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Excited states of quantum many-body interacting systems: a variational coupled-cluster description

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Abstract

We extend the recently proposed variational coupled-cluster method to describe excitation states of quantum many-body interacting systems. We discuss, in general terms, both quasiparticle excitations and quasiparticle-density-wave excitations (collective modes). In application to quantum antiferromagnets, we reproduce the well-known spin-wave excitations, i.e. quasiparticle magnons of spin ± 1. In addition, we obtain new, spin-zero magnon-density-wave excitations, which have been missing in Anderson's spin-wave theory. Implications of these new collective modes are discussed.

1. Introduction

In previous papers ([1, 2], hereafter referred to as paper I and paper II), we proposed a general variational theory for ground states of quantum many-body interacting systems. Our analysis extends the well-established coupled-cluster method (CCM) [3–5] to a variational formalism in which bra and ket states are now Hermitian to one another, in contrast to the traditional CCM where they are not [6]. Ever since the CCM was first proposed, attempts have been made to extend it to a standard variational formalism, for example, in the 1970s in nuclear physics [7] and later in quantum chemistry [8]. It is perhaps fair to say that progress of this variational approach is slow, particularly when comparing with a plethora of applications made by the traditional CCM over the last 35 years [9], including its recent state-of-the-art application to spin-lattice models [10]. The main difficulties in this variational approach include ad hoc approximation truncations and slow convergent numerical results. In I and II, we provided a new systematic scheme to overcome these difficulties. In particular, we introduced two sets of important *bare* distribution functions and derived self-consistency equations for these functions; calculations of physical quantities can all be done in terms of these functions. This strategy is similar to that employed by another well-established variational theory, the method of correlated basis functions (CBFs) [11], where density distribution functions are key ingredients. We showed that the traditional CCM is a simple *linear* approximation to one set of bare distribution functions. We introduced diagrammatic techniques to calculate those distribution functions to high orders for achieving convergent results; resummations of infinite (reducible) diagrams can now be done by a practical, self-consistent technique. Furthermore,

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in our diagrammatic approach, a close relation with the CBF method was established and exploited; a possible combination of these two methods was also proposed. We demonstrated the efficacy of our variational method by applying it to quantum antiferromagnets. The ground-state properties of spin-wave theory (SWT) [12] was reproduced in a simple approximation. Approximation beyond SWT by including higher-order, infinite sets of reducible diagrams produced the convergent, improved numerical results for square and cubic lattices and, interestingly, it also cures the divergence by SWT in one-dimensional systems.

In this paper we extend our variational CCM to describe excitation states. A brief report of some preliminary results has been published [13]. We investigate two different types of excitation state using two approaches. In the first approach, we follow the traditional CCM [14, 15] to investigate quasiparticle excitations, but keeping our ket and bra excited states Hermitian to one another. We then investigate collective modes by adapting Feynman's excitation theory of the phonon-roton spectrum of helium liquid [16] to our method. In application to antiferromagnets, we find that quasiparticle excitations correspond to Anderson's spin-wave excitations which are often referred to as magnons with spin $+1$ or -1 [12]. We find that collective modes in these quantum antiferromagnets are longitudinal, spin-zero magnon-density-wave excitations which have been missing in Anderson's theory. In our approximation, the energy spectra of these spin-zero excitations show a large gap for a cubic lattice (three dimensions) and are gapless in a square lattice (two dimensions). These spectra are similar to those of charge-density-wave excitations (plasmons) in quantum plasmas such as electron gases at low temperature [17]. More discussion on these collective modes will be given in section 5 of this paper.

2. Ground states investigated by the variational coupled-cluster method

We briefly summarize in this section our variational approach for describing the ground state of a many-body interacting system. Details can be found in I and II. We take a spin-s antiferromagnetic Heisenberg model on a bipartite lattice as our model system. The Hamiltonian is given by

$$H = \tfrac{1}{2}\sum_{l,n} \mathbf{s}_l \cdot \mathbf{s}_{l+n}, \tag{1}$$

where index l runs over all lattice sites, and n runs over all z nearest-neighbour sites. We use the Coester representation for both ket and bra ground states, and write

$$|\Psi_{\rm g}\rangle = {\rm e}^{S}|\Phi\rangle, \qquad S = \sum_I F_I C_I^\dagger; \qquad \langle\tilde{\Psi}_{\rm g}| = \langle\Phi|{\rm e}^{\tilde{S}}, \qquad \tilde{S} = \sum_I \tilde{F}_I C_I, \tag{2}$$

where the model state $|\Phi\rangle$ is given by the classical Néel state, and $C_I^\dagger$ and C_I with nominal index I are the so-called configurational creation and destruction operators and are given by, for the spin lattice of equation (1),

$$\sum_I F_I C_I^\dagger = \sum_{k=1}^{N/2} \sum_{i_1\cdots,j_1\cdots} f_{i_1\cdots,j_1\cdots} \frac{s_{i_1}^- \cdots s_{i_k}^- s_{j_1}^+ \cdots s_{j_k}^+}{(2s)^k}, \tag{3}$$

for the ket state. The bra state operators are given by the corresponding Hermitian conjugate of equation (3), using the notation $\tilde{F}_I = \tilde{f}_{i_1\cdots,j_1\cdots}$ for the bra-state coefficients. As before, we have used index i exclusively for the spin-up sublattice of the Néel state and index j for the spin-down sublattice. The coefficients $\{F_I, \tilde{F}_I\}$ are then determined by the standard variational equations as

$$\frac{\delta\langle H\rangle}{\delta\tilde{F}_I} = \frac{\delta\langle H\rangle}{\delta F_I} = 0, \qquad \langle H\rangle \equiv \frac{\langle\tilde{\Psi}_{\rm g}|H|\Psi_{\rm g}\rangle}{\langle\tilde{\Psi}_{\rm g}|\Psi_{\rm g}\rangle}. \tag{4}$$

The important bare distribution functions, $g_I \equiv \langle C_I \rangle$ and $\tilde{g}_I \equiv \langle C_I^\dagger \rangle$, can be expressed in self-consistency equations as

$$g_I = G(\tilde{g}_J, F_J), \qquad \tilde{g}_I = G(g_J, \tilde{F}_J), \tag{5}$$

where G is a function containing up to linear terms in $\tilde{g}_J$ (or g_J) and finite-order terms in F_J (or $\tilde{F}_J$). The Hamiltonian expectation $\langle H \rangle$ of equation (4) can be expressed as, in general, a function containing up to linear terms in g_I and $\tilde{g}_I$ and a finite-order polynomial in F_I (or in $\tilde{F}_I$),

$$\langle H \rangle = \mathcal{H}(g_I, \tilde{g}_I, F_I) = \mathcal{H}(\tilde{g}_I, g_I, \tilde{F}_I). \tag{6}$$

In I and II, as a demonstration, we considered a simple truncation approximation in which the correlation operators S and $\tilde{S}$ of equations (2) and (3) retain only the two-spin-flip operators as

$$S \approx \sum_{i,j} f_{ij} C_{ij}^\dagger = \sum_{i,j} f_{ij} \frac{s_i^- s_j^+}{2s}, \qquad \tilde{S} \approx \sum_{i,j} \tilde{f}_{ij} C_{ij} = \sum_{i,j} \tilde{f}_{ij} \frac{s_i^+ s_j^-}{2s}. \tag{7}$$

The spontaneous magnetization (order parameter) in this two-spin-flip approximation is given by the one-body density function ρ_{ij} as

$$\langle s_i^z \rangle = s - \rho, \qquad \rho = \sum_j \rho_{ij} = \sum_j f_{ij} \tilde{g}_{ij}, \tag{8}$$

where we have taken the advantage of translational invariance of the lattice system. For the j-sublattice, $\langle s_j^z \rangle = \rho - s$. Within this approximation the SWT result for the correlation coefficient can be derived from equation (4) as

$$f_q = \tilde{f}_q = \frac{1}{\gamma_q} \left[\sqrt{1 - (\gamma_q)^2} - 1 \right], \qquad \gamma_q = \frac{1}{z} \sum_n \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}_n}, \tag{9}$$

where f_q is the sublattice Fourier transformation of f_{ij} with $\mathbf{q}$ restricted to the magnetic zone, z is the coordination number of the lattice, and n is the nearest-neighbour index. The Fourier component of the one-body bare distribution function is derived as

$$\tilde{g}_q = \frac{\tilde{f}_q}{1 - \tilde{f}_q f_q}. \tag{10}$$

Finally, the two-body distribution functions is approximated by, in the same order,

$$\tilde{g}_{ij,i'j'} \approx \tilde{g}_{ij} \tilde{g}_{i'j'} + \tilde{g}_{ij'} \tilde{g}_{i'j}. \tag{11}$$

Approximation beyond these SWT formulae produced improved results, and these are given in detail in section 2. For simplicity of our first attempt to discuss excitation states, we shall restrict ourselves to these approximations of equations (7)–(11) in the following.

3. Quasiparticle excitations

As mentioned in section 1, inspired by the close relation between our approach and the CBF method, we can investigate quasiparticle-density-wave excitations by adapting Feynman's excitation theory, as well as usual quasiparticle excitations by a similar approach to that in the traditional CCM. One well-known example of a quantum system exhibiting two similar kinds of excitation is quantum electron gases [17], where quasiparticle excitations are electron or hole excitations and collective modes are plasmon excitations representing longitudinal, charge-neutral density fluctuations of those quasielectrons and holes. In this section we focus on

quasiparticle excitations, and we leave the discussion of collective modes to the next section. We will first discuss these excitations in general terms and then apply them to the spin-lattice model of equation (1) as a demonstration.

Following Emrich in the traditional CCM [14, 15], we express the excitation ket-state $|\Psi_e\rangle$ by a linear operator X constructed from creation operators acting onto the ground state $|\Psi_g\rangle$ as

$$|\Psi_e\rangle = X|\Psi_g\rangle = Xe^S|\Phi\rangle, \qquad X = \sum_L x_L C_L^\dagger, \tag{12}$$

and, unlike the traditional CCM, our bra excitation state is the corresponding Hermitian conjugate, involving only destruction operators such as

$$\langle\tilde{\Psi}_e| = \langle\tilde{\Psi}_g|\tilde{X} = \langle\Phi|e^{\tilde{S}}\tilde{X}, \qquad \tilde{X} = \sum_L \tilde{x}_L C_L. \tag{13}$$

In equations (12) and (13), the ground-state operators S and $\tilde{S}$ are as given by equation (2); x_L and its Hermitian conjugate $\tilde{x}_L$ are excitation coefficients. For quasiparticle creation and destruction operators $C_L^\dagger$ and C_L of equations (12) and (13), we use the index L to mark the following important difference from the ground-state counterparts $C_I^\dagger$ and C_I of equations (2). Due to symmetry considerations, some configuration operators are not included in the correlation operators S and $\tilde{S}$ of the ground states but they are important in the excited states. In our spin-lattice example of equation (1), the ground-state operators of equation (3) always contain an even number of spin-flip operators (each spin-flip-up operator for the i-sublattice always pairs up with one spin-flip-down operator for the j-sublattice) to ensure the total z-component of angular momentum $s^z_{\text{total}} = 0$. For the excitation operators, however, the constraints are different. The single spin-flip operator s_i^- for the i-sublattice (or s_j^+ for the j-sublattice) will be the important first term in equation (12) to be discussed in the following; the corresponding excitation state $|\Psi_e\rangle$ is in the $s^z_{\text{total}} = -1$ sector (or $+1$ if s_j^+ is used). Therefore, these excitations are referred to as quasiparticles carrying spin ± 1. For our spin-lattice models, we expect that these quasiparticles are the well-known magnons of spin-wave excitations [12].

If the ground state $|\Psi_g\rangle$ is exact with energy E_0, the energy difference between the excitation state of equation (12) and the ground state can be written as

$$\epsilon = \frac{\langle\tilde{\Psi}_g|\tilde{X}HX|\Psi_g\rangle}{\langle\tilde{\Psi}_e|\Psi_e\rangle} - E_0 = \frac{\langle\tilde{\Psi}_g|\tilde{X}[H,X]|\Psi_g\rangle}{\langle\tilde{\Psi}_e|\Psi_e\rangle}, \tag{14}$$

which involves a commutation. In general, $|\Psi_g\rangle$ is not exact but is calculated by approximations. For our variational ground states of equations (2), equation (14) can be shown to remain valid after replacing the exact energy E_0 by the variational energy E_g, which obeys the following optimal conditions:

$$E_g = \langle H\rangle = \frac{\langle HC_I^\dagger\rangle}{\tilde{g}_I} = \frac{\langle C_I H\rangle}{g_I}, \tag{15}$$

derived from equation (4).

To prove equation (14) after replacing the exact E_0 by the variational E_g, we first express the normalization of excited states of equations (12) and (13) as an expectation value in the ground states of equation (2) as

$$I_e = \langle\tilde{\Psi}_e|\Psi_e\rangle = I_g\langle\tilde{X}X\rangle = I_g\sum_{L,L'}\tilde{x}_{L'}x_L\langle C_{L'}C_L^\dagger\rangle, \tag{16}$$

where $I_g = \langle\tilde{\Psi}_g|\Psi_g\rangle$. We now consider a general linear operator $O = O(C_I^\dagger, C_I)$ (a polynomial of $C_I^\dagger$ and/or C_I), and write

$$O|\Psi_g\rangle = Oe^S|\Phi\rangle = e^S\bar{O}|\Phi\rangle, \tag{17}$$

where the similarity-transformed operator $\bar{O} \equiv e^{-S}Oe^S = O(\bar{C}_I^\dagger, \bar{C}_I)$, $\bar{C}_I^\dagger = C_I^\dagger$ and

$$\bar{C}_I = e^{-S}Oe^S = C_I + [C_I, S] + \frac{1}{2!}[[C_I, S], S] + \cdots, \tag{18}$$

which always terminates for a finite-order operator C_I. In each term of such $\bar{O}$ expansion series, by shifting all destruction operators C_I to the right, and using the property $C_I|\Phi\rangle = 0$, we conclude that only terms containing constants or only creation operators survive. We therefore have a general expression

$$O(C_I^\dagger, C_I)|\Psi_g\rangle = \mathcal{O}(C_J^\dagger, F_J)|\Psi_g\rangle, \tag{19}$$

where $\mathcal{O}(C_J^\dagger, F_J)$ is a function containing up to linear terms in $C_J^\dagger$ and finite-order terms in F_J. We shall refer to equation (19) as the *linear theorem* in our variational approach as it is useful for general analysis. In fact, the important equations (5) and (6) in section 2 are two specific application of this linear theorem. Therefore we can write, for a special case of equation (19),

$$C_{L'}C_L^\dagger|\Psi_g\rangle = Y_{L'L}(C_I^\dagger, F_I)|\Psi_g\rangle, \tag{20}$$

where $Y_{L',L}(C_I^\dagger, F_I)$ is a function containing up to linear terms in $C_I^\dagger$ and finite-order terms in F_I. Using equation (20), equation (16) can be written as

$$I_e = I_g \sum_{L,L'} \tilde{x}_{L'} Y_{L'L}(\tilde{g}_I, F_I) x_L. \tag{21}$$

Combining with the optimal condition of equation (15), it is easy to show that

$$\frac{1}{I_e}\langle\tilde{\Psi}_g|H\tilde{X}X|\Psi_g\rangle = E_g. \tag{22}$$

Hence, we obtain a similar equation to equation (14) for the energy difference,

$$\epsilon = \frac{1}{I_e}\langle\tilde{\Psi}_g|\tilde{X}HX|\Psi_g\rangle - E_g = \frac{I_g}{I_e}\langle\tilde{X}[H, X]\rangle. \tag{23}$$

We now apply the above formulae to discuss quasiparticle excitations of spin systems of equation (1). For simplicity, we consider an approximation in which we retain only single-spin-flip operators in X and $\tilde{X}$ of equations (12) and (13),

$$X \approx \sum_i x_i s_i^-, \qquad \tilde{X} \approx \sum_i \tilde{x}_i s_i^+, \tag{24}$$

with coefficients chosen as

$$x_i = x_i(q) = \sqrt{\frac{2}{N}}e^{i\mathbf{q}\cdot\mathbf{r}_i}, \qquad \tilde{x}_i = \tilde{x}_i(q) = \sqrt{\frac{2}{N}}e^{-i\mathbf{q}\cdot\mathbf{r}_i}, \tag{25}$$

to define a linear momentum $\mathbf{q}$. Such an excited state, $|\Psi_e\rangle = X|\Psi_g\rangle$, is therefore in the sector of $s^z_{\text{total}} = -1$ and has a linear momentum $\mathbf{q}$. The normalization integral of equation (24) is easily calculated as

$$\frac{I_e}{I_g} = \langle\tilde{X}X\rangle = 2\sum_i \tilde{x}_i x_i\langle s_i^z\rangle + 2s\sum_{i,i',j}\tilde{x}_{i'}x_i f_{i'j}\tilde{g}_{ij} - \sum_{i,i',j,j'}\tilde{x}_{i'}x_i f_{i'j}f_{i'j'}\tilde{g}_{ij,i'j'}, \tag{26}$$

and using equations (8) and (11) we derive

$$\frac{I_e}{I_g} = 2(s-\rho)(1+\rho_q), \tag{27}$$

where $\rho_q \equiv f_q \tilde{g}_q$. Using approximations of equations (9)–(11), we obtain, for the isotropic point $A = 1$,

$$I_e \propto \frac{1}{q}, \qquad q \to 0, \tag{28}$$

in all dimensions.

Calculation of the numerator in equation (23) is slightly more complicated. We quote the result here, to the order of $(2s)^2$, as

$$\langle \tilde{X}[H, X] \rangle \approx 2s^2 z(1 + \rho_q + \gamma_q g_q). \tag{29}$$

The energy spectrum of equation (23) is therefore given, to the order of $(2s)$, by

$$\epsilon_q = \frac{I_g}{I_e} \langle \tilde{X}[H, X] \rangle \approx sz \frac{1 + \rho_q + \gamma_q g_q}{1 + \rho_q} \ . \tag{30}$$

Using equations (9)–(11), we obtain the energy spectrum as

$$\epsilon_q = sz\sqrt{1 - (\gamma_q)^2}, \tag{31}$$

which agrees exactly with the spin-wave theory [12]. The spectrum of equation (31) is gapless in any dimension because $\epsilon_q \propto q$ as $q \to 0$. Similar calculations using spin-flip operators $s_j^\dagger$ and s_j^- for the j-sublattice in equation (24) will produce the same spectrum as equation (31), except that the corresponding excitation state has spin $s^z_{\text{total}} = +1$. These spin-wave excitations are often referred to as magnons.

4. Quasiparticle-density-wave excitations

In the previous section, by using quasiparticle operators (i.e., spin-flip operators $s^\pm$), we have reproduced the magnon excitations with spin equal to $+1$ or -1. These quasiparticles in general interact with one another, thus producing quasiparticle density fluctuations. Excitation states due to these fluctuations are usually referred to as collective modes and are best discussed in terms of the corresponding density operator. For our spin models, density operators are clearly given by operators s^z as they measure the number of spin-flips with respect to the Néel model state, and the expectation value is the order parameter as given by equation (8). For general purposes, we use the notation C_L^0 for the quasiparticle density operators as opposed to the quasiparticle operators $C_L^\dagger$ and C_L used earlier. At this point, it is interesting to note that a general theory of elementary excitations (collective modes) for Fermi systems has been formulated by extending the random-phase approximation to strongly interacting Fermi systems within the framework of the CBF method [18], where a single particle–hole operator is employed, in contrast to the explicit density operator employed here. The efficiency and advantage of using explicit density operators to investigate collective modes of a quantum interacting system was demonstrated by Feynman for the phonon-roton spectrum of quantum fluid helium-4 [16]; he extended Bijl's theory [19] in a much simpler and clearer fashion. Feynman's excitation formula, involving a double commutation of the so-called f-sum rule, was also derived by Pines for the plasmon spectrum of three-dimensional (3D) metals [17]. The 2D plasmon spectrum first derived by Stern [20] can also be derived by using a density operator, as shown in [21]. It is interesting to note that both the CBF method for the ground state and Feynman's theory for excitation states have been successfully applied to fractional quantum Hall effects [22, 23]. Feynman's excitation theory is now often referred to as a single-mode approximation [23].

Following Feynman, we write the quasiparticle density-wave excitation state as

$$|\Psi_{\rm e}^0\rangle = X^0|\Psi_{\rm g}\rangle, \qquad X^0 = \sum_L x_L C_L^0, \tag{32}$$

where, as defined earlier, C_L^0 are the quasiparticle density operators. The bra state is given by the Hermitian conjugate of equation (32), $\langle\tilde{\Psi}_{\rm e}| = \langle\tilde{\Psi}_{\rm g}|\tilde{X}^0$. Using the same argument as before for the quasiparticle excitation of equation (23), we obtain a similar equation for the energy difference for our collective modes as

$$\epsilon^0 = \frac{I_{\rm g}}{I_{\rm e}^0}\langle\tilde{X}^0[H, X^0]\rangle, \tag{33}$$

where $I_{\rm e}^0 = \langle\tilde{\Psi}_{\rm e}^0|\Psi_{\rm e}^0\rangle$. We notice that, by definition, the density operator C_L^0 is a Hermitian operator, $(C_L^0)^\dagger = C_L^0$. By considering a similar excited state $\tilde{X}^0|\Psi_{\rm g}\rangle$, it is straightforward to derive the following double commutation formula,

$$\epsilon^0 = \frac{I_{\rm g}}{2I_{\rm e}^0}\langle[\tilde{X}^0, [H, X^0]]\rangle. \tag{34}$$

The double commutation in the above equation is the key to the efficiency of Feynman's excitation theory. It is often referred to as the f-sum rule in other quantum systems such as electron gases [17].

Before we apply equation (34) for collective modes in spin lattices, it is useful to discuss sum rules in our spin models, as density operators normally obey sum rule equations [11, 24]. The order parameter of equation (8) can also be calculated through two-body functions as

$$(\langle s_i^z\rangle)^2 = \frac{\langle\tilde{\Psi}_{\rm g}|(s_a^z)^2|\Psi_{\rm g}\rangle}{\langle\tilde{\Psi}_{\rm g}|\Psi_{\rm g}\rangle}, \tag{35}$$

where $s_a^z = \sum_l (-1)^l s_l^z/N$ is the staggered spin operator. We introduce the total magnon-density operator $\hat{n}_i$ as

$$2\hat{n}_i = 2s - s_i^z + \frac{1}{z}\sum_{n=1}^{z} s_{i+n}^z, \tag{36}$$

where, as before, summation over n is over all z nearest neighbours. Hence, the sum rule for the one-body function is simply $\frac{2}{N}\sum_i\langle\hat{n}_i\rangle = \rho$. The two-body equation (35) can now be written, using the translational invariant property $\rho_i = \rho$, as

$$\frac{2}{N}\sum_{i'=1}^{N/2}\langle\hat{n}_i\hat{n}_{i'}\rangle = \rho\rho_i = \rho^2, \tag{37}$$

which is the familiar two-body sum rule equation [11, 24]. In the approximations of equations (7)–(11), we find that this sum rule is obeyed in both cubic and square lattices in the limit $N \to \infty$. In particular, we find that $(\frac{2}{N}\sum_{i'}\langle\hat{n}_i\hat{n}_{i'}\rangle - \rho^2) \propto 1/N$ in a cubic lattice and $\propto (\ln N)/N$ in a square lattice. These asymptotic properties are important in the corresponding excitation states as will be discussed later. However, equation (37) is violated in the one-dimensional model, showing the deficiency of the two-spin-flip approximation of equation (7) for the one-dimensional model. We therefore leave further investigation elsewhere and focus on the cubic and square lattices in the following, using approximations of equations (7)–(11).

We therefore write our magnon-density-wave excitation state, using the total magnon density operator $\hat{n}_i$ of equation (36), as

$$|\Psi_{\rm e}^0\rangle = X_q^0|\Psi_{\rm g}\rangle, \qquad X_q^0 = \sum_i x_i(q)\hat{n}_i, \quad q > 0 \tag{38}$$

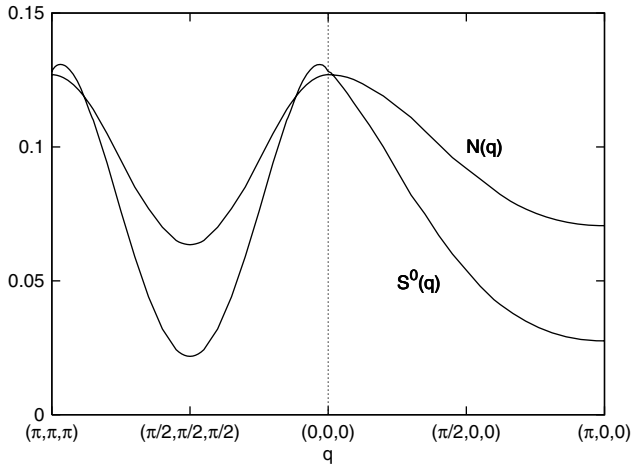

Figure 1. $N(q)$ and $S^0(q)$ of equations (40) and (41) for a cubic lattice. Shown are the values for two regions $\mathbf{q} = (0, 0, 0)$ to $(\pi, 0, 0)$ and to (π, π, π).

and its Hermitian counterparts for the bra state, $\langle\tilde{\Psi}^0_e| = \langle\tilde{\Psi}_g|\tilde{X}^0_q$. The coefficient $x_i(q) = \sqrt{\frac{2}{N}}e^{i\mathbf{q}\cdot\mathbf{r}_i}$, etc. The condition $q > 0$ in equation (38) ensures the orthogonality between this excited state and the ground state. The excitation energy difference is given by equation (34) as

$$\epsilon^0_q = \frac{N(q)}{S^0(q)}, \qquad q > 0 \tag{39}$$

where $N(q) \equiv \langle[\tilde{X}^0_q, [H, X^0_q]]\rangle/2$, and $S^0(q) \equiv \langle\tilde{X}^0_q X^0_q\rangle$ is the structure function. Both $N(q)$ and $S^0(q)$ can be straightforwardly calculated, using approximations of equations (7)–(11), as

$$N(q) = -\frac{sz}{2}\sum_{q'}(\gamma_{q'} + \gamma_q\gamma_{q-q'})\tilde{g}_{q'}, \tag{40}$$

and

$$S^0(q) = \tfrac{1}{4}(1+\gamma_q^2)\rho + \tfrac{1}{4}\sum_{q'}[(1+\gamma_q^2)\rho_{q'}\rho_{q-q'} + 2\gamma_q\tilde{g}_{q'}\tilde{g}_{q-q'}], \tag{41}$$

where $q > 0$. The energy spectrum ϵ^0_q of equation (39) can then be calculated numerically. We notice that equation (41) is closely related to the sum rule equation (37) which corresponds to the $q = 0$ case (with an additional term in equation (41) when $q \to 0$). Using the approximation of equations (9) and (10), it is not difficult to show that $N(q)$ of equation (40) has a nonzero, finite value for all values of q. Any special feature such as a gapless mode in the spectrum ϵ^0_q therefore comes from the structure function of equation (41), and hence is determined by the asymptotic behaviour of the sum rule equation (37) mentioned earlier.

For a cubic lattice, we show a plot of $N(q)$ and $S^0(q)$ for two regions of $\mathbf{q}$ in figure 1. In figure 2 we have plotted the corresponding spectra of equation (39), together with that of the magnon excitations of equation (31) for comparison. As can be seen from figure 2, the spectrum ϵ^0_q has a nonzero gap everywhere. The minimum gap is about $\epsilon^0_q \approx 0.96sz$ at $\mathbf{q} = (q_0, q_0, q_0)$ with $q_0 \approx 0.04\pi$. (This is slightly different to that reported in [13], where detailed calculations in this region had not been done.) This gap is about the same as the largest magnon energy, $\epsilon_q = sz$ at $\mathbf{q} = (\pi/2, \pi/2, \pi/2)$ from equation (31). At $\mathbf{q} = (\pi/2, \pi/2, \pi/2)$, we have the

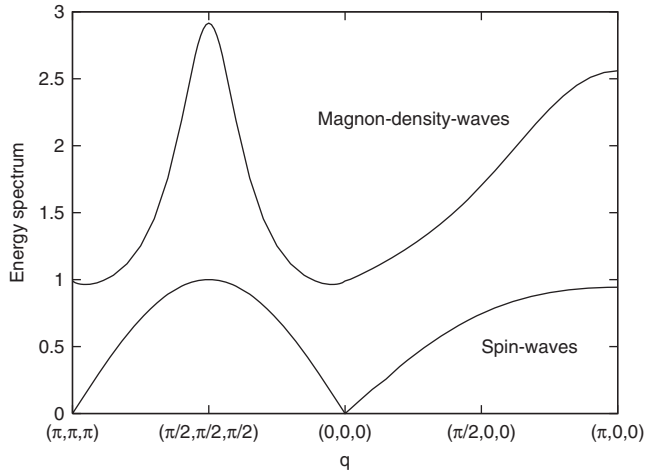

Figure 2. Excitation energy spectra in units of sz in a cubic lattice. The higher branch is for the plasmon-like excitation of equation (39) and the lower one is for the magnon excitation of equation (31).

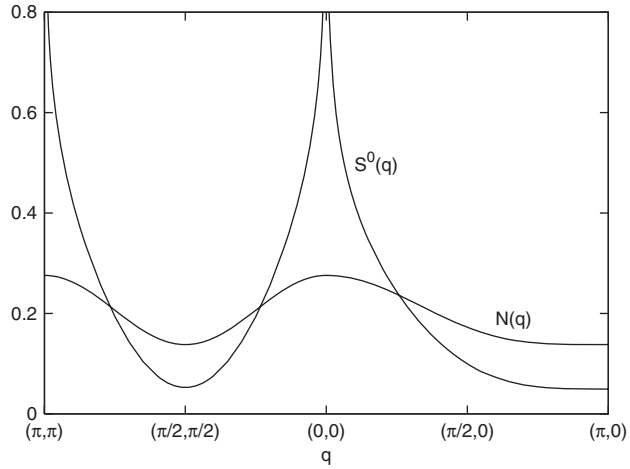

Figure 3. Similar to figure 1 but for a square lattice. The divergence of $S^0(q)$ at $\mathbf{q} = (0, 0)$ and (π, π) is given in the text.

largest energy, $\epsilon_q^0 \approx 2.92sz$. This is nearly three magnons' energy at this $\mathbf{q}$. At $\mathbf{q} = (\pi, 0, 0)$, we obtain $\epsilon_q^0 \approx 2.56sz$.

For a square lattice, the structure function $S^0(q)$ of equation (41) has a logarithmic behaviour $\ln q$ as $q \to 0$. This is not surprising as discussed earlier in the sum rule equation (37), where there occurs asymptotic behaviour of $(\ln N)/N$ as $N \to \infty$. For small values of q, $N(q)$ approaches a finite value: $N(q) \approx 0.275sz$ as $q \to 0$. The corresponding energy spectrum of equation (39) is therefore gapless as $q \to 0$. As with the cubic lattice, we show a plot of $N(q)$ and $S^0(q)$ of a square lattice in figure 3, and the corresponding spectra of equations (39) and (31) in figure 4. As can be seen from figure 4, the magnon-density-wave energy is always larger than the corresponding magnon energy. At small values of q ($q < 0.05\pi$), we find a good approximation by numerical calculations for the structure

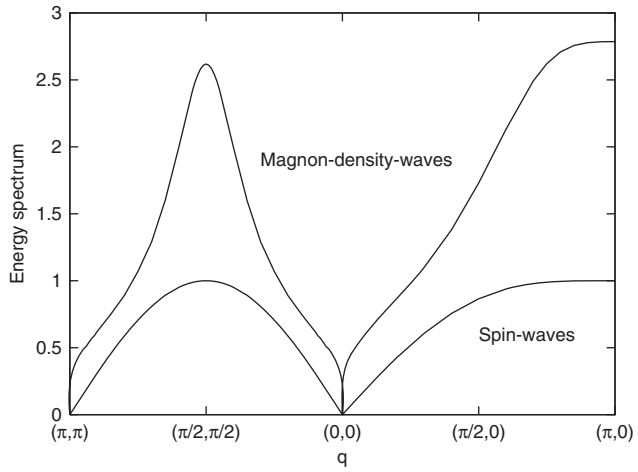

Figure 4. Similar to figure 2 but for a square lattice. The behaviour near $\mathbf{q} = (0, 0)$ and (π, π) for magnon density waves is given by equation (42).

function, $S^0(q) \approx 0.31 - 0.16 \ln q$ with $q_x = q_y$. Similar behaviour holds near $\mathbf{q} = (\pi, \pi)$. The energy spectrum of equation (39) in these region can therefore be approximated by

$$\epsilon_q^0 \approx \frac{0.275sz}{0.31 - 0.16 \ln q}, \qquad q \to 0 \tag{42}$$

for a square lattice with $q_x = q_y$. We notice the slight difference for the coefficients of equation (42) to that of equation (19) of [13] where we focused in the region with $q_y = 0$. Although our calculations clearly show that this spectrum of a square lattice is gapless at $q = 0$ and $\mathbf{q} = (\pi, \pi)$, it is nevertheless very 'hard' when compared with the magnon's soft mode $\epsilon_q \propto q$ at small q. For example, if we consider a system with lattice size $N = 10^{10}$, the smallest value for q is about $q \approx 10^{-10}\pi$, and we have energy $\epsilon_q^0 \approx 0.07sz$. Comparing this value with the corresponding magnon energy $\epsilon_q \approx 10^{-10}sz$, we conclude that the energy spectrum of equation (39) is 'nearly gapped' in a square lattice. We also notice that the largest energy in a square lattice $\epsilon_q^0 \approx 2.79sz$ at $\mathbf{q} = (\pi,\ 0)$, not at $\mathbf{q} = (\pi/2,\ \pi/2)$ as is the case in a cubic lattice. At $\mathbf{q} = (\pi/2,\ \pi/2)$, we obtain $\epsilon_q^0 \approx 2.62sz$ for the square lattice. We will discuss physical implications of these excitations in the next section.

5. Discussion

We have obtained two main results in this article. Firstly, we have succeeded in extending our recently proposed variational approach to describe, in general terms, excitation states of a quantum many-body system. Secondly, we have applied our technique to quantum antiferromagnets, thus reproducing the well-known magnon excitations and, in addition, we have obtained new, spin-zero longitudinal collective modes which have been missing in the spin-wave theory of Anderson [12]. In the following, we shall discuss further physical implications of these new excitations, and we conclude this article with a summary.

It is interesting to notice similar behaviours between collective modes of quantum antiferromagnets and plasmon excitations of electron gases as both spectra show a large energy gap in three dimensions and are gapless in two dimensions. In fact, further similarity between these two quantum systems can be made. It is generally accepted that, for many

purposes, a quantum antiferromagnet at zero temperature can be considered as a gas of weakly interacting, equal numbers of spin ± 1 magnons (the transverse spin-flip wave excitations with respect to the classical Néel state); also present in the system are the spin-zero, longitudinal fluctuations consisting of the multi-magnon continuum [25–28]. This is similar to quantum electron gases, which can also be considered as a gas of weakly interacting, equal numbers of quasielectrons and holes (the transverse excitations near the Fermi surfaces) and the charge-neutral, longitudinal fluctuations producing the quasielectron–hole continuum [17]. Plasmon excitations of electron gases have been well observed as sharp peaks over the electron–hole continuum [17]. However, plasmon-like collective modes of quantum antiferromagnets as discussed in this article have so far eluded observation, to our best knowledge. We can only draw some support by considering a finite-size Heisenberg model of equation (1). As the ground state of a finite antiferromagnetic Heisenberg lattice is spin-singlet, we expects that low-lying excitations are triplets with the z-component of spin equal to $0, \pm 1$. As the lattice size increases from finite to infinite, for cubic and square lattices, spontaneous symmetry breaking occurs, and the ground state is no longer a spin-singlet but has a long-ranged antiferromagnetic order. We expect that the triplet excitation splits into different branches. The magnon spectrum of equation (31) with spin ± 1 and the spectrum of equation (39) for spin-zero magnon-density waves are our approximation for these different branches of excitations. We also notice that recently modified spin-wave theories were applied to finite systems with results in reasonable agreements with exact finite-size calculations [29–31]. As pointed out in [30], however, a major deficiency in this theory is the missing spin-zero excitations as the low-lying excitations for a finite-lattice Heisenberg model are always triplets, as mentioned earlier. We believe that our magnon-density-wave excitation as discussed here corresponds to the missing branch; the energy gap in the cubic lattice and the nearly gapped spectrum in the square lattice of equation (39) reflect the nature of long-ranged Néel order in the ground states of infinite systems. Improvement for spectra of equation (39) can be done in similar fashion as was done for the ground state detailed in paper II, particularly for the square lattice. We will have more motivation to do so if we have experimental evidence of these collective modes.

In any case, this article concludes our general presentation of a new formalism of the variational coupled-cluster method for a quantum many-body system. Beginning in paper I, we introduced and discussed bare distribution functions, the key ingredient of this formalism. In paper II, we developed diagrammatic techniques for practical, high-order calculations of these functions. Application to quantum antiferromagnets has demonstrated the efficacy of this technique. The present article extends this formalism to excitation states. As discussed earlier, application to quantum antiferromagnets has produced new modes which have been missing in all spin-wave theories and are yet to be confirmed by experiment. Our next main focus is to combine our present variational approach with the CBF method, as first discussed in paper II. Hence we write our new ground state as

$$|\Psi_u\rangle = \mathrm{e}^{S^0}|\Psi_\mathrm{g}\rangle = \mathrm{e}^{S^0}\mathrm{e}^{S}|\Phi\rangle, \tag{43}$$

where S is as given by equation (2) and S^0 is the generalized Jastrow correlation operator involving quasiparticle density operators as

$$S^0 = \sum_{ij} f_{ij}^0 s_i^z s_j^z, \tag{44}$$

with f_{ij}^0 as new variational functions. Using the 2-spin-flip approximation of equation (7) for S, the new wavefunction of equation (43) can be understood as including both quasiparticle fluctuations described by the operator $\exp(S)$ and quasiparticle-density fluctuations described by the operator $\exp(S^0)$. The results of collective modes obtained in section 4 certainly make this new wavefunction of equation (43) much more appealing and imperative.

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References

[1] Xian Y 2001 *150 Years of Quantum Many-body Theories* ed R F Bishop, K A Gernoth and N R Walet (Singapore: World Scientific) p 107
Xian Y 2002 *Phys. Rev.* B **66** 184427
[2] Xian Y 2005 *Phys. Rev.* B **72** 224438
[3] Hubbard J 1957 *Proc. R. Soc.* A **240** 539
Hugenholtz A 1957 *Physica* **23** 481
Hugenholtz A 1957 *Physica* **23** 533
Coester F 1958 *Nucl. Phys.* **7** 421
[4] Coester F and Kümmel H 1960 *Nucl. Phys.* **17** 477
[5] Čížek J 1966 *J. Chem. Phys.* **45** 4256
Čížek J 1969 *Adv. Chem. Phys.* **14** 35
[6] Arponen J 1983 *Ann. Phys.* **151** 311
[7] da Providencia J and Shakin C M 1971 *Phys. Rev.* C **4** 1560
da Providencia J and Shakin C M 1971 *Phys. Rev.* C **5** 53
[8] Kutzelnig W 1998 *Mol. Phys.* **94** 65
Van Voorhis T and Head-Gordon M 2000 *J. Chem. Phys.* **113** 8873
[9] Bishop R F 1991 *Theor. Chim. Acta* **80** 95
Bartlett R J 1991 *Theor. Chim. Acta* **80** 71
[10] Zeng C, Farnell D J J and Bishop R F 1998 *J. Stat. Phys.* **90** 327
Farnell D J J and Bishop R F 2004 *Quantum Magnetism* (*Lecture Notes in Physics* vol 645) ed U Schollwöck, J Richter, D J J Farnell and R F Bishop (Berlin: Springer) p 307
[11] Clark J W and Feenberg E 1959 *Phys. Rev.* **113** 388
Feenberg E 1969 *Theory of Quantum Fluids* (New York: Academic)
[12] Anderson P W 1952 *Phys. Rev.* **86** 694
Oguchi T 1960 *Phys. Rev.* **117** 117
[13] Xian Y 2006 *Phys. Rev.* B **74** 212401
[14] Emrich K 1981 *Nucl. Phys.* A **351** 379
Emrich K 1981 *Nucl. Phys.* A **351** 397
[15] Bishop B F, Parkinson J B and Xian Y 1991 *Phys. Rev.* B **43** 13782
Bishop B F, Parkinson J B and Xian Y 1991 *Phys. Rev.* B **44** 9425
[16] Feynman R P 1954 *Phys. Rev.* **94** 262
Feynman R P and Cohen M 1956 *Phys. Rev.* **102** 1189
[17] Pines D 1963 *Elementary Excitations in Solids* (New York: Benjamin)
[18] Chen J M C, Clark J W and Sandler D G 1982 *Z. Phys.* A **305** 223
[19] Bijl A 1940 *Physica* **7** 869
[20] Stern F 1967 *Phys. Rev. Lett.* **18** 546
[21] Xian Y 1989 A study of two-dimensional quantum systems *PhD Thesis* University of Minnesota, Minneapolis
[22] Laughlin R B 1983 *Phys. Rev. Lett.* **50** 1395
[23] Girvin S M, MacDonald A H and Platzman P M 1985 *Phys. Rev. Lett.* **54** 581
Girvin S M 1990 *The Quantum Hall Effects* ed R E Prange and S M Girvin (New York: Springer) p 353
[24] Blaiza J-P and Ripka G 1986 *Quantum Many-Body Theory of Finite Systems* (London: MIT press)
[25] Braune S and Maleyev S V 1990 *Z. Phys.* B **81** 69
[26] Bunker A and Landau D P 2000 *Phys. Rev. Lett.* **85** 2601
[27] Schweika W, Maleyev S V, Brückel Th, Plakhty V P and Regnault L-P 2002 *Europhys. Lett.* **60** 446
[28] Huberman T *et al* 2005 *Phys. Rev.* B **72** 014413
[29] Arovas D P and Auerbach A 1988 *Phys. Rev.* B **38** 316
Auerbach A and Arovas D P 1988 *Phys. Rev. Lett.* **61** 617
[30] Hirsch J E and Tang S 1989 *Phys. Rev.* B **39** 2887
Tang S, Lazzouni M E and Hirsch J E 1989 *Phys. Rev.* B **40** 5000
[31] Takahashi M 1989 *Phys. Rev.* B **40** 2494