Order by disorder in the Heisenberg-compass model on the cubic lattice

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Starting from an anisotropic super-exchange Hamiltonian as is found for compounds with strongly correlated electrons in multi-orbital bands and subject to strong spin-orbit interaction we calculate the contribution of thermal and quantum spin fluctuations to the free energy. While the mean field solution of ordered states for such systems usually has full rotational symmetry, we show here that the fluctuations lead to a pinning of the spontaneous magnetization along some preferred direction of the lattice. The fluctuations choose preferred directions for the magnetic order parameter amongst the classically degenerate manifold of states.

I. INTRODUCTION

Recent research activities on transition metal oxides suggest that the interplay of the strong spin-orbit coupling (SOC), crystal field (CF) interactions and electron correlations may lead to compass-like anisotropic interactions between magnetic degrees of freedom. These anisotropic interactions have a generic form $J^\alpha S_i^\alpha S_j^\alpha$ in which $\alpha$ depends on the direction of the particular link or bond and $S$ denotes spin or pseudospin describing magnetic degrees of freedom.

The models in which compass-like anisotropies are dominating, or also the pure compass models, have been known for a long time. These models appear naturally in strongly correlated electron systems as minimal models to account for interactions between pseudospins describing orbital degrees of freedom. The compass-like anisotropies also arise as interactions between magnetic degrees of freedom in systems with strong SOC which might be realized in 4d and 5d transition metal oxides. However, in these systems, due to the extended nature of 4d and 5d orbitals, the compass interactions are always accompanied by the usual SU(2) symmetric Heisenberg-type exchange. These models are especially interesting because while the pure compass-like models are rare, the combined Heisenberg-compass models have been shown to be minimal models describing the magnetic properties of various materials. A review of the different realizations of compass models and their physical motivations, symmetries, unconventional orderings and excitations may be found in the recent paper by Nussinov and van den Brink.

One of the common features induced by compass-like anisotropies is frustration, arising from a competition of interactions along different directions and leading to the macroscopic degeneracy of the classical ground state and in addition rich quantum behavior. In many cases, the pure compass models do not support conventional magnetic ordering because the degeneracy of the classical ground state is connected to discrete sliding symmetries of the model. Because these symmetries are intrinsic symmetries of the model, they can not be lifted by order-by-disorder mechanisms. Instead, the direct consequence of the existence of these symmetries is that the natural order parameters for pure compass models are nematic, which are invariant under discrete sliding symmetries.

The nematic order present in the compass model is fragile and is easily destroyed by the presence of the isotropic Heisenberg interaction which breaks some of the intrinsic symmetries of the model. In Heisenberg-compass models, some of the degeneracies become accidental. In these models, the true magnetic order might be selected by fluctuations via an order by disorder mechanism, removing accidental degeneracies and determining both the nature and the direction of the order parameter. Despite the simplicity of these models, the interplay of the Heisenberg and compass interaction leads to very rich phase diagrams even in the simplest case of the square lattice. For classical systems this mechanism requires finite temperatures, where entropic contributions of fluctuations to the free energy become effective.

In this work, we will be interested in studying the directional-ordering transitions in the Heisenberg-compass model on the cubic lattice. From a historical perspective, the three-dimensional 90° compass model was the first model of this kind proposed by Kugel and Khomskii in the context of the ordering of the $t_{2g}$ orbitals in transition metal oxides with perovskite structure. The formal procedure which we will be using here is based on the derivation of the fluctuational part of the free energy by integrating out the leading fluctuations, and determining which orientations of the vector order parameter correspond to the free energy minimum. To do so, we first express the partition function as a functional integral over classical fields. Our starting point in evaluating this exact representation of the partition function is the mean-field solution. This approach usually does not reflect the anisotropic character of the interaction referring to the crystal lattice axes. As a next step, we evaluate the contribution of Gaussian fluctuations to the free energy of the mean field ordered state. The latter carries the information embodied in the anisotropic spin interaction and may therefore be used to define preferred directions of the spin order with respect to the lattice. We will not go beyond the simple evaluation of the contribution of fluctuations, e.g. by incorporating...
the fluctuation contribution self-consistently.

For simplicity, we choose the parameters of the model such that the ground state is ferromagnetic, i.e. we consider the Heisenberg interaction to be ferromagnetic and allow the compass interaction to be both ferromagnetic and antiferromagnetic. Our analysis shows that the profile of the fluctuation part of the free energy exhibits significant changes when the compass interactions become antiferromagnetic and exceed some critical value. For any ferromagnetic and weak antiferromagnetic compass interactions, the minima of the fluctuation part of the free energy are attained if the spontaneous magnetization vector points along one of the cubic axes. Once the antiferromagnetic compass interactions become strong, the minima of the free energy and thus possible directions of the magnetization shift to one of the cubic body diagonals. Interestingly, this transition happens smoothly through an intermediate phase in which the locations of minima slide along the unit sphere in a very peculiar way.

As the compass interaction becomes more antiferromagnetic in the intermediate phase, the maxima and minima interchange in a symmetric manner. In order to do that, they continuously split and slide around each other. We found the intermediate phase to exist when the ratio of the compass to Heisenberg interactions is roughly $-1.2 < K/J < -1.45$. However, since the process is very smooth, it is difficult to determine the exact boundaries of the intermediate phase.

This paper is organized as follows. In section II we introduce the functional integral representation of the partition function for the spin systems with interactions described by the most general bilinear form of the superexchange Hamiltonian. In section III, we applied this framework to compute the angular dependence of the fluctuation part of the free energy for the ferromagnetic Heisenberg-compass model on the cubic lattice. Our results and discussions are given in Section IV.

II. REPRESENTATION OF THE PARTITION FUNCTION

We consider a system of identical spins on a lattice, interacting in an anisotropic fashion as indicated in the introduction, defined by the Hamiltonian

$$H = \sum_{j,j'} \sum_{\alpha,\alpha'} J_{j,j'}^{\alpha,\alpha'} S_j^\alpha S_{j'}^{\alpha'}$$

(1)

where $j,j'$ label the lattice sites and $\alpha,\alpha' = x, y, z$ label the three components of the spin. For the models with compass-like anisotropies and Heisenberg isotropic interactions of spins, the interaction is diagonal in the spin space, $\alpha = \alpha'$, and $J_{j,j'}^{\alpha,\alpha'}$-matrix elements are different for the $(j,j')$-bonds with $\gamma = \alpha$ and $\gamma \neq \alpha$. However, since our consideration is also valid for the case when $\alpha \neq \alpha'$, in the following we will keep both indices.

We will be interested in the long-range ordered phases of the system. The mean field approximation of the order parameter usually leads to a highly degenerate manifold of states, e.g. a FM state with spontaneous magnetization pointing in any direction. This degeneracy is lifted by anisotropic components of the spin interaction, but only at the level of the fluctuational contribution to the action $S_{fl}$. In the following we present a framework allowing to calculate $S_{fl}$.

The partition function of the system is given by a trace over the Boltzmann operator

$$Z = Tr \{ \exp[-\beta \sum_{j,j',\alpha,\alpha'} S_j^\alpha S_{j'}^{\alpha'}] \}$$

(2)

where $\beta = 1/kT$ is the inverse temperature, $S_j^\alpha$ are the components of the spin operator at site $j$. In order to compute $Z$, it is useful to introduce vector variables $\phi_j$ with components $\phi_j^\alpha$, where $\alpha = x, y, z$, by using the Hubbard-Stratonovich transformation of the partition function

$$Z = C Tr \{ \int [d\phi_j^\alpha] \exp \left[ \sum_{j,j',\alpha,\alpha'} \phi_j^\alpha (J^{-1})^{\alpha \alpha'}_{j,j'} \phi_{j'}^{\alpha'} + \sum_j \phi_j \cdot S_j \right] \}$$

(3)

where $[d\phi_j^\alpha] = \prod_{j,\alpha} d\phi_j^\alpha$. $(J^{-1})^{\alpha \alpha'}_{j,j'}$ is the matrix inverse of $J_{j,j'}^{\alpha,\alpha'}$ with respect to the combined indices $(j, \alpha)$ and $(j', \alpha')$. The constant $C$ is a function of $T$ and $J$, in the simplest case $C \propto (T T_e)^{1/2}$. Because $C$ gives only a constant shift of the free energy, we will neglect it in the following. Also, because spin operators of different sites commute, we need only trace over the Hilbert space of a single spin operator

$$W(\beta | \phi_j) = Tr_j \{ \exp[2\beta \phi_j \cdot n_j \cdot S_j] \}$$

(4)

Here, $|\phi_j| = [\phi_{jx}^2 + \phi_{jy}^2 + \phi_{jz}^2]^{1/2}$ and $n_j = \phi_j / |\phi_j|$ is the unit vector in the direction of the vector $\phi_j = (\phi_{jx}, \phi_{jy}, \phi_{jz})$. Because the trace is independent of the direction $n_j$, we may choose the quantization axis along $n_j$.

$$W(\beta | \phi_j) = \sum_{m=-S}^{S} \exp[2\beta |\phi_j| m],$$

(5)

where eigenvalues of $S_\alpha$ are denoted by $m$, in units where $\hbar = 1$. The partition function may thus be expressed as

$$Z = C \int [d\phi_j^\alpha] \exp[\beta \sum_{j,j',\alpha,\alpha'} \phi_j^\alpha (J^{-1})^{\alpha \alpha'}_{j,j'} \phi_{j'}^{\alpha'} + \sum_j \ln W(\beta | \phi_j)]$$

$$= C \int [d\phi_j] \exp[-\beta S],$$

(6)

where $l = (j, \alpha)$ is a combined index and the action is defined as

$$S = - \sum_{j,\alpha,j',\alpha'} \phi_j^\alpha (J^{-1})^{\alpha \alpha'}_{j,j'} \phi_{j'}^{\alpha'} - \beta^{-1} \sum_j \ln W(\beta | \phi_j).$$

(7)
In the special case of $S = 1/2$, we have
\[ W(\beta|\phi_j|) = 2 \cosh[\beta|\phi_j|]. \] (8)

III. FERROMAGNETIC HEISENBERG MODEL WITH COMPASS-LIKE ANISOTROPIES ON THE CUBIC LATTICE

A. Isotropic Heisenberg interaction

In order to demonstrate how to perform the evaluation of the above representation of the partition function, we consider the isotropic ferromagnetic Heisenberg model with nearest neighbor interactions on the cubic lattice. In this case, the model \([1]\) reads
\[ H = \sum_{j,j'} \sum_\alpha J_{j,j'}^\alpha \delta \phi_j^\alpha \delta \phi_{j'}^\alpha, \] (9)
where $J_{j,j'} = J$ and $J < 0$. A uniform mean field, or a saddle point solution, is found by taking $\delta \phi^\alpha = m_0^\alpha \phi_0 = m_0^\alpha \phi$, where $m_0^\alpha$ are the components of the unit vector $\mathbf{m}_0$. The saddle point equation, which is identical with the usual mean field equation (here we use $S = 1/2$),
\[ 0 = \frac{\partial}{\partial \phi} S = -\frac{\partial}{\partial \phi} \left[ \frac{2}{z} J \phi^2 + \beta^{-1} \ln(2 \cosh(\beta \phi)) \right] \] (10)
gives the following solution:
\[ -\frac{4}{z} J \phi = \tanh(\beta \phi), \] (11)
where $z$ is the number of nearest neighbors and $N$ is the number of lattice sites. Here we used $J^{-1}(q = 0) = 2/(zJ)$. At the transition, when $\phi \to 0$, we have $\beta_c = 1/T_c = -2J^{-1}(q = 0) = -4/zJ$. The mean field transition temperature $T_c$ is the characteristic energy which we may use as an energy unit. It is useful to define a dimensionless measure of magnetization (or rather spin polarization) by $t(T) = \beta_c \phi = \tanh(\beta \phi)$, which is zero at $T_c$ and rises monotonically upon cooling to the saturation magnetization $t = 1$ at $T = 0$.

The fluctuation contribution is obtained by expanding the action in the fluctuation field $\delta \phi_j = \phi_j - \phi_0$ about the mean field to lowest order
\[ S = S_0 + S_{\delta}, \] (12)
\[ S_0 = N \left[ \frac{T_c}{2} \left( 1 - t^2 \right) \right], \]
The mean field free energy $S_0$ is in complete agreement with the usual mean field theory of ferromagnets for spin $S = 1/2$. In particular the ground state energy $S_0 = N T_c$ and the transition temperature $T_c$ are correctly obtained. We note that $S_0$ does not depend on the direction of magnetization $\mathbf{m}_0 = \phi_0/|\phi_0|$. In order to derive the fluctuation part free energy, or equivalently the action $S_{\delta}$, we first note that $S_{\delta}$ is a bilinear function of $\delta \phi_j$. Thus, we need to calculate the second derivatives of $S$ and compute them at the mean field value of the order parameter. The fluctuation part of the free energy is given by
\[ S_{\delta} = -\sum_{j,\alpha} \sum_{j',\alpha'} \delta \phi_j^{\alpha} (J_{j,j'}^{\alpha\alpha'}) \delta \phi_{j'}^{\alpha'} \] (13)
\[ -\frac{1}{2\beta} \sum_j \sum_{\alpha\beta} \delta \phi_j^\alpha \delta \phi_j^\beta \left[ \frac{\partial^2}{\partial \delta \phi_j^\alpha \partial \delta \phi_j^\beta} \ln W(x) \right] _{\delta \phi_j^\alpha = \delta \phi_j^\beta = 0} \]
where $x = \beta|\phi_0 m_0 + \delta \phi_j|$. Using the second derivative of $W$ at the mean field value,
\[ \left[ \frac{\partial^2}{\partial \delta \phi_j^\alpha \partial \delta \phi_j^\beta} \ln W \right] _{\delta \phi_j^\alpha = \delta \phi_j^\beta = 0} = (1 - t^2) \beta^2 m_{0,\alpha} m_{0,\beta} + \beta \delta_{\alpha \beta} - m_{0,\alpha} m_{0,\beta} \]
one finds
\[ S_{\delta} = \sum_{j,\alpha} \sum_{j',\alpha'} \delta \phi_j^{\alpha} \left( - (J_{j,j'}^{\alpha\alpha'}) - J_{j,j'}^{\alpha\alpha'} \right) \frac{1}{2} (\beta_c \delta_{\alpha \alpha'}) \]
\[ + (\beta (1 - t^2) - \beta_c) m_{0,\alpha} m_{0,\alpha'} \delta \phi_j^{\alpha} \delta \phi_j^{\alpha'}, \]
\[ \text{We recall that } t = m_0 \tanh(\beta \phi_0) \text{ is the magnetization vector (in units of the saturation magnetization).} \]

It is easy to compute $S_{\delta}$ in the reciprocal space. To this end, we perform Fourier transformation $J_q = \sum_j e^{-i q \cdot R} J_{0,j}$ and $\cos q \theta$, where for the case of the simple cubic lattice $\alpha = x, y, z$, and get
\[ S_{\delta} = \sum_q \{ - J_{q}^{-1} \left( 1 - \frac{1}{2} |m_0| \right) (\phi_0 \cdot \delta \phi_{-q}) \} \]
\[ -\frac{1}{2} \left[ \beta (1 - t^2) - \beta_c \right] \left( m_0 \cdot \delta \phi_q \right) \left( m_0 \cdot \delta \phi_{-q} \right) \]
\[ - \sum_q A_{q}^{\alpha,\alpha'} \delta \phi_q^\alpha \delta \phi_{-q}^{\alpha'}, \]
where $J_{q}^{-1} = 1/J_q$. In this case $S_{\delta}$ is independent of the direction of magnetization $\mathbf{m}_0$. This is easy to see by considering longitudinal (along $\mathbf{m}_0$) and transverse fluctuations, $\delta \phi^l = \mathbf{m}_0 \cdot \delta \phi$ and $\delta \phi^{tr} = \sum_{\mu=1,2} \mathbf{m}_\mu \phi^\mu$, respectively. Here we defined $\delta \phi^{tr}_q = \mathbf{m}_\mu \cdot \delta \phi$, with $\mathbf{m}_1 = (\mathbf{m}_0 \times \mathbf{z})/|\sin \theta|$ and $\mathbf{m}_2 = \mathbf{m}_1 \times \mathbf{m}_0$, where $\cos \theta = \mathbf{m} \cdot \mathbf{z}$. In this new basis, the fluctuation part of the action can be written as
\[ S_{\delta} = \sum_q \sum_{\mu,\nu=0}^2 A_{q,\mu,\nu} \delta \phi_{q,\mu} \delta \phi_{-q,\nu}, \] (17)
where we defined $\delta \phi_{q,0} = \delta \phi^{l}_{q}$ and $\delta \phi_{q,1,2} = \delta \phi^{tr}_{q}$. It can be easily seen that the contribution of both, the transverse and the longitudinal fluctuations, is independent of the orientation of $\mathbf{m}_0$. The longitudinal fluctuations contribute to the action as
\[ S_{\delta,1} = \sum_q \left[ - J_{q}^{-1} \left( 1 - t^2 \right) \right] \left( m_0 \cdot \delta \phi^l_q \right) \left( m_0 \cdot \delta \phi^l_{-q} \right) \] (18)
For sufficiently small \( q \), the coefficient function \( \tilde{A}_{q,00} = J_q^{-1} + \frac{1}{2} \beta (1 - t^2) \geq 0 \), so fluctuations are energetically unfavorable. The transverse fluctuations also vanish in agreement with Goldstone’s theorem: both terms \( \tilde{A}_{q,11} \) and \( \tilde{A}_{q,22} \) are zero in the limit \( q \to 0 \) because \( m_0 \delta \phi_{tr} = 0 \) and \( -J_q^{-1} - \frac{1}{2} \beta \lambda \to 0 \) when \( q \to 0 \).

Note that while the coefficients \( \tilde{A}_{q,00}, \tilde{A}_{q,11} \) and \( \tilde{A}_{q,22} \) are all positive at sufficiently small \( q \), this is not the case near the Brillouin zone boundary. The reason is that \( J(q) \) has zeros on a certain surface in momentum space and changes sign. The way to transform the integration over fluctuations in those regions of momentum space where the eigenvalues of the coefficient matrix \( \tilde{A}_{q,\nu\nu} \) are negative is to deform the integration contour \( \delta \gamma \) into the definition of \( \tilde{A}_{q,\nu\nu} \), traversed along the imaginary axis. This amounts to replacing the eigenvalues by their modulus.

### B. Fluctuations due to anisotropic compass interactions

Next, in addition to the isotropic Heisenberg term, let us take into consideration an anisotropic compass interaction, \( K \). The constraint that the ferromagnetic solution remains stable is satisfied for all negative (ferromagnetic) values of \( K \) and for positive values \( K < 3 |J| \).

In the presence of anisotropic compass interaction, the model \([1]\) reads

\[
H = \sum_j \sum_{j'} \sum_{\alpha} J_{q,j,j'}^{\alpha} S_{j}^{\alpha} S_{j'}^{\alpha},
\]

where exchange interactions are given by

\[
J_{q,j,j'}^{\alpha} = \frac{1}{2} \delta_{\alpha,j,j'} \gamma_j + K \delta_{\alpha,|\tau|},
\]

the index \( \tau = \pm x, \pm y, \pm z \) labels nearest neighbor sites and \( |\tau| \) denotes a direction in spin space. We obtain the Fourier transform of the interaction as

\[
J_q^{\alpha} = \sum_j e^{-i q \cdot R_j} J_{0, j}^{\alpha} = \sum_{\alpha'} \left( J + K \delta_{\alpha, \alpha'} \right) \cos q_{\alpha'}
\]

Noting that the Fourier transform of the inverse of the operator \( J_q^{\alpha} \) is \( (J^{-1})^{\alpha}(q) = \frac{1}{J_q^{\alpha}} \), we have a representation of the partition function \( Z \) as a functional integral over Fourier components of \( \phi, \phi_q = (\phi_x, \phi_y, \phi_z) \).

\[
Z = C \int [d\phi_q] \exp \left[ \beta \sum_q \sum_{\alpha} \left( \frac{1}{J_q^{\alpha}} |\phi_q| \right)^2 + \ln W(\beta |\phi_j|) \right]
\]

\[
= C \int [d\phi_q] \exp \left[ -\beta S \right]
\]

Given as before, \( \phi_0 = m_0 \phi_0 \) and \( \phi_0 = \beta^{-1} \), where \( \beta \lambda = 1/T_c = -2J^{-1}(q=0) = -2/(\gamma J + K) \). We get

\[
Z = C \exp \left( -\beta S_0 \right) \int [d\phi_q] \exp \left( -\beta S_\lambda \{ \delta \phi^\alpha_q \} \right),
\]

where the fluctuation part of the action is given by

\[
S_\lambda = \sum_q \left[ -\sum_{\alpha} \delta \phi_q^\alpha \delta \phi_q^\alpha - \frac{1}{2} \beta \delta \phi_q \cdot \delta \phi_q \right] - \frac{1}{2} (\beta (1 - t^2) - \beta \lambda) (m_0 \cdot \delta \phi_q) (m_0 \cdot \delta \phi_q - q)
\]

\[
= - \sum_{q,\alpha, \alpha'} A_{q, \alpha, \alpha'} \delta \phi_q^\alpha \delta \phi_q^\alpha
\]

where \( \delta \phi_q \) are the Fourier components of the fluctuating fields. By comparison to the isotropic model, Eq. \([24]\) manifestly breaks rotational invariance which results at the selected directions of the order parameter which minimize the free energy.

In the cubic basis, the elements of \( A_{q, \alpha, \alpha'} \) are given by

\[
A_{q, \alpha, \alpha'} = \delta_{\alpha, \alpha'} \frac{1}{J_q^{\alpha}}
\]

\[
+ \frac{1}{2} \sum_{\mu, \nu} m_{\mu, \alpha} m_{\nu, \alpha'} \delta_{\mu, \nu} [\beta \lambda + \delta_{\mu \alpha} (\beta (1 - t^2) - \beta \lambda)]
\]

The \( 3 \times 3 \)-matrix \( A_{q, \alpha, \alpha'} \) may be diagonalized and it has eigenvalues \( \lambda_{\gamma, q} \) and eigenvectors \( v_{\gamma, q} \), \( \gamma = 0, 1, 2 \). This allows to express \( \sum_{\alpha, \alpha'} A_{q, \alpha, \alpha'} \delta \phi_q^\alpha \delta \phi_q^\alpha = \sum_{\gamma} \lambda_{\gamma, q} \delta \phi_q^\alpha \delta \phi_q^\alpha \), where \( \delta \phi_q^\alpha = v_{\gamma, q} \cdot \delta \phi_q \). The integration over the fluctuation amplitudes may now be performed and gives

\[
S_\lambda = \beta^{-1} \sum_{q} \{ \ln(\lambda_0, q \lambda_1, q \lambda_2, q) \}
\]

Alternatively, we may use that \( \lambda_{0, q} \lambda_1, q \lambda_2, q = \det \{ A_{q, \alpha, \alpha'} \} \), saving the trouble of having to determine the eigenstates of \( A_{q, \alpha, \alpha'} \). In the case that one of the eigenvalues is seemingly negative, we may distort the integration contour in the complex \( \delta \phi_q \gamma \)-plane such that the eigenvalue turns positive, as discussed above. Assuming this transformation to be done whenever it is necessary, we may replace the eigenvalues by their moduli and

\[
\det \{ A_{q, \alpha, \alpha'} \} \approx \det \{ |A_{q, \alpha, \alpha'}| \}.
\]

Let us now derive the explicit expression for the fluctuation contribution for arbitrary orientation of \( m_0 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \). In this case the triad of unit vectors \( m_0, m_1, m_2 \) is given by

\[
m_0 = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)
\]

\[
m_1 = (\sin \phi, -\cos \phi, 0)
\]

\[
m_2 = (-\cos \theta \cos \phi, -\cos \theta \sin \phi, \sin \theta)
\]

Inserting \( m_0, m_1, m_2 \) into the definition of \( A_{q, \alpha, \alpha'} \), we find
its elements to be

\[
\begin{align*}
A_{q,00} &= -J_{q,x}^{-1} - b^l s_\theta^2 c_\phi^2 - b^{tr} (s_\theta^2 + c_\theta^2 c_\phi^2) \\
A_{q,01} &= c_\phi s_\theta s_{\phi}^2 (-b^l + b^{tr}) \\
A_{q,10} &= A_{q,01} \\
A_{q,02} &= c_\phi c_\theta s_\theta (-b^l + b^{tr}) \\
A_{q,20} &= A_{q,02} \\
A_{q,11} &= -J_{q,y}^{-1} - b^l s_\theta^2 s_\phi^2 - b^{tr} (c_\theta^2 + c_\theta^2 s_\phi^2) \\
A_{q,12} &= s_\phi c_\theta s_\theta (-b^l + b^{tr}) \\
A_{q,21} &= A_{q,12} \\
A_{q,22} &= -J_{q,z}^{-1} - b^l c_\phi^2 - b^{tr} s_\phi^2.
\end{align*}
\]

where, to shorten notations, we denote \( \sin \theta(\phi) \equiv s_{\theta(\phi)} \) and \( \cos \theta(\phi) \equiv c_{\theta(\phi)} \), \( b^l = \frac{1}{2} \beta (1 - t^2) \) and \( b^{tr} = \frac{1}{2} \beta_c \). The interactions are defined as \( J_{q,x}^{-1} = 1/((J + K) \cos q_x + J \cos q_y + J \cos q_z) \), \( J_{q,y}^{-1} = 1/((J + K) \cos q_y + J \cos q_x + J \cos q_z) \) and \( J_{q,z}^{-1} = 1/((J + K) \cos q_z + J \cos q_y + J \cos q_x) \). We see that the matrix \( A_{\alpha \alpha'} \) has a rather complex structure as a function of \( q \) and angles \( \theta \) and \( \phi \). This gives rise to a complex behavior of the eigenvalues \( \lambda_{0,q} \), \( \lambda_{1,q} \) and \( \lambda_{2,q} \).

IV. RESULTS AND DISCUSSIONS

We now present the results we obtained for \( S_B(\theta, \phi) \) by performing numerical integration in Eq. \( (26) \). The angular dependencies of \( S_B(\theta, \phi) \) for various values of \( K \) are presented in Fig. 1 and Fig. 3, where the magnitude of \( S_B(\theta, \phi) \) as a function of orientation of the spontaneous magnetization is shown as a color-coded plot on the unit sphere. The calculations for all the plots in Fig. 1 and Fig. 3 are performed at temperature \( \beta = \beta_c + 1 \) and assuming \( J = -1 \). We see that \( S_B(\theta, \phi) \) has a non-trivial dependence on the direction of the order parameter defined by angles \( \theta \) and \( \phi \) which is modified when we change the parameters of the model. This peculiar angular dependency of \( S_B(\theta, \phi) \) is inherited from non-trivial angular dependencies of \( \lambda_{0,q} \), \( \lambda_{1,q} \) and \( \lambda_{2,q} \).

In Fig. 1 (a), we present the profile of \( S_B(\theta, \phi) \) computed for \( K = 0.75 \). We can see, that \( S_B(\theta, \phi) \) is minimized when the magnetization is directed along one of the cubic axes. We note that the cubic directions are also selected for other values of ferromagnetic compass interactions (\( K < 0 \)) and up to the limit of the pure ferromagnetic compass model. In Fig. 1 (b), we increased the compass interaction to be equal to \( K = 1.5 \). We see that the minima of \( S_B(\theta, \phi) \) are achieved when the magnetization is directed along one of the \([1,1,1] \) axes, i.e. along the cubic diagonals, indicating that a rotation of the order parameter takes place as a function of \( K \).

Let us understand how the transition between these two ferromagnetic phases with cubic easy axes and easy axes along cubic diagonals takes place. In Fig. 2, we presented the finite temperature phase diagram of the model \((19)\). The ferromagnetic order is stable for \( K < 3|J| \). The mean field transition temperature is shown by a blue line. At small \( K \), the magnetization points along cubic axes.
The maxima are moving towards cubic face diagonals and the minima are moving towards cubic diagonals. (c) $J = -1$ and $K = 1.25$. The free energy shows the early stages of the splitting of the each maximum along one of the cubic diagonals into three maxima and the splitting of the each minimum along one of the cubic directions into four minima. (b) $J = -1$ and $K = 1.3$. The full splitting of each maximum into three and each minimum into four minima. The maxima are moving towards cubic face diagonals and the minima are moving towards cubic diagonals. (c) $J = -1$ and $K = 1.4$. The minima of the free energy reach cubic diagonal directions. The maxima of the free energy along [1,1,0], [1,0,1], [0,1,1] are splitting into two and going towards cubic directions.

At large $K$, the magnetization points along cubic diagonals. These two phases are separated by a phase in which the magnetization points along some intermediate direction. The borders of the intermediate phase are shown by red dashed lines. The characteristic profiles of the fluctuation free energy in the intermediate phase are shown in Fig. 3 (a)-(c). Fig. 3 (a) shows $S_{H}(\theta, \phi)$ computed for $K = 1.25$. The free energy shows the early stage of the splitting of each maximum along one of the cubic diagonals into three maxima and the splitting of each minimum along one of the cubic directions into four minima. For example, the maximum along [1,1,1] direction continuously splits into three maxima which slide towards the cubic face diagonals [1,1,0], [1,0,1], and [0,1,1]. At the same time the minima at cubic directions slide towards cubic diagonals. For example, the minimum at the [1,0,0] direction splits into four minima, which slide to replace the maxima along [1,1,1], [1,-1,1], [1,1,-1], [1,-1,-1] directions. At Fig. 3(b) we slightly increased the value of the compass interaction and set it equal to $K = 1.3$. Here we see the full splitting of each maximum into three and each minimum into four minima. The maxima are moved towards cubic face diagonals and the minima are moved towards cubic diagonals. In Fig. 3(c) we set $K = 1.4$, which corresponds to the final stage of the deformation of the free energy profile before it has the structure shown in Fig. 1 (b). Here we see that the maxima of the free energy along [1,1,0], [1,0,1], [0,1,1] are splitting into two and are going towards the cubic axes directions but do not yet reach it. So in this way the maxima and minima slide around each other to replace each other as we change the parameters.

V. CONCLUSION

The magnetic properties of heavy transition metal oxides such as iridates and others are emerging as a new fascinating field offering opportunities to realize strongly frustrated quantum spin systems in the laboratory. In these systems the combination of multi-band electronic structure and strong Coulomb and Hund’s couplings with strong spin-orbit interaction can give rise to extremely anisotropic spin exchange interactions of the compass type. Mean field solutions of these models are often untouched by the anisotropies of the model and show the full isotropy of pure Heisenberg models, in contrast with experimental observation. In this paper we addressed the question how the system selects special preferred directions of the mean field order parameter vector. We restricted ourselves to the case of a ferromagnetic order parameter, but the analogous question exists for antiferromagnetic or more complicated ordered structures. We find that the high degeneracy of the ferromagnetic mean field solution is lifted by the free energy contribution from thermal (or quantum) fluctuations. We calculated the fluctuation contribution for a Heisenberg-compass model of spins $S = 1/2$ on a three dimensional cubic lattice with nearest neighbor interactions - an isotropic Heisenberg coupling $J < 0$ (which we take as the energy unit), and a compass coupling $K$. The ferromagnetic state is found if $K < 3|J|$. Rather than exploring the full phase diagram, we focused on one typical temperature $T = T_c/(1 + T_c)$ where $T_c$ is the mean field transition temperature and show a qualitative phase diagram in Fig. 2. For values of $K < 1.2$ the system is found to choose preferred directions of the spontaneous magnetization along one of the cubic axes. For $1.5 < K < 3|J|$ the preferred directions are found to be along the space diagonals. The two do-
mains are separated by a region in which the minima and maxima of the free energy split into four and three, respectively, and perform an interesting dance around each other. In these intermediate phase thus has not only six equilibrium orientations, but twenty four. Exactly how these transitions happen, in particular as a function of temperature, will be the subject of future work. The thermodynamic properties of these intermediate phases at elevated temperature, when thermally activated transitions between different orientations of finite domains may occur is another field to be explored.

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