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Field-induced spin supersolidity in frustrated $S=\frac{1}{2}$ spin-dimer models

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By means of the recently developed algorithm based on the tensor product states, the magnetization process of frustrated spin-1/2 spin-dimer models on a square lattice is investigated. Clear evidence of a supersolid phase over a finite regime of magnetic field is observed. Besides, critical fields at various field-induced transitions are determined accurately. Our work hence sheds light on the search of the supersolid phase in real frustrated spin-dimer compounds.

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Over the last decade, dimerized quantum antiferromagnets have attracted much attention since rich field-induced quantum phases can appear in these compounds.[1] In the absence of magnetic field, the system exhibits spin-singlet ground state, consisting of dimers for closely spaced pairs of spins $S=1/2$. By applying a large enough field such that the energy gap to spin-triplet excitations closes, the lowest triplet excitation starts to condense and the system develops a spin superfluid (SF) state, which supports a staggered magnetization transverse to the field direction. When the effective repulsion between triplets overwhelms their kinetic energy, instead of the Bose-Einstein condensation of triplet excitations, incompressible commensurate crystals of triplets with broken translational symmetry can be stabilized,[2] which are signaled by magnetization plateaus.

Recently, an even more exotic *supersolid* (SS) phase is found in the vicinity of a magnetization plateau for some spin-dimer models.[3] This generated an enormous interest in the study of quantum and thermal phase transitions out of these spin SS states.[4–6] The main character of the SS phase is that its ground states possess both solid and SF long-range orders. It has been proposed that correlated hopping of triplets may play a crucial role in forming this phase.[7] At the SF-SS transition point, a magnetization anomaly and thereby a discontinuity in magnetic susceptibility appears. This indicates that the SF-SS transition is of second order. Moreover, approaching the edge of the magnetization plateau from the SS phase, the spin stiffness vanishes linearly,[4] in agreement with the superfluid-insulator universality class.[8]

For the spin-1/2 spin-dimer models studied previously, large Ising-like exchange anisotropy is necessary for the existence of the SS phase,[3–5] which is unrealistic for most magnetic systems. Under some kind of approximation, such an anisotropy can be considered as an effective interaction resulting from frustrated spin-isotropic couplings.[3,6] Thus, the results for the spin-anisotropic cases suggest that the SS phase can appear also in frustrated spin-isotropic models. Nevertheless, because of underlying approximation, quantitative predictions of the needed frustrated coupling and magnetic field for the appearance of this phase cannot be determined accurately in the preceding studies. To provide a useful guide to the experimental search of the SS phase in real frustrated spin-dimer compounds, investigations directly within the frustrated spin-isotropic models are called for.

In this Rapid Communication, various field-induced quantum phase transitions in frustrated spin-1/2 spin-dimer Heisenberg models are explored by using the combined algorithm[9] of the infinite time-evolving block decimation (iTEBD) method[10] and the tensor renormalization-group (TRG) approach.[11] In this combined algorithm, the ground states are assumed in the form of the tensor product state (TPS) or the projected entangled-pair state (PEPS).[12] The power of the TPS- or PEPS-based approach in studying first-order quantum phase transitions has been demonstrated by several groups.[13–15] We note that, in contrast to quantum Monte Carlo simulation which is plagued by the sign problem in studying frustrated spin systems, the numerical approach employed here is appropriate because frustration does not introduce additional difficulties to the TPS- or PEPS-based method.[15,16] By using the combined iTEBD and TRG method, the existence of the SS phase in the frustrated systems under consideration is firmly established, and the critical fields bounding this phase are determined precisely. These results provide further theoretical support on searching the SS phases in the neighborhood of magnetization plateaus observed in some spin-dimer compounds with frustration. Moreover, the success in obtaining precise results for frustrated spin systems clearly demonstrates that the combined algorithm can be an efficient and accurate numerical tool with wide applications including even frustrated systems.

We consider the following spin-1/2 bilayer Heisenberg Hamiltonian under a uniform magnetic field h on a square lattice with a strong interlayer exchange $J_{\perp}$, a weaker intralayer coupling J, and a frustrating interlayer interaction J_d [see Fig. 1(a)],

$$H = J_{\perp}\sum_{i}\mathbf{S}_{i,1}\cdot\mathbf{S}_{i,2} - h\sum_{i,\alpha}S^{z}_{i,\alpha} + J\sum_{\langle i,j\rangle,\alpha}\mathbf{S}_{i,\alpha}\cdot\mathbf{S}_{j,\alpha} + J_d\sum_{\langle i,j\rangle,\alpha}\mathbf{S}_{i,\alpha}\cdot\mathbf{S}_{j,\bar{\alpha}}. \tag{1}$$

Here, the antiferromagnetic couplings are assumed $(J_{\perp},J,J_d>0)$. The indices i and j denote rungs of the bilayer lattice and $\alpha=1,\ 2$ labels the two different layers. The summation $\langle i,j\rangle$ runs over pairs of nearest-neighbor rungs. Henceforth, $J_{\perp}\equiv 1$ is set to be the energy unit. To character-

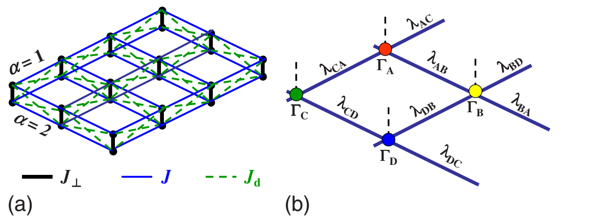

FIG. 1. (Color online) (a) Square lattice of $S=1/2$ dimers with an intradimer interaction $J_\perp$ and interdimer interactions J and J_d. (b) The construction of periodic tensor network with a 2×2 unit cell.

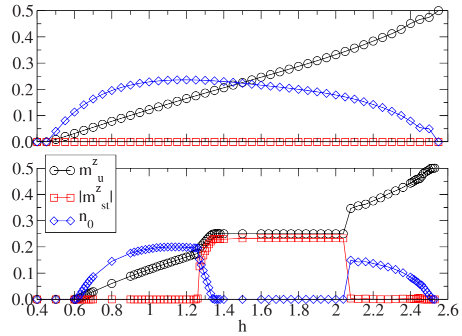

FIG. 2. (Color online) Values of $m_{\rm u}^z$, $|m_{\rm st}^z|$, and $n_0=2|m_{\rm st}^x|^2$ for the ground states at $J_d=0.15$ (upper panel) and 0.21 (lower panel) with $J=0.38$ as functions of external field h for systems of size $2^7\times 2^7$ with $D=4$ and $D_{\rm cut}=16$. The J_d independence of the saturation field h_s can be observed.

ize different phases, several local order parameters are calculated. First, when systems undergo the dimer-SF transition, the z-component uniform magnetization per site $m_{\rm u}^z \equiv (1/2N)\Sigma_i\langle S_{i,1}^z+S_{i,2}^z\rangle$ begins to be nonzero, where N is the total number of rungs on the bilayer. Second, the SF states with nonzero in-plane antiferromagnetic magnetization along the x direction can be detected by the x-component staggered magnetization per site $m_{\rm st}^x\equiv(1/2N)\Sigma_i\langle S_{i,1}^x-S_{i,2}^x\rangle e^{i\mathbf{Q}\cdot\mathbf{r_i}}$. Using the mapping for the triplets to the semi-hard-core bosons $b_i^\dagger=(S_{i,1}^+-S_{i,2}^+)e^{i\mathbf{Q}\cdot\mathbf{r_i}}/\sqrt{2}$,[3] the condensate density n_0 of triplet excitations can be related to $m_{\rm st}^x$ by $n_0\equiv|\langle b^\dagger\rangle|^2=2|m_{\rm st}^x|^2$. Finally, the checkerboard solid (CBS) order will be signaled by a finite value of the z-component staggered magnetization per site $m_{\rm st}^z\equiv(1/2N)\Sigma_i\langle S_{i,1}^z+S_{i,2}^z\rangle e^{i\mathbf{Q}\cdot\mathbf{r_i}}$, where $\mathbf{Q}=(\pi,\pi)$. In the thermodynamic limit, this quantity has a direct relation, $|m_{\rm st}^z|^2=S(\mathbf{Q})/2N$, to the static structure factor $S(\mathbf{Q}) \equiv(1/2N)\Sigma_{i,j}\langle(S_{i,1}^z+S_{i,2}^z)(S_{j,1}^z+S_{j,2}^z)\rangle e^{i\mathbf{Q}\cdot(\mathbf{r_i}-\mathbf{r_j})}$.

These quantities are evaluated under the combined iTEBD and TRG algorithm,[9,14] where the ground-state wave function is approximated by a TPS or PEPS ansatz.[12] Our construction of TPS for these bilayer systems on a square lattice is to attach a rank-five tensor $[\Gamma_i]^s_{lrud}$ to each *rung* i and a diagonal singular value matrix $[\lambda_{\langle i,j\rangle}]_l$ to each bond of nearest-neighboring rungs i and j, as sketched in Fig. 1(b). Here, s is the physical index with $s=1,\ldots,4$ for the present spin-dimer case and $l,r,u,d(=1\cdots D)$ denote the virtual bond indices in four directions. The approximation can be systematically improved simply by increasing the bond dimension D of the underlying tensors. The optimized TPS or PEPS is determined through the power method via iterative projections for a given initial state. This procedure can be considered as a generalization of the one-dimensional iTEBD method[10] to the two-dimensional cases. To improve the stability the algorithm, the calculated ground state for a lower field h is usually employed as the initial state for the higher-h case.[17] By means of TRG method,[11] the expectation values for a TPS or PEPS ground state of very large systems can be calculated efficiently, where the accuracy can be systematically improved by increasing the TRG cutoff $D_{\rm cut}$. In the present work, we consider the bond dimension up to $D=5$ and keep $D_{\rm cut}\geq D^2$ to ensure the accuracy of the TRG calculation.

The results of the local order parameters defined above as functions of magnetic field h for $J_d=0.15$ and 0.21 with $J=0.38$ and systems size $N=2^7\times 2^7$ are shown in Fig. 2. Here, we take the bond dimension $D=4$ and the TRG cutoff $D_{\rm cut}=16$. We note that results for $D=3,\ 5$ are very similar to those for $D=4$ (see below). Upon increasing the field, the ground state of the model in Eq. (1) goes through a succession of distinct quantum phases. For the case of weak frustration ($J_d=0.15$), the ground state evolves first from the dimer phase ($m_{\rm u}^z,n_0=0$) to the SF phase ($m_{\rm u}^z,n_0\neq 0$), and finally to the fully polarized (FP) phase ($m_{\rm u}^z=1/2$ and $n_0=0$). Such a behavior is consistent with the results of the unfrustrated ($J_d=0$) case.[18]

For the larger-J_d case ($J_d=0.21$), apart from aforementioned phases, a magnetization plateau and a peculiar SS phase with both the CBS and the SF orders are found. The general feature of our results for $J_d=0.21$ is quite similar to what have been discovered in the previous works for the spin-anisotropic systems.[3–5] Within the regime of magnetization plateau, we find that the uniform magnetization is $m_{\rm u}^z\simeq 0.25$ together with a nonzero CBS order parameter $|m_{\rm st}^z|\simeq 0.23$. Thus, this plateau state describes the CBS phase with long-range diagonal order at wave vector $\mathbf{Q}=(\pi,\pi)$. The observed CBS phase can be understood as formed by half filling the system with triplet excitations, so that $m_{\rm u}^z=0.25$. Its stability comes from the strong effective repulsion between nearest-neighbor triplets generated by interdimer frustrated couplings J and J_d. We note that, as in the anisotropic cases studied previously,[3–5] the calculated CBS order parameter $|m_{\rm st}^z|$ is also slightly smaller than its classical value $|m_{\rm st}^z|=1/4$, which is caused by quantum fluctuations therein. At higher fields, the melting of the CBS is found to be of first order and the SF phase reappears. At this transition, the magnetization changes abruptly from $m_{\rm u}^z\simeq 0.25$ to $m_{\rm u}^z\simeq 0.35$, and the condensate fraction n_0 jumps from zero to $n_0\simeq 0.15$. On the other hand, when decreasing the field from the plateau, a SS phase emerges in the present frustrated spin-dimer system, where both the CBS order parameter $m_{\rm st}^z$ *and* the Bose condensate density n_0 are nonzero. At even lower fields, the CBS order disappears and a standard SF phase with only $n_0\neq 0$ is recovered.

As a check on our prescription of the TRG cutoff $D_{\rm cut}$ and bond dimension D, the dependence of the evaluated order parameters on them is shown in Fig. 3. Here, we consider two typical values of $h=1.2$ and 1.3, which are corresponding to the SF and the SS phases, respectively. It is expected

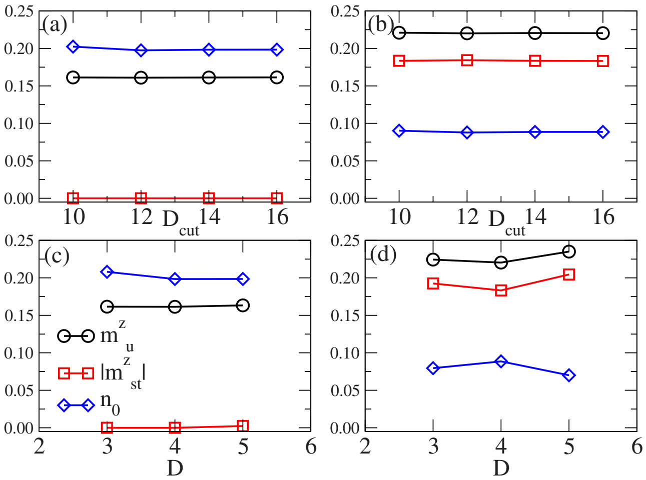

FIG. 3. (Color online) Dependence of the calculated order parameters on $D_{\rm cut}$ (upper panels) and D (lower panels): (a) h=1.2 and (b) 1.3 with D=4; (c) h=1.2 and (d) 1.3 with $D_{\rm cut}$=16 for $D \leq 4$ and $D_{\rm cut}$=25 for D=5.

that the ground states in these two cases are more entangled than those in the dimer or the CBS phases. Consequently, reliable results can be reached only when D and $D_{\rm cut}$ are large enough. As seen from Fig. 3, there is almost no dependence on $D_{\rm cut}$ from $D_{\rm cut}$=10 to 16 for D=4, and the dependence on D is small. (The variance of each order parameter is less than 0.025 even in the SS phase with h=1.3.) These results indicate that the bond dimension and the TRG cutoff used in this work are large enough to provide accurate findings for the present case.

To explore the behaviors around the transition points to the SS phase, results around this phase with an enlarged scale are shown in Fig. 4(a). We find that the transition between the SF and the SS phases occurs at the critical field $h_{c2} \approx 1.26$, at which the CBS order $m^z_{\rm st}$ begins to vanish. As observed in Fig. 4(a) (also in Fig. 2), this transition is also signaled by a kink in the magnetization curve, which implies a discontinuity in magnetic susceptibility $\chi \equiv dm^z_{\rm u}/dh$. The field-induced transition between the SS and the CBS phases occurs at another critical field $h_{c3} \approx 1.34$, at which the condensate fraction n_0 begins to vanish. Moreover, we observe that n_0 vanishes linearly as h approaches h_{c3} from below. This behavior is in agreement with the SF-insulator universality class[8] since the density of the bosonic excitations (triplet *holes*) should be small around h_{c3} and the condensate fraction roughly equals the spin stiffness in this dilute-boson limit. In the inset of Fig. 4(a), the dependence of the critical fields h_{c2} and h_{c3} on the bond dimension D is presented. The values show only a minor dependence on D, which again supports the validity of the present approach.

Now we turn our attention to the cases near the dimer-SF transition at the critical field h_{c1} and around the saturation field h_s. In both cases, some analytical results are available. As same as the unfrustrated (J_d=0) case,[18] the instability of the dimer phase is triggered by the energy gap closing of the bosonic *one-triplet* excitation above the dimer state. On the other hand, the FP state becomes unstable when the lowest bosonic excited state *with a single spin flip* is degenerate with the FP state. Thus, both transitions are expected to be of second order and in the universality class of the dilute Bose gas quantum-critical point.[19] By using the expression of the excitation spectrum of the one-triplet states up to the third-order perturbation expansion,[20] the critical field h_{c1} of the dimer-SF transition is achieved, $h_{c1} \simeq 1-2(J-J_d)-\frac{3}{2}J(J-J_d)^2$. To determine the saturation field h_s, one notes that the states with a single spin flip are the eigenstates of our model in Eq. (1) and their energy eigenvalues can be calculated *exactly*. Thus, the exact expression for h_s can be derived. We find that, when $J_d < J$ and $J_d < 1/4$, the saturation field $h_s = 1+4J$, which is independent of the magnitude of the frustrated coupling J_d. A closer look around the transitions at h_{c1} and h_s is shown in Figs. 4(b) and 4(c). In agreement with the SF-insulator universality class,[8] we find that the condensate fraction n_0 vanishes linearly also around these two field-induced transition points. The dimer-SF transition occurs at $h_{c1} \approx 0.61$, where the uniform magnetization $m^z_{\rm u}$ and the condensate fraction n_0 start to be nonzero. Above the saturation field $h_s \approx 2.52$, all spins are polarized in the z direction and the uniform magnetization saturates at the value of $m^z_{\rm u}$=0.5. Our findings of h_{c1} and h_s agree well with the values ($h_{c1} \simeq 0.64$ and h_s=2.52) given by the analytic formulas with J=0.38 and J_d=0.21. Moreover, as seen from Fig. 2, the calculated values of the saturation field h_s for the cases of J_d=0.15 and 0.21 are identical. Thus, the independence of the saturation field on the frustrated coupling J_d is indeed preserved in our approach. These observations further substantiate that the employed method can provide reliable results even for the frustrated spin systems.

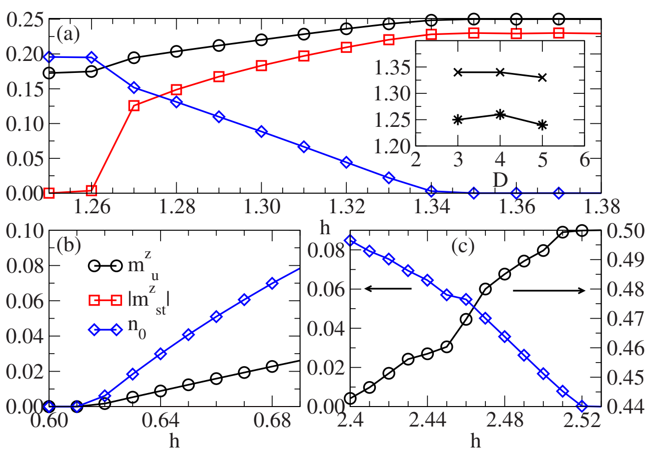

FIG. 4. (Color online) Details of local order parameters around (a) the SS phase, (b) the dimer-SF, and (c) the SF-FP transition points with enlarged scale. The parameters are the same as those for the lower panel of Fig. 2. The inset in (a) shows the critical fields h_{c2} ($\times$) and h_{c3} ($*$) for various D ($D_{\rm cut}$=16 for $D \leq 4$ and $D_{\rm cut}$=25 for D=5).

As shown in Fig. 2, a SS phase can exhibit as ground states of frustrated spin-dimer models when the frustrated coupling J_d becomes large enough. One may wonder how the SS phase becomes if J_d increases further. In Fig. 5, two values of even larger J_d (J_d=0.23 and 0.27) are considered. We find that the width in h of the SS state slightly decreases from $h_{c3}-h_{c2} \approx 0.08$ for J_d=0.21 (see Fig. 4) down to about

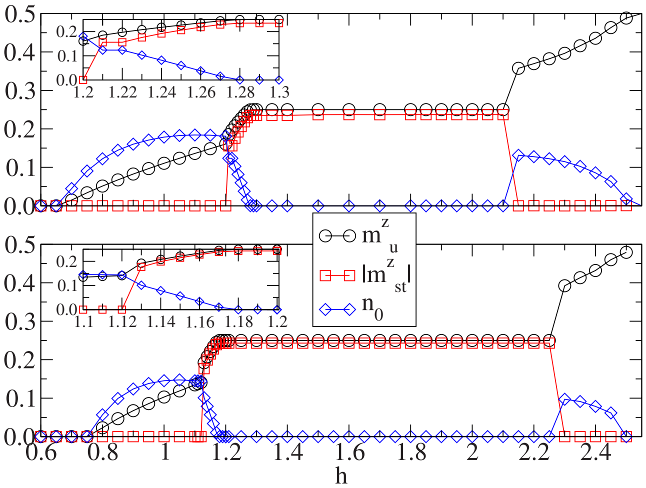

FIG. 5. (Color online) Local order parameters at J_d=0.23 (upper panel) and 0.27 (lower panel) as functions of external field h. Other parameters are the same as those for Fig. 2. Insets of both panels show the details of local order parameters around their SS phases with enlarged scales.

0.06 for J_d=0.27 (see Fig. 5). Nevertheless, as seen from Fig. 5, the regime for the plateau state expands upon increasing J_d. Moreover, the width in h of the SF phase shrinks and the magnitude of n_0 in this state decreases as J_d increases. These outcomes indicate that the SS state may eventually disappear for large enough frustration. That is, the SS phase may be stabilized only within a limited region of the h-J_d phase diagram. Therefore, carefully tuning system parameters into the suggested parameter regime are necessary to uncover experimentally this phase in real frustrated spin-dimer compounds.

To summarize, the field-induced quantum phase transitions in frustrated spin-1/2 spin-dimer models are studied under the combined iTEBD and TRG algorithm.[9,14] Clear evidence of a SS phase over a finite regime of magnetic field is provided. Critical fields at various field-induced transitions are evaluated accurately by using merely a moderate bond dimension D. Besides providing quantitative predictions of the needed frustrated coupling and magnetic field for the appearance of the SS phase, the present work also demonstrates clearly the potential in applying the current formalism even to frustrated spin systems.

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