Nematic and supernematic phases in Kagome quantum antiferromagnets under a magnetic field

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Optimizing translationally invariant infinite-Projected Entangled Pair States (iPEPS), we investigate the spin-2 Affleck-Kennedy-Lieb-Tasaki (AKLT) and spin-1 Heisenberg models on the Kagome lattice as a function of magnetic field. We found that the magnetization curves offer a wide variety of compressible and incompressible phases. Incompressible nematic phases breaking the lattice $C_3$ rotation for which we propose simple qualitative pictures – give rise to magnetization plateaux at reduced magnetization $m_z = 5/6$ and $m_z = 1/3$ for spin-2 and spin-1, respectively, in addition to the $m_z = 0$ plateaux characteristic of zero-field gapped spin liquids. Moving away from the plateaux we observe a rich variety of compressible superfluid nematic – named “supernematic” – phases breaking spontaneously both point group and spin-$U(1)$ symmetries, as well as a superfluid phase preserving lattice symmetries. We also identify the nature – continuous or first-order – of the various phase transitions. Possible connections to experimental spin-1 systems are discussed.

Introduction – In the field of quantum magnetism, the magnetic field is a key control parameter which enables to explore exotic phase diagrams of spin systems. In a spin ladder, one of the simplest spin system where spin-1/2 pair up into singlets on the rungs, the magnetic field, by playing the role of a chemical potential for triplet excitations on the rungs (triplons), can induce a transition to the spin-analog of the one-dimensional Luttinger Liquid (LL) [1]. In two dimensions (2D), finite-energy triplons can Bose-Einstein condense [2] and lead to a spin superfluid phase when the Zeeman coupling to the field overcomes the triplon energy. Field-induced Bose-Einstein condensation (BEC) of triplons have indeed been experimentally observed in 2D quantum antiferromagnets (AFM) such as TiCuCl$_3$ [3], Cs$_2$CuCl$_4$ [4] and BaCuSi$_2$O$_6$ [5]. Another spectacular effect of the magnetic field, in the presence of magnetic frustration, is to give rise to magnetization plateaux in the magnetization curve. Such states with a fractional magnetization (when normalized w.r.t. the saturated value) are characterized by a gap towards spin excitations: therefore, similarly to their charge analogs – the Mott insulators – they are incompressible. In celebrated examples such as the Shastry-Sutherland quantum spin-1/2 AFM for strontium-copper-borate [6] or the spin-1/2 Kagome AFM (possibly) relevant for volborthite and vesignieite [7], it has been predicted that incompressible plateaux are stabilized under an applied magnetic field by spontaneous breaking translation symmetry [6, 8]. In such cases, the stability of the plateau is generically associated to an order by disorder (OBD) mechanism [9] where the semi-classical long range (LR) spin order possesses a macroscopic entropy and maximizes quantum fluctuations. Whether plateau physics can occur in spin systems which preserve translation symmetry is still unknown although such a translation invariant incompressible state can formally be constructed based on an Affleck-Kennedy-Lieb-Tasaki (AKLT) [10] framework involving resonating triplets polarized along the field [11].

In addition, search for plateaux whose stabilization goes beyond the OBD mechanism is another motivation for our work.

In this Letter we consider the spin-2 AKLT model

$$H_{\text{AKLT}} = \sum_{\langle ij \rangle} P_{ij}^{(4)} - h \sum_i S_i^z$$

(1)

where $P_{ij}^{(4)}$ is the projector onto the $S = 4$ subspace of the nearest-neighbor $\langle ij \rangle$ bond and the spin-1 quantum Heisenberg model

$$H_H = \sum_{\langle ij \rangle} S_i \cdot S_j - h \sum_i S_i^z$$

(2)

on the Kagome lattice in the presence of an applied magnetic field $h$ (chosen along the $z$ direction). We use infinite-Projected Entangled Pair States (iPEPS) [12, 13] in the thermodynamic limit and find very rich phase diagrams. Although we restrict to translationally invariant states, we allow for non-equivalent A, B and C sites in the unit cell (see Fig.1(a)). Hence, point group symmetries may be spontaneously broken (while translation symmetry is preserved by construction). Such symmetry broken phases named “nematics” are characterized by fractional magnetization plateaux resulting from a gap towards spin excitations. Hence, the “spin compressibility” (the derivative of the magnetization w.r.t. the field) vanishes and these phases can be viewed as “incompressible” (like “solid” phases). In addition, the Hamiltonian (spin) $U(1)$ symmetry around the field direction may (independently) be spontaneously broken resulting in superfluid phases – or “supernematic” phases whenever nematic order coexists with superfluidity. In contrast, in the incompressible nematic phases the $U(1)$ symmetry is preserved and the transverse magnetization vanishes on every site. A summary of the new phases found in this work and their symmetries – compared to the more traditional solid and supersolid phases not investigated here – are shown in Table I.
| Compressible | $U(1)$ | $C_3$ | $C_2$ | $G_T$ |
|-------------|--------|-------|-------|-------|
| Bose Glass  | ✓      | ✓     | ✓     | ✓     |
| Valence Bond Solid (VBS) | ×      | ✓     | ✓     | ✓     |
| Simplex Solid (SiSo) | ×      | ✓     | ✓     | ✓     |
| Superfluid (SF) | ✓      | ×     | ✓     | ✓     |
| Solid (S) | ×      | ✓     | ✓     | ✓     |
| Nematic (N) | ×      | ✓     | ✓     | ✓     |
| Supersolid (SS) | ✓      | ×     | ✓     | ✓     |
| Supernematic (SN) | ✓      | ×     | ✓     | ✓     |

TABLE I: Comparison between different field-induced phases in term of preserved (✓) or broken (×) point group ($C_3$ and $C_2$ rotations), translation group ($G_T$) or spin-U(1) symmetries. Compressibility (✓) or incompressibility (×) is also indicated.

Our iPEPS representation \[ A_{k,l}^s, B_{m,n}^s, C_{o,p}^s \] involves three tensors $A_{k,l}^s$, $B_{m,n}^s$, and $C_{o,p}^s$ located on the lattice sites and two tensors $R_{i}^\updownarrow$ and $R_{p,q,r}^\updownarrow$, which connect the above three site-tensors on the down- and up-triangles, as shown in Fig. 1. The five tensors are optimized through an imaginary time evolution procedure, starting from random initial states. The various phases are then determined by analyzing (i) the magnetizations $\langle S^z_\mu \rangle$ on the 3 sites of the unit cell - both along ($\alpha = z$) and transverse ($\alpha = x, y$) to the magnetic field - and (ii) the bond-energy densities on the six non-equivalent bonds of the unit cell. For convenience, we define reduced magnetizations by normalizing the longitudinal and transverse components by the spin $S$, i.e. $m_z^\alpha = \langle S^z_\mu \rangle / S$ and $m_\perp^\alpha = \sqrt{\langle S^x_\mu \rangle^2 + \langle S^y_\mu \rangle^2} / S$ respectively. The total (reduced) longitudinal magnetization is obtained by adding the (algebraic) contributions from the 3 sites, $m_z = \sum_\mu \langle S^z_\mu \rangle / 3S$. Note that the total planar magnetization always vanishes, $\sum_\mu \langle S^\alpha_\mu \rangle = 0$ for $\alpha = x$ or $y$. Spontaneous breaking of the $2\pi/3$-rotation (named $C_3$) is directly revealed by a difference in the longitudinal magnetization on some of the A, B or C sites and characterizes nematic (or supernematic) phases. Note that we find that, generically, at least 2 of the 3 sites still have the same magnetization, i.e. a mirror symmetry is preserved. Note also that the inversion (i.e. the $\pi$-rotation named $C_2$) transforming up- into down-triangles can be broken in the case of a “simplex solid” for which the bond energies differ on the two types of triangles.

Spin-2 AKLT model – We first start with a description of the phase diagram of the $S=2$ AKLT model shown in Fig. 2. Turning on the field, we first observe a $m_z = 0$ magnetization plateau corresponding to the well-known fully symmetric singlet Valence Bond Solid (VBS), stable up to a critical field of $h_c = \Delta_z / S \approx 0.245$ where $\Delta_z$ is the spin gap of the AKLT (zero-field) phase \[10\]. The AKLT VBS is an exact $D = 2$ PEPS : on each site four spin-1/2 ancillas (or virtual states) are paired up into singlets with their neighbors and a map projects the virtual spin representation $\mathbb{S}^2$ onto the physical spin-2 subspace. Above the critical field (where a more complex PEPS based upon the simplex tensors $R^\updownarrow$ and $R^\triangle$ is needed) we observe a compressible phase characterized by transverse components of the magnetization at $120°$-degrees breaking the spin-U(1) symmetry – a characteristic of a superfluid (SF) phase – and a uniform longitudinal magnetization. At larger field we find a magnetization plateau at $m_z = 5/6$ characteristic of an exotic incompressible phase. This remarkable phase is a nematic which can be qualitatively pictured as a simple (D=3) PEPS as shown in Fig. 1(c) : in the unit cell all spin-1/2 ancillas are polarized ($S_z = +1/2$) except two which form a resonating singlet around site C. As in the usual $h = 0$ AKLT state, local maps onto the spin-2 physical subspace are applied on every site. Such a simple picture enables to understand the broken point group symmetries of the nematic state : the A and B sites remain equivalent, as well as the 4 diagonal bonds and the 2 horizontal bonds. The transition (or crossover) between the SF and the nematic phases is subtle and will be discussed later. Then, increasing the field further above a new critical value, transverse magnetic order smoothly appears while nematic order persists but with a finite compressibility $\partial m_z / \partial h$. This supernematic I phase is characterized by equal collinear transverse magnetizations on the A and B sites. In contrast, in the supernematic II phase at larger field the transverse magnetizations are opposite on A and B (and hence there is no transverse magnetization on site C). Finally, we observe a jump of $m_z$ to the fully saturated value $m_z = 1$ (1st order transition).
FIG. 2: Phase diagram of the Kagome AKLT model vs magnetic field obtained from the analysis of the longitudinal and transverse magnetizations. First-order phase transitions are shown by red dashed lines. Reduced magnetization along the field (a) and transverse to the field (b) are shown for the three sites of the unit cell. The total (reduced) magnetization is also shown in (a) as a continuous black line. Schematic pictures of the magnetization patterns (along and perpendicular to the field) are provided for each phase. The \( m_z = 0 \) and \( m_z = 5/6 \) magnetization plateaux are characterized by \( m_\perp = 0 \) in contrast to the superfluid and supernematic phases.

**Spin-1 Heisenberg model** – We now turn to the description of the phase diagram of the spin-1 Heisenberg AFM as a function of the magnetic field, shown in Fig. 3. As for the AKLT model, we find a magnetization plateau at \( m_z = 0 \), which is characteristic of a gapped phase. The corresponding (two-fold degenerate) simplex solid ground state (GS) depicted on Fig. 1(d) is SU(2) invariant but breaks the \( (C_2) \) symmetry between up- and down-triangles due to different bond energies. Remarkably, the magnetization curve of the spin-1 AFM also shows a plateau at \( m_z = 1/3 \). The corresponding incompressible state is a semi-classical ordered state, as pictured in Fig. 1(e), with a favored direction (horizontal in the figure) of ferromagnetic chains \( (m^{A}_z = m^{B}_z \simeq +1) \) and Néel chains in the two other directions \( (m^{C}_z \simeq -1) \). We expect this nematic state (breaking the \( 2\pi/3 \)-rotation) to be stabilized by quantum fluctuations via an OBD mechanism, in contrast to the AKLT plateau state. On each side of the magnetization plateau, we find supernematic phases with transverse components of the magnetization coexisting with the longitudinal magnetic order inherited from the \( m_z = 1/3 \) nematic phase. As for the spin-2 AKLT model, we find two types of supernematic phase depending whether the transverse components of the magnetization are opposite (SN I, SN II and SN IV) or collinear and equal (SN III) on the A and B sites. Note that there is a transition between SN I and SN II (although they are of the same type) due to a sudden change of sign of all the components of the magnetization along the field.

**Nature of phase transitions** – Our phase diagrams offer
a rich variety of phase transitions which can be classified according to the behavior of the magnetization, a thermodynamic quantity, $m_z(h) = \partial E_{GS}/\partial h$. (i) The transition from the VBS AKLT state to the SF is a continuous transition with $m_z \sim (h-h_c)^{1/2}$ and $m_\perp \sim m_z^{1/2}$ as shown in Fig. 4(a). We can view it as a traditional BEC of triplons. (ii) We observe a second class of (2nd order) continuous transitions on the right edges of the two magnetization plateaux clearly characterized by $m_z-m_{\text{plateau}} \propto (h-h_c)$ and $m_z^{\text{plateau}} \propto (m_z-m_{\text{plateau}})^{1/2}$, as shown in Fig. 4(b,c), where $m_{\text{plateau}}$ corresponds to the fractional magnetization 5/6 and 1/3 of the plateaux of the AKLT and Heisenberg models, respectively.

(iii) The transitions on the left edges of the plateaux are more unconventional. For the spin-1 Heisenberg AFM, the transition between SN II and the nematic phase may be weakly first order, or $m_z(h)$ may have a vertical slope. For the AKLT model there is a narrow intermediate region between the superfluid and the nematic phase which might correspond to another supernematic phase (similar to SN IV). We also identify a narrow interval of superfluid phase between the simplex solid and SN I in the spin-1 AFM involving at least a first order transition. Also, we observe that the transition to the fully polarized state is generically of first order with a jump of the total magnetization (and of other observables).

(iv) Transitions between the supernematic phases, i.e. between SN I and SN II (in both phase diagrams) and between SN III and SN IV are remarkably smooth. Indeed, they do not seem to involve a discontinuity of the slope of $m_z(h)$ (a second derivative of the energy) – strictly speaking they would correspond to 3rd order phase transitions – although observables like the individual site magnetizations are all discontinuous.

**Discussions and conclusions** – In this Letter, we study the very rich phase diagrams under a magnetic field of two Kagome quantum antiferromagnets described by the S=2 AKLT and the S=1 Heisenberg models. Besides known phases, such as superfluid, valence bond solid or fully polarized phases, we establish the existence of new remarkable field-induced phases, namely, nematic phases which break $2\pi/3$-rotation and preserve all other symmetries, and supernematic phases which break, in addition, the spin-U(1) symmetry. Nematic phases are incompressible and, therefore, give rise to magnetization plateaux – at $m_z = 5/6$ and $m_z = 1/3$ for S=2 and S=1, respectively. A wide variety of phase transitions are revealed and discussed. We also find that the zero-field GS of the S=1 AFM (using a translationally-invariant ansatz) is gapped and trimmerized ($\pi/2$-rotation symmetry breaking), realizing a new form of incompressible state named simplex solid.

It is interesting to discuss here the relevance of this work to experiments on some Nickelate or Vanadate compounds consisting of (weakly coupled) S=1 Kagome AFM layers. Reduced spin fluctuations (compared to spin-1/2 analogs) and possible existence of single-ion anisotropy might restrict the observation of a spin liquid behavior in such systems. For example, BaNi$_3$(OH)$_2$(VO$_4$)$_2$ shows a glassy behavior at low temperature whose origin is still unknown [17]. Nevertheless, experimental behaviors suggestive of a spin gap have been seen in YCa$_3$(VO)$_3$(BO$_3$)$_4$ [18] and KV$_3$Ge$_2$O$_9$ [19], and Kagome compounds based on spin-1 $V^{3+}$ ions. Although current single crystals might still contain a sizable amount of impurities [18] or competing ferromagnetic interactions might be present [19], such materials might nevertheless be good candidate to observe the exotic physical behaviors described here.

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