Long-range order in the XY model on the honeycomb lattice

Jacek Wojtkiewicz,[1] Krzysztof Wohlfeld,[1] and Andrzej M. Oleś[2,3,*]

[1]*Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL-02093 Warsaw, Poland*
[2]*Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[3]*Institute of Theoretical Physics, Jagiellonian University, Prof. Stanisława Łojasiewicza 11, PL-30348 Kraków, Poland*

(Received 23 November 2022; accepted 30 January 2023; published 9 February 2023)

Using the reflection positivity method, we provide rigorous proof of the existence of long-range magnetic order for the XY model on the honeycomb lattice for large spins $S \geqslant 2$. This is in contrast with the result obtained using the *same* method but on the square lattice—which gives a stable long-range order for spins $S \geqslant 1$. We suggest that the difference between these two cases stems from the enhanced quantum spin fluctuations on the honeycomb lattice. Using linear spin-wave theory, we show that the enhanced fluctuations are due to the overall much higher kinetic energy of the spin waves on the honeycomb lattice (with Dirac points) than on the square lattice (with good nesting properties).

DOI: 10.1103/PhysRevB.107.064409

I. INTRODUCTION

One of the main questions concerning the nature of a quantum spin model is whether long-range order (LRO) of any kind could stabilize in a certain range of parameters. Models with finite magnetic anisotropies have discrete symmetries and order more easily, which agrees with our intuition. An occurrence of phase transition in the two-dimensional (2D) Ising model, established on the basis of exact solution of interacting spins S at a square lattice is the most prominent example. The LRO sets in the Ising model at positive temperature $T < T_c$, where T_c is the critical temperature, though the order parameter is reduced by thermal fluctuations [1]. The spin-order parameter becomes maximal in the ground state, i.e., $\langle S^z \rangle \equiv S$ at $T = 0$. On the other hand, the one-dimensional (1D) Ising model orders *only* at $T = 0$.

Models with continuous symmetries, such as the Heisenberg SU(2)-symmetric or the XY U(1)-symmetric one, are quite different. In this case the Mermin-Wagner theorem prevents the LRO at positive temperatures in all low dimensions, i.e., not only in a 1D but also a 2D model [2–4]. This is due to the proliferation of the Goldstone modes, i.e., gapless spin waves, which enhances the thermal fluctuations and kills the LRO. Moreover, the $T = 0$ version of the above theorem, the Coleman theorem [4], states that at $T = 0$ the ground state of such models typically [5] does not carry LRO in one dimension, for the order parameter is completely destroyed by quantum fluctuations triggered by the spin waves. This happens, for instance, in the 1D antiferromagnetic (AFM) Heisenberg model [3,6].

This shows that 2D spin models with continuous symmetries are special, since they never order at positive temperature but may order at $T = 0$. Note that the Coleman theorem merely *allows* for the onset of the LRO but does *not* guarantee it. This is probably best exemplified by the search for the spin-liquid ground state of Heisenberg models on 2D frustrated lattices [7,8]. But an intriguing situation arises already in the 2D AFM Heisenberg model on the square lattice. Here the linear spin-wave theory (LSWT) expansion suggests that at least for a large-enough size of spin S, the quantum corrections to the order parameter (Δm) should be small enough to allow for LRO. In fact, several numerical and analytical methods suggest that the LRO exists (already) for spin $S = 1/2$ [9–13]. However, it is both an amusing and irritating circumstance that its existence has not been rigorously confirmed: the proof shows that the LRO can be stable only for spins $S \geqslant 1$ [14]. This fragility of the long-range spin order is further strengthened by the research on the low-lying excited states which suggests that these may partially be better described in terms of excitations from a spin liquid state (spinons) [15–17] than from the symmetry-broken state with LRO (spin waves or magnons) [18–20].

Experimentally, the 2D spin models with continuous symmetries can basically be realized in the van der Waals crystals [21–23]. These materials are a subject of intensive research and one of the main questions is whether the thermal fluctuations kill the magnetic order. In principle, this should not be the case, for the assumptions of the Mermin-Wagner theorem are never strictly fulfilled in the materials that are solely *quasi*-2D and always have finite magnetic anisotropies. Yet, the applicability of the Mermin-Wagner theorem as well as the potential onset of the large thermal corrections to the order parameter are a subject of intensive discussion [21–23]. It is thus natural to investigate what the role played by the quantum fluctuations is in the onset of the LRO in the ground state of

*a.m.oles@fkf.mpg.de

such a van der Waals spin model which is approximately 2D and has continuous symmetry. Here the salient feature is that the van der Waals materials support the honeycomb [21–29], rather than the square, lattice. Although honeycomb lattice is bipartite, just as the square lattice is, it is not obvious *how the LRO spin order would survive in the ground state of a spin model with continuous symmetry on the honeycomb lattice at* $T = 0$—which is the main question of this paper.

Indeed, the spin LRO is likely to be less stable on the honeycomb than for the square lattice as there are three outgoing exchange bonds from each site and this may amplify the effects of quantum fluctuations which could destroy the ordered state. (Notably, for the 1D Heisenberg model there are just two exchange bonds outgoing from each site and the LRO is then destroyed, as just discussed above.) In fact, for the Heisenberg model on the honeycomb lattice, there is proof of the existence of LRO for $S \geqslant 3/2$ [30], whereas for the square lattice case the *analogous* proof applies already to spins $S \geqslant 1$ [14], see above. Another argument in favor of diminished stability of the ordered AFM state on the honeycomb lattice is provided by the LSWT: Quantum corrections to the order parameter Δm for the Heisenberg model are substantially larger on the honeycomb lattice than on the square lattice, (i.e., $\Delta m \simeq 0.28$ versus $\Delta m \simeq 0.197$ [31]).

In this paper, we shall investigate the existence of LRO on the honeycomb lattice in the spin model and discuss why the order may be less stable than on the square lattice. To this end, we choose to work with the XY model. While this model has a lower symmetry than the Heisenberg model [32] and one expects that it orders more easily, there is no proof of the existence of the LRO using the same method as the one used for its square lattice counterpart and yielding LRO for $S \geqslant 1$ [33] either [34]. It is thus of crucial importance to verify whether the LRO is stable in this model for the same *or* for the higher spin S value than on the square lattice. Moreover, the LSWT corrections calculated to the order parameter of the XY model for the honeycomb lattice are also larger than for the square lattice (i.e., $\Delta m \simeq 0.08$ versus $\Delta m \simeq 0.06$ [32,35]), making it an ideal case to compare the stability of the LRO on these two distinct 2D lattices.

The paper is organized as follows. We shall start from the reflection positivity (RP) method applied to the XY spin model on the honeycomb lattice in Sec. II. Next we use the LSWT method to intuitively understand why the LRO on the honeycomb lattice is less stable than on the square lattice, see Sec. III. The summary and conclusions are presented in Sec. IV.

II. RESULTS: REFLECTION POSITIVITY METHOD

In this section, we rigorously prove that Néel order exists in the ground state of the XY model on the honeycomb lattice with AFM interactions, for a large enough value of spins. The proof is based on the RP technique. Note that, while we consider below solely the AFM case, the proof is valid for the ferromagnetic XY model as well—since these models are in fact isomorphic, unlike in the Heisenberg case.

For quantum spin systems, the RP technique originated in a seminal paper [36]. This paper treated spin systems in three dimensions at positive temperature. In two dimensions, there is no LRO at positive temperature in systems with continuous symmetry group due to Mermin-Wagner theorem [2], but there remains non-trivial question of the ground-state ordering. In Ref. [37], authors have shown that technique of Ref. [36] can be adapted to prove the existence of Néel order in the ground state of an AFM Heisenberg model on the square lattice provided $S \geqslant 3/2$. Later on, it was noticed that the authors of Ref. [37] made a numerical error and in fact LRO exists for all spins $S \geqslant 1$ [14]. Similarly, the LRO in the Heisenberg model on the honeycomb lattice was proven for spins $S \geqslant 3/2$ [30].

For reasons presented in the previous section, it would be desirable to settle the question of ground-state ordering for the XY model on the honeycomb lattice. This problem has been answered in a positive manner for the square lattice: Whereas using an *analogous* method as presented below it was shown that the LRO exists in the ground state for spins $S \geqslant 1$ [33], a distinct calculation showed that the ground state is ordered for an arbitrary value of spin [38]. However, we are not aware of such a result for the honeycomb lattice, and this opportunity encouraged us to undertake attempts to prove this. Below we supply such a proof. The calculation is based on an adaptation of the AKLT technique [30], with heavy use of results given in Ref. [36], as well as in Ref. [37], so we do not include here all the details.

We write the Hamiltonian as

$$\mathcal{H}_\Lambda = \sum_{\langle \mathbf{m},\mathbf{n}\rangle} h^{\mathrm{YZ}}_{\langle \mathbf{mn}\rangle}, \tag{1}$$

where $\mathbf{m}$ and $\mathbf{n}$ are two connected sites, $\langle \mathbf{m}, \mathbf{n}\rangle$ is a bond between nearest neighbors, and the summation is performed over such bonds on the honeycomb lattice, and we define

$$h^{\mathrm{YZ}}_{\langle \mathbf{mn}\rangle} = S^2_{\mathbf{m}} S^2_{\mathbf{n}} + S^3_{\mathbf{m}} S^3_{\mathbf{n}}. \tag{2}$$

Note that we take for convenience exchange couplings between components 2 and 3 (or {Y, Z}, respectively) instead of conventional 1 and 2 (or {X, Y}). Both models are, of course, physically equivalent. Our choice is dictated by an easier comparison with results for an isotropic Heisenberg model. In particular, we define as the order parameter the average of the third (or Zth) component, in analogy to Ref. [30].

The first step of calculation is to compute eigenvalues and eigenvectors of the Laplacian $-\Delta$ on the honeycomb lattice. It is defined as

$$(-\Delta\psi)(\mathbf{m}) = 3\psi(\mathbf{m}) - \sum_{\mathbf{n}:||\mathbf{m}-\mathbf{n}||=1} \psi(\mathbf{n}), \tag{3}$$

where $||\mathbf{m} - \mathbf{n}|| = 1$ means that $\{\mathbf{m}, \mathbf{n}\}$ are nearest-neighbor sites. The honeycomb lattice is periodic with period 2, so eigenvectors cannot be found by ordinary Fourier transform. Instead, observe that the honeycomb lattice is bipartite, i.e., it can be represented as a disjoint union of two sublattices, with any nearest neighbors belonging to different sublattices. We will refer to these sublattices as even and odd ones; yet they are strictly periodic. One performs two Fourier transforms associated with these sublattices.

Let $\boldsymbol{\delta}_i$, for $i = 1, 2, 3$, be unit lattice vectors such that for every even site $\mathbf{m}$, the nearest neighbors are given by $\mathbf{m} + \boldsymbol{\delta}_i$. The nearest neighbors of an odd site $\mathbf{n}$ are then $\mathbf{n} - \boldsymbol{\delta}_i$. We take explicitly $\boldsymbol{\delta}_1 = (0, -1)$, $\boldsymbol{\delta}_2 = (\frac{\sqrt{3}}{2}, \frac{1}{2})$, and

$\boldsymbol{\delta}_3 = (-\frac{\sqrt{3}}{2}, \frac{1}{2})$. For a finite lattice Λ with periodic boundary conditions, the eigenvalues of the Laplacian are grouped in two $\pm$ bands:

$$E^{\pm}_{\mathbf{k}} = 3 \pm |\epsilon(\mathbf{k})|, \quad \text{where} \quad \epsilon(\mathbf{k}) = \sum_{j=1}^{3} \exp(i\mathbf{k}\cdot\boldsymbol{\delta}_j). \quad (4)$$

In an explicit manner,

$$\epsilon(\mathbf{k}) = \exp(-i\,k_2) + 2\exp\left(i\,\frac{k_2}{2}\right)\cos\left(\frac{\sqrt{3}k_1}{2}\right), \quad (5)$$

and therefore

$$|\epsilon(\mathbf{k})| = \sqrt{1 + 4\cos\frac{\sqrt{3}k_1}{2}\left(\cos\frac{\sqrt{3}k_1}{2} + \cos\frac{3k_2}{2}\right)}. \quad (6)$$

Here, the momentum $\mathbf{k} \equiv (k_1, k_2)$ takes values in the Brillouin zone (BZ) for one of the two sublattices. Corresponding eigenvectors $h^{\pm}_{\mathbf{k}}(\mathbf{m})$ are

$$h^{+}_{\mathbf{k}}(\mathbf{m}) = \text{sgn}(\mathbf{m})\frac{1}{\sqrt{|\Lambda|}}\exp\left[i\mathbf{k}\cdot\mathbf{m} + \text{sgn}(\mathbf{m})\frac{\phi(\mathbf{k})}{2}\right], \quad (7)$$

$$h^{-}_{\mathbf{k}}(\mathbf{m}) = \frac{1}{\sqrt{|\Lambda|}}\exp\left[i\mathbf{k}\cdot\mathbf{m} + \text{sgn}(\mathbf{m})\frac{\phi(\mathbf{k})}{2}\right], \quad (8)$$

where the phase $\phi(\mathbf{k})$ is determined from

$$\epsilon(\mathbf{k}) = |\epsilon(\mathbf{k})|\exp\left(i\phi(\mathbf{k})\right).$$

Following Ref. [36], and in particular Lemma 6.1 therein, one proves the *Gaussian domination* inequality common for both Heisenberg and YZ models:

$$\left(\sum_{\mathbf{m}}\text{sgn}(\mathbf{m})S^3_{\mathbf{m}}\overline{(-\Delta\text{f})(\mathbf{m})} \times \sum_{\mathbf{n}}\text{sgn}(\mathbf{n})S^3_{\mathbf{n}}(-\Delta f)(\mathbf{n})\right) \leqslant \beta^{-1}\sum_{\mathbf{m}}\overline{f(\mathbf{m})}(-\Delta f)(\mathbf{m}), \quad (9)$$

where $(\cdot,\cdot)$ is Duhamel two-point function [36], the bar denotes the complex conjugation, $f(\mathbf{m})$ is arbitrary function on the lattice, and β is inverse temperature (below we shall take the limit $\beta \to \infty$).

Define

$$S^{\pm}_{\mathbf{k}} = \sum_{\mathbf{m}} h^{\pm}_{k}(\mathbf{m})S^3_{\mathbf{m}}. \quad (10)$$

(Note that $S^{\pm}_{\mathbf{k}}$ are *not* related to the spin raising and lowering operators.) The sum in Eq. (10) includes only third components of spin operator, and $\pm$ is a band index. Choosing now eigenvectors $h^{\pm}_{\mathbf{k}}$ as a function f in Eq. (9), we get

$$\left(\overline{S^{\pm}_{\mathbf{k}}}, S^{\pm}_{\mathbf{k}}\right) \leqslant \frac{1}{\beta E^{\mp}_{\mathbf{k}}}. \quad (11)$$

So far, the calculations for YZ model (1) are very similar to those for the Heisenberg model [30]. Substantial difference appears when one calculates the average of the *double commutator* $\langle[S^{\pm}_{\mathbf{k}}, [H, \overline{S^{\pm}_{\mathbf{k}}}]]\rangle$. The double commutator is calculated in a standard manner:

$$\left[S^{\pm}_{\mathbf{k}}, [H, \overline{S^{\pm}_{\mathbf{k}}}]\right] = \frac{1}{|\Lambda|}\sum_{\mathbf{m}}\sum_{\mathbf{n}:||\mathbf{m}-\mathbf{n}||=1}\left(e^{i\mathbf{k}\cdot(\mathbf{m}-\mathbf{n})}S^1_{\mathbf{m}}S^1_{\mathbf{n}} - S^2_{\mathbf{m}}S^2_{\mathbf{n}}\right). \quad (12)$$

The average of $\langle S^2_{\mathbf{m}}S^2_{\mathbf{n}}\rangle$ is expressed easily by the ground-state energy per site e_{gs},

$$\left\langle S^2_{\mathbf{m}}S^2_{\mathbf{n}}\right\rangle = \frac{1}{2}\left\langle h^{\text{YZ}}_{\langle\mathbf{mn}\rangle}\right\rangle = \frac{1}{2}\frac{|\Lambda|}{\mathcal{N}}e_{\text{gs}}, \quad (13)$$

where $\mathcal{N}$ is the number of bonds of the lattice. The average of $\langle S^1_{\mathbf{m}}S^1_{\mathbf{n}}\rangle$ can be estimated as in Refs. [14,33]:

$$\left|\left\langle S^1_{\mathbf{m}}S^1_{\mathbf{n}}\right\rangle\right| \leqslant \left|\left\langle S^2_{\mathbf{m}}S^2_{\mathbf{n}}\right\rangle\right|. \quad (14)$$

Putting all together, the average of double commutator can be estimated as

$$\langle[S^{\pm}_{\mathbf{k}}, [H, \overline{S^{\pm}_{\mathbf{k}}}]]\rangle \leqslant \frac{1}{3}\tilde{E}_{\mathbf{k}}\,|E_0|, \quad (15)$$

where

$$\tilde{E}_{\mathbf{k}} = 3 + \sqrt{1 + 4\left|\cos\frac{\sqrt{3}k_1}{2}\right|\left(\left|\cos\frac{\sqrt{3}k_1}{2}\right| + \left|\cos\frac{3k_2}{2}\right|\right)}, \quad (16)$$

and E_0 is a lower bound on the ground state energy. We have also used $\cos x \leqslant |\cos x|$ and $\mathcal{N}/|\Lambda| = 3/2$ for the honeycomb lattice.

A crude approximation for E_0 can be obtained with aid of inequalities, expressing the free energy of the YZ model by the free energy of the Ising model, in a similar manner as in Ref. [39], see p. 57:

$$f^{\text{Is}}(\beta) \geqslant f^{\text{YZ}}(\beta) \geqslant f^{\text{Is}}(2\beta).$$

Passing to the limit $\beta \to \infty$, one obtains

$$E^{\text{YZ}}_{\text{gs}} \geqslant E^{\text{Is}}_{\text{gs}} = -2S^2\mathcal{N}, \quad (17)$$

so for the honeycomb lattice, one finds the lower bound E_0 for the ground-state energy per site:

$$E_0 = -3S^2. \quad (18)$$

Following the arguments of Refs. [30,36], i.e., the Gaussian domination inequality Eq. (9), and the Falk-Bruch inequality, the usual sum rule and $\langle S^3_{\mathbf{m}}S^3_{\mathbf{m}}\rangle = \langle\mathbf{S_m}\cdot\mathbf{S_m}\rangle/3 = S(S+1)/3$ imply that there is Néel order in the ground state if

$$\frac{2S(S+1)}{3} > S(I_+ + I_-), \quad (19)$$

where

$$I_{\pm} = \lim_{|\Lambda|\to\infty}\sum_{\mathbf{k}}\sqrt{\frac{\tilde{E}_{\mathbf{k}}}{E^{\pm}_{\mathbf{k}}}} = \frac{1}{2|\text{BZ}|}\int_{\text{BZ}}d^2\mathbf{k}\sqrt{\frac{\tilde{E}_{\mathbf{k}}}{E^{\pm}_{\mathbf{k}}}}. \quad (20)$$

Here BZ stands for the Brillouin zone for one of two sublattices and |BZ| is its area. The integrand of I_+ is a regular function, whereas integrands of I_- possess singularities, but they are integrable. One finds a numerical value of $I_+ + I_- = 1.777$, which implies that the condition (19) is fulfilled for $S = 2$ or larger. In other words, we have proved that the AFM XY *model on the honeycomb lattice possesses Néel* *order in the ground state for $S \geqslant 2$.* We suggest that future research should allow us to improve an estimation for the average of double commutator (12), as well as for the lower bound of the ground-state energy.

III. DISCUSSION: LINEAR SPIN-WAVE THEORY INSIGHT

In this section, we would like to provide better understanding why, as the RP result suggests, the LRO seems to be softer on the honeycomb than on the square lattice (since the spin for which the LRO exists is proved to be higher for the honeycomb than for the square lattice). To this end, we analyze in detail the well-known LSWT result which gives the quantum correction to the order parameter on the square (honeycomb) lattice $\Delta m = 0.06$ ($\Delta m = 0.08$), respectively [35]. Thus, we follow the calculations of Ref. [35] and write down the expression for the LSWT quantum corrections to the order parameter by performing the Holstein-Primakoff expansion around the Néel state to bosonic operators for each spin at site $\mathbf{m}$ of the ↑-spin sublattice [31],

$$S^-_{\mathbf{m}} \simeq a^\dagger_{\mathbf{m}}, \quad S^+_{\mathbf{m}} \simeq a_{\mathbf{m}}, \quad S^z_{\mathbf{m}} = S - a^\dagger_{\mathbf{m}} a_{\mathbf{m}}, \tag{21}$$

and similarly for the ↓-spin sublattice. Keeping only the linear terms in the bosonic operators and performing successive Fourier and Bogoliubov transformations, one finds then the quantum corrections to the order parameter [35], $\langle S^z_{\mathbf{m}}\rangle = S - \Delta m$, where

$$\Delta m = \tfrac{1}{4}\left| C^+_1 + C^-_1 + C^+_{-1} + C^+_{-1} \right|. \tag{22}$$

Here

$$C^\pm_1 = \frac{z}{2\mathcal{N}} \sum_{\mathbf{k}} C^\pm_1(\mathbf{k}), \quad C^\pm_{-1} = \frac{z}{2\mathcal{N}} \sum_{\mathbf{k}} C^\pm_{-1}(\mathbf{k}), \tag{23}$$

and

$$C^\pm_1(\mathbf{k}) = \sqrt{1 \pm |\gamma(\mathbf{k})|} - 1, \tag{24}$$

$$C^\pm_{-1}(\mathbf{k}) = \frac{1}{\sqrt{1 \pm |\gamma(\mathbf{k})|}} - 1. \tag{25}$$

A constant z stands for the coordination number of the lattice ($z = 3$ for the honeycomb and $z = 4$ for the square) and $\gamma(k)$ is the structure factor that for the honeycomb lattice is given by

$$\gamma(\mathbf{k}) = \frac{1}{3}\left[\exp\left(-i\,\frac{2k_2}{3}\right) + 2\exp\left(i\,\frac{k_2}{3}\right)\cos\left(\frac{k_1}{2}\right)\right], \tag{26}$$

and for the square lattice by

$$\gamma(\mathbf{k}) = \tfrac{1}{2}\,[\cos(k_1) + \cos(k_2)]. \tag{27}$$

Note that above we used the two-sublattice BZ of the *same* range for both the honeycomb and square lattice, namely, $-\pi < k_{1,2} \leqslant \pi$. The use of the same BZ enables us to easily compare any momentum-dependent function on the honeycomb and on the square lattice. Note that the structure factor for the honeycomb lattice can be obtained from the bands defined by Eq. (5) after substituting $k_1 \to k_1/\sqrt{3}$ and $k_2 \to 2k_2/3$.

The important observation is that the modulus of any of the four contributions to the quantum corrections to the order parameter Δm (22), i.e., $|C^\pm_{1,-1}|$, is always by a factor $q \simeq 1.3$ times larger for the honeycomb lattice than for the square lattice—i.e., just as Δm. Hence, despite the fact that $C^\pm_{1,-1}$ have different signs and overall scales to understand why Δm is q times larger for the honeycomb than for the square lattice, it is enough to investigate why the moduli $|C^\pm_{1,-1}|$ are always q times larger on the honeycomb lattice.

To this end, we plot in Figs. 1(a)–1(d) the functions $C^\pm_{1,-1}(\mathbf{k})$ in the first BZ of the square and honeycomb lattice (note that the BZs are the same due to the rescaled momenta of the standard rectangular BZ of the honeycomb lattice, see above). We observe that for all momenta in the substantial (central) part of the BZ the functions $|C^+_1(\mathbf{k})|$, $|C^-_{-1}(\mathbf{k})|$, and $|C^+_{-1}(\mathbf{k})|$ all take a higher value for the honeycomb lattice than for the square lattice. It is only for relatively small areas around the corners of the BZ [i.e., close to $(\pm\pi, \pm\pi)$ and $(\pm\pi, \mp\pi)$ momenta] that the opposite situation takes place. At first sight, a bit more intricate situation takes place for the $|C^-_{-1}(\mathbf{k})|$ function, see Fig. 1(e). In that case, one should also take into account the distinct singularities for both lattices. However, their contributions are in the end roughly equal and we end up with a similar conclusion for $|C^-_{-1}(\mathbf{k})|$, as for the case of $|C^+_1(\mathbf{k})|$, $|C^-_{-1}(\mathbf{k})|$, and $|C^+_{-1}(\mathbf{k})|$.

To fully track the origin of the larger quantum corrections to the order parameter Δm on the honeycomb lattice, we try to understand why in the large part of the BZ all of the relevant functions $|C^\pm_{1,-1}(\mathbf{k})|$ take a higher value for the honeycomb lattice than for the square lattice. To this end, we turn our attention to the moduli of the structure factors $\pm|\gamma(\mathbf{k})|$ for the honeycomb and square lattice—since these are the crucial quantities entering Eqs. (24) and (25). Figures 1(c)–1(f) show that in the large part of the BZ, also the modulus of the structure factors takes a higher value for the honeycomb lattice than for the square lattice. Mathematically, this situation is to a large extent controlled by the fact that the sets of zeros of the structure factor functions are very distinct for the honeycomb and for the square lattice: Whereas for the honeycomb lattice there are just two independent momenta for which $|\gamma(\mathbf{k})| \equiv 0$ (at the Dirac points), for the square lattice there is a whole range of momenta for which $|\gamma(\mathbf{k})| \equiv 0$ (note that the nesting property occurs along the magnetic BZ boundary). Physically, this indicates the noticeably larger mobility of the spin waves on the honeycomb than on the square lattice.

IV. SUMMARY AND OUTLOOK

Motivated by recent studies of the van der Waals materials with *quasi*-2D honeycomb magnetism, we have investigated the onset of the LRO at $T = 0$ of a continuous spin model on the honeycomb lattice. Thereby, we have shown that the order in the XY model occurs on the honeycomb lattice but is softer than for the square lattice: Using the RP method, we have shown that the magnetic LRO occurs for the honeycomb lattice in the XY model for sufficiently large spin value $S \geqslant 2$. This is in contrast with the result obtained using the *same* method for the square lattice which gives LRO for spin $S \geqslant 1$ [33].

The intuitive understanding of the above result can be achieved using the (approximate) LSWT. We show that the enhanced quantum spin fluctuations on the honeycomb lattice, as calculated using the spin waves, are due to the overall much

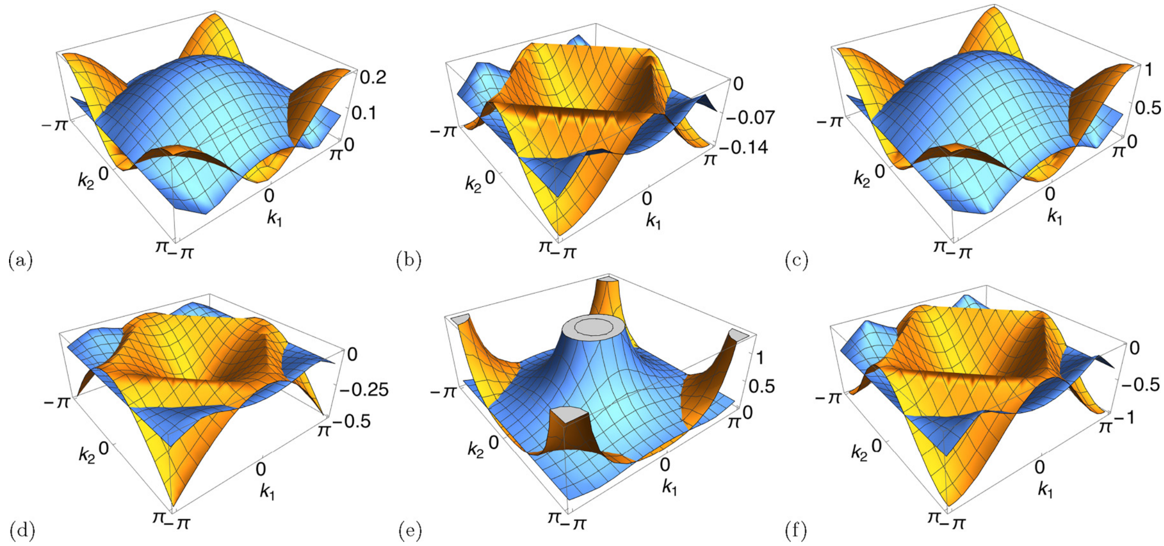

FIG. 1. Dependence of the four contributions to the order parameter renormalization Δm (22) on the momentum components $\{k_1, k_2\}$ in the LSWT approach: (a) $C_1^+(\mathbf{k})$, (b) $C_{-1}^+(\mathbf{k})$, (d) $C_1^-(\mathbf{k})$, (e) $C_{-1}^-(\mathbf{k})$. For comparison, the relevant moduli of the structure factors are also shown in (c) $|\gamma(\mathbf{k})|$ and (f) $-|\gamma(\mathbf{k})|$ (see text for further details). The blue (yellow) color indicates for the results found for the honeycomb (square) lattice, respectively.

higher kinetic energy of the spin waves on the honeycomb lattice than on the square lattice. The latter can largely be traced back to the large qualitative differences between the (nearest-neighbor) structure factors: Whereas on the honeycomb lattice the structure factor has Dirac points and hence rarely vanishes, the good nesting properties of the square lattice yield a whole range of momenta for which the structure factor vanishes. We note that the here-obtained intuition goes beyond the simple argument, which suggests that the order is less stable on the honeycomb than on the square lattice due to the lower coordination number z of the former lattice (see Introduction).

We conclude by suggesting two open problems: First, finding rigorous proof of the existence of LRO in the XY model on the honeycomb lattice *below* the spin value $S = 2$ remains a challenging open problem in the theory of magnetism. It is a bit surprising that LRO here has this constraint while a qualitative argument that this should be the case is missing.

Second, rigorously verifying the existence of the ordered state for the Heisenberg model on the honeycomb lattice *with* small Kitaev interactions may be an important, but supposedly also quite challenging, exercise. So far, it is known that the interplay of Heisenberg and Kitaev interactions gives an interesting phase diagram with several ordered phases competing with spin liquids [40,41], and an experimental realization of the spin liquid was recently proposed [42]. However, the border lines between particular phases depend on the accuracy with which one treats quantum fluctuations [43,44]. It would be interesting to control quantum fluctuations in perturbation theory for the Kitaev-Heisenberg (or Kitaev-XY) model with weak Kitaev interactions.

ACKNOWLEDGMENTS

We thank Wojciech Brzezicki and Hosho Katsura for their interest and insightful discussions. We kindly acknowledge financial support by National Science Centre (NCN, Poland) under Projects No. 2016/23/B/ST3/00839 (J.W. and A.M.O.) and No. 2016/22/E/ST3/00560 (K.W.). A.M.O. is grateful for support via the Alexander von Humboldt Foundation Fellowship (Humboldt-Forschungspreis).

[1] L. Onsager, Crystal statistics. I. A two-dimensional model with an order-disorder transition, Phys. Rev. **65**, 117 (1944).

[2] N. D. Mermin and H. Wagner, Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models, Phys. Rev. Lett. **17**, 1133 (1966).

[3] A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer-Verlag, New York, 1994).

[4] A. J. Beekman, L. Rademaker, and J. van Wezel, An introduction to spontaneous symmetry breaking, SciPost Phys. Lect. Notes, 11 (2019).

[5] It means in magnets with type-A Goldstone modes [4]. Note that below we consider solely magnets with such Goldstone modes, i.e., we exclude those with type-B Goldstone models (as best exemplified by the Heisenberg ferromagnet).

[6] H. Bethe, To the theory of metals. I. Eigenvalues and Eigenfunctions of a linear atomic chain, Z. Phys. **71**, 205 (1931).

[7] L. Balents, Spin liquids in frustrated magnets, Nature (London) **464**, 199 (2010).

[8] L. Savary and L. Balents, Quantum spin liquids: A review, Rep. Prog. Phys. **80**, 016502 (2017).

[9] R. R. P. Singh, Thermodynamic parameters of the $T = 0$, spin-1/2 square-lattice Heisenberg antiferromagnet, Phys. Rev. B **39**, 9760 (1989).

[10] C. J. Hamer, Zheng Weihong, and P. Arndt, Third-order spin-wave theory for the Heisenberg antiferromagnet, Phys. Rev. B **46**, 6276 (1992).

[11] S. R. White and A. L. Chernyshev, Néel order in square and triangular lattice Heisenberg models, Phys. Rev. Lett. **99**, 127004 (2007).

[12] A. W. Sandvik and H. G. Evertz, Loop updates for variational and projector quantum Monte Carlo simulations in the valence-bond basis, Phys. Rev. B **82**, 024407 (2010).

[13] M. Kadosawa, M. Nakamura, Y. Ohta, and S. Nishimoto, Study of staggered magnetization in the spin-s square-lattice Heisenberg model using spiral boundary conditions, J. Phys. Soc. Jpn. **92**, 023701 (2023).

[14] T. Kennedy, E. H. Lieb, and S. Shastry, Existence of Néel order in some spin-1/2 Heisenberg antiferromagnets, J. Stat. Phys. **53**, 1019 (1988).

[15] O. F. Syljuåsen and P. A. Lee, Anomalous Spin Excitation Spectrum of the Heisenberg Model in a Magnetic Field, Phys. Rev. Lett. **88**, 207207 (2002).

[16] B. Dalla Piazza, M. Mourigal, N. B. Christensen, G. J. Nilsen, P. Tregenna-Piggott, T. G. Perring, M. Enderle, D. F. McMorrow, D. A. Ivanov, and H. M. Rønnow, Fractional excitations in the square-lattice quantum antiferromagnet, Nat. Phys. **11**, 62 (2015).

[17] F. Ferrari and F. Becca, Spectral signatures of fractionalization in the frustrated Heisenberg model on the square lattice, Phys. Rev. B **98**, 100405(R) (2018).

[18] M. Powalski, G. S. Uhrig, and K. P. Schmidt, Roton Minimum as a Fingerprint of Magnon-Higgs Scattering in Ordered Quantum Antiferromagnets, Phys. Rev. Lett. **115**, 207202 (2015).

[19] M. Powalski, K. P. Schmidt, and G. S. Uhrig, Mutually attracting spin waves in the square-lattice quantum antiferromagnet, SciPost Phys. **4**, 001 (2018).

[20] R. Verresen, F. Pollmann, and R. Moessner, Quantum dynamics of the square-lattice Heisenberg model, Phys. Rev. B **98**, 155102 (2018).

[21] C. Gong, L. Li, Z. Li, H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia, and X. Zhang, Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals, Nature (London) **546**, 265 (2017).

[22] K. S. Burch, D. Mandrus, and J.-G. Park, Magnetism in two-dimensional van der Waals materials, Nature (London) **563**, 47 (2018).

[23] C. Gong and X. Zhang, Two-dimensional magnetic crystals and emergent heterostructure devices, Science **363**, eaav4450 (2019).

[24] P. A. Joy and S. Vasudevan, Magnetism in the layered transition-metal thiophosphates MPS_3 (M=Mn, Fe, and Ni), Phys. Rev. B **46**, 5425 (1992).

[25] K. Kim, S. Y. Lim, J.-U. Lee, S. Lee, T. Y. Kim, K. Park, G. S. Jeon, C.-H. Park, J.-G. Park, and H. Cheong, Suppression of magnetic ordering in XXZ-type antiferromagnetic monolayer $NiPS_3$, Nat. Commun. **10**, 345 (2019).

[26] K. Kim, S. Y. Lim, J. Kim, J.-U. Lee, S. Lee, P. Kim, K. Park, S. Son, C.-H. Park, and J.-G. Park, Antiferromagnetic ordering in van der Waals 2D magnetic material $MnPS_3$ probed by Raman spectroscopy, 2D Mater. **6**, 041001 (2019).

[27] C. Kim, J. Jeong, P. Park, T. Masuda, S. Asai, S. Itoh, H.-S. Kim, A. Wildes, and J.-G. Park, Spin waves in the two-dimensional honeycomb lattice XXZ-type van der Waals antiferromagnet $CoPS_3$, Phys. Rev. B **102**, 184429 (2020).

[28] M. J. Coak, D. M. Jarvis, H. Hamidov, A. R. Wildes, J. A. M. Paddison, C. Liu, C. R. S. Haines, N. T. Dang, S. E. Kichanov, B. N. Savenko, S. Lee, M. Kratochvílová, S. Klotz, T. C. Hansen, D. P. Kozlenko, J.-G. Park, and S. S. Saxena, Emergent Magnetic Phases in Pressure-Tuned van der Waals Antiferromagnet $FePS_3$, Phys. Rev. X **11**, 011024 (2021).

[29] C. Autieri, G. Cuono, C. Noce, M. Rybak, K. M. Kotur, C. E. Agrapidis, K. Wohlfeld, and M. Birowska, Limited ferromagnetic interactions in monolayers of MPS_3 (M = Mn and Ni), J. Phys. Chem. C **126**, 6791 (2022).

[30] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Valence bond ground states in isotropic quantum antiferromagnets, Commun. Math. Phys. **115**, 477 (1988).

[31] D. C. Mattis, *The Theory of Magnetism I* (Springer, Berlin, 1981).

[32] G. Gomez-Santos and J. D. Joannopoulos, Application of spin-wave theory to the ground state of XY quantum Hamiltonians, Phys. Rev. B **36**, 8707 (1987).

[33] K. Kubo, Existence of Long-Range Order in the XY Model, Phys. Rev. Lett. **61**, 110 (1988).

[34] In fact, the LRO has been proven for $S \geqslant 1/2$ for the square lattice [38]—but using a distinct method than the one here, see discussion in Sec. II.

[35] Zheng Weihong, J. Oitmaa, and C. J. Hamer, Second-Order Spin-Wave Results for the Quantum XXZ and XY Models with Anisotropy, Phys. Rev. B **44**, 11869 (1991).

[36] F. J. Dyson, E. H. Lieb, and B. Simon, Phase transitions in quantum spin systems with isotropic and nonisotropic interactions, J. Stat. Phys. **18**, 335 (1978).

[37] E. J. Neves and J. F. Perez, Long range order in the ground state of two-dimensional antiferromagnets, Phys. Lett. A **114**, 331 (1986).

[38] T. Kennedy, E. H. Lieb, and B. S. Shastry, The XY model has long-range order for all spins and all dimensions greater than one, Phys. Rev. Lett. **61**, 2582 (1988).

[39] B. Simon, *Mathematical Theory of Lattice Gases* (Princeton University Press, Princeton, 1993).

[40] J. Chaloupka, G. Jackeli, and G. Khaliullin, Zigzag Magnetic Order in the Iridium Oxide Na_2IrO_3, Phys. Rev. Lett. **110**, 097204 (2013).

[41] S. M. Winter, A. A. Tsirlin, M. Daghofer, J. van den Brink, Y. Singh, P. Gegenwart, and R. Valentí, Models and materials for generalized Kitaev magnetism, J. Phys.: Condens. Matter **29**, 493002 (2017).

[42] S. K. Takahashi, J. Wang, A. Arsenault, T. Imai, M. Abramchuk, F. Tafti, and P. M. Singer, Spin Excitations of a Proximate Kitaev Quantum Spin Liquid Realized in Cu_2IrO_3, Phys. Rev. X **9**, 031047 (2019).

[43] D. Gotfryd, J. Rusnačko, K. Wohlfeld, G. Jackeli, J. Chaloupka, and A. M. Oleś, Phase diagram and spin correlations of the Kitaev-Heisenberg model: Importance of quantum effects, Phys. Rev. B **95**, 024426 (2017).

[44] K. Morita, M. Kishimoto, and T. Tohyama, Ground-state phase diagram of the Kitaev-Heisenberg model on a kagome lattice, Phys. Rev. B **98**, 134437 (2018).