Paired-magnon analysis of quantum antiferromagnets

Efstratios Manousakis
Department of Physics, Center for Materials Research and Technology, and Supercomputer Computations Research Institute, Florida State University, Tallahassee, Florida 32306
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We study the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on an infinite square lattice. The calculational scheme known as "paired-phonon analysis" developed for strongly correlated quantum fluids is extended to a "paired-magnon analysis" to study quantum antiferromagnets. We define a complete and orthonormal set of multimagnon states and calculate the matrix elements of the Hamiltonian using a separability approximation. Our results obtained by diagonalizing the Hamiltonian matrix analytically are very similar to those obtained in spin-wave theory. We obtain -0.3290, for the ground-state energy per bond in units of the antiferromagnetic coupling and 0.303 for the ground-state staggered magnetization. These results compare well with the best-known estimates -0.334 ± 0.001 and 0.313, respectively. We derive the analytic form of the ground-state wave function in this approximation and find it to be of the same form as that assumed by Marshall in his variational studies.. The zero-point motion of long-wavelength excitations (spin waves) in the model, however, reflects a long-range tail in our wave function. We discuss the separability approximation by giving quantitative arguments which justify its validity.

I. INTRODUCTION

The discovery of copper-oxide superconductors has renewed the interest in certain quantum spin and fermion models. The examination of these materials by neutron scattering experiments[1] shows long-range antiferromagnetic (AF) correlations which may be understood[2,3] in terms of the dynamics of a simple two-dimensional (2D) spin-$\frac{1}{2}$ AF Heisenberg model

$$H=J\sum_{\langle \mathbf{R},\mathbf{R}'\rangle}\mathbf{S}_{\mathbf{R}}\cdot\mathbf{S}_{\mathbf{R}'} \ . \tag{1.1}$$

In this model $\mathbf{S}_{\mathbf{R}}$ describes the Pauli spin-$\frac{1}{2}$ operator of one electron of the ith CuO_2 cell being in a linear combination of the orbitals $d_{x^2-y^2}$ of the copper and p_x and p_y of the two oxygen atoms of the CuO_2 plane. This model can be obtained as the strong-coupling limit of the Hubbard model, when the conduction band is half filled.

Contrary to its simplicity the model (1.1) lacks an exact solution in two or higher space dimensions and a growing number of numerical,[3,4] analytical,[5] or semianalytical[6] techniques of an approximate nature have been employed. Even though there is no exact statement yet,[7] based upon the above methods, it is believed that the spin-$\frac{1}{2}$ AF Heisenberg model on the square lattice develops AF long-range order at zero temperature. Moreover, the general picture emerging from these studies is that one may obtain a relatively good quantitative description of the ground state of the AF Heisenberg model by treating small spin fluctuations above the Nèel state perturbatively.

The Hamiltonian (1.1) can be written as

$$H=H_1+H_2 \ , \tag{1.2a}$$

$$H_1=\frac{1}{4}\sum_{\langle \mathbf{R},\mathbf{R}'\rangle}\sigma^z_{\mathbf{R}}\sigma^z_{\mathbf{R}'} \ , \tag{1.2b}$$

$$H_2=\frac{1}{2}\sum_{\langle \mathbf{R},\mathbf{R}'\rangle}(S^+_{\mathbf{R}}S^-_{\mathbf{R}'}+S^-_{\mathbf{R}}S^+_{\mathbf{R}'}) \ , \tag{1.2c}$$

where $\sigma^z=2S^z$, $S^+=S_x+iS_y$ and $S^-=S_x-iS_y$, and by letting $J=1$ we measure the energy in units of J.

We define the set of "multimagnon" states in the following way:

$$|\cdots n(k)\cdots\rangle\equiv\prod_{\mathbf{k}}(\sigma^z_{\mathbf{k}})^{n(k)}|\phi\rangle \ , \tag{1.3a}$$

$$\sigma^z_{\mathbf{k}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{R}}e^{i\mathbf{k}\cdot\mathbf{R}}\sigma^z_{\mathbf{R}} \ , \tag{1.3b}$$

where the sum runs over all N lattice vectors $\mathbf{R}$ and $n(k)=0,1,2,\ldots,N$. The state $|\phi\rangle$ is defined as follows:

$$|\phi\rangle\equiv\frac{1}{(2^N)^{1/2}}\sum_c(-1)^{L(c)}|c\rangle \ . \tag{1.4}$$

Here the sum is over all possible spin configurations c of the lattice and $L(c)$ is the number of down spins in one sublattice contained in the configuration c. Therefore, the state $|\phi\rangle$ is

$$|\phi\rangle=\prod_{\mathbf{R}\in A}|\mathbf{R}\rangle_+\prod_{\mathbf{R}\in B}|\mathbf{R}\rangle_- \ , \tag{1.5a}$$

$$|\mathbf{R}\rangle_\pm\equiv\frac{1}{\sqrt{2}}(|+\rangle\pm|-\rangle) \ , \tag{1.5b}$$

where A and B represent the two sublattices and $|+\rangle$ and $|-\rangle$ are eigenstates of $\sigma^z_{\mathbf{R}}$ with eigenvalues $+1$ and -1, respectively. The operator $\sigma^z_{\mathbf{R}}$ acting on $|\mathbf{R}\rangle_\pm$ gives

$$\sigma^z_{\mathbf{R}}|\mathbf{R}\rangle_+=|\mathbf{R}\rangle_- \ , \tag{1.6a}$$

$$\sigma^z_{\mathbf{R}}|\mathbf{R}\rangle_-=|\mathbf{R}\rangle_+ \ . \tag{1.6b}$$

Since the states $|\mathbf{R}\rangle_+$ and $|\mathbf{R}\rangle_-$ form a complete basis of the Hilbert space of the electron at $\mathbf{R}$, all possible states

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of the Hilbert space for N spins can be obtained by acting on $|\phi\rangle$ by all products of $\sigma_{\mathbf{R}_1},\ldots,\sigma^z_{\mathbf{R}_l}$ for any l $(0<l\le N)$ different sites. It can be easily verified that the state (1.4) [or (1.5)] has zero staggered magnetization in the z and y directions but has full staggered magnetization in the x direction. In fact, if we rotate the Nèel state around the y axis by $\pi/2$ we obtain the state (1.4) [or (1.5)].

The set of states defined by (1.3) form a nonorthogonal basis. In the next section of this paper we orthonormalize them and calculate the matrix elements of H in a separability approximation. This approximation was introduced in the theory of quantum fluids[8] in the context of "paired-phonon analysis" of strongly correlated Bose liquids. Following Ref. 8 we extend the method of "paired-phonon analysis" to a "paired-magnon analysis" to study the spin-$\frac{1}{2}$ Heisenberg antiferromagnet. The separability approximation neglects the coupling of paired multimagnon states. In Sec. III we diagonalize the Hamiltonian matrix and find the ground-state and elementary excitations. We obtain -0.3290 J for the ground-state energy per bond of the infinite square lattice, which is in $<2\%$ agreement with the most accurate estimates.[6] In Sec. IV we derive the analytic form of the ground-state wave function and show that it has the form assumed by Marshall in his variational studies. Our wave function, however, has long-distance behavior consistent with the existence of low-lying long-wavelength excitations (spin waves) in the model and their zero-point motion. In Sec. V, we calculate the staggered magnetization and find 0.303 the same value with the results of spin-wave theory.[5] In the same section, we give quantitative justification of our separability approximation. Since the ground-state properties of the spin-$\frac{1}{2}$ Heisenberg antiferromagnetic can be analytically and accurately calculated with this technique, it will be interesting to study the presence of one, two, or more holes with the effective Hamiltonian obtained from the Hubbard model in the strong coupling limit.

II. MULTIMAGNON STATES AND MATRIX ELEMENTS

Let us start from the following states:

$$|m,n)\equiv(\sigma^z_{\mathbf{k}})^m(\sigma^z_{-\mathbf{k}})^n|\phi\rangle \ . \tag{2.1}$$

These states, however, do not form an orthogonal set. We modify the definition as follows:

$$|m,n\rangle\equiv\left[\frac{[N-(m+n)]!}{m!n!N!}\right]^{1/2}\sum_{\{\mathbf{R}_i,\mathbf{r}_j\}_C} e^{i\mathbf{k}\cdot(\mathbf{R}_1+\cdots+\mathbf{R}_m)}e^{-\mathbf{k}\cdot(\mathbf{r}_1+\cdots+\mathbf{r}_n)}\sigma^z_{\mathbf{R}_1}\cdots\sigma^z_{\mathbf{R}_m}\sigma^z_{\mathbf{r}_1}\cdots\sigma^z_{\mathbf{r}_n}|\phi\rangle \ , \tag{2.2}$$

with $\mathbf{k}\neq0$. Here, $\{\mathbf{R}_i,\mathbf{r}_j\}_C$ means that the sum is over all $\{\mathbf{R}_1,\ldots,\mathbf{R}_m,\mathbf{r}_1,\ldots,\mathbf{r}_n\}$ with the constraint $\mathbf{R}_i\neq\mathbf{R}_j\neq\mathbf{r}_k\neq\mathbf{r}_l\neq\mathbf{R}_1$. The overlap between such states is given by

$$\begin{aligned}\langle m',n'|m,n\rangle=&\frac{1}{N!}\left[\frac{[N-(m+n)]![N-(m'+n')]!}{m!m'!n!n'!}\right]^{1/2}\\&\times\sum_{\{\mathbf{R}_i,\mathbf{r}_j\}_C,\{\mathbf{R}'_i,\mathbf{r}'_j\}_C}e^{i\mathbf{k}\cdot(\mathbf{R}_1+\cdots+\mathbf{R}_m)}e^{-i\mathbf{k}\cdot(\mathbf{R}'_1+\cdots+\mathbf{R}'_{m'})}e^{-i\mathbf{k}\cdot(\mathbf{r}_1+\cdots+\mathbf{r}_n)}e^{i\mathbf{k}\cdot(\mathbf{r}'_1+\cdots+\mathbf{r}_{n'})}\\&\times\langle\phi|\sigma^z_{\mathbf{R}'_1}\cdots\sigma^z_{\mathbf{R}'_{m'}}\sigma^z_{\mathbf{r}'_1}\cdots\sigma^z_{\mathbf{r}'_{n'}}\sigma^z_{\mathbf{R}_1}\cdots\sigma^z_{\mathbf{R}_m}\sigma^z_{\mathbf{r}_1}\cdots\sigma^z_{\mathbf{r}_n}|\phi\rangle\\=&\delta_{n,n'}\delta_{m,m'} \ .\end{aligned} \tag{2.3}$$

In order to obtain nonzero contribution, the σ's must occur in pairs such that $(\sigma^z)^2=1$ (because $\langle\phi|\sigma^z|\phi\rangle=0$). However, all the sites $\{\mathbf{R}_1,\ldots,\mathbf{R}_m,\mathbf{r}_1,\ldots,\mathbf{r}_n\}$ are different and no two sites in the set $\{\mathbf{R}'_1,\ldots,\mathbf{R}'_{m'},\mathbf{r}'_1,\ldots,\mathbf{r}'_{n'}\}$ are the same. Moreover, $\mathbf{R}_i\neq\mathbf{r}'_j$ and $\mathbf{R}'_i\neq\mathbf{r}_j$, because if $\mathbf{R}_i=\mathbf{r}'_j$ or $\mathbf{R}_i=\mathbf{r}'_j$ we obtain $\mathbf{k}=\mathbf{0}$ by summing over $\mathbf{R}_i$ or $\mathbf{R}'_i$ respectively. Hence $m'=m$, $n'=n$ and the sites $\mathbf{R}_1,\ldots,\mathbf{R}_m$ must be identical to any permutation of $\mathbf{R}'_1,\ldots,\mathbf{R}'_m$ and the sites $\mathbf{r}_1,\ldots,\mathbf{r}_n$ must be identical to any permutation of $\mathbf{r}'_1,\ldots,\mathbf{r}'_n$. There are $m!n!$ such permutations. The matrix element of σ's is unity for each such term and the summation over all different $\mathbf{R}_1,\ldots,\mathbf{R}_m$ and $\mathbf{r}_1,\ldots,\mathbf{r}_n$ gives a factor of $N(N-1)(N-2)\cdots[N-(m+n-1)]$. Therefore, the states $|m,n\rangle$ defined by (2.2) form an orthonormal set.

The states defined by Eq. (2.2), however, do not form a complete set. The entire Hilbert space is spanned by

$$|\cdots m_{\mathbf{k}},m_{-\mathbf{k}}\cdots\rangle\equiv\prod_{\mathbf{k},k_x>0}\left[\left[\frac{[N-(m_{\mathbf{k}}+m_{-\mathbf{k}})]!}{m_{\mathbf{k}}!m_{-\mathbf{k}}!N!}\right]^{1/2}\sum_{\{\mathbf{R}_i,\mathbf{r}_j\}_C}e^{i\mathbf{k}\cdot(\mathbf{R}_1+\cdots+\mathbf{R}_{m_\mathbf{k}})}e^{-i\mathbf{k}\cdot(\mathbf{r}_1+\cdots+\mathbf{r}_{m_{-\mathbf{k}}})}\times\sigma^z_{\mathbf{R}_1}\cdots\sigma^z_{R_{m_\mathbf{k}}}\sigma^z_{\mathbf{r}_1}\cdots\sigma_{\mathbf{r}_{m_{-\mathbf{k}}}}\right]|\phi\rangle \ , \tag{2.4}$$

where $m_{\mathbf{k}}$ and $m_{-\mathbf{k}}$ are the number of magnons in the momentum states $\mathbf{k}$ and $-\mathbf{k}$, respectively. These paired-multimagnon states are nonorthogonal. We can proceed further by introducing a separability approximation[8] in the calculation of the matrix elements of the unit operator and the Hamiltonian. Namely

$$\langle \cdots m'_{\mathbf{k}}, m'_{-\mathbf{k}} \cdots | \cdots m_{\mathbf{k}}, m_{-\mathbf{k}} \cdots \rangle \rightarrow \prod_{\mathbf{k}, k_x > 0} \langle m'_{\mathbf{k}}, m'_{-\mathbf{k}} | m_{\mathbf{k}}, m_{-\mathbf{k}} \rangle = \prod_{\mathbf{k}, k_x > 0} \delta_{m'_{\mathbf{k}}, m_{\mathbf{k}}} \delta_{m'_{-\mathbf{k}}, m_{-\mathbf{k}}} , \tag{2.5}$$

and

$$\langle \cdots m'_{\mathbf{k}}, m'_{-\mathbf{k}} \cdots | H - E_\phi | \cdots m_{\mathbf{k}}, m_{-\mathbf{k}} \cdots \rangle \rightarrow \sum_{\mathbf{q}, q_x > 0} \langle m'_{\mathbf{q}}, m'_{-\mathbf{q}} | H - E_\phi | m_{\mathbf{q}}, m_{-\mathbf{q}} \rangle \times \prod_{\mathbf{k} \neq \mathbf{q}, k_x > 0} \langle m'_{\mathbf{k}}, m'_{-\mathbf{k}} | m_{\mathbf{k}}, m_{-\mathbf{k}} \rangle . \tag{2.6}$$

where $E_\phi = \langle \phi | H | \phi \rangle$. Since we have orthogonalized the states (1.2) for all $\mathbf{k}$, within the separability approximation the states (2.4) are orthogonal. This approximation neglects the matrix elements which couple a subspace defined by (2.2) for a definite value of $m_{\mathbf{k}}, m_{-\mathbf{k}}$ with another subspace defined by (2.2) and characterized by different values. This approximation makes sense only in a limited function space characterized by

$$\sum_{\mathbf{k}} m_{\mathbf{k}} \ll N . \tag{2.7}$$

Our results are subject to the validity of the approximation (2.5) and (2.6). In the rest of the treatment we do not introduce any further approximation. In Sec. V, we will come back to this point and show that our solution satisfies the condition (2.7) to a reasonable degree.

The expectation value of the Hamiltonian (1.1) with the state $|\phi\rangle$ is given by

$$E_\phi \equiv \langle \phi | H | \phi \rangle = \frac{1}{2} \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} \langle \phi | S^+_{\mathbf{R}} S^-_{\mathbf{R}'} + S^+_{\mathbf{R}'} S^-_{\mathbf{R}} | \phi \rangle = -\frac{dN}{4} . \tag{2.8}$$

Here, it requires the same effort to work on a generalization of the square lattice to a hypercubic one in d dimensions.

In the Appendix we calculate the matrix elements of H in the separability approximation (2.6). We find that the nonzero matrix elements are

$$\langle m, n | H - E_\phi | m, n \rangle = d(m+n) \left[1 - \frac{3}{4} \frac{m+n}{N} \right] , \tag{2.9}$$

$$\langle m-1, n-1 | H - E_\phi | m, n \rangle = d\sqrt{mn} \left[1 - \frac{m+n}{N} \right] \gamma(k) , \tag{2.10}$$

$$\langle m+1, n+1 | H - E_\phi | m, n \rangle = d\sqrt{(m+1)(n+1)} \left[1 - \frac{m+n}{N} \right] \gamma(k) , \tag{2.11}$$

where

$$\gamma(k) = \frac{1}{d} \sum_{\mu=1}^{d} \cos(k_\mu) . \tag{2.12}$$

III. DIAGONALIZATION. GROUND-STATE AND ELEMENTARY EXCITATIONS

In the approximation (2.5) and (2.6), the ground-state wave function can be written as

$$|\psi_0\rangle = \prod_{\mathbf{k}, k_x > 0} F_{\mathbf{k}} |\phi\rangle . \tag{3.1}$$

The state $F_{\mathbf{k}} |\phi\rangle$ can be written as a linear superposition of states (2.2) with $m = n$, namely

$$F_{\mathbf{k}} |\phi\rangle = \sum_{m=0}^{\infty} C_m | m, m \rangle . \tag{3.2}$$

This function is the eigenstate of $\hat{H}$ with the lowest eigenvalue in the subspace spanned by (2.2) for a specific value of $\mathbf{k}$ and all $m = n$. The matrix elements of the Hamiltonian in this subspace are

$$\langle m, m | H - E_\phi | m, m \rangle = 2dm \left[1 - \frac{3}{2} \frac{m}{N} \right] , \tag{3.3}$$

$$\langle m-1, m-1 | H - E_\phi | m, n \rangle = dm \left[1 - 2\frac{m}{N} \right] \gamma(k) , \tag{3.4}$$

$$\langle m+1, m+1 | H - E_\phi | m, m \rangle = d(m+1) \left[1 - 2\frac{m}{N} \right] \gamma(k). \tag{3.5}$$

We need to diagonalize $H - E_\phi$ in this subspace. First we neglect the terms of order m/N. We will show that their contribution to the ground-state energy vanishes in the limit $N \rightarrow \infty$. The eigenvalue problem

$$\langle n, n | (H - E_\phi) F_{\mathbf{k}} | \phi \rangle = E \langle n, n | F_{\mathbf{k}} | \phi \rangle \tag{3.6}$$

reduces to the following recursion relation:

$$2dnC_n + d\gamma(k)(n+1)C_{n+1} + d\gamma(k) n C_{n-1} = EC_n . \tag{3.7}$$

It can be verified that the normalized solution of Eq. (3.7) is

$$C_n = C_0 D(k)^n , \tag{3.8}$$

$$C_0 = [1 - D(k)^2]^{1/2} \tag{3.9}$$

with

$$D(k) = \frac{-1 \pm [1 - \gamma(k)^2]^{1/2}}{\gamma(k)} , \tag{3.10}$$

$$E=\langle\phi|F_{k}^{\dagger}HF_{k}|\phi\rangle=d\{-1\pm[1-\gamma(k)^{2}]^{1/2}\} \quad (3.11)$$

and we must choose the solution with the plus sign because the other leads to an unstable ground state against creation of excitations (see the discussion of the excitation spectrum below).

Using (3.1) and the approximation (2.5) and (2.6), the ground-state energy is given by

$$E_{0}=E_{\phi}+d\sum_{\mathbf{k},k_{x}>0}\{-1+[1-\gamma(k)^{2}]^{1/2}\} . \quad (3.12)$$

Evaluation of this expression for a large enough square lattice gives $E_0/dN=-0.3290$. This value is in $<2\%$ agreement with the best estimates[6] of -0.334 ± 0.001. For the one-dimensional lattice we find $E_0/N=-0.4317$, which is within 3% of its exact value, even though we do not except the separability approximation to be accurate in 1D for arguments given in Sec. IV. For an infinite three-dimensional cubic lattice we find $E_0/dN=-0.2986$. Our expression (3.12) is the same as that obtained with linear spin-wave theory.[5]

Next, we examine the contribution of the terms neglected in (3.3)–(3.5). First, let us calculate the expectation value with $F_{\mathbf{k}}|\phi\rangle$ of the neglected parts $\hat{H}_r$ of $\hat{H}$:

$$\begin{aligned}\langle\phi|F_{k}^{\dagger}H_{r}F_{\mathbf{k}}|\phi\rangle=&-3d\frac{1}{N}\sum_{m}C_{m}^{2}m^{2}\\&-2d\frac{1}{N}\gamma(k)\sum_{m}C_{m}C_{m-1}m^{2}\\&-2d\frac{1}{N}\gamma(k)\sum_{m}C_{m}C_{m+1}m(m+1) ,\end{aligned} \quad (3.13)$$

and using Eqs. (3.8) and (3.9) we obtain

$$\langle\phi|F_{\mathbf{k}}^{\dagger}H_{r}F_{\mathbf{k}}|\phi\rangle=d\frac{1}{N}\langle m^{2}\rangle-2d\frac{1}{N}\gamma(k)D\langle m\rangle , \quad (3.14a)$$

$$\langle m^{p}\rangle\equiv\sum_{m}|C_{m}|^{2}m^{p}=(1-D^{2})\sum_{m}D^{2m}m^{p} . \quad (3.14b)$$

We find

$$\langle m\rangle=\frac{D^{2}}{1-D^{2}}=\frac{1}{2(1-\gamma^{2})^{1/2}}-\frac{1}{2} , \quad (3.15a)$$

$$\langle m^{2}\rangle=\frac{D^{2}(1+D^{2})}{(1-D^{2})^{2}}=\frac{1}{2(1-\gamma^{2})}-\frac{1}{2(1-\gamma^{2})^{1/2}} . \quad (3.15b)$$

The contribution of H_r to the ground-state expectation value per bond is obtained as

$$\begin{aligned}&\frac{1}{dN}\sum_{\mathbf{k},k_{x}>0}\langle\phi|F_{\mathbf{k}}^{\dagger}H_{r}F_{\mathbf{k}}|\phi\rangle\\&=\frac{1}{N^{2}}\sum_{\mathbf{k},k_{x}>0}\langle m^{2}\rangle-2\frac{1}{N^{2}}\sum_{\mathbf{k},k_{x}>0}\gamma D\langle m\rangle .\end{aligned} \quad (3.16)$$

The sum $(1/N)\sum\gamma D\langle m\rangle$ converges for a square lattice and therefore the second term vanishes in the limit $N\to\infty$. For large N, the sum of $(1/N)\sum\langle m^2\rangle\sim\ln(N)$ (i.e., logarithmically divergent with the size of the lattice). Hence, the first term vanishes in the limit $N\to\infty$ as $(1/N)\ln(N)$.

A single-magnon excitation of momentum $\mathbf{q}$ can be defined as

$$|\psi_{\mathbf{q}}\rangle=G_{\mathbf{q}}\prod_{\mathbf{k}\neq\mathbf{q},k_{x}>0}F_{\mathbf{k}}|\phi\rangle , \quad (3.17)$$

where $F_{\mathbf{k}}$ for $\mathbf{k}\neq\mathbf{q}$ is identical to the ground-state operator defined by (3.2) and $G_{\mathbf{q}}$ is defined as

$$G_{\mathbf{q}}|\phi\rangle=\sum_{m=0}^{\infty}B_{m}|m+1,m\rangle . \quad (3.18)$$

The excitation energy $e(q)$ in the separability approximation (2.5) and (2.6) is given by

$$\begin{aligned}e(q)&\equiv\langle\psi_{\mathbf{q}}|H|\psi_{\mathbf{q}}\rangle-\langle\psi_{0}|H|\psi_{0}\rangle\\&=\langle\phi|G_{\mathbf{q}}^{\dagger}HG_{\mathbf{q}}|\phi\rangle-\langle\phi|F_{\mathbf{q}}^{\dagger}HF_{\mathbf{q}}|\phi\rangle ,\end{aligned} \quad (3.19)$$

because the expectation values in the separability approximation are sums over all $\mathbf{k}$. Therefore, we need to determine $G_{\mathbf{q}}$ in the subspace of $|m+1,m\rangle$. Neglecting the $1/N$ terms in (2.9)–(2.11), the eigenvalue problem

$$(H-E_{\phi})G_{\mathbf{q}}|\phi\rangle=EG_{\mathbf{q}}|\phi\rangle \quad (3.20)$$

reduces to the following recursion relation:

$$\begin{aligned}d(2n+1)B_{n}+d\gamma(q)\sqrt{(n+1)(n+2)}B_{n+1}\\+d\gamma(q)\sqrt{n(n+1)}B_{n-1}=EB_{n} .\end{aligned} \quad (3.21)$$

It can be verified that the solution to this recursion relation is

$$B_{n}=B_{0}\sqrt{n+1}D(q)^{n} , \quad (3.22)$$

$$B_{0}=1-D(q)^{2} . \quad (3.23)$$

$D(q)$ is the same as that found for the ground state and given by (3.10). The eigenvalue is given by

$$E=\sqrt{\phi}|G_{\mathbf{q}}^{\dagger}HG_{\mathbf{q}}|\phi\rangle=-d\pm2d[1-\gamma(q)^{2}]^{1/2} , \quad (3.24)$$

and choosing the plus sign (3.19) takes the form

$$e(q)=d[1-\gamma(q)^{2}]^{1/2} . \quad (3.25)$$

We need to choose the solution with the positive sign for the stability of the ground state.

IV. THE FORM OF THE GROUND-STATE WAVE FUNCTION

Next, we determine the form of the ground-state wave function. The normalized states defined by (2.2) for $m=n$ can be expressed as

$$|m,m\rangle=\sum_{n=0}^{m}C_{n}^{m}|n,n) , \quad (4.1)$$

where $|n,n)$ are nonorthonormal states given by Eq. (2.1). We can determine C_n^m by projecting both sides to $\langle m',m'|$. We obtain

$$\delta_{m,m'}=\sum_{n=m'}^{m}C_{n}^{m}\langle m',m'|n,n) . \quad (4.2)$$

For $N \gg n$ and $N \gg m'$ we obtain

$$\langle m',m'|n,n\rangle = \frac{(n!)^2}{m'!(n-m')!}, \quad n \geq m'$$
$$=0, \quad n < m' . \tag{4.3}$$

It can be verified that the solution to (4.2) is

$$C_n^m = \frac{(-1)^{m-n}}{n!}\begin{bmatrix} m \\ n \end{bmatrix} . \tag{4.4}$$

Here

$$\begin{bmatrix} m \\ n \end{bmatrix} \equiv \frac{m!}{(m-n)!n!} .$$

Therefore, the ground-state wave function (3.1) is given by

$$|\psi_0\rangle = \prod_{\mathbf{k},k_x>0} (1-D^2)^{1/2} \sum_{m=0}^{\infty}\sum_{n=0}^{m} D^m \frac{(-1)^{m-n}}{n!}\begin{bmatrix} m \\ n \end{bmatrix} \times (|\sigma_{\mathbf{k}}^z|^2)^n|\phi\rangle . \tag{4.5}$$

The $\sum_{m=0}^{\infty}\sum_{n=0}^{m}$ can be changed to $\sum_{n=0}^{\infty}\sum_{m\geq n}^{\infty}$, and by changing the summation variable m to $l=m-n$, we obtain

$$|\psi_0\rangle = \prod_{\mathbf{k},k_x>0} (1-D^2)^{1/2} \sum_{n=0}^{\infty} \frac{D^n}{n!}(|\sigma_{\mathbf{k}}^z|^2)^n \times \sum_{l=0}^{\infty} (-D)^l \begin{bmatrix} l+n \\ n \end{bmatrix} |\phi\rangle . \tag{4.6}$$

The last summation gives $1/(1+D)^{n+1}$ and therefore

$$|\psi_0\rangle = \prod_{\mathbf{k},k_x>0} \left[\frac{1-D}{1+D}\right]^{1/2} \sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{D}{1+D}|\sigma_{\mathbf{k}}^z|^2\right]^n |\phi\rangle$$
$$=\Lambda \exp\left[\sum_{\mathbf{k},k_x>0}\frac{D(k)}{1+D(k)}|\sigma_{\mathbf{k}}^z|^2\right]|\phi\rangle$$
$$=\Lambda \exp\left[-\tfrac{1}{2}\sum_{i<j} u_{ij}\sigma_i^z\sigma_j^z\right]|\phi\rangle , \tag{4.7}$$

where

$$u_{ij} \equiv \frac{1}{N}\sum_{\mathbf{k}}\left[\left[\frac{1+\gamma(k)}{1-\gamma(k)}\right]^{1/2} - 1\right] e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} . \tag{4.8}$$

Variational wave functions of similar form were introduced and studied by Hulthen[9] and Kastelijn[10] for one dimension and Marshall[11] for one, two, and three dimensions. Starting from perturbation theory, similar variational studies were also performed by Bartkowski.[12] More recently, the same form was studied by Huse and Elser[13] using the variational Monte Carlo (VMC) approach. They took $u(1)=u_1$ and $u(r)=c/r^p$ for $r>1$, where $r=|\mathbf{R}_i-\mathbf{R}_j|$, and treated u_1, c, and p as variational parameters. The best energy obtained in this approach[14] is -0.3319 J for $u_1 \sim 0.65$, $c \sim 0.475$, and $p \sim 0.7$. Similar VMC studies were carried out by Horsch and Linden[14] where using only $u(1)$ as a variational parameter [and $u(r>1)=0$] they found -0.322 J for the ground-state energy in our units. Notice that our u is not a function of the distance r between two points on the lattice but rather a function of the two components x and y of the vector $\mathbf{R}_{ij}$. In Fig. 1 we plot our $u(x,y=0)$ (open circles) and compare it with the results of VMC (solid line). The form (4.7) and (4.8) has long-distance behavior consistent with the existence of long-wavelength spin-wave excitations. From Eq (4.8) we find that

$$u(r\to\infty) = \frac{\sqrt{2}}{\pi r} . \tag{4.9}$$

This form [Eq. (4.9)] is shown by the dashed line in Fig. 1 and we see that the onset of the asymptotic form starts from essentially $r=2$. The question of the long-range tails is well known in liquid ^{4}He where the existence of long-wavelength excitations (zero sound) influence the long-range behavior of the Jastrow correlation factor.[15] In the helium case the long-range behavior of the wave function does not give significant contribution to the ground-state energy. However, it has important consequencies to the spectrum of elementary excitations when the same wave function is used to define the Feynman-Cohen states or to construct a correlated basis.[16] We notice that the tails of the wave function of Ref. 13 and that of Eqs. (4.7) and (4.8) are quite different. The reason for that may be that the ground-state energy is not sensitive to the exact tail of the wave function. The numerical results of Ref. 14 does not seem to support the significance of the tail of the wave function for the long-wavelength excitations in the system since they find that the numerically calculated structure factor and the excitation spectrum are linear at low momenta. While this work was reviewed for publication, however, we have received the Green's-function Monte Carlo work of Ref. 17, where the conclusions of the authors confirm the results of our analytical calculations. It will be interesting to perform a variational calculation using a wave function where one treats u for the first few neighbors as variational parame-

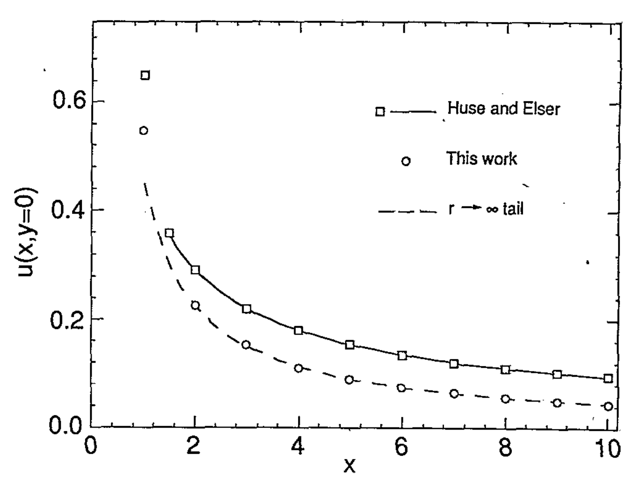

FIG. 1. Our results for the exponent $u(x,y)$ of the correlation factors in the ground-state wave function [Eqs. (4.7) and (4.8)] (open circles) for $y=0$. The solid line represents the results of the variational Monte Carlo calculation (Ref. 13).

ters and a tail proportional to that of (4.7) and (4.8) to account for low-lying spin-wave excitations. The proportionality constant can be found by requiring consistency of the calculation and sum rules.[18]

V. STAGGERED MAGNETIZATION. VALIDITY OF THE SEPARABILITY APPROXIMATION

We define the z component of the staggered magnetization operator as

$$\hat{M}^z_{st} \equiv \frac{1}{N} \sum_{x,y} (-1)^{x+y} S^z_{\mathbf{R}} , \tag{5.1}$$

where x and y are the two components of the vector $\mathbf{R}$ in units of the lattice spacing. The expectation value of $\hat{M}^z_{st}$ with the wave function (4.7) and (4.8) vanishes.

Let us consider the x component of the staggered magnetization

$$\hat{M}^x_{st} \equiv \frac{1}{N} \sum_{x,y} (-1)^{x+y} \frac{S^+_{\mathbf{R}} + S^-_{\mathbf{R}}}{2} , \tag{5.2}$$

where we have used the identity $S^x = (S^+ + S^-)/2$. We would like to calculate its expectation value with the ground wave function (4.7) and (4.8). Since (4.7) and (4.8) is a superposition of states with the same number of magnons in states having $\mathbf{k}$ and $-\mathbf{k}$, let us consider the matrix elements of (5.2) with such states

$$\langle m',m' | (-1)^{x+y} S^-_R | m,m \rangle = \frac{(-1)^{x+y}}{N! m! m'!} \sqrt{(N-2m)!(N-2m')!} \times \sum_{\{\mathbf{R}_i,\mathbf{r}_j\}_C, \{\mathbf{R}'_i,\mathbf{r}'_j\}_C} e^{i\mathbf{k}\cdot(\mathbf{R}_1+\cdots+\mathbf{R}_m)} e^{-i\mathbf{k}\cdot(\mathbf{R}'_1+\cdots+\mathbf{R}'_{m'})} e^{-i\mathbf{k}\cdot(\mathbf{r}_1+\cdots+\mathbf{r}_m)} e^{i\mathbf{k}\cdot(\mathbf{r}'_1+\cdots+\mathbf{r}'_{m'})}$$
$$\times \langle \phi | \sigma^z_{\mathbf{R}'_1} \cdots \sigma^z_{\mathbf{R}'_{m'}} \sigma^z_{\mathbf{r}'_1} \cdots \sigma^z_{\mathbf{r}'_{m'}} S^+_{\mathbf{R}} \sigma^z_{\mathbf{R}_1} \cdots \sigma^z_{\mathbf{R}_m} \sigma^z_{\mathbf{r}_1} \cdots \sigma^z_{\mathbf{r}_m} | \phi \rangle . \tag{5.3}$$

There are terms in which $\mathbf{R}$ is none of the $\{\mathbf{R}_i\}$ and $\{\mathbf{r}_i\}$. These matrix elements are nonzero if $m = m'$ and the set $\{\mathbf{R}_i\}$ is identical to any permutation of the set $\{\mathbf{R}'_i\}$ and the set $\{\mathbf{r}_i\}$ is identical to any permutation of the set $\{\mathbf{r}'_i\}$. The expectation value $(-1)^{x+y}\langle\phi|S^+_{\mathbf{R}}|\phi\rangle = \frac{1}{2}$ and summing over all $\mathbf{R}$ we obtain

$$\tfrac{1}{2}(1-2m/N)\delta_{m,m'}$$

There are also nonzero terms in which one of the $\{\mathbf{R}_i\}$ and one of the $\{\mathbf{R}'_i\}$ are equal to $\mathbf{R}$. In this case we obtain a nonzero contribution if $m = m'$ and the remaining $m-1$ elements of $\{\mathbf{R}_i\}$ are identical to any permutation of the remaining $m-1$ elements of $\{\mathbf{R}'_i\}$ and the $\{\mathbf{r}_i\}$ are identical to any permutation of $\{\mathbf{r}'_i\}$. The expectation value $\langle\phi|(-1)^{x+y}\sigma_{\mathbf{R}} S^+_{\mathbf{R}} \sigma_{\mathbf{R}}|\phi\rangle = -\frac{1}{2}$, hence summing over all $\mathbf{R}$ we obtain

$$-\frac{1}{2}\frac{m}{N}\delta_{m,m'} .$$

We obtain the same contribution if one of the $\{\mathbf{r}_i\}$ and one of the $\{\mathbf{r}'_i\}$ are the same with $\mathbf{R}$. The operator $(-1)^{x+y}S^-_R$ has the same matrix elements and therefore we conclude that

$$\langle m',m' | \hat{M}_x | m,m \rangle = \tfrac{1}{2} \left[1 - \frac{4m}{N} \right] \delta_{m,m'} . \tag{5.4}$$

Hence, the ground-state expectation value of the operator $\hat{M}_x$ is given by

$$\langle \psi_0 | \hat{M}_x | \psi_0 \rangle = \tfrac{1}{2} - \frac{1}{N} \sum_{\mathbf{k},k_x>0} \left[\frac{1}{[1-\gamma(k)^2]^{1/2}} - 1 \right] . \tag{5.5}$$

Evaluation of this expression for a square lattice and sufficiently large N gives $\langle \psi_0 | \hat{M}_x | \psi_0 \rangle = 0.303$ which is $\sim 61\%$ of its classical value. In 1D the correction diverges, and in 3D we obtain 0.422, which is closer to its classical value. The expectation value of the y component of the staggered magnetization is zero. Note that the expression (5.5) is identical to that obtained in spin-wave theory.[5]

Next, we check the criterion for the validity of our separability approximation. The average number of virtually excited magnons in the interacting ground state for an infinite square lattice is small as compared to the number of sites. We find that their ratio is [see Eq. (3.15a)]

$$R = \frac{1}{N} \sum_{\mathbf{k},k_x>0} \left[\frac{1}{[1-\gamma(k)^2]^{1/2}} - 1 \right] = 0.197 , \tag{5.6}$$

which is a rather small number. In 1D this integral diverges and therefore the separability approximation can not be justified. Our estimate, however, for the ground-state energy per bond for 1D is within 3% of its exact value. For an infinite 3D lattice the ratio $R = 0.078$.

Therefore, we expect the corrections due to our separability approximation in 3D to be even smaller than those in two dimensions.

In analogy with other interacting Bose systems $m_{\mathbf{k}}$, given by (3.15a), is the momentum distribution of the spin degrees of freedom in the interacting ground state. We demonstrate this as follows. We define the following operators:

$$a_{\mathbf{k}}^{\dagger}|m,n\rangle_{\mathbf{k}} \equiv \sqrt{(m+1)}|m+1,n\rangle_{\mathbf{k}} , \quad (5.7)$$

$$a_{\mathbf{k}}|m,n\rangle_{\mathbf{k}} \equiv \sqrt{m}\,|m-1,n\rangle_{\mathbf{k}} , \quad (5.8)$$

$$a_{-\mathbf{k}}^{\dagger}|m,n\rangle_{\mathbf{k}} \equiv \sqrt{(n+1)}|m,n+1\rangle_{\mathbf{k}} , \quad (5.9)$$

$$a_{-\mathbf{k}}|m,n\rangle_{\mathbf{k}} \equiv \sqrt{n}\,|m,n-1\rangle_{\mathbf{k}} . \quad (5.10)$$

It is straightforward to show that these operators satisfy

$$[a_{\mathbf{k}},a_{\mathbf{k}}^{\dagger}]=[a_{-\mathbf{k}},a_{-\mathbf{k}}^{\dagger}]=1 , \quad (5.11)$$

$$[a_{\mathbf{k}}^{\dagger},a_{-\mathbf{k}}^{\dagger}]=[a_{\mathbf{k}},a_{-\mathbf{k}}]=0 . \quad (5.12)$$

Neglecting the terms of order $(m+m)/N$ the Hamiltonian (2.9)–(2.11) is given by

$$H_{\mathbf{k}}=d(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+a_{-\mathbf{k}}^{\dagger}a_{-\mathbf{k}})+d\gamma(k)(a_{\mathbf{k}}a_{-\mathbf{k}}+a_{\mathbf{k}}^{\dagger}a_{-\mathbf{k}}^{\dagger}) . \quad (5.13)$$

This Hamiltonian can be exactly diagonalized by means of a canonical transformation:

$$\begin{aligned} A_{\mathbf{k}} &\equiv \lambda(k)a_{\mathbf{k}}-\mu(k)a_{-\mathbf{k}}^{\dagger} , \\ A_{\mathbf{k}}^{\dagger} &\equiv \lambda(k)a_{\mathbf{k}}^{\dagger}-\mu(k)a_{-\mathbf{k}} , \end{aligned} \quad (5.14)$$

with $A_{\mathbf{k}}^{\dagger}$ and $A_{\mathbf{k}}$ satisfying

$$[A_{\mathbf{k}},A_{\mathbf{k}}^{\dagger}]=[A_{-\mathbf{k}},A_{-\mathbf{k}}^{\dagger}]=1 , \quad (5.15)$$

$$[A_{\mathbf{k}}^{\dagger},A_{-\mathbf{k}}^{\dagger}]=[A_{\mathbf{k}},A_{-\mathbf{k}}]=0 \quad (5.16)$$

by choosing

$$\lambda(k)=\frac{1}{[1-D(k)^2]^{1/2}} , \quad (5.17)$$

$$\mu(k)=\frac{D(k)}{[1-D(k)^2]^{1/2}} . \quad (5.18)$$

The full Hamiltonian (1.2) in the separability approximation takes the following diagonal form:

$$H=E_{\phi}+\sum_{\mathbf{k},k_x>0}[-d+e(k)] + \sum_{\mathbf{k},k_x>0} e(k)(A_{\mathbf{k}}^{\dagger}A_{\mathbf{k}}+A_{-\mathbf{k}}^{\dagger}A_{-\mathbf{k}}) , \quad (5.19)$$

where $e(k)$ is given by (3.25). Therefore, these results are the same as those obtained in Sec. III.

Hence the momentum distribution of "bare" magnons is

$$\langle\psi_0|a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}|\psi_0\rangle=m_{\mathbf{k}} . \quad (5.20)$$

The "condensate fraction," i.e., fraction of degrees of freedom occupying the zero momentum state for the square lattice, is

$$m_0=1-\frac{1}{N}\sum_{\mathbf{k}\neq 0} m_k=0.803 . \quad (5.21)$$

Namely, there is a significant fraction of degrees of freedom at $\mathbf{k}=0$, even in the interacting ground state. We can conclude that the spin-$\frac{1}{2}$ Heisenberg antiferromagnet relative to helium is not as strongly interacting a system. In the former the "condensate" fraction is ~80%, whereas in helium the strong interactions leave only ~9% of the atoms in the condensate.[19]

It will be interesting to attempt extending this approach to the case of the effective Hamiltonian obtained from the Hubbard model in the strong-coupling limit.[20] Below half filling and at half filling, this Hamiltonian operates in a subspace of the Hilbert space having states with singly occupied sites. At half filling, it is equivalent to the Hamiltonian (1.1). The next obvious step is to study the case of one, two, or more holes with this Hamiltonian.

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APPENDIX

In this appendix we calculate the matrix elements of the Hamiltonian with the set of states (2.2). First we consider the z term

$$\langle m',n'|\sigma_{\mathbf{R}}^z\sigma_{\mathbf{R}'}^z|m,n\rangle=\frac{1}{N!}\left[\frac{[N-(m+n)]![N-(m'+n')]!}{m!m'!n!n'!}\right]^{1/2}$$

$$\times\sum_{\{\mathbf{R}_i,\mathbf{r}_j\}_C,\{\mathbf{R}_i',\mathbf{r}_j'\}_C} e^{i\mathbf{k}\cdot(\mathbf{R}_1+\cdots+\mathbf{R}_m)}e^{-i\mathbf{k}\cdot(\mathbf{R}_1'+\cdots+\mathbf{R}_{m'}')}e^{-i\mathbf{k}\cdot(\mathbf{r}_1+\cdots+\mathbf{r}_n)}e^{i\mathbf{k}\cdot(\mathbf{r}_1'+\cdots+\mathbf{r}_{n'}')}$$

$$\times\langle\phi|\sigma_{\mathbf{R}_1'}^z\cdots\sigma_{\mathbf{R}_{m'}'}^z\sigma_{\mathbf{r}_1'}^z\cdots\sigma_{\mathbf{r}_{n'}'}^z\sigma_{\mathbf{R}}^z\sigma_{\mathbf{R}'}^z\sigma_{\mathbf{R}_1}^z\cdots\sigma_{\mathbf{R}_m}^z\sigma_{\mathbf{r}_1}^z\cdots\sigma_{\mathbf{r}_n}^z|\phi\rangle . \quad (\mathrm{A1})$$

(1) We obtain nonzero diagonal matrix elements with $m'=m$, $n'=n$, in the following cases: (a) $\mathbf{R}$ is one of $\{\mathbf{R}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i'\}$, (b) $\mathbf{R}$ is one of $\{\mathbf{R}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i\}$, (c) $\mathbf{R}$ is one of $\{\mathbf{r}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i'\}$, and (d) $\mathbf{R}$ is one of $\{\mathbf{r}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i\}$. In the first case there are m^2 terms because $\mathbf{R}$ can be any one of $\{\mathbf{R}_i\}$ and $\mathbf{R}'$ any one of $\{\mathbf{R}_i'\}$. Let us consider for example the first term where $\mathbf{R}=\mathbf{R}_1$ and $\mathbf{R}'=\mathbf{R}_1'$. In order to obtain nonzero contribution the σ's must occur in pairs and hence the sites $\mathbf{R}_2,\ldots,\mathbf{R}_m$ must be identical to any permutation of $\mathbf{R}_2',\ldots,\mathbf{R}_m'$ and the sites $\mathbf{r}_1,\ldots,\mathbf{r}_n$ must be identical to any permutation of $\mathbf{r}_1',\ldots,\mathbf{r}_n'$. There are $(m-1)!n!$ such permutation. The summation over all different $\mathbf{R}_2,\ldots,\mathbf{R}_m$ and $\mathbf{r}_1,\ldots,\mathbf{r}_n$ gives a factor of $(N-2)(N-3)\cdots[N-(m+n)]$. The contribution of the first case to (A1) is obtained as

$$\delta_{m',m}\delta_{n',n}\frac{m[N-(m+n)]}{N(N-1)}e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} .$$

In the limit $N\gg 1$ we obtain

$$\delta_{m',m}\delta_{n',n}\frac{m}{N}\left[1-\frac{m+n}{N}\right]e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} .$$

The contribution of the other three cases can be obtained in a similar way. Summing up the contribution of the above four cases, we obtain

$$\langle m,n|\sigma_{\mathbf{R}}^z\sigma_{\mathbf{R}'}^z|m,n\rangle=\frac{(m+n)}{N}\left[1-\frac{m+n}{N}\right]\times(e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}+e^{-i\mathbf{k}(\mathbf{R}-\mathbf{R}')}) . \tag{A2}$$

(2) We can also have nonzero off-diagonal matrix elements with $m'=m-1$, $n'=n-1$, in the following cases: (a) $\mathbf{R}$ is one of $\{\mathbf{R}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i\}$ and (b) $\mathbf{R}$ is one of $\{\mathbf{r}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i\}$. It can be easily verified that the contribution of both cases for $N\gg 1$ is

$$\langle m-1,n-1|\sigma_{\mathbf{R}}^z\sigma_{\mathbf{R}'}^z|m,n\rangle=\frac{\sqrt{mn}}{N}\left[1-\frac{m+n}{N}\right]\times(e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}+e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}) . \tag{A3}$$

(3) We can also have off-diagonal matrix elements with $m'=m+1$, $m'=n+1$ when (a) $\mathbf{R}$ is one of $\{\mathbf{R}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i'\}$ and (b) $\mathbf{R}$ is one of $\{\mathbf{r}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i'\}$. In these cases we obtain

$$\langle m+1,n+1|\sigma_{\mathbf{R}}^z\sigma_{\mathbf{R}'}^z|m,n\rangle=\frac{\sqrt{(m+1)(n+1)}}{N}\left[1-\frac{m+n}{N}\right]\times(e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}+e^{-i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}) . \tag{A4}$$

Summing over all nearest neighbors $\mathbf{R}$, $\mathbf{R}'$ we find

$$\langle m,n|H_1|m,n\rangle=\frac{d}{2}(m+n)\left[1-\frac{m+n}{N}\right]\gamma(k) , \tag{A5}$$

$$\langle m-1,n-1|H_1|m,n\rangle=\frac{d}{2}\gamma(k)\sqrt{mn}\left[1-\frac{m+n}{n}\right] , \tag{A6}$$

$$\langle m+1,n+1|H_1|m,n\rangle=\frac{d}{2}\gamma(k)\sqrt{(m+1)(n+1)}\times\left[1-\frac{m+n}{n}\right] , \tag{A7}$$

where

$$\gamma(k)=\frac{1}{d}\sum_{\mu=1}^{d}\cos(k_\mu) . \tag{A8}$$

The second term of the Hamiltonian (1.2) is

$$\langle m',n'|\tfrac{1}{2}(S_{\mathbf{R}}^+S_{\mathbf{R}'}^-+S_{\mathbf{R}}^-S_{\mathbf{R}'}^+)|m,n\rangle=\frac{1}{N!}\left[\frac{[N-(m+n)]![N-(m'+n')]!}{m!m'!n!n'!}\right]^{1/2}$$
$$\times\sum_{\{\mathbf{R}_i,\mathbf{r}_j\}_C,\{\mathbf{R}_i',\mathbf{r}_j'\}_C} e^{i\mathbf{k}\cdot(\mathbf{R}_1+\cdots+\mathbf{R}_m)}e^{-i\mathbf{k}\cdot(\mathbf{R}_1'+\cdots+\mathbf{R}_{m'}')}e^{-i\mathbf{k}\cdot(\mathbf{r}_1+\cdots+\mathbf{r}_n)}e^{i\mathbf{k}\cdot(\mathbf{r}_1'+\cdots+\mathbf{r}_{n'}')}$$
$$\times\langle\phi|\sigma_{\mathbf{R}_1'}^z\cdots\sigma_{\mathbf{R}_{m'}'}^z\sigma_{\mathbf{r}_1'}^z\cdots\sigma_{\mathbf{r}_{n'}'}^z\tfrac{1}{2}(S_{\mathbf{R}}^+S_{\mathbf{R}'}^-+S_{\mathbf{R}}^-S_{\mathbf{R}'}^+)$$
$$\times\sigma_{\mathbf{R}_1}^z\cdots\sigma_{\mathbf{R}_m}^z\sigma_{\mathbf{r}_1}^z\cdots\sigma_{\mathbf{r}_n}^z|\phi\rangle . \tag{A9}$$

(1) We can have nonzero diagonal contributions with $m'=m$ and $n'=n$ in one of the following cases. (a) None of $\mathbf{R}$ and $\mathbf{R}'$ is one of the $\{R_i\},\{R_i'\},\{r_i\},\{r_i'\}$. In this case after summing over $\mathbf{R}$ and $\mathbf{R}'$, we obtain

$$-\tfrac{1}{4}dN\left[1-\frac{m+n}{N}\right]^2 .$$

(b) One of the $\mathbf{R},\mathbf{R}'$ is a member of the sets $\{\mathbf{R}_i\},\{\mathbf{r}_i\},\{\mathbf{R}_i'\},\{\mathbf{r}_i'\}$, and the other is not. In this case summing over all $\mathbf{R}$ and $\mathbf{R}'$ we obtain

$$\frac{d(m+n)}{2}\left[1-\frac{m+n}{N}\right] .$$

(c) Also the following four cases give diagonal elements: (i) $\mathbf{R}$ is one of $\{\mathbf{R}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i'\}$. (ii) $\mathbf{R}$ is one of $\{\mathbf{r}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i'\}$. (iii) $\mathbf{R}$ is one of $\{\mathbf{R}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i\}$. (iv) $\mathbf{R}$ is one of $\{\mathbf{r}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i\}$.

Summing over all $\mathbf{R}$ and $\mathbf{R}'$ the contribution of the above four cases combined is

$$-\frac{d}{2}\gamma(k)(m+n)\left[1-\frac{m+n}{N}\right].$$

(2) We obtain off-diagonal elements having $m'=m-1$ and $n'=n-1$ in the following cases. (a) $\mathbf{R}$ is one of $\{\mathbf{R}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i\}$. (b) $\mathbf{R}$ is one of $\{\mathbf{r}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i\}$. Summing over all $\mathbf{R},\mathbf{R}'$ we obtain

$$\frac{d}{2}\gamma(k)\left[1-\frac{m+n}{N}\right]\sqrt{mm}\,\delta_{m',m-1}\delta_{n',n-1}\,.$$

(3) We obtain nonzero off-diagonal matrix elements having $m'=m+1$ and $n'=n+1$ when (a) $\mathbf{R}$ is one of $\{\mathbf{R}_i'\}$ and $\mathbf{R}'$ one of $\{\mathbf{r}_i'\}$, (b) $\mathbf{R}$ is one of $\{\mathbf{r}_i\}$ and $\mathbf{R}'$ one of $\{\mathbf{R}_i'\}$. We obtain

$$\frac{d}{2}\gamma(k)\left[1-\frac{m+n}{N}\right]\sqrt{(m+1)(n+1)}\delta_{m',m+1}\delta_{n',n+1}\,.$$

Collecting all the terms contributing to the matrix elements of the second terms of (1.2), we obtain

$$\langle m,n|H_2|m,n\rangle=-\left[1-\frac{m+n}{N}\right]^2+\frac{d(m+n)}{2}[1-\gamma(k)]\left[1-\frac{m+n}{N}\right], \quad \text{(A10)}$$

$$\langle m-1,n-1|H_2|m,n\rangle=\frac{d}{2}\sqrt{mn}\left[1-\frac{m+n}{N}\right]\gamma(k), \quad \text{(A11)}$$

$$\langle m+1,n+1|H_2|m,n\rangle=\frac{d}{2}\sqrt{(m-1)(n+1)}\times\left[1-\frac{m+n}{N}\right]\gamma(k)\,. \quad \text{(A12)}$$

Adding the terms (A5)–(A7) and (A10)–(A12) we obtain

$$\langle m,n|H-E_\phi|m,n\rangle=d(m+n)\left[1-\frac{3}{4}\frac{m+n}{N}\right], \quad \text{(A13)}$$

$$\langle m-1,n-1|H|m,n\rangle=d\sqrt{mn}\left[1-\frac{m+n}{N}\right]\gamma(k), \quad \text{(A14)}$$

$$\langle m+1,n+1|H|m,n\rangle=d\sqrt{(m+1)(n+1)}\times\left[1-\frac{m+n}{N}\right]\gamma(k), \quad \text{(A15)}$$

where $E_\phi\equiv\langle\phi|H|\phi\rangle$ is given by Eq. (2.8).

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