Available online at www.sciencedirect.com
ScienceDirect
Journal of Magnetism and Magnetic Materials 310 (2007) 1371–1373
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Field-induced supersolid phase in spin dimer XXZ systems

Kwai-Kong Ng[a,b,*], T.K. Lee[a]

[a]Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan, ROC
[b]Physics department, Tunghai University, Taichung 40704, Taiwan, ROC

Available online 15 November 2006

Abstract

We study the ground state phase diagram of the two-dimensional spin $S=\frac{1}{2}$ dimer model with an anisotropic intra-plane coupling. A supersolid phase characterized by a non-uniform bose condensate density that breaks translational symmetry is found when the anisotropy $4 \gtrsim \Delta \gtrsim 3$. The rich phase diagram contains a checkerboard solid and two different types of superfluid phase with finite staggered magnetization in z-axis and in-plane direction, respectively. We show that the model can be realized if next nearest neighbor (n.n.n.) coupling among dimers is taken into account.

PACS: 75.10.Jm; 5.45.+j; 05.30.Jp; 75.40.Mg

Keywords: Supersolid; Spin dimer; Quantum Monte Carlo

1. Introduction

Recent experiments on spin dimer compounds, such as $TlCuCl_3$, $KCuCl_6$ and $BaSiCu_2O_6$ [1], have confirmed the formation of superfluid (SF) of the spin triplets under an external magnetic field. These spin bosons have also previously been found to be crystallized, signaled by the magnetization plateau, in dimer compounds such as $SrCu_2(BO_3)_2$ [2]. The competition between repulsive interaction and kinetic motion decides whether the ground state is a solid or is a SF [3]. This raises the possibility of a supersolid (SS) [4] state with simultaneous off-diagonal and diagonal long-range orders. While SS is unstable against phase separation for hardcore bosons in a square lattice [5,6], the spin bosons are shown to be semi-hardcore [7]. Using quantum Monte Carlo method we demonstrate that the ground state of a spin dimer XXZ model could be SF of two kinds of triplets, a quantum solid (QS) or, most importantly, a SS. This XXZ anisotropy can be easily realized if the n.n.n. interaction among dimers is considered.

In particular, we study the two-dimensional bilayer AF spin dimer XXZ model

$$H_{XXZ} = -h\sum_{l,i} S^z_{l,i} + J\sum_i \mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i} \quad (1)$$

$$+ J'\sum_{l,\langle i,j\rangle}(S^x_{l,i}S^x_{l,j} + S^y_{l,i}S^y_{l,j} + \Delta S^z_{l,i}S^z_{l,j}), \quad (2)$$

where $l=1,2$ denotes the layer index and the third term sums over all nearest neighbors (n.n.) in the xy plane for both layers. Since $J \gg J'$ (we take $J'/J = 0.29$ in this paper), the low energy physics is conveniently described by the interaction of the four spin states, singlet ($|s\rangle$) and triplets $S^z = 0, \pm 1$ ($|t_{0,\pm}\rangle$) of each dimer. Although $|s\rangle$ and $|t_0\rangle$ mix in the presence of h, their densities are still well defined and can be deduced from the relations $n_{t0} - n_s = \langle S^+_1 S^-_2 + S^+_2 S^-_1\rangle$ and $n_s + n_{t+} + n_{t-} + n_{t0} = 1$. While $n_{t\pm}$ can be easily measured, n_{t_0} and n_s are obtained by calculating the spin correlation function. The difference of $n_{t+} - n_{t-}$ gives the uniform magnetization m_z.

To study the phase diagram, we focus on the following order parameters:

$$m^s_z = \left\langle \sum_i \frac{(-1)^i}{N}(S^z_{1i} - S^z_{2i})\right\rangle, \quad (3)$$

*Corresponding author.
E-mail address: kkng@thu.edu.tw (K.-K. Ng).

0304-8853/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2006.10.730

$$m_{xy} = \sqrt{m_x^2 + m_y^2}, \quad m_\alpha = \sum_i \frac{(-1)^i}{N\sqrt{2}} \langle S^\alpha_{1,i} - S^\alpha_{2,i} \rangle, \tag{4}$$

$$\frac{1}{N} S(\mathbf{Q}) = \frac{1}{N^2} \sum_{ij} \langle n_{i,t+} n_{j,t+} \mathrm{e}^{\mathrm{i}\mathbf{Q}\mathbf{r}_{ij}} \rangle, \tag{5}$$

which are the staggered magnetization in z direction, in the xy direction, and the structure factor of $|t_+\rangle$ state, respectively. As shown before [7,8], the square of m^z_s and m_{xy} represent the condensate densities of hardcore boson $a^\dagger$, which creates a $|t_0\rangle$ state, and of semi-hardcore boson $b^\dagger_i = (-1)^i/\sqrt{2}(S^+_{1,i} - S^+_{2,i})$. The finite values of m^z_s and m_{xy} signal the condensation of these two different types of bosons and we name the resulted superfluids as SFI and SFII, respectively. At wavevector $\mathbf{Q} = (\pi, \pi)$, the structure factor S($\mathbf{Q}$)/N is non-vanishing when there exists a checkerboard solid ordering in which translational symmetry is broken. In the case where both condensate density and structure factor are finite, the system is a SS. Our numerical simulation using the original individual spin basis of Hamiltonian H_{XXZ} indeed shows the presence of SS phase from $\Delta \approx 3-4$.

2. Results and discussion

Fig. 1(a) shows the field dependence of the order parameters. SFI and SFII are found at low and high fields, respectively, where there is no solid ordering. Note that m^s_z is field independent since the energy of $|t_0\rangle$ is not affected by the applied field. The SFII condensate density $n_0 = m^2_{xy}$ reduces to zero at a saturated field where all spins are polarized in z-direction. Lowering h/J from SFII phase, via a first order phase transition the system becomes a checkerboard QS of $|t_+\rangle$ states. To reduce interaction energy, $|t_+\rangle$ has more occupation in one sublattice than the other.

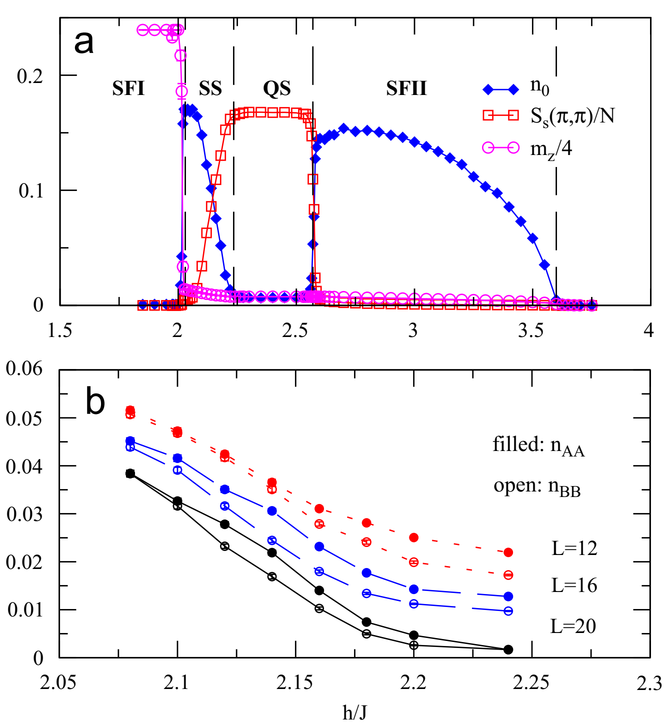

Fig. 1. (a) The condensate density n_0, structure factor $S(\pi,\pi)/N$, and out-of-plane staggered magnetization $m^s_z/4$ for $\Delta = 3.5$ of lattice size $20 \times 20 \times 2$. (b) The sublattice condensates n_{AA} and n_{BB} in the SS phase for different linear size L, $\Delta = 3.3$.

Between the phase QS and SFI, there is a second order phase transition that the structure factor reduces gradually as n_0 increases. This is the SS phase that breaks both diagonal (translational) and off-diagonal (U(1) gauge) symmetries. Finite size scaling indicates that the SS phases is stable in the thermodynamic limit [8]. To examine the condensate more closely, we define the sublattice condensates n_A and n_B as $n_\alpha = \sum_{i\in\alpha} \langle b^\dagger_i \rangle / N$, where $\alpha = A, B$. In our simulation, we compute the products of sublattice condensate $n_{\alpha\beta} = \sum_{i\in\alpha, j\in\beta} \langle b^\dagger_i b_j \rangle / N^2$. We found that $n_{AA} \neq n_{BB}$ (Fig. 1(b)) and $n_{AB} = n_{BA} = \sqrt{n_{AA} n_{BB}}$ in the SS phase, which means $n_{\alpha\beta} = n_\alpha n_\beta$, and $n_A \neq n_B$. It indicates that the condensate has a checkerboard ordering on its own, which is the intrinsic nature of a SS state. The full phase diagram of Δ vs. h/J is shown in Fig. 2. The SS phase is stable in a parameter region $4 \gtrsim \Delta \gtrsim 3$.

As mentioned, these phases can be realized in real material when n.n.n. coupling $J'' \mathbf{S}_{1,i} \mathbf{S}_{2,j}$ (i, j are n.n.) is taken into account. In bond operator representation, when the $|t_0\rangle$ states is ignored, spin operators $S^z_{1,2} \approx \frac{1}{2}(t^\dagger_+ t_+ - t^\dagger_- t_-)$ and $S^+_{1,2} \approx \pm \frac{1}{\sqrt{2}}(s^\dagger t_- - t^\dagger_+ s)$. Then the n.n.n. coupling is approximately given by

$$\mathbf{S}_{1,i} \mathbf{S}_{2,j} \approx S^z_{1,i} S^z_{1,j} - \tfrac{1}{2}(S^+_{1,i} S^-_{1,j} + S^-_{1,i} S^+_{1,j}). \tag{6}$$

Together with n.n. coupling $J' \mathbf{S}_{1,i} \mathbf{S}_{1,j}$, it leads to an XXZ model with effective n.n. coupling of $J^* = J' - J''$ and anisotropy Δ given by $J^* \Delta = J' + J''$. The inclusion of J'' now breaks the spin rotational symmetry. Therefore, if $J'' = J'/2$ one has a spin dimer XXZ model with $\Delta = 3$, close to the SS phase.

In summary, we demonstrate that the spin dimer XXZ model, a natural semi-hardcore boson system with defects, contains a SS phase that characterized by the bipartite

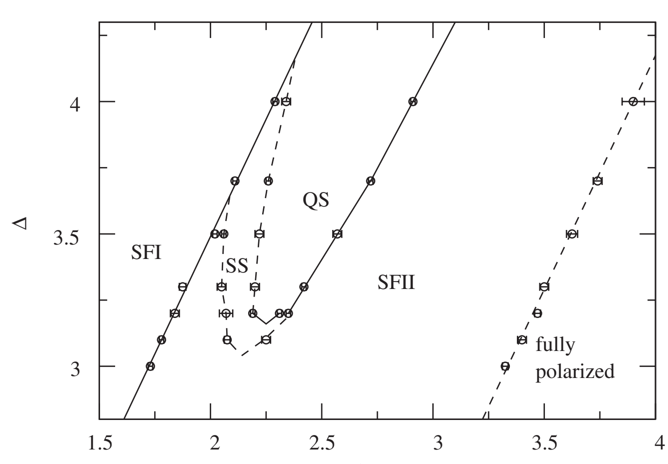

Fig. 2. Ground state phase diagram ($L \to \infty$) of Δ vs. h/J.

condensate density. The anisotropy can be a consequence of including the n.n.n. coupling among dimers. We propose that spin dimer compounds may be a natural place to realize the SS state of semi-hardcore bosons.

Acknowledgments

We acknowledges financial support by the NSC (ROC), Grant no. NSC 94-2112-M-001-003.

References

[1] Ch. Ruegg, et al., Nature 423 (2003) 62;
N. Cavadini, et al., Phys. Rev. B 65 (2002) 132415;
A. Oosawa, et al., Phys. Rev. B 66 (2002) 104405;
M. Jaime, et al., Phys. Rev. Lett. 93 (2004) 87203.
[2] H. Kageyama, et al., Phys. Rev. Lett. 82 (1999) 3168.
[3] T.M. Rice, Science 298 (2002) 760.
[4] O. Penrose, L. Onsager, Phys. Rev. 104 (1956) 576.
[5] P. Sengupta, L.P. Pryadko, F. Alet, M. Troyer, G. Schmid, Phys. Rev. Lett. 94 (2005) 207202.
[6] G. Schmid, S. Todo, M. Troyer, A. Dorneich, Phys. Rev. Lett. 88 (2002) 167208.
[7] K.K. Ng, T.K. Lee, Phys. Rev. B 73 (2006) 014433.
[8] K.K. Ng, T.K. Lee, Phys. Rev. Lett. 97 (2006) 127204.