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Flow equations and extended Bogoliubov transformation for the Heisenberg antiferromagnet near the classical limit

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Abstract. The Heisenberg spin-S quantum antiferromagnet is studied near the large-spin limit, applying a new *continuous* unitary transformation which extends the usual Bogoliubov transformation to higher order in the $1/S$-expansion of the Hamiltonian. This allows to diagonalize the bosonic Hamiltonian resulting from the Holstein-Primakoff representation beyond the conventional spin-wave approximation. The zero-temperature flow equations derived from the extension of the Bogoliubov transformation to order $\mathcal{O}(1/S^2)$ for the ground-state energy, the spin-wave velocity, and the staggered magnetization are solved exactly and yield results which are in agreement with those obtained by a perturbative treatment of the magnon interactions.

Dedicated to Professor Heinz Horner on the occasion of his 60th birthday

PACS. 75.10.Jm Quantized spin models – 71.27.+a Strongly correlated electrons

1 Introduction

The quantum Heisenberg model with antiferromagnetic coupling of neighboring spins on a lattice is one of the most fundamental models in the theory of magnetism. Besides its basic and longstanding role for the theoretical understanding of magnetic quantum systems, it has also gained renewed interest in the description of the undoped cuprates, where low dimensionality and small spin quantum number cause an enhanced importance of quantum fluctuations. A quite clear physical picture for the low-temperature phase diagram of the Heisenberg quantum antiferromagnet has emerged from a variety of methods [1], including spin-wave theory, Schwinger boson mean-field theory, renormalization-group calculations and various numerical and perturbative techniques.

Generally, a standard approach in the study of low-temperature magnetic systems [2] is spin-wave theory [3], which assumes magnetic ordering in the ground-state and applies an expansion of the spin interaction around the classical limit of large spin quantum number S, utilizing a spin-boson transformation. In the leading order of $1/S$, the resulting Hamiltonian is then bilinear in the boson operators and can be diagonalized by a usual Bogoliubov transformation eliminating terms which do not conserve the number of particles. In this approximative approach, which already yields quite good results for a number of physical quantities even in the $S = 1/2$ case [4], higher-order interaction terms representing scattering of spin-waves may be included in the analysis only perturbatively [5]. Such a treatment of the magnon interactions is performed in extended spin-wave theory, where the contributions to the bosonic Hamiltonian in next-to-leading order of $1/S$ are considered in first-order perturbation theory after the Bogoliubov transformation has been applied.

It is thus a natural question to ask whether one can devise an extended transformation which diagonalizes the bosonic Hamiltonian also in higher orders of the inverse spin. Although this is hardly feasible for a "single-step" transformation, a *continuous* transformation of the Hamiltonian with this desired property is much easier to construct. The method of continuous unitary transformations has been formulated originally by Wegner [6] and independently also by Głazek and Wilson [7]. It has been successfully applied to a variety of physical problems, including the Anderson impurity Hamiltonian [8], the spin-boson model of quantum dissipation [9], systems with electron-phonon interactions [10], the strong-coupling Hubbard Hamiltonian [11], and the low-dimensional n-orbital model [12], often yielding new and surprising results and clarifying problems of other approaches. On the other hand, the antiferromagnetic Heisenberg model near the classical limit also provides an instructive example how the $1/S$-expansion imposes a peculiar linear structure on the flow equations derived for the couplings of the Hamiltonian and makes their solutions perfectly controlled by a systematic parameter.

In the present work a new continuous unitary transformation is applied to the large-S Heisenberg antiferromagnet in the Holstein-Primakoff representation. This allows to go beyond conventional spin-wave theory and to diagonalize the resulting bosonic Hamiltonian also in higher orders of $1/S$, removing interactions which connect subspaces with a different number of spin excitations. Near the classical limit the inverse of the spin is small and may thus serve as a systematic expansion parameter. Due to this classification of the spin interactions in terms of $1/S$, the resulting flow equations derived from the continuous transformation are closed, and exact results for a number of physical quantities can be obtained. To be more precise, for every order of the $1/S$-expanded Hamiltonian one obtains an inhomogeneous system of linear differential equations involving the coupling functions of that particular order, while the inhomogeneous contributions exclusively result from the transformation and normal ordering of terms in other orders. We present results with the diagonalization being performed to order $\mathcal{O}(1/S^2)$. In contrast to the usual (leading order) Bogoliubov transformation, up to this order the proposed novel continuous transformation does not generate new types of nondiagonal interaction terms which were not present in the original Hamiltonian. The second-order flow equations for the ground-state energy, the spin-wave velocity, and the staggered magnetization are derived and solved exactly for the zero-temperature case. Although the continuous transformation is not based on perturbation theory around the leading-order magnon Hamiltonian, the corresponding results are in agreement with those obtained by the perturbative approach of extended spin-wave theory.

2 The flow equations

We consider the spin-S Heisenberg quantum antiferromagnet

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where the sum $\langle i,j \rangle$ is over all bonds of a general bipartite lattice with N sites and sublattices A and B, with $i \in A$ and $j \in B$. To be more specific, in the following we will always consider the special case of a simple cubic lattice with $z = 2d$ nearest neighbors, lattice spacing a, and the lattice dispersion $\gamma_q = \frac{1}{d}\sum_{l=1}^{d} \cos q_l a$, although most of the results obtained below are also valid for a more general bipartite lattice. The case of dimensionality $d = 2$, *i.e.* the square lattice, will be of special interest. To study this quantum model (1) near the classical limit where $S \gg 1$, we adopt the Holstein-Primakoff boson representation [13] of spin operators on the two sublattices,

$$\begin{aligned} S_i^z &= S - n_i \quad & S_i^+ &= \sqrt{2S - n_i}\, a_i \quad & S_i^- &= a_i^\dagger \sqrt{2S - n_i} \\ S_j^z &= -S + n_j \quad & S_j^+ &= b_j^\dagger \sqrt{2S - n_j} \quad & S_j^- &= \sqrt{2S - n_j}\, b_j, \end{aligned} \tag{2}$$

where the a_i and b_j are local Bose operators. Inserting these expressions in (1) and expanding the square roots results in an expansion of the Hamiltonian in powers of the inverse spin,

$$H(\ell) = E_0(\ell) + \Delta \sum_{k=1}^{\infty} \frac{:H_k(\ell):}{S^k}, \tag{3}$$

where $\Delta = zJS^2$ sets the energy scale of the problem. Due to the continuous transformation which is applied to the Hamiltonian, $H(\ell) = U(\ell)HU^\dagger(\ell)$, the couplings depend on the non-negative flow parameter ℓ. The interaction contributions $:H_k:$ are written in normal-ordered form and the normal ordering $:\ldots:$ is initially performed with respect to the classical vacuum $|0\rangle$, with $a_i|0\rangle = b_j|0\rangle = 0$. Since the classical vacuum is mapped to the (approximate) quantum ground state in the course of the transformation flow, generally (*i.e.* for $\ell > 0$) normal ordering is with respect to the actual transformed ground state $|0_\ell\rangle$, which incorporates quantum fluctuations to some order of $1/S$. We use the convention that the interaction terms of the Hamiltonian (3) are assigned to that H_k in which they appear at lowest order in k. As a consequence, the couplings of the interactions will in general also have contributions which are of higher order in $1/S$ and which originate from normal ordering of higher-order interaction terms. The normal ordering also ensures that $\langle 0_\ell| :H_k(\ell): |0_\ell\rangle = 0$ and thus $\langle 0_\ell|H(\ell)|0_\ell\rangle = E_0(\ell)$. The initial value $E_0(0) = -N\Delta/2$ of the ground-state energy corresponds to the classical Néel ground-state.

The transformation flow of the Hamiltonian is then described by the differential equation [6]

$$\frac{\mathrm{d}}{\mathrm{d}\ell} H(\ell) = [\eta(\ell), H(\ell)], \tag{4}$$

where the antihermitean flow generator $\eta(\ell)$ is also expanded in powers of $1/S$,

$$\eta(\ell) = \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} U^\dagger(\ell) = \sum_{k=0}^{\infty} \frac{\eta_k(\ell)}{S^k}. \tag{5}$$

Instead of the canonical form of the generator of the transformation, given by the commutator of the diagonal and nondiagonal parts of the Hamiltonian [6], the $\eta_k(\ell)$ employed here are somewhat simpler. At k-th order of the $1/S$-expansion, the corresponding $\eta_k(\ell)$ is chosen as the nondiagonal contribution to the Hamiltonian at that order, albeit brought in antihermitean form. Thus, $\eta_k(\ell)$ is simply given by the difference of the terms in $H_k(\ell)$ which raise and lower the number of particles by two, respectively. An analogous form for the generator has also been proposed for the block-diagonalizing strong-coupling transformation of the Hubbard model [11], and for the diagonalization of general band matrices [14].

It is also worth noting that utilizing the Dyson-Maleev [15] instead of the Holstein-Primakoff spin-boson transformation eventually generates the same types of interaction terms. However, due to the non-hermiteicity of the operators involved in the Dyson-Maleev representation, in higher orders the resulting flow equations are less symmetric and the Holstein-Primakoff transformation appears to be more suitable to the problem.

2.1 Linear spin-wave theory

To recover the results of linear spin-wave theory, only terms up to order $\mathcal{O}(1/S)$ are retained in the $1/S$-expansion of the Hamiltonian (3),

$$H_1(\ell) = \sum_q \big(f_q(\ell)\big(a_q^\dagger a_q + b_q^\dagger b_q\big) \\ +g_q(\ell)\big(a_q^\dagger b_{-q}^\dagger + a_q b_{-q}\big)\Big), \tag{6}$$

where one initially has $f_q(0) = 1$ and $g_q(0) = \gamma_q$. This leading correction beyond the classical contribution is bilinear in the boson operators and may be diagonalized directly in a single step by a conventional Bogoliubov rotation. However, since we are finally aiming at a diagonalization at order $\mathcal{O}(1/S^2)$ which requires some results of the continuous transformation in the leading order, we will present here a continuous version of the Bogoliubov transformation. In order $\mathcal{O}(1/S)$ the "single-step" and the continuous version yield the same final results for the transformed bosonic Hamiltonian.

In the framework of the continuous transformation the terms in (6) which do not conserve the number of spin excitations are eliminated by choosing

$$\eta_0(\ell) = \frac{1}{2}\sum_q g_q(\ell)\big(a_q^\dagger b_{-q}^\dagger - a_q b_{-q}\big), \tag{7}$$

resulting in the leading-order flow equation

$$\frac{\mathrm{d}}{\mathrm{d}\ell}H_1(\ell) = [\eta_0(\ell), H_1(\ell)]. \tag{8}$$

The differential equations which describe the transformation of the coupling functions of (6) are then given by

$$\frac{\mathrm{d}}{\mathrm{d}\ell}f_q(\ell) = -g_q^2(\ell) \qquad \frac{\mathrm{d}}{\mathrm{d}\ell}g_q(\ell) = -f_q(\ell)\, g_q(\ell). \tag{9}$$

The quantum corrections to the ground-state energy give rise to the flow of $E_0(\ell)$,

$$\frac{\mathrm{d}}{\mathrm{d}\ell}E_0(\ell) = -\frac{\Delta}{S}\sum_q g_q^2(\ell). \tag{10}$$

Introducing the bare spin-wave dispersion $\epsilon_q = (1-\gamma_q^2)^{1/2}$, one finds that $f_q^2(\ell) - g_q^2(\ell) = \epsilon_q^2$ is an invariant of the transformation flow. This invariant immediately suggests the hyperbolic parametrization which is usually employed in the Bogoliubov transformation. The solutions of (9) are thus readily obtained

$$f_q(\ell) = \epsilon_q \coth\big(\ell\epsilon_q + \ell_0(q)\big) \quad g_q(\ell) = \frac{\epsilon_q\,\mathrm{sgn}\gamma_q}{\sinh\big(\ell\epsilon_q + \ell_0(q)\big)} \tag{11}$$

with the initial values correctly reproduced by

$$\ell_0(q) = \frac{1}{2}\ln\frac{1+\epsilon_q}{1-\epsilon_q}. \tag{12}$$

Since $\ell_0(q) \geq 0$, the $f_q(\ell)$ and $g_q(\ell)$ are continuous and monotonically decreasing functions in the whole range $\ell \geq 0$. When $H_1(0)$ is already diagonal, *i.e.* $\gamma_q = 0$, the transformation does not give anything new, since then $f_q(\ell) \equiv 1$ and $g_q(\ell) \equiv 0$. Generally, the asymptotic behavior for $\ell \to \infty$ is governed by exponential convergence to the values $f_q(\infty) = \epsilon_q$ and $g_q(\infty) = 0$. In the degenerate case when $\epsilon_q = 0$, one finds a weaker algebraic decay of the coupling functions,

$$f_q(\ell) = \pm g_q(\ell) = \frac{1}{\ell+1} \qquad \text{for} \quad \gamma_q = \pm 1. \tag{13}$$

Therefore, the choice (7) for the generator of the transformation also ensures the elimination of bosonic spin excitations which are degenerate with the quantum groundstate.

2.2 The spin-wave interactions

Expanding the Hamiltonian (3) to next higher order in $1/S$ yields additional two-particle interactions of the spin-wave excitations,

$$H_2(\ell) = -\tfrac{2}{N}\sum_{q,q_1,q_2}\Big(h_{q,q_1,q_2}(\ell)a_{q+q_1}^\dagger a_{q_1} b_{-q+q_2}^\dagger b_{q_2} \\ +\xi_{q,q_1,q_2}(\ell)\big(a_{q+q_1}^\dagger a_{-q+q_2}^\dagger a_{q_1}a_{q_2} + b_{q+q_1}^\dagger b_{-q+q_2}^\dagger b_{q_1}b_{q_2}\big) \\ +\tfrac{1}{4}\zeta_{q,q_1,q_2}(\ell)\big(a_{q+q_1+q_2}^\dagger a_{q_1}a_{q_2}b_q + a_{q_1}^\dagger a_{q_2}^\dagger a_{q+q_1+q_2}b_q^\dagger \\ +a_q b_{q+q_1+q_2}^\dagger b_{q_1}b_{q_2} + a_q^\dagger b_{q_1}^\dagger b_{q_2}^\dagger b_{q+q_1+q_2}\big)\Big). \tag{14}$$

The interaction terms related to h_{q,q_1,q_2} and ξ_{q,q_1,q_2} involve t-channel scattering of magnons with initial momenta q_1 and q_2 and momentum transfer q, while ζ_{q,q_1,q_2} describes the creation or annihilation of spin excitations with total momentum $q+q_1+q_2$. Only the contributions given by the couplings h_{q,q_1,q_2} and ζ_{q,q_1,q_2} are initially present in the bosonized Heisenberg Hamiltonian. Accordingly, the coupling functions of the interaction terms (14) obey the initial conditions $h_{q,q_1,q_2}(0) = \zeta_{q,q_1,q_2}(0) = \gamma_q$ and $\xi_{q,q_1,q_2}(0) = 0$. One also finds the invariance properties

$$h_{q,q_1,q_2}(\ell) = h_{-q,q_2,q_1}(\ell), \quad \xi_{q,q_1,q_2}(\ell) = \xi_{-q,q_2,q_1}(\ell), \\ \text{and} \quad \zeta_{q,q_1,q_2}(\ell) = \zeta_{q,q_2,q_1}(\ell) \tag{15}$$

which are related to permutation symmetry, whereas hermiteicity of the Hamiltonian enforces the additional symmetry relations

$$h_{q,q_1,q_2}(\ell) = h_{-q,q+q_1,-q+q_2}(\ell), \\ \xi_{q,q_1,q_2}(\ell) = \xi_{-q,q+q_1,-q+q_2}(\ell). \tag{16}$$

At this point, usual spin-wave theory does not involve any further transformation of the interactive part of the Hamiltonian which is beyond the linear Bogoliubov transformation considered in the preceding section. As a consequence, in $H_2(\ell)$ nondiagonal terms are not removed. Correspondingly, the flow of $H_2(\ell)$, as completely described by the generator $\eta_0(\ell)$ only, does not eventually lead to a particle-conserving expression. However, the interaction terms which connect subspaces with a different number of spin excitations can be transformed away by an extension of the continuous generator. Choosing

$$\eta_1(\ell) = \tfrac{1}{4N}\sum_{q,q_1,q_2}\zeta_{q,q_1,q_2}(\ell)\big(a^\dagger_{q+q_1+q_2}a_{q_1}a_{q_2}b_q + a_q b^\dagger_{q+q_1+q_2}b_{q_1}b_{q_2} - a^\dagger_{q_1}a^\dagger_{q_2}a_{q+q_1+q_2}b^\dagger_q - a^\dagger_q b^\dagger_{q_1}b^\dagger_{q_2}b_{q+q_1+q_2}\big) \tag{17}$$

at second order in $1/S$ the flow equation for the Hamiltonian reads

$$\frac{\mathrm{d}}{\mathrm{d}\ell}H_2(\ell) = [\eta_0(\ell), H_2(\ell)] + [\eta_1(\ell), H_1(\ell)]. \tag{18}$$

The transformation (18) does not generate new types of nondiagonal interaction terms in the Hamiltonian, in contrast to the usual linear Bogoliubov transformation which at order $\mathcal{O}(1/S^2)$ leads to new interactions of the form $(aabb + a^\dagger a^\dagger b^\dagger b^\dagger)$ [*cf.* (25) below]. This is due to a cancellation of the corresponding contributions in (18), which does not occur without the term related to $\eta_1(\ell)$. Moreover, it seems to be peculiar for the specific choice of the generator, since also in related work [11,14] it was observed that an analogous type of transformation is able to avoid the population of initially empty off-diagonals.

As a consequence of normal ordering, the coupling functions appearing in $H_1(\ell)$ acquire a $\mathcal{O}(1/S)$ correction, $\tilde f_q(\ell) = f_q(\ell) + \frac{1}{S}f_q^{(1)}(\ell)$ and $\tilde g_q(\ell) = g_q(\ell) + \frac{1}{S}g_q^{(1)}(\ell)$. The corresponding second-order flow equations then read

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\tilde f_q(\ell) = -\tilde g_q^2(\ell) + \frac{1}{S}\int_Q g_Q(\ell)\,\zeta_{-Q,Q,q}(\ell) \tag{19}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\tilde g_q(\ell) = -\tilde f_q(\ell)\,\tilde g_q(\ell) + \frac{1}{2S}\int_Q g_Q(\ell)\,h_{Q-q,q,-q}(\ell), \tag{20}$$

where momentum integration $\int_Q$ extends over the entire Brillouin zone of the lattice. The coupling functions of $H_2(\ell)$ with general momenta are determined by the equations

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\ell}h_{q,q_1,q_2}(\ell) = -\frac{1}{2}\big(&g_{q_1}(\ell)\,\zeta_{q+q_1,-q+q_2,-q_1}(\ell)\\ &+g_{q_2}(\ell)\,\zeta_{-q+q_2,q+q_1,-q_2}(\ell)\\ &+g_{q+q_1}(\ell)\,\zeta_{q_1,q_2,-q-q_1}(\ell)\\ &+g_{q-q_2}(\ell)\,\zeta_{q_2,q_1,q-q_2}(\ell)\big),\end{aligned} \tag{21}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\ell}\xi_{q,q_1,q_2}(\ell) = -\frac{1}{8}\big(&g_{q_1}(\ell)\,\zeta_{-q_1,q+q_1,-q+q_2}(\ell)\\ &+g_{q_2}(\ell)\,\zeta_{-q_2,-q+q_2,q+q_1}(\ell)\\ &+g_{q+q_1}(\ell)\,\zeta_{-q-q_1,q_1,q_2}(\ell)\\ &+g_{q-q_2}(\ell)\,\zeta_{q-q_2,q_2,q_1}(\ell)\big),\end{aligned} \tag{22}$$

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}\ell}\zeta_{q,q_1,q_2}(\ell) = \tfrac{1}{2}&\zeta_{q,q_1,q_2}(\ell)\times\\ &\big(f_{q+q_1+q_2}(\ell) - f_q(\ell) - f_{q_1}(\ell) - f_{q_2}(\ell)\big)\\ &-g_{q_1}(\ell)\,h_{q+q_1,q_2,q}(\ell) - g_{q_2}(\ell)\,h_{q+q_2,q_1,q}(\ell)\\ &-2g_q(\ell)\big(\xi_{q+q_1,q_2,q_1}(\ell) + \xi_{q+q_2,q_1,q_2}(\ell)\big).\end{aligned} \tag{23}$$

The energetic stability of the spin-wave excitations, $\epsilon_{q_1+q_2} \le \epsilon_{q_1} + \epsilon_{q_2}$, ensures that $\zeta_{q,q_1,q_2}(\ell)$ decays exponentially in the asymptotic limit $\ell \to \infty$, apart from the highly degenerate situation when at least two momenta involved in the interaction vanish. Also the functions h_{q,q_1,q_2} and ξ_{q,q_1,q_2} converge exponentially fast to their asymptotic values in this regime.

This system of coupled linear differential equations (21-23) is substantially simplified, if one considers only those coupling functions with momenta entering into the $\mathcal{O}(1/S)$ corrections of $f_q(\ell)$ and $g_q(\ell)$. The reason for this, which will become more clear in the next section, is that only these coupling functions contribute to the ground-state properties in which we are eventually interested. Introducing $\vartheta_{0,q,Q}(\ell) = h_{0,-q,Q}(\ell) + 4\xi_{0,q,Q}(\ell)$, one thus obtains

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\begin{pmatrix}\zeta_{-q,q,Q}(\ell)\\ \zeta_{-Q,Q,q}(\ell)\\ \vartheta_{0,q,Q}(\ell)\\ h_{Q-q,q,-q}(\ell)\end{pmatrix} = -\begin{pmatrix}f_q(\ell) & 0 & g_q(\ell) & g_Q(\ell)\\ 0 & f_Q(\ell) & g_Q(\ell) & g_q(\ell)\\ 2g_q(\ell) & 2g_Q(\ell) & 0 & 0\\ g_Q(\ell) & g_q(\ell) & 0 & 0\end{pmatrix}\begin{pmatrix}\zeta_{-q,q,Q}(\ell)\\ \zeta_{-Q,Q,q}(\ell)\\ \vartheta_{0,q,Q}(\ell)\\ h_{Q-q,q,-q}(\ell)\end{pmatrix} \tag{24}$$

Unfortunately, the eigenvectors of the matrix in (24) are ℓ-dependent, so that this system of differential equations is not easily solved. Let us therefore first consider the somewhat simpler situation when only the linear spin-wave transformation is employed. Thus, without the elimination of the nondiagonal terms at order $\mathcal{O}(1/S^2)$ as performed by the introduction of $\eta_1(\ell)$, the corresponding flow equations for $H_2(\ell)$ are determined completely by the first commutator in (18), while the second one does not contribute. One then obtains a modified expression for the second-order Hamiltonian,

$$\begin{aligned}H_2'(\ell) = -\tfrac{2}{N}\sum_{q,q_1,q_2}\Big(&k_{q,q_1,q_2}(\ell)a^\dagger_{q+q_1}a_{q_1}b^\dagger_{-q+q_2}b_{q_2}\\ &+x_{q,q_1,q_2}(\ell)\big(a^\dagger_{q+q_1}a^\dagger_{-q+q_2}a_{q_1}a_{q_2} + b^\dagger_{q+q_1}b^\dagger_{-q+q_2}b_{q_1}b_{q_2}\big)\\ &+\tfrac{1}{4}z_{q,q_1,q_2}(\ell)\big(a^\dagger_{q+q_1+q_2}a_{q_1}a_{q_2}b_q + a^\dagger_{q_1}a^\dagger_{q_2}a_{q+q_1+q_2}b^\dagger_q\\ &\quad+a_q b^\dagger_{q+q_1+q_2}b_{q_1}b_{q_2} + a^\dagger_q b^\dagger_{q_1}b^\dagger_{q_2}b_{q+q_1+q_2}\big)\\ &+y_{q,q_1,q_2}(\ell)\big(a_{q_1}a_{q_2}b_q b_{-q-q_1-q_2} + a^\dagger_{q_1}a^\dagger_{q_2}b^\dagger_q b^\dagger_{-q-q_1-q_2}\big)\Big).\end{aligned} \tag{25}$$

Besides the terms related to k_{q,q_1,q_2}, x_{q,q_1,q_2}, and z_{q,q_1,q_2}, which are already present due to the extended transformation (17), the linear Bogoliubov transformation generates additional nondiagonal spin-wave interactions with coupling y_{q,q_1,q_2}. Therefore, one has the new initial conditions $k_{q,q_1,q_2}(0) = z_{q,q_1,q_2}(0) = \gamma_q$ and $x_{q,q_1,q_2}(0) = y_{q,q_1,q_2}(0) = 0$. As above, the determination of the ground state properties again requires only a partial knowledge of the complete set of flow equations for the coupling functions in (25). One introduces $t_{0,q,Q}(\ell) = k_{0,-q,Q}(\ell) + 4x_{0,q,Q}(\ell)$ and $r_{Q-q,q,-q}(\ell) = k_{Q-q,q,-q}(\ell) + 4y_{-q,q,Q}(\ell)$ to arrive at the system of linear differential equations

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\begin{pmatrix} z_{-q,q,Q}(\ell) \\ z_{-Q,Q,q}(\ell) \\ t_{0,q,Q}(\ell) \\ r_{Q-q,q,-q}(\ell) \end{pmatrix} = -\begin{pmatrix} 0 & 0 & g_q(\ell) & g_Q(\ell) \\ 0 & 0 & g_Q(\ell) & g_q(\ell) \\ g_q(\ell) & g_Q(\ell) & 0 & 0 \\ g_Q(\ell) & g_q(\ell) & 0 & 0 \end{pmatrix}\begin{pmatrix} z_{-q,q,Q}(\ell) \\ z_{-Q,Q,q}(\ell) \\ t_{0,q,Q}(\ell) \\ r_{Q-q,q,-q}(\ell) \end{pmatrix}. \tag{26}$$

Although the second-order Hamiltonian (25) resulting from the linear Bogoliubov transformation is more complicated in structure than the one which is derived in presence of $\eta_1(\ell)$, the corresponding system of flow equations (26) is simpler and can be solved easily. Noting that $t_{0,q,Q}(0) = 1$ and $r_{Q-q,q,-q}(0) = \gamma_{Q-q}$, one finds that the solutions are most conveniently written in terms of the functions $F_q(\ell)$ and $G_q(\ell)$ which are introduced below and are explicitly given in (54). Thus,

$$\begin{aligned} z_{-q,q,Q}(\ell) &= \gamma_q F_q(\ell)F_Q(\ell) + \gamma_Q G_q(\ell)G_Q(\ell) \\ &\quad + F_Q(\ell)G_q(\ell) + \gamma_{Q-q}F_q(\ell)G_Q(\ell) \\ t_{0,q,Q}(\ell) &= \gamma_q G_q(\ell)F_Q(\ell) + \gamma_Q G_Q(\ell)F_q(\ell) \\ &\quad + F_q(\ell)F_Q(\ell) + \gamma_{Q-q}G_q(\ell)G_Q(\ell) \\ r_{Q-q,q,-q}(\ell) &= \gamma_q F_q(\ell)G_Q(\ell) + \gamma_Q F_Q(\ell)G_q(\ell) \\ &\quad + G_q(\ell)G_Q(\ell) + \gamma_{Q-q}F_q(\ell)F_Q(\ell) \end{aligned} \tag{27}$$

From these solutions of the coupling functions the values for the transformed interactions in the linear spin-wave approximation are finally given by

$$\begin{aligned} z_{-q,q,Q}(\infty) &= \frac{\gamma_Q}{\epsilon_q\epsilon_Q}\left(\gamma_q\gamma_Q - \gamma_{Q-q}\right) \\ k_{0,q,Q}(\infty) &= \frac{1}{2} + \frac{1}{2\epsilon_q\epsilon_Q}\left(\epsilon_q^2 + \epsilon_Q^2 - 1 + \gamma_q\gamma_Q\gamma_{Q-q}\right) \\ k_{Q-q,q,-q}(\infty) &= \frac{\gamma_{Q-q}}{2} - \frac{1}{2\epsilon_q\epsilon_Q}\left(\gamma_q\gamma_Q - \gamma_{Q-q}\right) \\ x_{0,q,Q}(\infty) &= -\frac{1}{8} + \frac{1}{8\epsilon_q\epsilon_Q}\left(\epsilon_q^2 + \epsilon_Q^2 - 1 + \gamma_q\gamma_Q\gamma_{Q-q}\right) \\ y_{-q,q,Q}(\infty) &= -\frac{\gamma_{Q-q}}{8} - \frac{1}{8\epsilon_q\epsilon_Q}\left(\gamma_q\gamma_Q - \gamma_{Q-q}\right). \end{aligned} \tag{28}$$

The terms related to $k_{0,q,Q}$ and $x_{0,q,Q} = x_{Q-q,q,Q}$ correspond to and are in agreement with the diagonal interactions included in the second-order Hamiltonian derived from extended spin-wave theory.

Having solved the flow equations (26) for the purely linear transformation, one may now proceed to (24) and treat the terms which are different in these two systems of coupled differential equations as inhomogenities of (26). In this way, some additional information is available which is sufficient to determine the ground-state energy and the one-particle excitation spectrum. As will turn out in the next section, the solutions of the homogeneous system (26) are also fundamental for solving the flow equations of the second-order contributions to the occupation number of the Holstein-Primakoff bosons [*cf.* (59) below]. As a feature of the solutions which is most important for the determination of ground-state properties, one finds that the functions $\vartheta_{0,q,Q}(\ell)$ and $t_{0,q,Q}(\ell)$ converge to the same value in the asymptotic limit of the transformation,

$$\begin{aligned} \vartheta_{0,q,Q}(\infty) &= t_{0,q,Q}(\infty) = \\ &= \tfrac{1}{\epsilon_q\epsilon_Q}\left(\epsilon_q^2 + \epsilon_Q^2 - 1 + \gamma_q\gamma_Q\gamma_{Q-q}\right), \end{aligned} \tag{29}$$

and

$$\int_Q \vartheta_{0,q,Q}(\infty) = \epsilon_q \int_Q \epsilon_Q. \tag{30}$$

Furthermore, one obtains results for some of the transformed diagonal couplings of the second-order Hamiltonian,

$$\begin{aligned} \zeta_{-q,q,Q}(\infty) &= 0 \\ \xi_{0,q,Q}(\infty) &= x_{0,q,Q}(\infty) \\ \xi_{Q-q,q,Q}(\infty) &= x_{0,q,Q}(\infty) \\ h_{0,q,Q}(\infty) &= k_{0,q,Q}(\infty). \end{aligned} \tag{31}$$

3 Ground-state properties and one-particle excitations

To extract the physical properties of the quantum ground-state and the one-particle excitation spectrum from the flow equations presented in the preceding section, one first notes that (19) and (20) at order $\mathcal{O}(1/S)$ result in the equations

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\begin{pmatrix} f_q^{(1)}(\ell) \\ g_q^{(1)}(\ell) \end{pmatrix} = -\begin{pmatrix} 0 & 2g_q(\ell) \\ g_q(\ell) & f_q(\ell) \end{pmatrix}\begin{pmatrix} f_q^{(1)}(\ell) \\ g_q^{(1)}(\ell) \end{pmatrix} + \begin{pmatrix} b_{1;q}(\ell) \\ b_{2;q}(\ell) \end{pmatrix} \tag{32}$$

with initial conditions $f_q^{(1)}(0) = g_q^{(1)}(0) = 0$ and where the inhomogeneous contribution to this system of differential equations is given by

$$\begin{aligned} b_{1;q}(\ell) &= \int_Q g_Q(\ell)\zeta_{-Q,Q,q}(\ell), \\ b_{2;q}(\ell) &= \frac{1}{2}\int_Q g_Q(\ell)h_{Q-q,q,-q}(\ell). \end{aligned} \tag{33}$$

The integral basis for the homogeneous part of (32) consists of the two independent solutions

$$\begin{pmatrix} g_q^2(\ell) \\ f_q(\ell)\,g_q(\ell) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} f_q(\ell) - \ell\, g_q^2(\ell) \\ g_q(\ell) - \ell\, f_q(\ell)\, g_q(\ell) \end{pmatrix}. \tag{34}$$

Utilizing these expressions (34) and including the inhomogenities of (32), one derives the asymptotic values

$$\begin{aligned} g_q^{(1)}(\infty) &= 0 \qquad \text{and} \\ f_q^{(1)}(\infty) &= \tfrac{1}{\epsilon_q}\int_0^\infty \mathrm{d}\ell\,\left(f_q(\ell)\, b_{1;q}(\ell) - g_q(\ell)\, b_{2;q}(\ell)\right). \end{aligned} \tag{35}$$

Inserting here (33) and using (24), this yields the result

$$f_q^{(1)}(\infty) = \frac{1}{2}\big(\epsilon_q - \int_Q \vartheta_{0,q,Q}(\infty)\big), \quad (36)$$

which directly enters into the calculations for the ground-state energy and the spin-wave velocity.

3.1 Ground-state energy

Classifying also the contributions to the ground-state energy according to their power in the inverse spin,

$$E_0(\ell) = \sum_{k=0}^{\infty} \frac{E_0^{(k)}(\ell)}{S^k}, \quad (37)$$

from the result (10) of linear spin-wave theory one finds the flow equation for the leading-order quantum correction,

$$\frac{\mathrm{d}}{\mathrm{d}\ell} E_0^{(1)}(\ell) = -\Delta \sum_q g_q^2(\ell), \quad (38)$$

with the solution

$$E_0^{(1)}(\ell) = -\frac{N\Delta}{2}\big(1 - \int_q f_q(\ell)\big). \quad (39)$$

With the numerical result for the $d=2$ simple cubic lattice

$$\int_q \epsilon_q \simeq 0.842053, \quad (40)$$

the $\mathcal{O}(1/S)$ ground-state energy of the $S=1/2$ square lattice Heisenberg antiferromagnet is given by $E_0 \simeq -0.6579J$. Also the second-order correction of E_0 is entirely encapsulated in (10), since there are no further contributions to the flow equation for the ground-state energy arising from contractions of the magnon interaction terms. Including $g_q^{(1)}(\ell)$, one thus obtains

$$\frac{\mathrm{d}}{\mathrm{d}\ell} E_0^{(2)}(\ell) = -2\Delta \sum_q g_q(\ell)\, g_q^{(1)}(\ell). \quad (41)$$

With the integral

$$\begin{aligned} &\textstyle\int_0^\infty \mathrm{d}\ell\; g_q(\ell)\, g_q^{(1)}(\ell) = \\ -&\tfrac{1}{2\epsilon_q} \textstyle\int_0^\infty \mathrm{d}\ell\; \big((f_q(\ell)-\epsilon_q)\, b_{1;q}(\ell) - g_q(\ell)\, b_{2;q}(\ell)\big) \end{aligned} \quad (42)$$

and (24), this equation is solved by

$$\begin{aligned} E_0^{(2)}(\infty) &= -\frac{N\Delta}{8}\big(1 - \int_q \int_Q \vartheta_{0,q,Q}(\infty) \\ -4\int_q f_q^{(1)}(\infty)\big) &= -\frac{N\Delta}{8}\left(1 - \int_q \epsilon_q\right)^2, \end{aligned} \quad (43)$$

where we have made use of (30) and (36). With the numerical result (40), the total ground-state energy per site of the square-lattice Heisenberg antiferromagnet at order $\mathcal{O}(1/S^2)$ is then finally given,

$$E_0 = -2JS^2\big(1 + 0.15795/S + 0.00623/S^2 + \mathcal{O}(1/S^3)\big). \quad (44)$$

For $S=1/2$, one recovers the result of extended spin-wave theory, $E_0 = -0.6704\,J$.

3.2 Spin-wave velocity

From the diagonalized one-particle Hamiltonian (6) one can read off the excitation spectrum and the leading-order magnon dispersion $\omega_q(\infty) = 2dJS\epsilon_q$, which is linear for low momenta and is related to the spin-wave velocity, $c = \omega_q/q$ in the limit $q \to 0$. One thus obtains the bare value $c_0 = 2\sqrt{d}\,JSa$, in agreement with the standard linear spin-wave approximation. To obtain the quantum correction to the spin-wave velocity, one notes that

$$\omega_q(\ell) = 2dJS\,\big(f_q(\ell) + \frac{1}{S} f_q^{(1)}(\ell)\big). \quad (45)$$

Using (30) and the result (36) for $f_q^{(1)}(\infty)$, this yields

$$\omega_q(\infty) = 2dJS\epsilon_q\left(1 + \frac{1}{2S}\int_Q (1-\epsilon_Q)\right). \quad (46)$$

Together with (40), the enhancement of the spin-wave velocity by quantum fluctuations is then given by the factor $Z_c = c/c_0 \simeq 1.15795$ in the $S=1/2$ case, which again is in agreement with the result of extended spin-wave theory.

3.3 Staggered magnetization

The magnetic order in the ground-state of the Heisenberg antiferromagnet leads to a nonvanishing zero-temperature staggered or mean sublattice magnetization

$$m_\dagger = \frac{1}{N}\left(\sum_{i\in A}\langle S_i^z\rangle - \sum_{j\in B}\langle S_j^z\rangle\right) = S\big(1 - \frac{1}{2}\int_q n_q^{(0)}(\infty)\big), \quad (47)$$

where $n_q^{(0)}(\ell)$ represents the ground-state occupation of the Holstein-Primakoff bosons, with $n_q^{(0)}(0) = 0$ corresponding to the classical value. The total occupation number is again expressed by a series containing the quantum contributions,

$$n(\ell) = \sum_{k=0}^{\infty}\sum_q \frac{:n_q^{(k)}(\ell):}{S^k}, \quad (48)$$

where the leading bilinear term is given by

$$n_q^{(1)}(\ell) = F_q(\ell)\big(a_q^\dagger a_q + b_q^\dagger b_q\big) + G_q(\ell)\big(a_q^\dagger b_{-q}^\dagger + a_q b_{-q}\big), \quad (49)$$

with the initial values $F_q(0) = 1$ and $G_q(0) = 0$. In close analogy to the form of $H_2'(\ell)$ in (25), the second-order contribution to the number operator reads

$$\begin{aligned} n_q^{(2)}(\ell) = -\tfrac{2}{N}\textstyle\sum_{q_1,q_2} \Big(& H_{q,q_1,q_2}(\ell) a^\dagger_{q+q_1} a_{q_1} b^\dagger_{-q+q_2} b_{q_2} \\ & + X_{q,q_1,q_2}(\ell)\big(a^\dagger_{q+q_1} a^\dagger_{-q+q_2} a_{q_1} a_{q_2} + b^\dagger_{q+q_1} b^\dagger_{-q+q_2} b_{q_1} b_{q_2}\big) \\ & + \tfrac{1}{4} Z_{q,q_1,q_2}(\ell)\big(a^\dagger_{q+q_1+q_2} a_{q_1} a_{q_2} b_q + a^\dagger_{q_1} a^\dagger_{q_2} a_{q+q_1+q_2} b^\dagger_q \\ & + a_q b^\dagger_{q+q_1+q_2} b_{q_1} b_{q_2} + a^\dagger_q b^\dagger_{q_1} b^\dagger_{q_2} b_{q+q_1+q_2}\big) \\ & + Y_{q,q_1,q_2}(\ell)\big(a_{q_1} a_{q_2} b_q b_{-q-q_1-q_2} + a^\dagger_{q_1} a^\dagger_{q_2} b^\dagger_q b^\dagger_{-q-q_1-q_2}\big)\Big). \end{aligned} \tag{50}$$

In contrast to the $\mathcal{O}(1/S^2)$ contribution to the Hamiltonian, however, the two-particle terms of (50) are initially not present in $n(0)$, so that $H_{q,q_1,q_2}(0) = X_{q,q_1,q_2}(0) = Z_{q,q_1,q_2}(0) = Y_{q,q_1,q_2}(0) = 0$. Of course, these terms are due to $\eta_1(\ell)$ and are not generated in the linear spin-wave approximation.

The transformation of the total bosonic occupation number is described by the flow equation

$$\frac{\mathrm{d}}{\mathrm{d}\ell} n(\ell) = [\eta(\ell), n(\ell)], \tag{51}$$

which for the terms linear in $1/S$ encapsulates

$$\frac{\mathrm{d}}{\mathrm{d}\ell} n_q^{(1)}(\ell) = [\eta_0(\ell), n_q^{(1)}(\ell)]. \tag{52}$$

This leads to the differential equations

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}\ell} F_q(\ell) = -g_q(\ell)\, G_q(\ell) \qquad & \tfrac{\mathrm{d}}{\mathrm{d}\ell} G_q(\ell) = -g_q(\ell)\, F_q(\ell) \\ \tfrac{\mathrm{d}}{\mathrm{d}\ell} n_q^{(0)}(\ell) = -\tfrac{1}{S} & g_q(\ell)\, G_q(\ell). \end{aligned} \tag{53}$$

With the results (11), one obtains the solutions for the couplings

$$\begin{aligned} F_q(\ell) &= \frac{1}{\epsilon_q^2}\big(f_q(\ell) - \gamma_q\, g_q(\ell)\big) \\ G_q(\ell) &= \frac{1}{\epsilon_q^2}\big(g_q(\ell) - \gamma_q\, f_q(\ell)\big) \end{aligned} \tag{54}$$

and for the ground-state occupation number

$$n_q^{(0)}(\ell) = \frac{1}{S}\big(F_q(\ell) - 1\big). \tag{55}$$

Inserted in (47), this expression together with the square-lattice result

$$\int_q \frac{1}{\epsilon_q} \simeq 1.393 \tag{56}$$

yields the linear spin-wave value for the sublattice magnetization

$$m_\dagger = S\left(1 - \frac{1}{2S}\int_q (\epsilon_q^{-1} - 1)\right). \tag{57}$$

Thus, for $S = 1/2$ one has the well-known result $m_\dagger \simeq 0.303$.

Extending the transformation of $n(\ell)$ to order $\mathcal{O}(1/S^2)$, the flow of the interaction contributions to the total bosonic occupation number is described by

$$\frac{\mathrm{d}}{\mathrm{d}\ell} n_q^{(2)}(\ell) = [\eta_0(\ell), n_q^{(2)}(\ell)] + [\eta_1(\ell), n_q^{(1)}(\ell)], \tag{58}$$

which results in the system of coupled differential equations

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}\ell}\begin{pmatrix} Z_{-q,q,Q}(\ell) \\ Z_{-Q,Q,q}(\ell) \\ T_{0,q,Q}(\ell) \\ R_{q,Q}(\ell) \end{pmatrix} = - \begin{pmatrix} 0 & 0 & g_q(\ell) & g_Q(\ell) \\ 0 & 0 & g_Q(\ell) & g_q(\ell) \\ g_q(\ell) & g_Q(\ell) & 0 & 0 \\ g_Q(\ell) & g_q(\ell) & 0 & 0 \end{pmatrix} \times \\ \begin{pmatrix} Z_{-q,q,Q}(\ell) \\ Z_{-Q,Q,q}(\ell) \\ T_{0,q,Q}(\ell) \\ R_{q,Q}(\ell) \end{pmatrix} - \begin{pmatrix} C_{1;q,Q}(\ell) \\ C_{1;Q,q}(\ell) \\ C_{2;q,Q}(\ell) \\ 0 \end{pmatrix} \end{aligned} \tag{59}$$

where again only those couplings have been kept which enter into the calculation of the ground-state occupation. Furthermore, we have introduced $T_{0,q,Q}(\ell) = H_{0,-q,Q}(\ell) + 4X_{0,q,Q}(\ell)$ and $R_{q,Q}(\ell) = H_{Q-q,q,-q}(\ell) + 4Y_{-q,q,Q}(\ell)$. The inhomogeneous contributions in (59) read

$$\begin{aligned} C_{1;q,Q}(\ell) &= F_q(\ell)\zeta_{-q,q,Q}(\ell) \qquad \text{and} \\ C_{2;q,Q}(\ell) &= G_q(\ell)\zeta_{-q,q,Q}(\ell) + G_Q(\ell)\zeta_{-Q,Q,q}(\ell). \end{aligned} \tag{60}$$

Naturally, if only the linear spin-wave transformation is applied, in the flow equation (58) the second commutator does not contribute and the inhomogeneous part of (59) vanishes, so that all the coupling functions are identically zero. To determine the higher-order contribution to $n_q^{(0)}$, first one has to evaluate the $\mathcal{O}(1/S)$ corrections of the coupling functions in the bilinear contributions (49) to the total magnon occupation number. For the couplings $\tilde{F}_q(\ell) = F_q(\ell) + \frac{1}{S}F_q^{(1)}(\ell)$ and $\tilde{G}_q(\ell) = G_q(\ell) + \frac{1}{S}G_q^{(1)}(\ell)$ one finds

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}\ell}\begin{pmatrix} F_q^{(1)}(\ell) \\ G_q^{(1)}(\ell) \end{pmatrix} = \\ -\begin{pmatrix} 0 & g_q(\ell) \\ g_q(\ell) & 0 \end{pmatrix}\begin{pmatrix} F_q^{(1)}(\ell) \\ G_q^{(1)}(\ell) \end{pmatrix} + \begin{pmatrix} B_{1;q}(\ell) \\ B_{2;q}(\ell) \end{pmatrix}, \end{aligned} \tag{61}$$

with the initial conditions $F_q^{(1)}(0) = G_q^{(1)}(0) = 0$ and the inhomogenities

$$\begin{aligned} B_{1;q}(\ell) = -g_q^{(1)}(\ell)G_q(\ell) + \tfrac{1}{2}\textstyle\int_Q G_Q(\ell)\zeta_{-Q,Q,q}(\ell) \\ + \tfrac{1}{2}\textstyle\int_Q g_Q(\ell) Z_{-Q,Q,q}(\ell), \\ B_{2;q}(\ell) = -g_q^{(1)}(\ell)F_q(\ell) + \tfrac{1}{2}\textstyle\int_Q g_Q(\ell) R_{q,Q}(\ell). \end{aligned} \tag{62}$$

From the integral basis of (61),

$$\begin{pmatrix} f_q(\ell) \\ g_q(\ell) \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} g_q(\ell) \\ f_q(\ell) \end{pmatrix}, \tag{63}$$

and from the equations (59) one now extracts

$$F_q^{(1)}(\infty) = \frac{1}{\epsilon_q}\int_0^\infty \mathrm{d}\ell\,\big(f_q(\ell)\,B_{1;q}(\ell) - g_q(\ell)\,B_{2;q}(\ell)\big) = -\frac{1}{2}\int_Q T_{0,q,Q}(\infty), \quad (64)$$

where the latter equality is based on a useful integral relation derived from (32) for the second-order nondiagonal interactions,

$$\int_0^\infty \mathrm{d}\ell\,\left(g_q^{(1)}(\ell) + \frac{1}{2}\int_Q \zeta_{-q,q,Q}(\ell)\right) = 0. \quad (65)$$

The total contribution to $n_q^{(0)}$ is then given by

$$\frac{\mathrm{d}}{\mathrm{d}\ell}n_q^{(0)}(\ell) = -\frac{1}{S}g_q(\ell)\,G_q(\ell) - \frac{1}{S^2}\big(g_q^{(1)}(\ell)\,G_q(\ell) + g_q(\ell)\,G_q^{(1)}(\ell)\big). \quad (66)$$

With the result (64), and using (59) and (61), the ground-state occupation of the Holstein-Primakoff bosons is finally derived

$$\int_q n_q^{(0)}(\infty) = \frac{1}{S}\int_q \big(F_q(\infty) - 1\big) - \frac{1}{4S^2}\int_q\int_Q T_{0,q,Q}(\infty). \quad (67)$$

Thus, the second-order correction to the staggered magnetization is completely encapsulated in the coupling $T_{0,q,Q}$. While for the transformation linear in $1/S$ one has trivially $T_{0,q,Q}(\ell) \equiv 0$, from (59) follows

$$T_{0,q,Q}(\infty) = \frac{1}{\epsilon_q\epsilon_Q}\int_0^\infty \mathrm{d}\ell\,\big(\gamma_q\,f_Q(\ell)\zeta_{-q,q,Q}(\ell) + \gamma_Q\,f_q(\ell)\zeta_{-Q,Q,q}(\ell)\big). \quad (68)$$

This expression can be evaluated exactly, since from (24) and (26) one derives

$$\int_0^\infty \mathrm{d}\ell\,f_Q(\ell)\zeta_{-q,q,Q}(\ell) = \frac{\epsilon_Q}{\epsilon_q}z_{-q,q,Q}(\infty), \quad (69)$$

which finally yields for the transformed coupling

$$T_{0,q,Q}(\infty) = \frac{\gamma_q\gamma_Q}{\epsilon_q^3\epsilon_Q^3}\big(\epsilon_q^2 + \epsilon_Q^2\big)\big(\gamma_q\gamma_Q - \gamma_{Q-q}\big). \quad (70)$$

Therefore, one has $\int_q\int_Q T_{0,q,Q}(\infty) = 0$, so that the linear spin-wave result (57) remains unchanged at order $\mathcal{O}(1/S^2)$.

4 Summary and conclusions

In this work a new continuous unitary transformation has been applied to the Heisenberg antiferromagnet, utilizing the Holstein-Primakoff representation near the large-spin limit. This continuous approach to devising a unitary transformation allows to exceed conventional spin-wave theory and to diagonalize the spin-boson transformed magnon Hamiltonian also in higher orders of $1/S$. Removing those two-particle interactions of spin-wave excitations which do not conserve the number of magnons, one arrives at a Hamiltonian diagonal to order $\mathcal{O}(1/S^2)$. The flow equations for the second-order quantum corrections of the ground-state energy, of the spin-wave velocity, and of the sublattice magnetization have been derived and solved exactly. Although non-perturbative in nature, the continuous transformation yields results which are in agreement with extended spin-wave theory with its perturbative treatment of magnon interactions around the leading-order Hamiltonian. This agreement of both approaches in second order of $1/S$ appears to be a consequence of the systematic expansion in the inverse spin which leads to a complete classification of the contributions to physical quantities.

However, the method of continuous transformations has certain conceptual advantages compared to extended spin-wave theory. With the appropriate choice of the generator which has been used in this work, it is possible to avoid the occurrence of new types of interaction terms in the higher-order contributions to the Hamiltonian. These new types of interactions destroy the block-tridiagonal structure of the original bosonized Heisenberg Hamiltonian. They are not generated in the continuously transformed model, but inevitably appear, if the usual linear Bogoliubov transformation is performed. Thus, the flow equation approach ensures that block-tridiagonality of the Hamiltonian is preserved to *all* orders in the $1/S$-expansion. It therefore reduces the number of terms to be handled in higher orders. Additionally, it allows to obtain explicitly the operator expressions for observables beyond the leading order treated in spin-wave theory, and not only the corresponding expectation values. In principle, this is also true for the explicit result for the quantum ground-state, involving the higher corrections to the Néel state. This, however, would require the complete solutions of the coupling functions, *i.e.* the solutions for general momenta.

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