Second-order spin-wave results for the quantum XXZ and XY models with anisotropy

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A second-order spin-wave analysis is given for the quantum Heisenberg antiferromagnet with anisotropy on the one-dimensional linear chain, two-dimensional honeycomb lattice, and three-dimensional simple-cubic and body-centered-cubic lattices. A similar analysis is given for the quantum XY model with anisotropy on the one-dimensional linear chain, two-dimensional triangular and honeycomb lattices, and three-dimensional simple-cubic, body-centered-cubic, and face-centered-cubic lattices. The singular behavior at the isotropic point is discussed in detail. We find that the quantum spin reduction of the isotropic Heisenberg antiferromagnet on a two-dimensional honeycomb lattice is much stronger than that on a square lattice.

I. INTRODUCTION

For comparison with the results of our series expansions about the Ising limit for the zero-temperature quantum XXZ and XY models on a square lattice, we [1,2] recently carried out a standard second-order spin-wave analysis for the above models, and its predictions were found to be in extremely good agreement with the results of the series expansions. In this paper we apply the general spin-wave results obtained in our previous papers[1,2] to other lattices. We present spin-wave predictions for the isotropic Heisenberg antiferromagnet on the two-dimensional honeycomb lattice, and the isotropic ferromagnetic XY model on the two-dimensional triangular and honeycomb lattice and three-dimensional face-centered-cubic lattice.

Spin-wave theory can provide us with a rather accurate picture of the low-lying states of quantum spin systems. There exist several different versions of the spin-wave theory. The standard spin-wave theory based on the Holstein-Primakoff representation for the Heisenberg model was proposed by Anderson,[3] and further extended to second order by Kubo[4] and Oguchi.[5] The singular behavior of the anisotropic model was discussed by Stinchcombe.[6] This spin-wave theory was previously thought to be unsatisfactory in the XY case,[7] but recently Gomez-Santos and Joannopoulos[8] have shown that, by a different choice of the quantized spin axis, one can obtain a good theoretical fit to the model. Another spin-wave theory using a special spin-wave representation was originally proposed by Villain,[9] and further extended up to second order by Nishimori and Miyake.[10] But up to second order, both traditional spin-wave theories give the same ground-state energy for the Heisenberg antiferromagnet. Recently, a sublattice symmetric spin-wave theory has been formulated by Takahashi,[11] Hirsch,[12] and Tang[13] where the total staggered magnetization is constrained to be zero, which yields excellent agreement with Bethe ansatz results for the $S=\frac{1}{2}$ Heisenberg antiferromagnetic in one dimension. In addition to this, Takahashi[14] has also developed another modified spin-wave theory by using the Dyson-Maleev transformation instead of the Holstein-Primakoff transformation: it predicted the perpendicular susceptibility for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice to be $\chi_\perp=0.065\,50$, which is in excellent agreement with our series expansion result[1] [$\chi_\perp=0.0659(10)$].

Recently, the discovery of the remarkable magnetic properties of high-T_c superconductors has led to a reexamination of quantum spin systems mainly in two dimensions (including the square lattice, triangular lattice,and perhaps the honeycomb lattice, although the honeycomb lattice has been less well studied). The standard first-order spin-wave analysis of the triangular Heisenberg quantum antiferromagnet with nearest-neighbor couplings was given by Jolicoeur and Le Guillou,[15] and then extended for both nearest-neighbor and next-nearest-neighbor interactions by Jolicoeur, Dagotto, Gagliano, and Bacci.[16] The standard spin-wave analysis of the Heisenberg antiferromagnet on a square lattice with both nearest-neighbor and next-nearest-neighbor couplings was discussed by Chandra and Doucot,[17] and Kubo and Kishi.[18]

In the present paper, we will not repeat the derivation of our general second-order spin-wave results in detail, but the notations here have the same meanings as in our previous papers.[1,2] The arrangement of the paper is as follows: in Sec. II we give the spin-wave results for the anisotropic Heisenberg antiferromagnet on a one-dimensional linear chain, two-dimensional honeycomb lattice, and three-dimensional simple-cubic and body-centered-cubic lattices. In Sec. III we discuss the spin-wave results for the XY model with anisotropy on a one-dimensional linear chain, two-dimensional triangular and honeycomb lattice, and three-dimensional simple-cubic, body-centered-cubic, and face-centered-cubic lattices. The XY model on a honeycomb lattice needs an analysis based on two sublattices.

II. SPIN-WAVE ANALYSIS OF THE ANISOTROPIC HEISENBERG ANTIFERROMAGNET

The Heisenberg antiferromagnet with anisotropy can be described by the following Hamiltonian:

$$H=\sum_{\langle lm\rangle}[S_l^zS_m^z+x(S_l^xS_m^x+S_l^yS_m^y)]\ , \tag{2.1}$$

where we have divided the lattice sites into two sublattices, denoted by l and m, respectively, and the sum over $\langle lm\rangle$ denotes a sum over all nearest-neighbor pairs. The points $x=0$ and 1 correspond to the antiferromagnetic Ising model and isotropic Heisenberg model, respectively. The second-order spin-wave theory[1] gives the ground-state energy E_0, the mass gap m, the staggered magnetization M^+, the parallel staggered susceptibility $\chi_\parallel^s$, the uniform perpendicular susceptibility $\chi_\perp$, and the staggered perpendicular susceptibility $\chi_\perp^S$ as follows:

$$\begin{aligned}
E_0/N&=-\frac{zS}{2}\left[S-C_1+\frac{1}{4S}\left[C_1^2+\frac{1-x^2}{x^2}(C_{-1}-C_1)^2\right]\right]\ ,\\
m&=z(1-x^2)^{1/2}(S-C_{-1}/2)\ ,\\
M^+&=S-\tfrac{1}{2}C_{-1}-\frac{1-x^2}{4Sx^2}(C_{-1}-C_1)(C_{-3}-C_{-1})\ ,\\
\chi_\parallel^S&=\frac{1}{2zS}(C_{-3}-C_{-1})+\frac{1}{4zS^2}\left[C_1(C_{-3}-C_{-1})+\frac{1-x^2}{x^2}[(C_{-3}-C_{-1})^2+(C_{-1}-C_1)(C_{-1}+3C_{-5}-4C_{-3})]\right]\ ,\\
\chi_\perp&=\frac{1}{z(1+x)}\left[1-\frac{C_{-1}-C_1}{2Sx}\right]\ ,\\
\chi_\perp^S(x)&=\chi_\perp(-x)\ ,
\end{aligned} \tag{2.2}$$

where z is the coordination number of the lattice, and C_n is defined by

$$C_n=\frac{2}{N}\sum_k[(1-x^2\gamma_k\gamma_k^*)^{n/2}-1]\ , \tag{2.3}$$

the sum over k denotes a sum over the first Brillouin zone of the sublattice l, and the structure factor γ_k is defined by

$$\gamma_k=\frac{1}{z}\sum_\rho e^{ik\cdot\rho}\ . \tag{2.4}$$

Note that if γ_k is complex (denote $\gamma_k=|\gamma_k|e^{i\delta_k}$), that is, $\gamma_k\neq\gamma_k^*=\gamma_{-k}$, the phase factor $e^{i\delta_k}$ in the Hamiltonian can be absorbed by the transformation $b_k\to b_ke^{-i\delta_k}$, or by the following Bogoliubov transformation:

$$\begin{aligned}
a_k&=\cosh\theta_k\,\alpha_k-\sinh\theta_ke^{-i\delta_k}\beta_k^*\ ,\\
b_k&=-\sinh\theta_k\,e^{-i\delta_k}\alpha_k^*+\cosh\theta_k\,\beta_k\ ,
\end{aligned} \tag{2.5}$$

instead of Eq. (2.9) in Ref. 1.

The results above are applicable to any bipartite lattice. Now we discuss the application of the above results to the one-dimensional linear chain, two-dimensional honeycomb lattice, and three-dimensional simple-cubic and body-centered-cubic lattice (a is the lattice spacing).

A. One-dimensional linear chain

The structure factor γ_k for the linear chain is

$$\gamma_k=\cos(k_xa)\ ,\quad -\pi/(2a)<k_x\le\pi/(2a)\ , \tag{2.6}$$

and

$$\frac{2}{N}\sum_k\gamma_k^{2n}=2^{-2n}\binom{2n}{n}\sim(\pi n)^{-1/2}\left[1-\frac{1}{8n}+O\left[\frac{1}{n^2}\right]\right]\quad\text{as } n\to\infty\ . \tag{2.7}$$

Using the same techniques applied in our calculation of XXZ model,[1] one can find the asymptotic expansion near $x^2=1$ of C_n:

$$\begin{aligned}
C_1&=-0.363\,38-\frac{1}{2\pi}(1-x^2)\ln(1-x^2)\\
&\quad+0.282\,12(1-x^2)\\
&\quad-\frac{3}{16\pi}(1-x^2)^2\ln(1-x^2)+\cdots\ ,\\
C_{-1}&=-\frac{1}{\pi}\ln(1-x^2)-0.117\,458\\
&\quad-\frac{1}{4\pi}(1-x^2)\ln(1-x^2)\\
&\quad+0.0615(1-x^2)+\cdots\ ,\\
C_{-3}&=\frac{2}{\pi(1-x^2)}-\frac{1}{2\pi}\ln(1-x^2)-0.718+\cdots\ ,\\
C_{-5}&=\frac{4}{3\pi}(1-x^2)^{-2}+\frac{1}{\pi}(1-x^2)^{-1}+\cdots\ .
\end{aligned} \tag{2.8}$$

The Heisenberg antiferromagnet on a one-dimensional linear chain has no long-range order, and the spin-wave theory here gives a divergent occupation number per site $\langle n_i \rangle$, so the spin-wave theory lacks intrinsic consistency. But the ground-state energy in the isotropic case is $E_0/N = -S^2 - 0.363\,38S - 0.033\,011$, which compares fairly well with the exact solution[19,20] ($E_0/N = -0.4430$ for $S=\frac{1}{2}$).

B. Two-dimensional honeycomb lattice

The two-dimensional honeycomb lattice is a bipartite lattice, consisting of sublattice l and sublattice m. The primitive lattice vectors of the l sublattice are

$$\mathbf{e}_1 = a(\tfrac{3}{2}, \sqrt{3}/2)\,, \qquad \mathbf{e}_2 = a(0, \sqrt{3})\,, \tag{2.9}$$

and the reciprocal-lattice vectors for the l sublattice are

$$\mathbf{h}_1 = \frac{2\pi}{a}(\tfrac{2}{3}, 0)\,, \qquad \mathbf{h}_2 = \frac{2\pi}{a}\left[-\frac{1}{3}, \frac{1}{\sqrt{3}}\right], \tag{2.10}$$

which correspond to the triangular lattice. The first Brillouin zone can be chosen as the rectangular region

$$-\frac{2\pi}{3a} < k_x \le \frac{2\pi}{3a}\,, \quad -\frac{\pi}{\sqrt{3}a} < k_y \le \frac{\pi}{\sqrt{3}a}\,. \tag{2.11}$$

Then the structure factor is

$$\gamma_k = \frac{1}{3}\left[e^{ik_xa} + 2e^{-ik_xa/2}\cos\left[\frac{\sqrt{3}}{2}k_ya\right]\right], \tag{2.12}$$

and it follows that

$$\begin{aligned}
\gamma_k\gamma_k^* &= \frac{1}{9}\left[1 + 4\cos^2\left[\frac{\sqrt{3}}{2}k_ya\right] + 4\cos\left[\frac{3k_xa}{2}\right]\cos\left[\frac{\sqrt{3}}{2}k_ya\right]\right],\\
\frac{2}{N}\sum_k(\gamma_k\gamma_k^*)^n &= \frac{3^{-2n}}{4\pi^2}\int_{-\pi}^{\pi}dx\int_{-\pi/2}^{\pi/2}dy\,(1 + 4\cos^2 y + 4\cos x\cos y)^n\\
&= \sum_{i=0}^{n/2}\sum_{j=0}^{n-2i}\frac{3^{-2n}[2(i+j)]!n!}{(i!)^2 j!(n-2i-j)![(i+j)!]^2}\\
&\sim \frac{3\sqrt{3}}{4\pi n}\left[1 - \frac{1}{4n} + O\left[\frac{1}{n^2}\right]\right] \quad \text{as } n\to\infty\,.
\end{aligned} \tag{2.13}$$

Therefore, one can deduce the asymptotic behavior near $x^2=1$ of C_n:

$$\begin{aligned}
C_1 &= -0.209\,8417 + 0.363\,114(1-x^2) - \frac{\sqrt{3}}{2\pi}(1-x^2)^{3/2} + 0.225\,61(1-x^2)^2 - \frac{7\sqrt{3}}{20\pi}(1-x^2)^{5/2} + \cdots\,,\\
C_{-1} &= 0.516\,386 - \frac{3\sqrt{3}}{2\pi}(1-x^2)^{1/2} + 0.5392(1-x^2) - \frac{3\sqrt{3}}{4\pi}(1-x^2)^{3/2} + \cdots\,,\\
C_{-3} &= \frac{3\sqrt{3}}{2\pi}(1-x^2)^{-1/2} - 0.5621 - \frac{3\sqrt{3}}{4\pi}(1-x^2)^{1/2} + \cdots\,,\\
C_{-5} &= \frac{\sqrt{3}}{2\pi}(1-x^2)^{-3/2} + \frac{5\sqrt{3}}{4\pi}(1-x^2)^{-1/2} + \cdots\,.
\end{aligned} \tag{2.14}$$

The asymptotic behavior of the physical quantities is then given by

$$\begin{aligned}
E_0/N &= -3S^2/2 - 0.314\,763S - 0.016\,5126 + (0.544\,67S - 0.140\,63)(1-x^2)\\
&\quad + (-0.413\,50S + 0.407\,05)(1-x^2)^{3/2} + \cdots\,,\\
m &= (1-x^2)^{1/2}[3S - 0.774\,579 + 1.2405(1-x^2)^{1/2} + \cdots]\,,\\
M^+ &= S - 0.258\,193 + (0.413\,4967 - 0.150\,1464/S)(1-x^2)^{1/2} + \cdots\,,\\
\chi_\parallel^S &= (0.137\,83/S + 0.035\,5873/S^2)(1-x^2)^{-1/2} - 0.179\,74/S + 0.018\,8589/S^2 + \cdots\,,\\
\chi_\perp &= \tfrac{1}{6} - 0.060\,5190/S + 0.097\,462(1-x)^{1/2}/S + \cdots\,,\\
\chi_\perp^S &= [\tfrac{1}{3} + 0.121\,038/S - 0.194\,92(1-x)^{1/2}/S + \cdots]/(1-x).
\end{aligned} \tag{2.15}$$

C. Three-dimensional simple-cubic lattice

The structure factor γ_k for a simple-cubic lattice is

$$\gamma_k = \tfrac{1}{3}[\cos(ak_x) + \cos(ak_y) + \cos(ak_z)]\,, \quad -\frac{\pi}{2a} < k_x, k_y \le \frac{\pi}{2a}\,, \quad |k_z| \le \frac{\pi}{a}\,. \tag{2.16}$$

It then follows that

$$\frac{2}{N}\sum_k \gamma_k^{2n} = 3^{-2n} 2^{-2n} \left[\begin{matrix} 2n \\ n \end{matrix} \right] \sum_{m=0}^{n} \left[\begin{matrix} 2m \\ m \end{matrix} \right] \left[\begin{matrix} n \\ m \end{matrix} \right]^2$$
$$\sim \frac{3\sqrt{3}}{4\pi^{3/2}} n^{-3/2} \left[1 - \frac{3}{8n} + O\left[\frac{1}{n^2} \right] \right] \quad \text{as } n \to \infty , \tag{2.17}$$

and one can deduce the asymptotic behavior of C_n:

$$\begin{aligned} C_1 &= -0.097\,158 + 0.126\,937(1-x^2) + \frac{3\sqrt{3}}{16\pi^2}(1-x^2)^2 \ln(1-x^2) \\ &\quad + 3.9624 \times 10^{-3}(1-x^2)^2 + \frac{3\sqrt{3}}{16\pi^2}(1-x^2)^3 \ln(1-x^2) + \cdots , \\ C_{-1} &= 0.156\,715 + \frac{3\sqrt{3}}{4\pi^2}(1-x^2)\ln(1-x^2) - 0.0453(1-x^2) + \frac{9\sqrt{3}}{16\pi^2}(1-x^2)^2 \ln(1-x^2) + \cdots , \\ C_{-3} &= -\frac{3\sqrt{3}}{2\pi^2}\ln(1-x^2) - 0.015\,9704 + 0.0236(1-x^2) + \cdots , \\ C_{-5} &= \frac{\sqrt{3}}{\pi^2}(1-x^2)^{-1} - \frac{3\sqrt{3}}{2\pi^2}\ln(1-x^2) - 0.207 + \cdots . \end{aligned} \tag{2.18}$$

The asymptotic behavior near $x=1$ of the physical quantities is

$$\begin{aligned} E_0/N &= -3S^2 - 0.291\,474S - 0.007\,079\,76 + (0.380\,810S - 0.029\,8394)(1-x^2) \\ &\quad + (0.098\,715S - 0.045\,327)(1-x^2)^2 \ln(1-x^2) + \cdots , \\ m &= [6S - 0.470\,146 - 0.394\,860(1-x^2)\ln(1-x^2) + \cdots](1-x^2)^{1/2} , \\ M^+ &= S - 0.078\,3577 + \left[-0.065\,810 + \frac{0.016\,707}{S} \right](1-x^2)\ln(1-x^2) + \cdots , \\ \chi_\parallel^S &= \left[-\frac{0.021\,9367}{S} + \frac{0.001\,065\,66}{S^2} \right] \ln(1-x^2) - \frac{0.014\,3905}{S} + \frac{0.006\,268\,22}{S^2} + \cdots , \\ \chi_\perp &= \frac{1}{12} - \frac{0.010\,5781}{S} - \frac{0.005\,484\,17}{S}(1-x^2)\ln(1-x^2) + \cdots , \\ \chi_\perp^S &= [\tfrac{1}{6} + 0.021\,1561/S + 0.010\,9683(1-x^2)\ln(1-x^2)/S + \cdots]/(1-x) . \end{aligned} \tag{2.19}$$

D. Three-dimensional body-centered-cubic lattice

The structure factor γ_k for a bcc lattice is

$$\gamma_k = \cos\left[\frac{ak_x}{2} \right] \cos\left[\frac{ak_y}{2} \right] \cos\left[\frac{ak_z}{2} \right] , \quad -\frac{\pi}{a} < k_x, k_y, k_z \le \frac{\pi}{a} . \tag{2.20}$$

Then,

$$\frac{2}{N}\sum_k \gamma_k^{2n} = 2^{-6n} \left[\begin{matrix} 2n \\ n \end{matrix} \right]^3 \sim (\pi n)^{-3/2} \left[1 - \frac{3}{8n} + O\left[\frac{1}{n^2} \right] \right] \quad \text{as } n \to \infty , \tag{2.21}$$

and, therefore, one can deduce the asymptotic behavior of C_n:

$$
\begin{aligned}
C_1 &= -0.073\,037\,67+0.095\,8370(1-x^2)+\frac{1}{4\pi^2}(1-x^2)^2\ln(1-x^2) \\
&\quad +0.003\,2057(1-x^2)^2+\frac{1}{4\pi^2}(1-x^2)^3\ln(1-x^2)+\cdots\,, \\
C_{-1} &= 0.118\,6364+\frac{1}{\pi^2}(1-x^2)\ln(1-x^2)-0.032\,35(1-x^2)+\frac{3}{4\pi^2}(1-x^2)^2\ln(1-x^2)+\cdots\,, \\
C_{-3} &= -\frac{2}{\pi^2}\ln(1-x^2)-0.019\,298\,85+0.0291(1-x^2)+\cdots\,, \\
C_{-5} &= \frac{4}{3\pi^2}(1-x^2)^{-1}-\frac{2}{\pi^2}\ln(1-x^2)-0.1738+\cdots\,.
\end{aligned}
\tag{2.22}
$$

The asymptotic behavior near $x=1$ of the physical quantities is

$$
\begin{aligned}
E_0/N &= -4S^2-0.292\,151S-0.005\,3345+(0.383\,35S-0.022\,739)(1-x^2) \\
&\quad +(0.101\,32S-0.035\,141)(1-x^2)^2\ln(1-x^2)+\cdots\,, \\
m &= [8S-0.474\,545-0.405\,285(1-x^2)\ln(1-x^2)+\cdots](1-x^2)^{1/2}\,, \\
M^+ &= S-0.059\,3192-(0.050\,6606-0.009\,710\,32/S)(1-x^2)\ln(1-x^2)+\cdots\,, \\
\chi_\parallel^S &= (-0.012\,665/S+4.6252\times10^{-4}/S^2)\ln(1-x^2)-0.008\,6209/S+2.7424\times10^{-3}/S^2+\cdots\,, \\
\chi_\perp &= \frac{1}{16}-\frac{0.005\,9898}{S}-\frac{0.003\,1663}{S}(1-x^2)\ln(1-x^2)+\cdots\,, \\
\chi_\perp^S &= \left[\frac{1}{8}+\frac{0.011\,9796}{S}+\frac{0.006\,332\,57}{S}(1-x^2)\ln(1-x^2)+\cdots\right]\Big/(1-x)\,.
\end{aligned}
\tag{2.23}
$$

III. SPIN-WAVE ANALYSIS OF THE ANISOTROPIC XY MODEL

The XY model with anisotropy can be described by the following Hamiltonian:

$$
H=-\sum_{\langle lm\rangle}(S_l^xS_m^x+xS_l^yS_m^y)\,,
\tag{3.1}
$$

where the sum over $\langle lm\rangle$ denotes a sum over all nearest-neighbor pairs. The points $x=0$ and 1 correspond to the ferromagnetic Ising model and isotropic ferromagnetic XY model (F), respectively. For a bipartite lattice, the isotropic antiferromagnetic XY model (A) is related to the ferromagnetic one by a simple spin rotation on one sublattice. Hence, there exist the following relations between the isotropic ferromagnet (F), antiferromagnet (A), and the model described by Eq. (3.1):

$$
\begin{aligned}
&E_0(x=1)=E_0(x=-1)=E_0^A=E_0^F\,, \\
&M_x(x=1)=M_x(x=-1)=M_x^F=M_x^{A,S}\,, \\
&\chi_{xx}(x=1)=\chi_{xx}(x=-1)=\chi_{xx}^F=\chi_{xx}^{A,S}\,, \\
&\chi_{yy}(x=1)=\chi_{yy}^{A,S}=\chi_{yy}^F\,,\quad \chi_{yy}(x=-1)=\chi_{yy}^A=\chi_{yy}^{F,S}\,, \\
&\chi_{zz}(x=1)=\chi_{zz}^A=\chi_{zz}^F\,,\quad \chi_{zz}(x=-1)=\chi_{zz}^{A,S}=\chi_{zz}^{F,S}\,,
\end{aligned}
\tag{3.2}
$$

where the superscript S denotes the staggered magnetization and susceptibility.

The second-order spin-wave theory[2] gives the ground-state energy E_0, the mass gap m, the magnetization M_x, and the susceptibility χ_{xx}, χ_{yy}, χ_{zz} as follows:

$$\frac{E_0}{N} = -\frac{zS^2}{2} + \frac{zSC_1}{2} - \frac{z}{16}\left[\frac{1-x^2}{x^2}(C_1-C_{-1})^2 + 2C_1^2 + \frac{1}{x^2}(C_1-C_3)^2\right],$$

$$m = \left[zS - \frac{z}{4}\left[C_1 - \frac{C_3}{x} + \frac{1+x}{x}C_{-1}\right]\right](1-x)^{1/2},$$

$$\begin{aligned} M_x = S - \tfrac{1}{4}(C_1+C_{-1}) + \frac{1}{32S}\Bigg[&\frac{4-3x^2}{x^2}(C_1-C_{-1})^2 + \frac{2}{x^2}(C_1-C_3)(C_3-2C_1+C_{-1}) \\ &+ 2\frac{1-x^2}{x^2}(C_1-C_{-1})(C_{-3}-C_1)\Bigg], \end{aligned} \tag{3.3}$$

$$\begin{aligned} \chi_{xx} = {}& \frac{1}{8zS}(C_1+C_{-3}-2C_{-1}) \\ &+ \frac{1}{32zS^2}\Bigg[\frac{1-x^2}{x^2}(C_1-C_{-1})(3C_1-C_{-1}+C_{-3}-3C_{-5}) \\ &\quad + \frac{4}{x^2}(C_1-C_{-1})^2 + 2\frac{4-x^2}{x^2}(C_1-C_{-1})(C_{-3}-C_1) \\ &\quad + \frac{1-x^2}{x^2}(C_{-3}-C_1)^2 + 2(C_{-1}-C_1)(C_{-1}-2C_1) + \frac{1}{x^2}(C_{-1}-4C_1+3C_3)^2 \\ &\quad + 2(C_{-1}-C_{-3})(C_1-2C_{-1}) + \frac{1}{x^2}(C_1-C_3)(-C_{-3}+3C_{-1}-7C_1+5C_3)\Bigg] \end{aligned}$$

$$\chi_{yy} = \frac{1}{z(1-x)}\left[1 + \frac{C_{-1}-C_1}{2Sx}\right],$$

$$\chi_{zz} = \frac{1}{z}\left[1 - \frac{C_3-C_1}{2Sx}\right],$$

where z is again the coordination number of the lattice, and C_n is defined by

$$C_n = \frac{1}{N}\sum_k [(1-x\gamma_k)^{n/2} - 1], \tag{3.4}$$

the sum over k denotes a sum over the first Brillouin zone, and the structure factor

$$\gamma_k = \frac{1}{z}\sum_\rho e^{ik\cdot\rho} \tag{3.5}$$

is required to satisfy the condition

$$\frac{1}{N}\sum_k \gamma_k = 0. \tag{3.6}$$

The results above are applicable to the ferromagnetic XY model on any lattice, or to the antiferromagnetic XY model on any bipartite lattice following a simple spin rotation. Now we discuss the application of the above results to the one-dimensional linear chain, two-dimensional triangular lattice, and three-dimensional simple-cubic, body-centered-cubic, and face-centered-cubic lattices. For the two-dimensional honeycomb lattice, the simplest unit cell contains two sites, so the spin-wave theory based on one sublattice in the form given above is invalid for it despite the fact that it is a bipartite lattice. In Sec. III F, we develop a second-order spin-wave theory for the XY model on the honeycomb lattice, based on a two-sublattice decomposition.

A. One-dimensional linear chain

The structure factor of the linear chain is

$$\gamma_k = \cos(k_x a), \quad -\frac{\pi}{a} < k_x \le \frac{\pi}{a}, \tag{3.7}$$

and it follows that

$$\frac{1}{N}\sum_k \gamma_k^{2n} = 2^{-2n}\begin{bmatrix}2n\\ n\end{bmatrix} \sim (\pi n)^{-1/2}\left[1-\frac{1}{8n}+O\left[\frac{1}{n^2}\right]\right] \quad \text{as } n\to\infty , \tag{3.8}$$

and

$$\frac{1}{N}\sum_k \gamma_k^{2n+1}=0 , \quad n=0,1,2,\ldots . \tag{3.9}$$

From this, one can deduce the asymptotic behavior of C_n as

$$\begin{aligned}
C_3 &= 0.200\,4218-0.225\,079(1-x^2)-\frac{3}{32\sqrt{2}\pi}(1-x^2)^2\ln(1-x^2) \\
&\quad +6.869\,47\times10^{-3}(1-x^2)^2-\frac{35}{512\sqrt{2}\pi}(1-x^2)^3\ln(1-x^2)+\cdots , \\
C_1 &= -0.099\,684-\frac{\sqrt{2}}{8\pi}(1-x^2)\ln(1-x^2)+0.065\,21(1-x^2)-\frac{15\sqrt{2}}{256\pi}(1-x^2)^2\ln(1-x^2)+\cdots , \\
C_{-1} &= -\frac{1}{\sqrt{2}\pi}\ln(1-x^2)-0.063\,922-\frac{3}{16\sqrt{2}\pi}(1-x^2)\ln(1-x^2)+0.034\,85(1-x^2)+\ldots , \\
C_{-3} &= \frac{2\sqrt{2}}{\pi(1-x^2)}-\frac{\sqrt{2}}{8\pi}\ln(1-x^2)-0.935+\ldots , \\
C_{-5} &= \frac{8\sqrt{2}}{3\pi}(1-x^2)^{-2}-\frac{1}{\sqrt{2}\pi}(1-x^2)^{-1}+\ldots .
\end{aligned} \tag{3.10}$$

For the one-dimensional linear chain, as pointed out by Gomez-Santos *et al.*,[8] the spin-wave theory gives a divergent occupation number per site $\langle n_i\rangle$, and the theory lacks intrinsic consistency. But the ground-state energy ($E_0/N=-S^2-0.099\,684S-0.013\,7421$) compares fairly well with the exact solution[21,22] ($E_0/N=-0.318$ for $S=\frac{1}{2}$).

B. Two-dimensional triangular lattice

For the triangular lattice, we only find the asymptotic expansions near $x=1$ because the triangular lattice is not a bipartite lattice. The structure factor of the triangular lattice is

$$\gamma_k=\frac{1}{3}\left[\cos(k_x a)+2\cos\left[\frac{k_x a}{2}\right]\cos\left[\frac{\sqrt{3}k_y a}{2}\right]\right] , \quad |k_x|\le\frac{\pi}{a} , \ |k_y|\le\frac{2\pi}{a\sqrt{3}} . \tag{3.11}$$

From this it follows that

$$\frac{1}{N}\sum_k \gamma_k^{2n+1}=\sum_{j=1}^{n}\sum_{k=0}^{(j-1)/2}\frac{2^{j-2n-2k-2}(2n+1)!(2k+2n-2j+2)!}{3^{2n+1}[2(n-j)+1]!(2k+1)!(j-2k-1)!j![(n-j+k+1)!]^2} \quad n=1,2,\ldots,$$

and

$$\frac{1}{N}\sum_k \gamma_k^{2n}=\sum_{i=0}^{n}\sum_{j=0}^{i/2}\frac{2^{i-2j-2n}(2n)!i!}{3^{2n}(2n-2i)!(2i)!(i-2j)!(2j)!}\begin{bmatrix}2(j+n-i)\\ j+n-i\end{bmatrix}\begin{bmatrix}2i\\ i\end{bmatrix} , \quad n=1,2,\ldots,$$

the asymptotic behavior is

$$\frac{1}{N}\sum_k \gamma_k^{n} \sim \frac{\sqrt{3}}{2\pi n}\left[1-\frac{1}{2n}+O\left[\frac{1}{n^2}\right]\right] \quad \text{as } n\to\infty , \tag{3.12}$$

therefore, one can deduce the asymptotic behavior of C_n:

$$C_3 = 0.068\,9479 - 0.151\,808(1-x) + 0.139\,345(1-x)^2 - \frac{\sqrt{3}}{5\pi}(1-x)^{5/2} + 0.102\,61(1-x)^3 - \frac{6\sqrt{3}}{35\pi}(1-x)^{7/2} + \ldots,$$

$$C_1 = -0.032\,2577 + 0.135\,19(1-x) - \frac{\sqrt{3}}{3\pi}(1-x)^{3/2} + 0.158\,77(1-x)^2 - \frac{4\sqrt{3}}{15\pi}(1-x)^{5/2} + \ldots,$$

$$C_{-1} = 0.238\,124 - \frac{\sqrt{3}}{\pi}(1-x)^{1/2} + 0.5000(1-x) - \frac{2\sqrt{3}}{3\pi}(1-x)^{3/2} + \ldots, \tag{3.13}$$

$$C_{-3} = \frac{\sqrt{3}}{\pi}(1-x)^{-1/2} - 0.761\,63 + 0.2124(1-x) + \ldots,$$

$$C_{-5} = \frac{\sqrt{3}}{3\pi}(1-x)^{-3/2} + \frac{2\sqrt{3}}{3\pi}(1-x)^{-1/2} - 0.903 + \ldots,$$

and the asymptotic behavior of physical quantities:

$$E_0/N = -3S^2 - 0.096\,773S - 0.004\,6214 + (0.405\,57S - 0.034\,186)(1-x) + (-0.551\,33S + 0.20076)(1-x)^{3/2} + \ldots,$$

$$m = [6S - 0.562\,56 + 1.6540(1-x)^{1/2} + \ldots](1-x)^{1/2},$$

$$M_x = S - 0.051\,4666 - 6.5848\times 10^{-5}/S + (0.137\,83 - 0.024\,463/S)(1-x)^{1/2} + \ldots, \tag{3.14}$$

$$\chi_{xx} = \left[\frac{0.011\,486}{S} + \frac{1.0536}{10^4 S^2}\right](1-x)^{-1/2} - \frac{0.026\,461}{S} + \frac{7.0461}{10^3 S^2} + \ldots,$$

$$\chi_{yy} = (1-x)^{-1}[\tfrac{1}{6} + 0.022\,532/S - 0.045\,944(1-x)^{1/2}/S + \ldots],$$

$$\chi_{zz} = \tfrac{1}{6} - 0.008\,4338/S + 0.015\,483(1-x)/S + \ldots .$$

C. Three-dimensional simple-cubic lattice

The structure factor of the simple-cubic lattice is

$$\gamma_k = \tfrac{1}{3}[\cos(ak_x) + \cos(ak_y) + \cos(ak_z)], \quad -\frac{\pi}{a} < k_x, k_y, k_z \le \frac{\pi}{a}, \tag{3.15}$$

and it follows that

$$\frac{1}{N}\sum_k \gamma_k^{2n} = 3^{-2n}2^{-2n}\binom{2n}{n}\sum_{m=0}^{n}\binom{2m}{m}\binom{n}{m}^2 \sim \frac{3\sqrt{3}}{4\pi^{3/2}}n^{-3/2}\left[1 - \frac{3}{8n} + O\left(\frac{1}{n^2}\right)\right] \quad \text{as } n\to\infty \tag{3.16}$$

and

$$\frac{1}{N}\sum_k \gamma_k^{2n+1} = 0 . \tag{3.17}$$

Therefore, one can deduce the asymptotic behavior of C_n:

$$
\begin{aligned}
C_3 &= 0.064\,5497 - 0.067\,3613(1-x^2) + 4.763\,53\times 10^{-3}(1-x^2)^2 + \frac{3\sqrt{6}}{256\pi^2}(1-x^2)^3\ln(1-x^2) \\
&\quad + 1.64\times 10^{-3}(1-x^2)^3 + \frac{261\sqrt{3}}{8192\sqrt{2}\pi^2}(1-x^2)^4\ln(1-x^2) + \dots , \\
C_1 &= -0.025\,265\,47 + 0.035\,1565(1-x^2) + \frac{3\sqrt{3}}{32\sqrt{2}\pi^2}(1-x^2)^2\ln(1-x^2) \\
&\quad + 2.512\times 10^{-3}(1-x^2)^2 + \frac{51\sqrt{3}}{512\sqrt{2}\pi^2}(1-x^2)^3\ln(1-x^2) + \dots , \\
C_{-1} &= 0.115\,3607 + \frac{3\sqrt{6}}{8\pi^2}(1-x^2)\ln(1-x^2) - 0.038\,836(1-x^2) + \frac{69\sqrt{6}}{256\pi^2}(1-x^2)^2\ln(1-x^2) + \dots , \\
C_{-3} &= -\frac{3\sqrt{3}}{\sqrt{2}\pi^2}\ln(1-x^2) - 0.101\,571 - \frac{9\sqrt{3}}{16\sqrt{2}\pi^2}(1-x^2)\ln(1-x^2) + \dots , \\
C_{-5} &= \frac{4\sqrt{3}}{\sqrt{2}\pi^2}(1-x^2)^{-1} - \frac{9\sqrt{3}}{4\sqrt{2}\pi^2}\ln(1-x^2) + \dots ,
\end{aligned}
\tag{3.18}
$$

and the asymptotic behavior of the physical quantities is

$$
\begin{aligned}
E_0/N &= -3S^2 - 0.075\,7964S - 0.003\,5038 + (0.105\,470S - 0.002\,2028)(1-x^2) \\
&\quad + (0.034\,901S - 0.008\,5914)(1-x^2)^2\ln(1-x^2) + \dots \quad (x\sim\pm 1) , \\
m &= [6S - 0.211\,359 - 0.279\,208(1-x^2)\ln(1-x^2) + \dots](1-x)^{1/2} \quad (x\sim 1) , \\
m &= [6S - 0.058\,9264 + 0.172\,831(1+x) + \dots](1-x)^{1/2} \quad (x\sim -1) , \\
M_x &= S - 0.022\,5238 - \frac{6.7558}{10^4 S} - \left[0.023\,2674 - \frac{3.5676}{10^3 S}\right](1-x^2)\ln(1-x^2) + \dots \quad (x\sim\pm 1) , \\
\chi_{xx} &= \left[-\frac{7.755\,79}{10^3 S} + \frac{4.6916}{10^4 S^2}\right]\ln(1-x^2) - \frac{7.449}{10^3 S} + \frac{1.935}{10^3 S^2} + \dots \quad (x\sim\pm 1) , \\
\chi_{yy} &= (1-x)^{-1}\left[\frac{1}{6} + \frac{0.011\,7188}{S} + \frac{0.007\,755\,79}{S}(1-x^2)\ln(1-x^2) + \dots\right] \quad (x\sim 1) , \\
\chi_{yy} &= \frac{1}{12} - \frac{0.005\,8594}{S} - \frac{0.003\,8778}{S}(1-x^2)\ln(1-x^2) + \dots \quad (x\sim -1) , \\
\chi_{zz} &= \tfrac{1}{6} - 0.007\,484\,60/S + 0.009\,601\,72(1-x)/S + \dots \quad (x\sim 1) , \\
\chi_{zz} &= \tfrac{1}{6} + 0.007\,484\,60/S - 0.009\,601\,72(1+x)/S + \dots \quad (x\sim -1) .
\end{aligned}
\tag{3.19}
$$

D. Three-dimensional body-centered-cubic lattice

The structure factor of the bcc lattice is

$$
\gamma_k = \cos\left[\frac{ak_x}{2}\right]\cos\left[\frac{ak_y}{2}\right]\cos\left[\frac{ak_z}{2}\right] , \quad -\frac{\pi}{a} < k_x, k_y \le \frac{\pi}{a} , \quad -\frac{2\pi}{a} < k_z \le \frac{2\pi}{a} ,
\tag{3.20}
$$

and it follows that

$$
\frac{1}{N}\sum_k \gamma_k^{2n} = 2^{-6n}\left[\begin{matrix}2n\\ n\end{matrix}\right]^3 \sim (\pi n)^{-3/2}\left[1 - \frac{3}{8n} + O\left[\frac{1}{n^2}\right]\right] \quad \text{as } n\to\infty ,
\tag{3.21}
$$

and

$$
\frac{1}{N}\sum_k \gamma_k^{2n+1} = 0 , \quad n = 0,1,2,\dots .
\tag{3.22}
$$

The asymptotic behavior of the C_n is given by

$$
\begin{aligned}
C_3 &= 0.048\,434\,50 - 0.050\,578\,82(1-x^2) + 0.003\,644\,61(1-x^2)^2 \\
&\quad + \frac{\sqrt{2}}{64\pi^2}(1-x^2)^3 \ln(1-x^2) + 0.001\,2683(1-x^2)^3 + \frac{87\sqrt{2}}{4096\pi^2}(1-x^2)^4 \ln(1-x^2) + \dots \,. \\
C_1 &= -0.019\,003\,93 + 0.026\,578\,57(1-x^2) + \frac{1}{8\sqrt{2}\pi^2}(1-x^2)^2 \ln(1-x^2) \\
&\quad + 0.001\,983\,965(1-x^2)^2 + \frac{17}{128\sqrt{2}\pi^2}(1-x^2)^3 \ln(1-x^2) + \cdots \,, \\
C_{-1} &= 0.087\,310\,34 + \frac{\sqrt{2}}{2\pi^2}(1-x^2)\ln(1-x^2) - 0.028\,042(1-x^2) + \frac{23\sqrt{2}}{64\pi^2}(1-x^2)^2 \ln(1-x^2) + \cdots \,, \\
C_{-3} &= -\frac{2\sqrt{2}}{\pi^2}\ln(1-x^2) - 0.087\,102\,62 - \frac{3\sqrt{2}}{8\pi^2}(1-x^2)\ln(1-x^2) + 0.053\,39(1-x^2) + \dots \,, \\
C_{-5} &= \frac{8\sqrt{2}}{3\pi^2}(1-x^2)^{-1} - \frac{3\sqrt{2}}{2\pi^2}\ln(1-x^2) - 0.468\,69 + \dots \,,
\end{aligned} \tag{3.23}
$$

and the asymptotic behavior of the physical quantities is

$$
\begin{aligned}
E_0/N &= -4S^2 - 0.076\,0157S - 0.002\,635\,12 + (0.106\,314S - 0.001\,711\,76)(1-x^2) \\
&\qquad + (0.035\,8224S - 0.006\,672\,54)(1-x^2)^2 \ln(1-x^2) + \dots \quad (x \sim \pm 1)\,, \\
m &= [8S - 0.214\,364 - 0.286\,580(1-x^2)\ln(1-x^2) + \dots](1-x)^{1/2}\,, \quad (x \sim 1)\,, \\
m &= [8S - 0.058\,8612 + 0.173\,753(1+x) + \dots](1-x)^{1/2} \quad (x \sim -1)\,, \\
M_x &= S - 0.017\,0766 - \frac{3.7914}{10^4 S} - \left[0.017\,911 - \frac{2.078}{10^3 S}\right](1-x^2)\ln(1-x^2) + \dots \quad (x \sim \pm 1)\,, \\
\chi_{xx} &= (-0.004\,477\,81/S + 2.050\,81 \times 10^{-4}/S^2)\ln(1-x^2) \\
&\qquad - 0.004\,386\,36/S + 8.4389 \times 10^{-4}/S^2 + \dots \quad (x \sim \pm 1)\,,
\end{aligned} \tag{3.24}
$$

$$
\begin{aligned}
\chi_{yy} &= (1-x)^{-1}\left[\frac{1}{8} + \frac{0.006\,644\,64}{S} + \frac{0.004\,477\,81}{S}(1-x^2)\ln(1-x^2) + \dots\right] \quad (x \sim 1)\,, \\
\chi_{yy} &= \frac{1}{16} - \frac{0.003\,322\,32}{S} - \frac{0.002\,238\,90}{S}(1-x^2)\ln(1-x^2) + \dots \quad (x \sim -1)\,, \\
\chi_{zz} &= \tfrac{1}{8} - 0.004\,214\,90/S + 0.005\,429\,77(1-x)/S + \dots \quad (x \sim 1)\,, \\
\chi_{zz} &= \tfrac{1}{8} + 0.004\,214\,90/S - 0.005\,429\,77(1+x)/S + \cdots \quad (x \sim -1)\,.
\end{aligned} \tag{3.25}
$$

E. Three-dimensional face-centered-cubic lattice

For the fcc lattice, we only find the asymptotic expansions near $x=1$ because the fcc lattice is not a bipartite lattice. The structure factor of the fcc lattice is

$$
\gamma_k = \frac{1}{3}\left[\cos\left[\frac{k_x a}{2}\right]\cos\left[\frac{k_y a}{2}\right] + \cos\left[\frac{k_y a}{2}\right]\cos\left[\frac{k_z a}{2}\right] + \cos\left[\frac{k_z a}{2}\right]\cos\left[\frac{k_x a}{2}\right]\right],
$$
$$
-\frac{2\pi}{a} < k_x, k_y \le \frac{2\pi}{a}\,, \quad -\frac{\pi}{a} < k_z \le \frac{\pi}{a}\,. \tag{3.26}
$$

It follows that

$$
\frac{1}{N}\sum_k \gamma_k^{2n+1} = \sum_{p+q+r=n-1} \frac{3^{-2n-1}2^{-4n-2}(2n+1)![2(p+q+1)]![2(q+r+1)]![2(r+p+1)]!}{(2p+1)!(2q+1)!(2r+1)![(p+q+1)!]^2[(q+r+1)!]^2[(r+p+1)!]^2}\,, \quad n=1,2,3,\dots \tag{3.27}
$$

and

$$
\frac{1}{N}\sum_k \gamma_k^{2n} = \sum_{p+q+r=n} \frac{3^{-2n}2^{-4n}(2n)![2(p+q)]![2(q+r)]![2(r+p)]!}{(2p)!(2q)!(2r)![(p+q)!]^2[(q+r)!]^2[(r+p)!]^2}\,, \quad n=1,2,3,\dots\,. \tag{3.28}
$$

The asymptotic behavior is

$$\frac{1}{N}\sum_k \gamma_k^n \sim \frac{3\sqrt{3}}{4\pi^{3/2}n^{3/2}}\left[1-\frac{3}{4n}+O\left[\frac{1}{n^2}\right]\right] \quad \text{as } n\to\infty\ , \tag{3.29}$$

and from this, one can deduce the asymptotic behavior near $x=1$ of C_n:

$$\begin{aligned}
C_3 &= 0.034\,033\,83-0.073\,070\,80(1-x)+0.051\,3015(1-x)^2\\
&\quad +\frac{3\sqrt{3}}{32\pi^2}(1-x)^3\ln(1-x)+0.006\,668(1-x)^3+\frac{117\sqrt{3}}{1024\pi^2}(1-x)^4\ln(1-x)+\cdots\ ,\\
C_1 &= -0.014\,680\,04+0.044\,045\,02(1-x)+\frac{3\sqrt{3}}{16\pi^2}(1-x)^2\ln(1-x)\\
&\quad +0.007\,204(1-x)^2+\frac{27\sqrt{3}}{128\pi^2}(1-x)^3\ln(1-x)+\cdots\ ,\\
C_{-1} &= 0.073\,4100+\frac{3\sqrt{3}}{4\pi^2}(1-x)\ln(1-x)+0.050\,58(1-x)+\frac{45\sqrt{3}}{64\pi^2}(1-x)^2\ln(1-x)+\ldots\ ,\\
C_{-3} &= -\frac{3\sqrt{3}}{2\pi^2}\ln(1-x)-0.290\,90-\frac{9\sqrt{3}}{16\pi^2}(1-x)\ln(1-x)+\ldots\ ,\\
C_{-5} &= \frac{\sqrt{3}}{\pi^2}(1-x)^{-1}-\frac{9\sqrt{3}}{8\pi^2}\ln(1-x)\ +\cdots\ .
\end{aligned} \tag{3.30}$$

The asymptotic behavior of the physical quantities near $x=1$ is then

$$\begin{aligned}
E_0/N &= -6S^2-0.088\,080S-0.002\,103\,04+(0.264\,27S-0.004\,702)(1-x)\\
&\quad +(0.197\,43S-0.030\,930)(1-x)^2\ln(1-x)+\ldots\ ,\\
m &= [12S-0.294\,318-0.7897(1-x)\ln(1-x)+\ldots](1-x)^{1/2}\ ,\\
M_x &= S-0.014\,6825-\frac{1.7402}{10^4S}-\left[0.032\,905-\frac{0.003\,2225}{S}\right](1-x)\ln(1-x)+\ldots\ ,\\
\chi_{xx} &= \left[-\frac{2.7421}{10^3S}+\frac{1.07508}{10^4S^2}\right]\ln(1-x)-\frac{4.713\,44}{10^3S}+\frac{4.867\,34}{10^4S^2}+\cdots\ ,\\
\chi_{yy} &= (1-x)^{-1}\left[\frac{1}{12}+\frac{0.003\,6704}{S}+\frac{0.005\,4842}{S}(1-x)\ln(1-x)+\ldots\right]\ ,\\
\chi_{zz} &= \frac{1}{12}-\frac{0.002\,0297}{S}+\frac{0.002\,8501}{S}(1-x)+\ldots\ .
\end{aligned} \tag{3.31}$$

F. Two-dimensional honeycomb lattice

For the honeycomb lattice, the smallest unit cell contains two sites and hence a spin-wave theory must be based on two sublattices. This can be developed as follows. For the following Hamiltonian,

$$H=-\sum_{\langle lm\rangle}(S_l^xS_m^x+xS_l^yS_m^y)+h\sum_i S_i^x\ , \tag{3.32}$$

first, we introduce Holstein-Primakoff transformation for two sublattices A and B:

$$\begin{aligned}
&S_l^+=(1S)^{1/2}f_l(S)a_l\ ,\quad S_l^-=(2S)^{1/2}a_l^*f_l(S)\ ,\quad S_l^x=S-a_l^*a_l\ ,\quad l\in A\ ,\\
&S_m^+=(2S)^{1/2}f_m(S)b_m\ ,\quad S_m^-=(2S)^{1/2}b_m^*f_m(S)\ ,\quad S_m^x=S-b_m^*b_m\ ,\quad m\in B\ ,
\end{aligned} \tag{3.33}$$

where $f_l(S)\simeq 1-a_l^*a_l/(4S)$.

Second, we introduce Bloch-type operators a_k, b_k by the Fourier transformation

$$a_k=\sqrt{2/N}\sum_l e^{ik\cdot l}a_l\ ,\quad b_k=\sqrt{2/N}\sum_m e^{ik\cdot m}b_m\ . \tag{3.34}$$

Note that, for the honeycomb lattice, the structure factor $\gamma_k=(1/z)\sum_\rho e^{i\rho\cdot k}$ is complex, that is, $\gamma_k\neq\gamma_k^*=\gamma_{-k}$ (denote $\gamma_k=|\gamma_k|e^{i\delta_k}$). The phase factor $e^{i\delta_k}$ in the Hamiltonian can be absorbed by a simple transformation:

$b_k \to b_k e^{i\delta_k}$, and the Hamiltonian can be diagonalized by the following Bogoliubov transformation:

$$a_k = (\cosh\theta_{1k}\,\alpha_k + \sinh\theta_{1k}\,\alpha^*_{-k} + \cosh\theta_{2k}\,\beta_k - \sinh\theta_{2k}\,\beta^*_{-k})/\sqrt{2}\ ,$$
$$b_k = (\cosh\theta_{1k}\,\alpha_k + \sinh\theta_{1k}\,\alpha^*_{-k} - \cosh\theta_{2k}\,\beta_k + \sinh\theta_{2k}\,\beta^*_{-k})/\sqrt{2}\ , \tag{3.35}$$

where $\tanh(2\theta_{1k}) = |D_k|/(1-|D_k|)$, $\tanh(2\theta_{2k}) = |D_k|/(1+|D_k|)$, and $|D_k| = x|\gamma_k|[1-(h/zS)]^{-1}/2$.

By a similar method as in Ref. 2, we can get the same results for ground-state energy E_0/N, the mass gap m, the magnetization M_x, and the susceptibility χ_{xx}, χ_{yy}, χ_{zz} as Eq. (3.3) except that, here, C_n is defined by

$$C_n = \frac{1}{N}\sum_k [(1-x|\gamma_k|)^{n/2} + (1+x|\gamma_k|)^{n/2} - 2]\ , \tag{3.36}$$

the sum over k denotes a sum over the first Brillouin zone of sublattice A. For the two-dimensional honeycomb lattice, the asymptotic behavior near $x^2=1$ of C_n is

$$\begin{aligned}
C_3 &= 0.130\,8252 - 0.139\,842(1-x^2) + 0.022\,928(1-x^2)^2 \\
&\quad - \frac{3\sqrt{6}}{80\pi}(1-x^2)^{5/2} + 0.030\,86(1-x^2)^3 - \frac{177\sqrt{6}}{4480\pi}(1-x^2)^{7/2} + \cdots\ , \\
C_1 &= -0.055\,630\,93 + 0.107\,7546(1-x^2) - \frac{\sqrt{3}}{4\sqrt{2}\pi}(1-x^2)^{3/2} + 0.085\,24(1-x^2)^2 - \frac{31\sqrt{3}}{160\sqrt{2}\pi}(1-x^2)^{5/2} + \cdots\ , \\
C_{-1} &= 0.375\,3874 - \frac{3\sqrt{6}}{4\pi}(1-x^2)^{1/2} + 0.358\,68(1-x^2) - \frac{11\sqrt{3}}{16\sqrt{2}\pi}(1-x^2)^{3/2} + \ldots\ , \\
C_{-3} &= \frac{3\sqrt{6}}{2\pi}(1-x^2)^{-1/2} - 1.059\,32 - \frac{3\sqrt{3}}{8\sqrt{2}\pi}(1-x^2)^{1/2} + \ldots\ , \\
C_{-5} &= \frac{\sqrt{6}}{\pi}(1-x^2)^{-3/2} + \frac{5\sqrt{6}}{8\pi}(1-x^2)^{-1/2} + \cdots\ ,
\end{aligned} \tag{3.37}$$

so the asymptotic behavior of the physical quantities are

$$\begin{aligned}
E_0/N &= -1.5S^2 - 0.083\,446S - 0.007\,679 + (0.161\,63S - 0.019\,544)(1-x^2) \\
&\qquad + (-0.1462S + 0.083\,64)(1-x^2)^{3/2} + \cdots \quad (x\sim\pm1)\ , \\
m &= [3S - 0.423\,239 + 1.2405(1-x)^{1/2} + \cdots](1-x)^{1/2} \quad (x\sim1)\ , \\
m &= [3S - 0.056\,396 + 0.231\,55(1+x) + \cdots](1-x)^{1/2} \quad (x\sim-1)\ , \\
M_x &= S - 0.079\,939 - 0.001\,3902/S + (0.146\,19 - 0.040\,444/S)(1-x^2)^{1/2} + \cdots \quad (x\sim\pm1)\ , \\
\chi_{xx} &= \left[\frac{0.048731}{S} + \frac{9.1607}{10^4S^2}\right](1-x^2)^{-1/2} - \frac{0.077\,738}{S} + \frac{0.033\,239}{S^2} + \cdots \quad (x\sim\pm1)\ , \\
\chi_{yy} &= (1-x)^{-1}[\tfrac{1}{3} + 0.071\,8364/S - 0.137\,832(1-x)^{1/2}/S + \cdots] \quad (x\sim1)\ , \\
\chi_{yy} &= \tfrac{1}{6} - 0.035\,9182/S + 0.068\,916(1+x)^{1/2}/S + \cdots \quad (x\sim-1)\ , \\
\chi_{zz} &= \tfrac{1}{3} - 0.031\,076/S + 0.051\,456(1-x)/S + \cdots \quad (x\sim1)\ , \\
\chi_{zz} &= \tfrac{1}{3} + 0.031\,076/S - 0.051\,456(1+x)/S + \cdots \quad (x\sim-1)\ .
\end{aligned} \tag{3.38}$$

IV. DISCUSSION

The general second-order spin-wave results for the XXZ and XY models have been found for several different lattices. Just as in the case of the Heisenberg antiferromagnet,[10] the ground-state energy for the isotropic XY model on a one-dimensional linear chain, and the three-dimensional simple-cubic lattice and body-centered-cubic lattice obtained here coincides with that of Nishimori and Miyake,[10] which is obtained from a special spin-wave representation rather than the traditional Holstein-Primakoff representation (a comparison of the ground-state energy on these lattices obtained by spin-wave theory and that obtained by other methods can be found in Nishimori and Miyake.)[10] For the $S=\frac{1}{2}$ isotropic XY ferromagnet on a triangular lattice, the ground-state energy is $E_0/N = -0.8030$, which is consistent with the result $E_0/N = -0.7989(45)$ obtained by Fujiki and Betts[23] using a finite-lattice method.

The XXZ Heisenberg antiferromagnet and XY model have very similar characteristics. The isotropic Heisenberg antiferromagnet at $x=1$ possesses a rational SU(2) symmetry for $S=\frac{1}{2}$ [or a rotational O(3) symmetry for integer S], which is broken when $x<1$ into a product of a $\mathbb{Z}(2)$ symmetry in the **z** direction times a U(1) symmetry in the **x**-**y** plane. The isotropic XY ferromagnet at $x=1$ possesses a rotational O(2) symmetry in the **x**-**y** spin plane, which is broken when $x<1$ into a $\mathbb{Z}(2)$ symmetry in the **z** direction times a U(1) symmetry in the **x**-**y** plane. The isotropic XY ferromagnet at $x=1$ possesses a rotational O(2) symmetry in the **x**-**y** spin plane, which is broken when $x<1$ into a $\mathbb{Z}(2)$ symmetry in the **x** direction. The ground state of both isotropic models exhibits spontaneous symmetry breaking by the Goldstone mechanism, so that, if the isotropic limit is approached from the Ising side ($x<1$), there is long-range order in the **z** direction for the XXZ model or in the **x** direction for the XY model. The mass gap goes to zero in the isotropic limit, corresponding to the appearance of a massless Goldstone mode. Therefore, C_n and the physical quantities have singularities at the isotropic point. For one- and three-dimensional lattices (in fact, for any odd-dimensional lattice), the singular terms have the form $(1-x^2)^m \ln(1-x^2)$ [or $(1-x)^m \ln(1-x)$ for the XY model on a nonbipartite lattice]. For even-dimensional lattices, the singular terms of C_n have the form $(1-x^2)^{m/2}$ [or $(1-x)^{m/2}$ for the XY model on a nonbipartite lattice].

For the spin-$\frac{1}{2}$ isotropic Heisenberg antiferromagnet (HAF) on a two-dimensional honeycomb lattice, the quantum effect reduces the staggered magnetization M^+ more than 50% from its classical value, which is much stronger than that for the square-lattice HAF which is $M^+=S-0.1966$, and is almost as strong as that of the triangular-lattice HAF which is[15] $M^+=S-0.216$.

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