The spin-$\frac{1}{2}$ $J_1$-$J_2$ model on the body-centered cubic lattice

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Using exact diagonalization (ED) and linear spin wave theory (LSWT) we study the influence of frustration and quantum fluctuations on the magnetic ordering in the ground state of the spin-$\frac{1}{2}$ $J_1$-$J_2$ Heisenberg antiferromagnet ($J_1$-$J_2$ model) on the body-centered cubic (bcc) lattice. Contrary to the $J_1$-$J_2$ model on the square lattice, we find for the bcc lattice that frustration and quantum fluctuations do not lead to a quantum disordered phase for strong frustration. The results of both approaches (ED, LSWT) suggest a first order transition at $J_2/J_1 \approx 0.7$ from the two-sublattice Néel phase at low $J_2$ to a collinear phase at large $J_2$.

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I. INTRODUCTION

The properties of the two-dimensional (2d) $J_1$-$J_2$ model have attracted a great deal of interest during the last decade (see e.g. Refs. and references therein). The Hamiltonian of the $J_1$-$J_2$ model is

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $J_1 = 1$ is the nearest-neighbor, and $J_2 \geq 0$ is the frustrating next-nearest-neighbor Heisenberg exchange. We are interested in the extreme quantum case, i.e. we consider the spin quantum number is $s = 1/2$. For the square lattice it seems to be well-accepted that there is a quantum spin-liquid phase between $J_2/J_1 \approx 0.38$ and $J_2/J_1 \approx 0.60$ and that the corresponding quantum phase transitions from the Néel ordered state to the spin-liquid state at $J_2/J_1 \approx 0.38$ is of second order. The nature of the transition from the spin-liquid state to the collinear state at $J_2/J_1 \approx 0.60$ is still under discussion but there are indications that it might be of first order. The Néel phase for small $J_2$ is characterized by an antiparallel alignment of nearest-neighbor spins with a corresponding magnetic wave vector $Q_{\text{Néel}} = (\pi, \pi)$. The collinear state for large $J_2$ is twofold degenerated and the corresponding magnetic wave vectors are $Q_{\text{col}}^1 = (\pi, 0)$ and $Q_{\text{col}}^2 = (0, \pi)$. The two collinear states are characterized by a parallel spin orientation of nearest neighbors in vertical (horizontal) direction and an antiparallel spin orientation of nearest neighbors in horizontal (vertical) direction and exhibit therefore Néel order within the initial sublattices $A$ and $B$. The properties of the spin-liquid phase are a current field of active research. Even additional quantum phase transitions at $(J_2/J_1) \approx 0.34$ and $(J_2/J_1) \approx 0.50$ are discussed.

The properties of quantum spin systems strongly depend on the dimensionality. So, contrary to the 2d model, the one-dimensional $J_1$-$J_2$ model does not have a Néel ordered ground state, but exhibits a transition from a critical state to a dimer phase at $J_2/J_1 = 0.241$ (see e.g. and references therein). Though the tendency to order is more pronounced in three-dimensional (3d) quantum spin systems than in low-dimensional ones a spin-liquid phase is also observed for frustrated 3d systems like the Heisenberg antiferromagnet on the pyrochlore lattice.

In this paper we consider the 3d version of the $J_1$-$J_2$ model. To cover the possibility to have in a 3d model both Néel phases found for the 2d model we need a 3d bi-bipartite lattice, i.e. a lattice consisting of two interpenetrating bipartite sublattices. The bcc lattice consists of two interpenetrating, identical simple cubic sublattices. Each simple cubic sublattice consists of two interpenetrating, identical fcc lattices. Therefore the bcc lattice is a 3d bi-bipartite cubic lattice.

The classical ground state for the bcc lattice corresponds to that of the square lattice: For $J_2/J_1 < \alpha_c$ it is a usual two-sublattice Néel state whereas for $J_2/J_1 > \alpha_c$ an antiferromagnet with four sublattices is realized. The transition point $\alpha_c$ depends on the coordination numbers $\alpha_c = z_1/(2z_2)$, where $z_1$ is the number of nearest-neighbors ($J_1$ bonds) and $z_2$ of the number of next-nearest-neighbors ($J_2$ bonds). Consequently we have $\alpha_c = 1/2$ for the square lattice but $\alpha_c = 2/3$ for the bcc lattice. Therefore we define as the appropriate parameter of frustration

$$p = \frac{J_2 z_2}{J_1 z_1}$$

and we have $p_{\text{square}} = p_{\text{bcc}} = 1/2$.

In what follows we use the exact diagonalization scheme and the linear spin wave theory to calculate the ground-state properties of the $J_1$-$J_2$ model on the bcc lattice and compare the results with the corresponding ones for the square lattice. We will present the ground-state energy, the violation of the Marshall-Peierls sign rule, the sublattice magnetizations and the spin gap of
finite lattices in section II. Properties of the infinite lattices will be given in section III, where the results of the extrapolation of the ground-state energy, the sublattice magnetizations (from ED data) and the corresponding results of the LSWT are shown.

II. EXACT DIAGONALIZATION

A. The generation of finite bcc lattices

The generation of finite 3d lattices with periodic boundary conditions is less transparent than for 2d lattices. As has been recently pointed out by Betts and coworkers, the use of a triple of edge vectors in upper triangular lattice form (utlf) leads to a systematic generation of finite 3d lattices. In this paper we use the utlf edge vectors and follow strictly Refs. 17, 18, 19. Finite parallelepipeds that build up the infinite bcc lattice can be defined by three edge vectors,

\[ \mathbf{L}_n = \sum_{\beta=1}^{3} n_{\alpha \beta} \mathbf{a}_{\beta}, \]

where \( n_{\alpha \beta} \) with \( \beta = 1, 2, 3 \) are integers and \( \mathbf{a}_1 = (1,1,-1), \mathbf{a}_2 = (1,-1,1), \mathbf{a}_3 = (-1,1,1) \) are the basis vectors of the lattice connecting nearest neighbors. The lattice vectors connecting next nearest neighbors are \( \mathbf{b}_1 = (\pm 2, 0, 0), \mathbf{b}_2 = (0, \pm 2, 0), \mathbf{b}_3 = (0, 0, \pm 2) \).

There are altogether 10 finite bcc lattices with \( N \leq 36 \) listed in Table I, which fulfill the following three conditions: (i) Every site \( i \) of the bcc lattices should have 8 nearest and 6 next-nearest neighbors, which means that they have the full number of nearest and next-nearest neighbors. (ii) The finite lattices should be bi-bipartite in order to avoid frustration due to boundary conditions for \( p = 0 \) and \( p \to \infty \). (Notice, that finite bcc lattices may be not bi-bipartite even though the infinite bcc lattice is.) (iii) Furthermore they should be topologically distinct, i.e. the spin Hamiltonian should exhibit different physical properties.

B. Ground-state energy

The ground-state energy gives first insight in the nature of possible zero-temperature phase transitions. In the thermodynamic limit a kink in \( E_0(p) \) (respectively a jump in the first derivative \( dE_0/dp \)) signals a first order transition, whereas a smooth \( dE_0/dp \) is compatible with second order transitions. Furthermore the maximum in \( E_0(p) \) indicates the point of maximal frustration. The ground-state energy for the classical model consists of two straight lines \( E_{0, \text{clas}}(p) = (p - 1)N \) for \( p \leq 0.5 \) and \( E_{0, \text{clas}}(p) = -pN \) for \( p \geq 0.5 \) with a kink (maximum) at \( p = 0.5 \).

The quantum ground state \( |\Psi_0 \rangle \) of finite bcc lattices with \( N \mod 8 = 0 \) has the same translational symmetry for small and large \( J_2 \) (\( \mathbf{k}_{gs} = (0,0,0) \)), whereas the translational symmetry of \( |\Psi_0 \rangle \) for lattices with \( N \ mod 4 = 0 \) but \( N \mod 8 \neq 0 \) is different for small and large \( J_2 \). The change of symmetry from \( \mathbf{k}_{gs} = (0,0,0) \) to \( \mathbf{k}_{gs} = (\pi, \pi, \pi) \) appears slightly right from the maximum of the ground-state energy.

For the quantum model we show exact-diagonalization results of \( E_0/N \) for three different values of frustration in Table II. While \( J_2 = 0 \) and \( J_2 = 1.3333 \) correspond to zero or small frustration, \( J_2 = 0.7 \) is in the region of strong frustration.

For the sake of clearness we present in the figures only results of selected finite lattices. To illustrate the finite-size effects in the most of the subsequent figures we present data for the smallest (\( N=24 \)) and the largest lattices we have calculated, where for \( N = 32, 36 \) we have chosen the lattices having highest symmetry. Note, that the curves for lattices of identical \( N \) look very similar.

For comparison with the square lattice we have calculated data of \( J_2 \) up to \( N = 6 \times 6 = 36 \). However, we think a square lattice with \( N = 4 \times 4 = 16 \) is comparably good.?
rable to a bcc lattice with \( N = 36 \). This can be seen if one looks at the characteristic lengths \( L_{3d} \propto N^{1/3} \) and \( L_{2d} \propto N^{1/2} \). Further, we mention that the square lattice of \( N = 16 \) contains 5 neighborhood shells, whereas some of the more dense finite bcc lattices with \( N = 32 \) and \( N = 36 \) contain even more.

In Fig. 1 one finds the ground-state energies of the bcc lattices 24C, 36C and for comparison the 24C, 36C lattices. To have comparable curves we scaled the ground-state energy of the square lattice with \( N = 36 \) (36sq) versus \( p \). The inset is an enlargement of the strongly frustrated region around \( p = 0.52 \).

As pointed out in [4, 5] and very recently in [11] the sign rule may survive some frustration but is clearly violated for the square lattice in the strongly frustrated spin-liquid region. Hence we can use the violation of the Marshall-Peierls sign rule as an indication of the breakdown of the two-sublattice Néel state.

In Fig. 2 one finds the weight \( g(X) = \sum_n (c_n)^2 \) of the Ising states \( |n\rangle \) fulfilling the Marshall-Peierls sign rule (i.e. the sum \( \sum_n \) is restricted to the subset of states having \( c_n > 0 \)) for two finite bcc lattices and two square lattices. For the \( J_1 - J_2 \) model on the bcc lattice the rule (4) is violated almost discontinuously at that point where the ground-state energy has its maximum. This is a hint to a very drastic change of the ground state on the bcc lattice around \( p = 0.52 \) which can be attributed to an abrupt breakdown of the two-sublattice Néel state. On the other hand for the \( J_1 - J_2 \) model on the square lattice the violation of the sign rule (4) starts smoothly and becomes significant near \( p = 0.4 \) where the second-order transition to the spin-liquid state takes place. The modified sign rule with \( g(A_1 \cup B_1) \) changes also discontinuously for the bcc lattice but smoothly for the square lattice. However, there is a violation of the modified rule also in the collinear phase, which can be attributed to the coupling between the both antiferromagnetic subsystems living on the initial sublattices \( A \) and \( B \). Only for large \( p \gg 1 \), where the ground state becomes a product state of both antiferromagnetic subsystems the modified rule is rigorously fulfilled.

![FIG. 1: Ground-state energy per site in units of \( J_1 \) for the bcc lattices 24C, 36C and for the square lattices (scaled) with \( N = 16 \) (16sq) and \( N = 36 \) (36sq) versus \( p \). The inset is an enlargement of the strongly frustrated region around \( p = 0.52 \).](image1)

![FIG. 2: The weight \( g(X) \) (that is 1 for \( p = 0 \)) and \( g(A_1 \cup B_1) \) (that is 1 for \( p \gg 1 \)) of basis states \( |n\rangle \) fulfilling the Marshall-Peierls sign rule for the bcc lattice 24C, 36C and the square lattice with \( N = 16 \) (16sq) and \( N = 32 \) (32sq) versus \( p \). On the bcc lattices the sign rule is completely fulfilled up to \( p = 0.4 \) and 99.8% fulfilled at \( p = 0.51 \).](image2)
D. Sublattice magnetizations

Of course the most important parameter to study Néel ordering is the sublattice magnetization. In finite systems the conventional antiferromagnetic LRO, that is realized for small \( p \), has to be described by the square of the sublattice magnetization of one spin component

\[
m^2(Q) = \langle \left( \frac{1}{N} \sum_{i=1}^{N} e^{iQ \cdot R_i} S_i^z \right)^2 \rangle
\]

with \( Q_{\text{Néel}} = (\pi, \pi, \pi) \) for the bcc lattice (and \( Q_{\text{Néel}} = (\pi, \pi) \) for the square lattice). For large values of \( p \) the magnetic wave vectors \( Q_{\text{col}}^1 = (\pm \pi/2, \pm \pi/2, \pm \pi/2) \) have to be used for the bcc lattice (and \( Q_{\text{col}}^1 = (\pi, 0) \) or \( Q_{\text{col}}^2 = (0, \pi) \) for the square lattice) to describe the collinear phase with antiferromagnetic order within the initial sublattices. We denote in the following the order parameter of the Néel phase calculated with \( Q_{\text{Néel}} \) with \( m^2 \) and that of the collinear phase calculated with \( Q_{\text{col}}^1 \) or \( Q_{\text{col}}^2 \) with \( m^2_\alpha \). Notice, that \( m^2_\alpha \) is identical for \( Q_{\text{col}}^1 \) and \( Q_{\text{col}}^2 \). In Table III we give the order parameters of the ten finite bcc lattices for \( J_2 = 0 \) and \( J_2 = 1.3333 \).

FIG. 3: Sublattice magnetizations \( m^2 \) (maximal for small \( p \)) and \( m^2_\alpha \) (maximal for large \( p \)) of the bcc lattices \( 24C \), \( 36C \) and the square lattices with \( N = 16 \) (16sq) and \( N = 36 \) (36sq) versus \( p \).

FIG. 4: Sublattice magnetizations \( m^2 \) (maximal for small \( p \)) and \( m^2_\alpha \) (maximal for large \( p \)) of the bcc lattice \( 36C \), \( 32D \), \( 28D \) and \( 24C \) near the phase transition point \( p \approx 0.52 \).

FIG. 5: Spin gap \( \Delta_{ST} \) in units of \( J_1 \), i.e. the gap to the first triplet excitation for the bcc lattices \( 24C \), \( 36C \) and the square lattices with \( N = 16 \) (16sq) and \( N = 32 \) (32sq) versus \( p \).
E. Spin gap

Another indication for a possible quantum disordered spin-liquid state is the spin gap, i.e. the gap $\Delta_{ST}$ between the singlet ground state and the first triplet excitation. In Néel ordered systems we have Goldstone modes and no spin gap is observed in the thermodynamic limit. Contrary to this, quantum disorder is accompanied by the opening of a spin gap. We show the gap $\Delta_{ST}$ of two finite bcc lattices in Fig. 5. The first triplet excitation relevant for the gap belongs to the translational symmetry $k_l = (\pi, \pi, \pi)$ for small $p$ and $k_l = (\pi/2, \pi/2, \pi/2)$ for large $p$. For comparison we show the gap for the square lattice of $N = 16$ and $N = 32$ sites. Of course, the gap of a finite lattice is finite. However, in the long-range ordered Néel and collinear phases the extrapolation to the thermodynamic limit yields a vanishing gap. Obviously there is no increase in the gap for the bcc lattices till about $p \approx 0.52$ where the transition from the two-sublattice Néel phase to the collinear phase takes place. In the collinear phase the relevant coupling parameter for excitations is $J_2$ instead of $J_1$ and consequently the gap increases linearly with $p$. Clearly we see that there is no special behavior of $\Delta_{ST}$ near the transition point $p \approx 0.52$. The gap for the square lattice shows a similar behavior for parameter regions where magnetic long-range order in the ground state is present, but around $p = 0.5$ the behavior of $\Delta_{ST}$ is in contrast to the bcc lattice. In this region a quantum disordered gapped phase for the square lattice is expected which is consistent with the significant increase of $\Delta_{ST}$ near $p = 0.5$.

We conclude from the examination of the spin gap that there are no indications for a quantum disordered gapped phase for the bcc lattice.

III. INFINITE BCC LATTICES

A. Finite-Size Extrapolation

To obtain properties of the infinite bcc lattice we extrapolate the ED data of all ten lattices listed in Table 1. The finite-size extrapolation is a well elaborated approximation scheme successfully applied to many 2d quantum spin systems like the $J_1 - J_2$ model on the square lattice [2]. But even for 3d lattices this scheme may lead to precise data for the infinite lattice [17, 18, 19]. The corresponding scaling laws are known from literature [22, 23, 24]. The scaling equation for ground-state energy per site $\epsilon = E_0/N$ of the bcc lattice is

$$\epsilon(L) = \epsilon(\infty) + A_1 L^{-4} + \ldots$$

(7)

and for the order parameter

$$m^2(L) = m^2(\infty) + B_2 L^{-2} + \ldots$$

(8)

with $L = N^{1/3}$.

The same relation is valid for $m_{ST}^2$. The results are presented in Figs. 6 and 7. The discussion of the data is given below.

B. Linear spin wave theory (LSWT)

1. LSWT for small $J_2$

Starting from the classical two-sublattice Néel state we choose a two-boson representation of the Hamiltonian [1]. Rewriting the spin operators of the Hamiltonian in terms of boson operators by using the usual Holstein-Primakoff transformation and taking into account only quadratic terms in the boson operators, we obtain a bosonic Hamiltonian in Fourier transformed representation

$$H = \frac{s^2}{2} \sum_k \left( A_k (a_k^+ a_k + b_k^+ b_k) + B_k (a_k b_{-k} + a_k^+ b_{-k}^+) \right)$$

(9)

with the coefficients

$$A_k = s (8 - 6p (1 - \gamma_{2k}))$$

(10)

$$B_k = 8s^2 \gamma_k$$

(11)

The structure factors of nearest neighbors and next-nearest neighbors are given by

$$\gamma_{1k} = \cos k_x \cos k_y \cos k_z$$

(12)

$$\gamma_{2k} = \frac{1}{3} (\cos 2k_x + \cos 2k_y + \cos 2k_z).$$

(13)

The ground-state energy per site is then

$$E_0/N = s^2 (-8 + 6p) + \frac{1}{N} \sum_k (\omega_k - A_k)$$

(14)

FIG. 6: LSWT data for the ground-state energies $E_0$ of the infinite bcc lattice (dashed line, LSWT bcc) and square lattice (dotted line, LSWT sq) as well as the extrapolated ED data for $E_0$ (solid line with data points) versus $p$. 
with $\omega_k = \sqrt{A_k^2 - B_k^2}$. The sublattice magnetization $m = \langle S_i^z \rangle$ is

$$m = s - \frac{1}{N} \sum_k \left( -\frac{1}{2} + \frac{A_k}{2\omega_k} \right), \quad (15)$$

2. LSWT for large $J_2$

The classical ground state of the $J_1 - J_2$ model on the bcc lattice for large $J_2$ consists of two interpenetrating Néel states each living on the initial sublattices $A$ and $B$. The two Néel states are energetically decoupled, i.e. the angle $\theta$ between the staggered magnetization on $A$ and $B$ is arbitrary for classical spins. For the quantum model we start with arbitrary $\theta$ and use as quantization axis the local orientation of the spins in the classical ground state. The further procedure is the same as for small $J_2$ but the bosonic Hamiltonian now contains the angle $\theta$. By means of the Hellmann-Feynman theorem \cite{kosterlitz} $\langle \partial H(\theta)/\partial \theta \rangle = \partial E(\theta)/\partial \theta$ it can be easily found that in the quantum model the collinear state ($\theta = 0$ or $\pi$) has lowest energy. This lifting of the continuous degeneracy of the classical ground state by quantum fluctuations \textit{('order from disorder effect')} is also found for the square lattice \cite{weinacht}. For $\theta = 0$ the bosonic Hamiltonian reads

$$H = -6Nps^2 + \sum_k \left\{ A(a_k^+a_k + b_k^+b_k) \right\}$$

$$+ [C_k(b_k^+a_k - b_k^+a_{-k}) - B_k(a_k a_{-k} + b_k b_{-k}) + h.c.] \right\},$$

where

$$A = 6sp \quad (17)$$

$$B_k = 3sp\gamma_2k \quad (18)$$

$$C_k = 4s(cos k_x cos k_y cos k_z$$

$$+ i sin k_x sin k_y sin k_z).$$

Then the ground-state energy per site is

$$E_0/N = -6s^2p + \frac{1}{N} \sum_k \left( \frac{\omega_{1k}}{2} + \frac{\omega_{2k}^2}{2} - A \right)$$

(20)

with the modes

$$\omega_{1k} = \sqrt{A^2 - 4B_k^2 + F_k} ; \quad \omega_{2k} = \sqrt{A^2 - 4B_k^2 - F_k}$$

(21)

and the function

$$F_k = \{(C_k^2 - C_k^2)^2 - 8B_k(C_k^2 + C_k^2)^2$$

$$+ 4C_kC_k^4(A^2 + 4B_k^2)^{1/2}.$$

The sublattice magnetization is written as

$$m_\alpha = s - \frac{1}{N} \sum_k \frac{D(k, \omega_{1k})}{2\omega_{1k}(\omega_{1k} - \omega_{2k})}$$

$$- \frac{1}{N} \sum_k \frac{D(k, \omega_{2k})}{2\omega_{2k}(\omega_{2k} - \omega_{1k})}$$

(23)

with

$$D(k, \omega_k) = -\omega_k^3 + A\omega_k^2 - (4B_k^2 - A^2)\omega_k$$

$$+ A(4B_k^2 + 2C_kC_k^4) - 2B_k(C_k^2 + C_k^2) - A^3.$$ \hfill (24)

The results of LSWT and the finite-size extrapolation are shown in Figs.9 and 10. For the limits $J_2 = 0$ and $J_1 = 0$ our LSWT results are in agreement with data for the bcc and the sc lattice given in [24]. Both methods yield similar results. For the ground-state energy we have a good quantitative agreement. Being in the size of the data points, the standard deviation of extrapolated ground-state energy is not shown. For the order parameter the finite-size effects are stronger and the agreement is only qualitative. Both methods suggest a first-order transition for the spin-$1/2$ $J_1$-$J_2$ model on the bcc lattice. The transition point obtained from the ED data is $J_2 \approx 0.7J_1$ (i.e. $p \approx 0.52$) while the LSWT becomes instable at the classical transition point.

IV. CONCLUSION

We have presented spin-wave and exact diagonalization results for the spin-$1/2$ $J_1$-$J_2$ model on the bcc lattice and compare them with those for the square lattice. In general, we observe that the physics for the 3d quantum model is closer to classical behavior since quantum fluctuations and finite-size corrections become less important for higher coordination number and larger dimension.
We are not sure whether the increase of the magnetization \( m_\alpha \) approaching the transition point from the right (shown in Fig. 7) is a real effect. A possible physical origin for an increase may be a stronger coupling of the Néel ordered subsystems A and B due to larger quantum fluctuations or finite-size effects that become more important in the region of strong frustration. From the data for the ground-state energy, the Marshall-Peierls sign rule, the sublattice magnetizations and the spin gap we conclude that the increase from dimension \( d=2 \) to \( d=3 \) changes the physical properties basically. The good agreement with the spin wave results support this conclusion. Contrary to the 2d model, where the quantum fluctuations and frustration lead to a second order transition from the two-sublattice Néel state to a disordered spin-liquid like phase, in the 3d model we find no indications for a disordered ground-state phase. The quantum \( J_1 - J_2 \) model on the bcc lattice shows one transition of first order induced by strong frustration from the two-sublattice Néel state directly to the collinear state, where the transition takes place at \( \alpha_c = (J_2/J_1)_c \approx 0.7 \).

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