The supersolid (SS) state of matter has attracted great interest lately following the experiments of Kim and Chan on solid $^4$He. While it is still unclear whether it can be stabilized in the continuum, there are several numerical studies which show that a SS phase can be realized in the presence of a periodic potential or underlying lattice for bosons [23, 48] as well as spins [3, 38]. The SS state is easier to stabilize on a lattice because the lattice parameter of the “solid phase” or charge density wave cannot relax to any arbitrary value (it has to be an integer multiple of the underlying lattice parameter). In this work we have studied a class of spin-SS on cubic lattices, focusing primarily on the unique signatures of the thermal melting of the SS in experimentally measurable observables. We also discuss different conditions under which a spin-SS can be realized in real spin compounds.

The minimal spin model that has a thermodynamically stable supersolid ground state on a bipartite lattice is the $S = 1$ Heisenberg model with uniaxial single–ion and exchange anisotropies and an external magnetic field:

$$H_H = J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) + \sum_i (D S_i^{zz} - B S_i^z)$$  \tag{1}

where $\langle i,j \rangle$ indicates that i and j are nearest neighbor sites, $D$ is the amplitude of the single ion-anisotropy and $\Delta$ determines the magnitude of the exchange uniaxial anisotropy. Note that although the exchange interaction is anisotropic, the longitudinal ($J$) and transverse ($\Delta$) couplings are both AFM (positive). Henceforth, $J$ is set to unity and all the parameters are expressed in units of $J$.

The ground state properties of the above model on a square lattice were studied in detail previously [8]. For $D, \Delta > 1$, the ground state is supersolid over a finite range of applied field $B$. In this work, we report the ground state and thermodynamic properties of (1) on a cubic lattice. While the quantum phase diagram remains qualitatively unchanged, the thermodynamic properties are different in three dimensions (3Ds) because the condensate (XY ordered antiferromagnetic phase) extends to finite temperatures. Additionally, the melting of this phase belongs to the XY universality class as opposed to Kosterlitz-Thouless (KT) type in two dimensions (2Ds). This has important consequences in any putative experimental detection of the SS phase, as we shall discuss below.

The Stochastic Series expansion (SSE) quantum Monte Carlo method [27] is used to study the Hamiltonian (1) on cubic lattices $N = L \times L \times L/2$, with $8 \leq L \leq 16$. To characterize the different phases, we compute the longitudinal component of the staggered static structure factor (SSSF),

$$S^{zz}(Q) = \frac{1}{N} \sum_{j,k} e^{-iQ\cdot(r_j - r_k)} \langle S_j^z S_k^z \rangle, \quad Q = (\pi, \pi, \pi),$$  \tag{2}

and the spin stiffness, $\rho_s$, defined as the response of the system to a twist in the boundary conditions. $S^{zz}(Q)$ measures the extent of diagonal (Ising like) long-range order (LRO) at the ordering wave vector $Q = (\pi, \pi, \pi)$, while the stiffness (superfluid density in particle language [5, 8]), indicates the presence of XY (off-diagonal) LRO (this is not true for $D < 3$). In 3D, the superfluid density is identical to the condensate fraction. In the simulations, the stiffness is obtained from the winding numbers of the world lines along the three axes: $\rho_s = (W_x^2 + W_y^2 + W_z^2)/3\beta^2$.

**Ground state (GS) phases** As the field, $B$, is varied, the GS of (1) goes through a succession of phases, including spin-gapped Ising-ordered (IS) and gapless XY-ordered (XY) states. The IS phase is marked by a diverging value of $S^{zz}(Q) \propto N$ in the thermodynamic limit, whereas a finite $\rho_s$ characterizes the gapless XY ordered phase. A spin SS phase is identified by a finite value of both $S^{zz}(Q)/N$ and $\rho_s$ [10]. Both quantities are always finite for finite size systems and estimates for $N \rightarrow \infty$ are obtained from finite-size scaling.

Fig. 1 shows the quantum phase diagram as a function of magnetic field, $B$, for $D = 3.0$ and $\Delta = 6.0$ – it is qualitatively similar to that obtained in 2Ds [6]. The $m_z(B)$ curve features two prominent plateaus corresponding to different IS phases. For small $B$, the GS is a gapped AFM solid (IS1) with no net magnetization. The stiffness, $\rho_s$, vanishes in the thermodynamic limit, while $S^{zz}(Q)/N \approx 1$ with the spins primarily in the $S_i^z = \pm 1$ states in the two sublattices. At a critical field, $B_{c1}$, there is a second order transition to a state with a finite fraction of spins in the $S_i^z = 0$ state. These $S^2 = 0$ “particles” Bose-Einstein condense (BEC) to give the
FIG. 1: (Color online) Quantum phase diagram of $H_H$ (Eq. 1) for $D = 3.0$ and $\Delta = 6.0$. The upper panel shows the magnetization as a function of field $B$. The SS phase appears between the two Ising-like phases IS1 and IS2. At higher fields, there is a first order transition to a pure XY–AFM phase. The lower panel shows the stiffness and the longitudinal component of the SSF. The SS phase has finite values of both observables.

GS a finite stiffness. The diagonal order is reduced but remains finite as well. The resulting GS thus has simultaneous long-range diagonal and off-diagonal order; in other words, it is a spin-supersolid. The complete phase diagram consists of a second gapped Ising phase (IS2) with diagonal order (all the spins in the $S^z = -1$ sublattice are flipped to $S^z = 0$) and an XY phase at high fields with pure off-diagonal ordering.

Finite temperature transitions Finite temperature properties of the SS has previously been examined for hard core bosons[8, 11, 12] and $S = \frac{1}{2}$ spins on a bilayer[13]. The melting of the SS phase proceeds via two steps – the superfluid order disappears at a lower temperature whereas the solid order persists up to a higher temperature. In 2Ds, the continuous U(1) symmetry cannot be broken at $T > 0$ and the SS has only a quasi long-range off-diagonal order for $T < T_{KT}$. The vanishing of the spin stiffness occurs via a KT transition. In contrast, true long-range off-diagonal order in the SS persists to finite temperatures in 3Ds and the melting of the superfluid order belongs to the XY universality class. The solid order disappears at a higher temperature via an Ising-like transition.

The results of simulations of thermal transitions associated with the SS phase are shown in fig.2. The top panel shows the variation of the solid and superfluid order parameters as a function of temperature. At low temperatures, both order parameters are finite. With increasing $T$, the SS “melts” into a pure solid. The disappearance of SF order is marked by an enhancement in the solid order. This apparently anomalous behavior reflects the fact that in the SS phase, the solid order is partially suppressed by the co-existing SF order. The longitudinal component of the SSF is accessible experimentally by neutron scattering and its non-monotonic behavior at the onset of superfluid order can serve as an important signature of the SS phase. The three dimensionality of the model implies that the two transitions should be accompanied by specific heat anomalies at the corresponding temperatures. The XY transition will manifest itself as a $\lambda$-anomaly while the Ising-like solid melting will be marked by a cusp. Indeed we find clear signatures of the two transitions in the calculated specific heat (lower panel of fig.2). While both the peaks are rounded by finite-size effects, their positions coincide unambiguously with the melting of the superfluid and Ising orders. Since it is one of the most readily measurable observables, having clear signatures in the specific heat is of great experimental relevance.

Next we discuss the relevance of these results for finding a SS phase in real magnets. The magnetic properties of spin compounds with spin-orbit interaction much smaller than the crystal field splitting can be adequately described by a U(1) invariant model (although this invariance is never perfect)[10]. The transition metal magnetic ions belong to this class. On the other hand, the exchange anisotropy is typically very small in these compounds. The above model with large $\Delta$ is not directly applicable to this class of real quantum magnets. We
shall show below that under appropriate conditions, an effective uniaxial exchange anisotropy can be generated in the low-energy subspace of a model with (realistic) isotropic interactions. To this end we consider coupled layers of dimers with only isotropic (Heisenberg) AFM interactions—an intra-dimer exchange $J_0$ and weaker inter-dimer frustrated couplings $J_1$ and $J_2$ (see Figs. 3(a) and 3(b)):

$$H_D = J_0 \sum_{i} S_i^+ \cdot S_i^- + J_1 \sum_{(i,j),\alpha} S_{i\alpha}^+ \cdot S_{j\alpha}^- + J_2 \sum_{(i,j),\alpha} S_{i\alpha}^- \cdot S_{j\bar{\alpha}}^- - B \sum_{i\alpha} S_{iz}^-.$$  (3)

The index $\alpha = \pm$ denotes the two spins on each dimer.

For $S = 1$ dimers, the low energy subspace of $H_D$ (for $J_1, J_2 \ll J_0$) consists of the singlet, the $S^z = 1$ triplet and the $S^z = 2$ quintuplet (see Fig. 3(a)). The low-energy effective model that results from restricting $H_D$ to this subspace supports a field-induced supersolid phase on a bipartite lattice for $J_0 > z(J_1 + J_2)/2$ and $J_0 \gg z(J_1 - J_2)/2$ ($z$ is the co-ordination number of the lattice) as was shown in Ref. [6].

$$H_{eff} = \sum_{(i,j)} (b_i^+ b_j + b_j^+ b_i) + V \sum n_i n_j - \mu \sum n_i.$$  (4)

$b_i^+$ creates a $S^z = 1$ triplet state at site $i$ whereas the singlet corresponds to the empty boson state; $n_i$ is the boson number operator $b_i^+ b_i$ and the parameters of the effective model are expressed in terms of those of the original Hamiltonian $H_D$ as $t = (J_1 - J_2)/2 V = (J_1 + J_2)/2$ and $\mu = -J_0 + B$. On many frustrated lattices, this model contains a SS phase in its quantum phase diagram for $t < 0$ and $V \gg |t|$ [3, 4, 5, 12]. In terms of the original model, this implies that $S = 1/2$ dimers with frustrated inter-dimer couplings, $J_2 \gtrsim J_1$ provides an alternative realization of a spin-SS on different frustrated lattices.

As a final example, we consider $S = 1$ Heisenberg model with large easy-plane single-ion anisotropy ($\Delta = 1$ and $D < 0$ in Eq.(1)). For $|D| \gg J$ the low energy subspace consists of the $S^z = \pm 1$ states (see Fig. 3(c)). The low-energy effective model is once again the $t - V$ Hamiltonian [3] with $t = -J^2/2D, V = J + J^2/D$ and $\mu = B - J^2/D - 2n_b J$, up to second order in $J/D$. $n_b$ is the number of bonds per site. As in the previous case, a SS phase is realized for $V \gg |t|$ on different frustrated lattices [3, 4, 12]. The BEC component corresponds to spin nematic ordering.

In conclusion, we have used numerical simulation to study the ground state and thermodynamic phase transitions involving the spin-supersolid phase in a $S = 1$ Heisenberg model with uniaxial exchange and single-ion anisotropies on a cubic lattice. The melting of the SS occurs in two steps with the $XY$ and Ising ordering disappearing at different temperatures. The transitions are marked by unique features in the structure factor and the specific heat which will be useful in any experimental detection of the SS. Finally, we discuss several different conditions under which a SS can be realized in real spin compounds.

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