtrsim 2.1$. The crossings occur with a clear discontinuity in slope, as is completely characteristic of a first-order phase transition, exactly as observed in the classical (i.e., $s\to\infty$) case. Furthermore, the direct first-order phase transition between the z-aligned Néel and stripe phases that is thereby indicated for all values of $\Delta\gtrsim 2.1$, occurs (for all such values of Δ) very close to the classical phase boundary $J_2=\frac{1}{2}$, the point of maximum (classical) frustration. Conversely, curves such as those shown in Fig. 2(a) for values of Δ in the range $1<\Delta\lesssim 2.1$ also illustrate clearly that the corresponding pairs of gs energy curves for the z-aligned Néel and stripe phases do not intersect one another. In this regime we thus have clear preliminary evidence for the opening up of an intermediate phase between the Néel and stripe phases. The corresponding curves in Fig. 2(b) for values of $\Delta<1$ tell a similar story, with an intermediate phase similarly indicated to exist between the xy-planar-aligned Néel and stripe phases for values of Δ in the range $-0.1\lesssim\Delta<1$.

We show in Fig. 3 corresponding indicative sets of CCM results, based on the same four model states, for the gs order parameter (viz., the staggered magnetization), to those shown in Fig. 2 for the gs energy. The staggered magnetization data completely reinforce the phase structure of the model as deduced above from the gs energy data. Thus, let us now denote by M_c the quantum phase transition point deduced from curves such as those shown in Fig. 3, where M_c is defined to be either (a) the point where corresponding pairs of CCM staggered magnetization curves (for the same value of Δ), based on the Néel and stripe model states, intersect one another if they do so at a physical value $M\geq 0$—or (b) if they do not so intersect at a value $M\geq 0$, the two points where the corresponding values of the staggered magnetization go to zero.

Clearly, case (a) here corresponds to a direct phase transition between the Néel and stripe phases, which will generally be first order if the intersection point has a value $M\neq 0$ (and, exceptionally, second order, if the crossing occurs exactly at $M=0$). On the other hand, case (b) corresponds to the situation where the points where the long-range order (LRO) vanishes for both quasiclassical (i.e., Néel-ordered and stripe-ordered) phases are, at least naively, indicative of a second-order phase transition from each of these phases to some unknown intermediate magnetically disordered phase. We return to a discussion of the actual order of such transitions in Sec. V. In summary, we hence define the staggered magnetization criterion for a quantum critical point as the point where there is an indication of a phase transition between the two states by their order parameters becoming equal, or where the order parameter vanishes, whichever occurs first. A detailed discussion of this order parameter criterion and its relation to the stricter energy crossing criterion may be found elsewhere.[59]

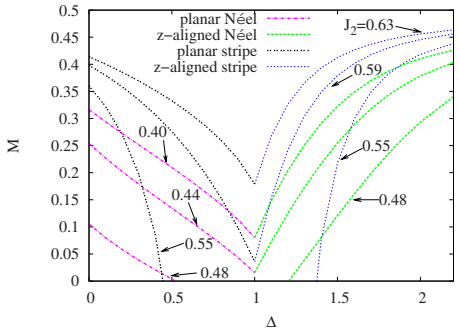

FIG. 4. (Color online) Extrapolated CCM LSUBn results using the z-aligned and planar x-aligned states for the staggered magnetization versus the anisotropy Δ for the $s=1/2$ $J_1^{XXZ}-J_2^{XXZ}$ model, for the NN exchange coupling $J_1=1$. The LSUBn results are extrapolated in the limit $n\to\infty$ using the sets $n=\{4,6,8,10\}$ for both the z-aligned model states and the planar x-aligned model states.

From curves such as those shown in Fig. 3(a) we see that for $\Delta\lesssim 1.95$ for the z-aligned states, there exists an intermediate region between the critical points at which $M\to 0$ for the Néel and stripe phases. Conversely, for $\Delta\gtrsim 1.95$ the two curves for the order parameters M of the quantum Néel and stripe phases for the same value of Δ meet at a finite value, $M>0$, as is typical of a first-order transition. Similarly, Fig. 3(b) shows that for the planar x-aligned states, there exists an intermediate region between the critical points at which $M\to 0$ for the Néel and stripe phases for all values of Δ in the range $-0.15\lesssim\Delta<1$. Again, the two curves for the order parameters M of the Néel and stripe phases for the same value of Δ intersect at a value $M>0$ for $\Delta\lesssim -0.15$. In order to show more explicitly how the quantum phase transitions are driven by anisotropy, Δ, we display the same data for the extrapolated results for the order parameter, M, somewhat differently in Fig. 4, where we plot M as a function of Δ for various values of J_2 around the value $J_2=0.5$, corresponding to the point of maximum (classical) frustration.

By putting together data of the sort shown in Figs. 2–4 we are able to deduce the gs phase diagram of our 2D spin-1/2 $J_1^{XXZ}-J_2^{XXZ}$ model on the square lattice, from our CCM calculations based on the four model states with quasiclassical antiferromagnetic LRO (viz., the Néel and stripe states for both the z-aligned and planar xy-aligned cases).

We show in Fig. 5 the zero-temperature gs phase diagram, as deduced from the order parameter criterion, and using our extrapolated LSUBn data sets with $n=\{4,6,8,10\}$, shown as the critical value J_2^c for the next-nearest-neighbor (NNN) exchange coupling J_2 as a function of anisotropy Δ [with nearest-neighbor (NN) exchange coupling strength $J_1=1$]. Very similar results are obtained from using the energy criterion, where it can be applied (viz., along the transition lines between quasiclassical states with magnetic LRO). In order to test the accuracy of our results, particularly the positions of the phase boundaries shown in Fig. 5, we have also performed extrapolations using the LSUBn data sets with $n=\{2,4,6,8,10\}$, $n=\{2,4,6,8\}$, and $n=\{4,6,8\}$ for both the energy criterion and the order parameter criterion. In general terms we find that the results are remarkably robust, and the error bars quoted below are based on such an analysis.

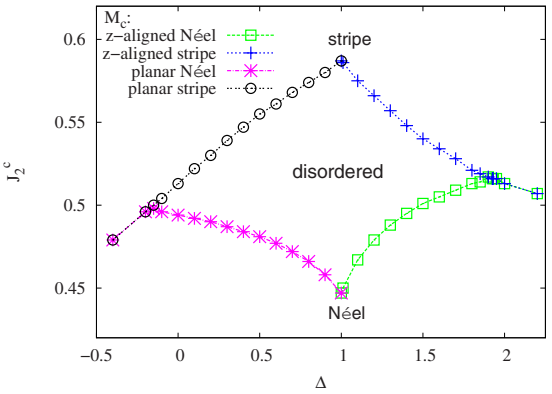

FIG. 5. (Color online) Extrapolated CCM LSUBn results using the z-aligned and planar x-aligned states for the ground-state phase diagram of the $s=1/2$ $J_1^{XXZ}-J_2^{XXZ}$ model, for the NN exchange coupling $J_1=1$. The LSUBn results for the staggered magnetization are extrapolated to the limit $n\to\infty$ using the sets $n=\{4,6,8,10\}$ for both the z-aligned model states and the planar x-aligned model states. $M_c\equiv$ magnetization critical point, defined in the text.

For the case of the z-aligned states, all of our results provide clear and consistent evidence for an upper *quantum triple point* (QTP) at $(\Delta^c=2.05\pm 0.15,\ J_2^c=0.530\pm 0.015)$ (for $J_1=1$). For $1<\Delta\lesssim 2.0$, there exists an intermediate paramagnetic (magnetically disordered) quantum phase, separating the Néel and stripe phases. This intermediate phase disappears for $\Delta\gtrsim 2.0$, and both our energy and order parameter criteria give clear and unequivocal evidence for a direct first-order quantum phase transition between the two quasiclassical antiferromagnetic states in this regime, just as in the corresponding classical model (i.e., with $s\to\infty$). The phase boundary approaches the classical line $J_2^c=0.5$ as $\Delta\to\infty$.

Similarly, for the case of the xy-planar-aligned phases, a second (lower) QTP occurs at $(\Delta^c=-0.10\pm 0.15,\ J_2^c=0.505\pm 0.015)$ (for $J_1=1$), with an intermediate disordered phase existing in the region $-0.1\lesssim\Delta<1$. The z-aligned and xy-planar-aligned phases meet precisely at $\Delta=1$, just as in the classical case. Exactly at the isotropic point $\Delta=1$, where the model becomes just the original J_1-J_2 model, the disordered phase exists for the largest range of values of J_2, $J_2^{c1}<J_2<J_2^{c2}$, as can be clearly seen from Fig. 5. For the pure J_1-J_2 model our calculations yield the values $J_2^{c1}/J_1=0.44\pm 0.01$ and $J_2^{c2}/J_1=0.59\pm 0.01$ that demarcate the phase boundaries for the disordered phase, in complete agreement with both our own earlier work and that of others that we have already discussed in Sec. I.

V. DISCUSSION AND CONCLUSIONS

We have shown in detail how, as expected, the quantum fluctuations present in the spin-1/2 J_1-J_2 model on the two-dimensional (2D) square lattice, that has become an archetypal model for studying the interplay between quantum fluctuations and frustration, can be tuned by the introduction of spin anisotropy. We have clearly confirmed our prior expectation that anisotropy reduces the quantum fluctuations.

Thus, for both the cases $\Delta > 1$ and $0 < \Delta < 1$, the intermediate paramagnetic phase present in the pure J_1–J_2 model is observed to shrink to a smaller range of values of J_2/J_1 centered near to the point of maximal classical frustration, $J_2^c/J_1 = \frac{1}{2}$, that marks the classical phase boundary between the Néel-ordered and collinear stripe-ordered phases.

We have seen that the intermediate disordered phase disappears precisely at two quantum triple points at $\Delta^c = -0.10 \pm 0.15$ and $\Delta^c = 2.05 \pm 0.15$, and that for values of Δ outside the range spanned by these values the intermediate phase is totally absent. In particular, for $\Delta \gtrsim 2.0$ we find unequivocal evidence for a first-order phase transition between the Néel and collinear stripe phases. This direct first-order phase transition between states of different quasiclassical antiferromagnetic ordering is very similar to what has been observed in another similar extension of the spin-1/2 J_1–J_2 model on a square lattice, namely the so-called J_1–J_2–$J_\perp$ model on a stacked square lattice, where we now introduce a (weak) interlayer coupling through NN bonds of strength $J_\perp$. The quantum fluctuations in the J_1–J_2 model are tuned here by the parameter $J_\perp$. An analysis of this model[59] found that the intermediate region of disordered paramagnetic phase, $\alpha^{c1} < J_2/J_1 < \alpha^{c2}$, in the pure J_1–J_2 model now shrinks as the interlayer coupling strength $J_\perp$ is increased. The second-order phase transition for the Néel-ordered phase to the paramagnetic phase disappears for $J_\perp/J_1$ above some critical value (estimated to be in the range 0.2–0.3) marking a QTP in the J_2–$J_\perp$ plane (with $J_1 \equiv 1$). Above the QTP there is again a direct first-order phase transition between the two phases of different quasiclassical antiferromagnetic LRO.

On the other hand this scenario of a first-order phase transition between the two states of different quasiclassical LRO may be contrasted with the situation observed in yet another generalization of the pure spin-1/2 J_1–J_2 model on a square lattice, namely the so-called J_1–J_1'–J_2 model that we have briefly discussed in Sec. I. In this case the quantum fluctuations are tuned by introducing a spatial anisotropy so that the NN bonds have different strengths in the intrachain (J_1) and interchain (J_1') directions on the square lattice. A similar CCM analysis of the spin-1/2 version of this model by some of the present authors[44] again found a QTP in the J_2–J_1' plane (with $J_1 \equiv 1$), now below which the disordered paramagnetic phase disappears, and there is again a direct phase transition between the quasiclassical Néel and stripe-ordered phases with magnetic LRO. However, the surprising situation found here was the existence of strong evidence for the phase transition in this case to be second order, and hence inexplicable by standard Ginzburg-Landau theory, as discussed more fully in Sec. I above.

Having discussed the transition line between the two phases of quasiclassical antiferromagnetic LRO in the phase diagram in the J_2–Δ plane of our spin-1/2 J_1^{XXZ}–J_2^{XXZ} model on the 2D square lattice, we turn our attention to the four phase boundary lines shown in Fig. 5 that delimit the region of existence for the intermediate disordered paramagnetic phase. As has been explained in Ref. 59 a judicious combination of the CCM energy data with the CCM order parameter data can shed light on the nature of the phase transitions between the quasiclassically long-range-ordered phases and the paramagnetic phase. The method for so doing relies essentially on the fact that although we perform our CCM calculations with model (or reference) states with quasiclassical LRO, one knows[12,54,55,58] that one can also reliably use such calculations in parameter regimes where all semblance of the quasiclassical LRO is destroyed. Thus, what is required for the CCM equations to converge to a solution is a sufficient overlap between the wave functions of the model (reference) state $|\Phi\rangle$ and the true ground state (GS) $|\Psi\rangle$. The termination points of the CCM LSUBn equations discussed above are indicators of where this condition breaks down. Thus, provided that the CCM LSUBn equations converge and yield extrapolated solutions far enough beyond the points M_c, where the order parameter vanishes, we can also determine whether the solution based on the Néel-ordered or the stripe-ordered model state has lower energy.

We find in this way that there are indicators of a very narrow region where the gs energy obtained with the Néel model state might be slightly lower in energy than that obtained with the collinear striped model state, even in regions (close to) where the Néel order parameter has already gone to zero, but where the stripe order parameter is still nonzero. As explained in more detail in Ref. 59, the use of this evidence here points toward the zero-temperature phase transitions from Néel LRO to quantum paramagnetic disorder being second order, while the transitions from quantum paramagnetic disorder to collinear stripe order are possibly (rather weakly) first order rather than second order. We stress, however, that the analysis here is very sensitive to the accuracy of our results, and the evidence for the nature of these quantum phase transitions involving the quantum paramagnetic state in the regime $-0.1 \lesssim \Delta \lesssim 2.0$ is less compelling than that for the transition between the two quasiclassically ordered states being first order in the regime $\Delta \gtrsim 2.0$.

The only other analysis of the current spin-1/2 J_1^{XXZ}–J_2^{XXZ} model on the square lattice of which we are aware[48] has been performed at the very low level of lowest-order spin-wave theory (LSWT). For the case studied here of equal spin-anisotropy parameters in the NN and NNN exchange bonds, these authors have only investigated the case $\Delta > 1$, for which they find an (upper) QTP at a very small value of the anisotropy parameter, $\Delta_{(u)}^c \approx 1.048$, much smaller than the corresponding value $\Delta_{(u)}^c = 2.05 \pm 0.15$ obtained by us for the upper QTP. Such an extreme fragility or sensitivity of the paramagnetic phase to spin anisotropy is not easy to understand. In the face of our own much more accurate calculations it would seem simply to be an artifact of the LSWT approximation. On the other hand, the LSWT analysis does give the same qualitative trends as found by us for the phase transitions in the range $\Delta > 1$, viz., a second-order transition between the Néel-ordered and disordered phases, and a first-order transition between the disordered and collinear stripe-ordered phases for $1 < \Delta < \Delta_{(u)}^c$, and a direct first-order transition between the Néel-ordered and collinear stripe-ordered phases for $\Delta > \Delta_{(u)}^c$.

It is perhaps worth noting at this point in the context of spin-wave theory (SWT) that Igarashi[11] has shown that whereas its lowest-order (or linear) version (LSWT) works quite well when applied to the isotropic Heisenberg model with NN couplings only, it consistently overestimates the quantum fluctuations in the pure (isotropic) J_1–J_2 model as

the frustration J_2/J_1 increases. Thus, he showed by going to higher orders in SWT in powers of $1/s$, where LSWT is the leading order, that the expansion converges reasonably well for values of $\alpha \equiv J_2/J_1 \lesssim 0.35$, but for larger values of the frustration parameter α, including the point $\alpha=0.5$ of maximum classical frustration, the series loses stability. He showed for the $s=\frac{1}{2}$ J_1-J_2 model that whereas LSWT predicts[6] a value of $\alpha^{c_1} \approx 0.38$ at which the transition from the Néel-ordered phase to the disordered phase occurs, the higher-order corrections to SWT for $\alpha \lesssim 0.4$ make the Néel-ordered phase more stable than predicted by LSWT. This is precisely in agreement with our own predicted value of $\alpha^{c_1} = 0.44 \pm 0.01$ for the $s=\frac{1}{2}$ J_1-J_2 model on the square lattice. He concludes that any predictions from SWT for the J_1-J_2 model on the square lattice are likely to be unreliable for values $J_2/J_1 \gtrsim 0.4$.

For reasons unclear to us, the authors of Ref. 48 never investigated the regime with $\Delta<1$, for which we find a lower QTP at $\Delta^c_{(l)}=-0.10\pm0.15$, $J^c_{2(l)}=0.505\pm0.015$. Clearly, our results are consistent with this lower QTP occurring exactly at the isotropic *XY* point (i.e., $\Delta=0$) of the model, and also exactly at the point of maximal classical frustration, $J_2=\frac{1}{2}$. A more detailed theoretical investigation of the corresponding $J_1^{XX}-J_2^{XX}$ model is clearly warranted by our results.

Finally, we note that in our analysis here we have relied on two of the unique strengths of the CCM, namely its ability to deal with highly frustrated systems as readily as unfrustrated ones, and its use from the outset of infinite lattices. Our own results, presented here, for the gs energy and staggered magnetization of the present model that have been obtained from four sets of independent calculations based on different reference states, provide us with a set of internal checks that lead us to believe that we now have a self-consistent and robust description of this rather challenging model system. However, the model is sufficiently complicated that one might not expect any single method or approach to solve it fully. For that reason alone it would be well worthwhile to apply other high-order many-body techniques to this same system. Nevertheless, we have presented here intriguing results that have been obtained with a method for which a great deal of work over the past decade that has employed it, has shown its ability to describe very reliably the quantum phase transitions present in a wide variety of spin-lattice systems.

ACKNOWLEDGMENTS

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