Coupled-cluster approximation in momentum space

F. Cornu
Laboratoire de Physique Théorique ENSLAPP, École Normale Supérieure de Lyon, 46 allée d'Italie, F-69364 Lyon, Cédex 07, France

Th. Jolicoeur
Service de Physique Théorique, C.E. Saclay, F-91191 Gif-sur-Yvette Cédex, France

J. C. Le Guillou
Laboratoire de Physique Théorique ENSLAPP, Université de Savoie et Institut Universitaire de France, Boîte Postale 110, F-74941 Annecy-le-Vieux Cédex, France

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A simple coupled-cluster-type approximation is introduced, which generalizes in momentum (k) space a method recently presented in the literature for real space, and tested on the exactly solvable XXZ anisotropic quantum antiferromagnetic spin-$\frac{1}{2}$ chain. We implement our approximation in k space on the fermionized version of this model, and obtain improved results, with remarkable quantitative and qualitative features.

I. INTRODUCTION

The coupled-cluster approximation (CCA) has been extensively used in a wide variety of fields ranging from quantum chemistry to nuclear physics.[1] Its application in quantum chemistry has proved to be especially successful: extremely accurate energies are given by the CCA, which is able to cope with correlation effects beyond the Hartree-Fock approximation. However, the CCA formulated in momentum space (k space) leads to very complicated calculations which necessitate the use of further and mostly uncontrolled approximations.[2]

Recently, several authors[3–7] have undertaken the application of the CCA to various problems involving strong correlations typical of solid-state physics. The application of a new coupled-cluster-type approximation in real space (x space) to quantum spin systems in one and two dimensions as well as to electronic models like the Hubbard model seems promising. At the expense of modest algebraic manipulations, one gets accurate ground-state energies that compare well with variational or *ab initio* Monte Carlo results. This CCA in x space has been tested on the XXZ anisotropic quantum antiferromagnetic spin-$\frac{1}{2}$ chain. This model is exactly solvable using the Bethe ansatz.[8–10]

The aim of this paper is to present a new CCA in k space in the same spirit as the method in x space. We work on the fermionized version of the XXZ model. Our method is much simpler that the usual CCA in k space, whose complexity is well known. We shall show that our CCA in k space leads to better results for the XXZ model than the x-space treatment. We obtain very accurate results in a wide range of values of the anisotropy parameter, and our results exhibit a clear signature of the true phase transition from the antiferromagnetic to the ferromagnetic regime.

The outline of this article is as follows. In Sec. II we present a brief summary of the coupled-cluster approximation in general and of its recent version in x space for spin and electronic models. In Sec. III we apply this CCA in x space to the fermionized version of the anisotropic quantum antiferromagnetic spin-$\frac{1}{2}$ chain, and we compare our results with those of the same real-space approach on the spin model. In Sec. IV we present our CCA in k space on the fermionized model and discuss the results for the ground-state energy.

II. COUPLED-CLUSTER APPROXIMATIONS

Let H be the quantum-mechanical Hamiltonian operator under consideration, $|\Psi\rangle$ its true ground-state and E the corresponding eigenvalue. If H contains a noninteracting part H_0 with ground state $|\Phi\rangle$, one can relate these two wave functions by

$$|\Psi\rangle=[\exp S]|\Phi\rangle \ . \tag{1}$$

The strategy of the CCA is to compute S as a sum $\sum_n S_n$, where the operator S_n describes the excitation of a cluster of n particles (by particles we mean the excitations above $|\Phi\rangle$: they are not the true many-body excitations above $|\Psi\rangle$). Introducing

$$\tilde{H}=[\exp(-S)]H[\exp S] \ , \tag{2}$$

the Schrödinger equation leads to a set of coupled equations:

$$\langle\Phi|\tilde{H}|\Phi\rangle=E \ , \quad \langle n|\tilde{H}|\Phi\rangle=0 \ , \tag{3}$$

where $|n\rangle$ is a noninteracting state with n excitations.

The coupled-cluster approximation then takes into account only the first few S_n. For instance, in the case of a system of fermions where $|\Phi\rangle$ is a Fermi-sea wave function (and where the effect of S_1 is only to change the

single-particle orbitals that form the Slater determinant $|\Phi\rangle$), the lowest-order coupled-cluster approximation takes into account only S_2, expressed in k space as

$$S_2=\sum_{k_1,k_2,k_1',k_2'}\alpha(k_1,k_2,k_1',k_2')\psi_{k_1'}^{\dagger}\psi_{k_2'}^{\dagger}\psi_{k_1}\psi_{k_2} \tag{4}$$

where momenta k_1,k_2 are holelike and momenta k_1',k_2' are particlelike. This leads to complicated equations on which various further approximations must be made.[2]

However Roger and Hetherington[3,4] recently considered the CCA method for strongly interacting spins on a regular lattice and then proposed in x space a new CCA, which was subsequently developed by Bishop, Parkinson, and Xian.[5–7] The idea is to take into account in S all possible terms that involve spins within a domain of n adjacent sites, defining the so-called LSUBn scheme. In the first LSUB2 step, one retains in S the lowest two-spin excitations (lowest means excitations which flip nearest-neighbor spin pairs). The next LSUB4 step of the approximation is then to include in S the lowest four-spin excitations, with terms which flip four first neighbors, together with the next-to-lowest two-spin excitations, with terms which flip third-neighbor pairs, and so on.

This method has been tested[3–7] for the exactly solvable[8–10] XXZ anisotropic quantum antiferromagnet spin-$\frac{1}{2}$ chain. We shall detail this approach on the fermionized version of this model in the next section.

III. CCA IN x SPACE FOR THE FERMIONIZED HEISENBERG CHAIN

Using standard conventions,[11] the initial Hamiltonian for an XXZ spin-$\frac{1}{2}$ chain is

$$H=J\sum_n[-\tfrac{1}{2}(S_n^+S_{n+1}^-+S_n^-S_{n+1}^+)+\Delta S_n^zS_{n+1}^z], \tag{5}$$

where Δ is the exchange anisotropy. At $\Delta=1$ one has the Heisenberg SU(2)-symmetric model. After a Jordan-Wigner transformation, H can be written in terms of spinless fermion operators as

$$H=J\sum_n[-\tfrac{1}{2}(\psi_n^{\dagger}\psi_{n+1}+\psi_{n+1}^{\dagger}\psi_n)+\Delta(\psi_n^{\dagger}\psi_n-\tfrac{1}{2})(\psi_{n+1}^{\dagger}\psi_{n+1}-\tfrac{1}{2})], \tag{6}$$

where a spin up corresponds to the presence of a fermion and a spin down to the absence of a fermion, since $S_n^z=\psi_n^{\dagger}\psi_n-\frac{1}{2}$. The XY model obtained when $\Delta=0$ is then mapped on a free-fermionic model.

The coupled-cluster method of Refs. 3–7 in x space has been introduced on the spin formulation of Eq. (5). It is interesting to apply this method to the fermionized version of the model given by Eq. (6). For our bipartite chain, the $|\Phi\rangle$ state is here taken as the Néel antiferromagnetic state, which in the fermionic version has a fermion on each site i of sublattice A and no fermion on each site j of sublattice B.

The first step of the method is to consider in S only the lowest one-fermion excitations, where lowest means one-site hopping, with conservation of the number of fermions:

$$S=\alpha\sum_{i\in A}(\psi_{i-1}^{\dagger}+\psi_{i+1}^{\dagger})\psi_i\equiv\alpha O_1 \tag{7}$$

and a constant α. With the same transformation as in Eq. (2), one gets

$$\begin{aligned}&\tilde{\psi}_i=\psi_i\ ,\quad \tilde{\psi}_i^{\dagger}=\psi_i^{\dagger}-\alpha(\psi_{i-1}^{\dagger}+\psi_{i+1}^{\dagger})\ ,\quad i\in A\ ,\\&\tilde{\psi}_j=\psi_j+\alpha(\psi_{j-1}+\psi_{j+1})\ ,\quad \tilde{\psi}_j^{\dagger}=\psi_j^{\dagger}\ ,\quad j\in B\ .\end{aligned} \tag{8}$$

Using $\psi_i^{\dagger}|\Phi\rangle=0$ and $\psi_j|\Phi\rangle=0$, one gets

$$\tilde{H}|\Phi\rangle=J[-(\alpha+\tfrac{1}{2}\Delta)N/2+\tfrac{1}{2}(-1+2\Delta\alpha+3\alpha^2)O_1+\tfrac{1}{2}\alpha^2O_2-\Delta\alpha^2O_3]|\Phi\rangle\ , \tag{9}$$

where N is the number of sites of the whole lattice, and where

$$O_2\equiv\sum_{i\in A}(\psi_{i-3}^{\dagger}+\psi_{i+3}^{\dagger})\psi_i\ , \tag{10}$$

$$O_3\equiv\sum_{i\in A}(\psi_{i-3}^{\dagger}\psi_{i-2}\psi_{i-1}^{\dagger}+\psi_{i+3}^{\dagger}\psi_{i+2}\psi_{i+1}^{\dagger})\psi_i\ . \tag{11}$$

The ground-state energy by site in units of J is

$$\frac{E}{NJ}=-\tfrac{1}{2}(\alpha+\tfrac{1}{2}\Delta)\ . \tag{12}$$

The procedure is now to ignore the generated operators

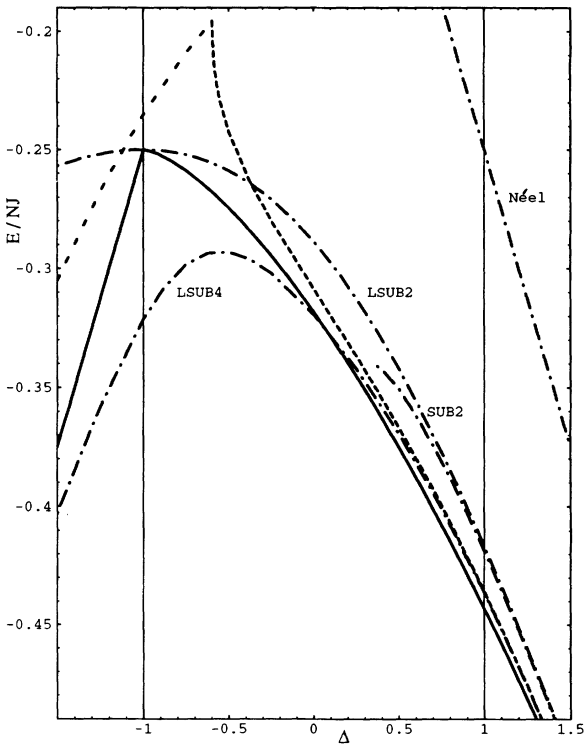

FIG. 1. Ground-state energy per spin for the anisotropic quantum antiferromagnet model in one dimension as a function of Δ: the solid curves are the exact results of Ref. 10; dashed curves are our results using Roger and Hetherington's method in x space on the fermionic version of the model; dot-dashed curves are the classical Néel result and results LSUB2, LSUB4, and SUB2 of Ref. 6 from CCA-type approximations in x space for the spin version of the model.

O_2 and O_3 in $\tilde{H}|\Phi\rangle$, which are not present in S, and to cancel the term involving O_1, which is present in S. This determines the constant α and gives a first approximation to E. As shown in Fig. 1, this approximation, which is identical to LSUB2 of Ref. 6 for the spin version of the model, is already a substantial improvement on the classical Néel result.

We can go a step further and take for S:

$$S=\alpha O_1+\beta O_2+\gamma O_3 \ , \tag{13}$$

containing, in addition to the lowest one-fermion excitations, the lowest two-fermion excitations, with two adjacent one-site hoppings, together with the next-to-lowest one-fermion excitations, with a three-site hopping, and where we take constant α, β, γ. With the new $\tilde{\psi}$ and $\tilde{\psi}^\dagger$ one gets

$$\tilde{H}|\Phi\rangle=J\{-(\alpha+\tfrac{1}{2}\Delta)N/2+\tfrac{1}{2}(-1+2\Delta\alpha+3\alpha^2+2\alpha\beta+2\beta^2-2\gamma)O_1+\tfrac{1}{2}(\alpha^2+4\alpha\beta+\gamma+4\Delta\beta)O_2$$
$$+[4\alpha\gamma-\beta\gamma+\Delta(-\alpha^2+2\alpha\beta+\gamma)]O_3+\cdots\}|\Phi\rangle \ , \tag{14}$$

ignoring more complicated operators that are also generated in this process. Cancellation of the O_1, O_2, O_3 terms in $\tilde{H}|\Phi\rangle$ determines α, β, γ, and one then obtains by Eq. (12) a second approximation for the ground-state energy. As shown in Fig. 1 this approximation is different from the corresponding LSUB4 of Ref. 6 for the spin version of the model. Though it presents quantitatively the same type of improvement, it has a more interesting qualitative behavior than the LSUB4: it has an end point at $\Delta_c \cong -0.6$, below which the energy becomes complex, its real part being shown in Fig. 1 for $\Delta<\Delta_c$. This behavior compares remarkably with the true antiferromagnetic-ferromagnetic transition of the exact solution of the spin system at $\Delta=-1$.

In the scheme of Refs. 3–7, one introduces recursively the operators generated at the previous order of approximation. In various examples, it appears that this strategy is much more tractable and fruitful than trying to solve first the lowest-order CCA equations with the most general ansatz for O_1 (e.g., $O_1=\sum_{i,j}\alpha_{ij}\psi_i^\dagger\psi_j$), and so on. At the expense of simplifying the O's, one is able to capture correlations involving a larger number of particles, albeit in a crude way.

IV. CCA IN k SPACE FOR THE FERMIONIZED HEISENBERG CHAIN

Let us now present our generalization for k space of the Roger and Hetherington method. By Fourier transformation the Hamiltonian (6) in terms of spinless fermion operators reads:

$$H=-J\sum_k(\cos k+\Delta)\psi_k^\dagger\psi_k+\frac{N}{4}J\Delta$$
$$+J\Delta\frac{1}{2N}\sum_{k,k'}\sum_t[\cos t-\cos(k-k'+t)]$$
$$\times\psi_{k+t}^\dagger\psi_{k'-t}^\dagger\psi_{k'}\psi_k \ , \tag{15}$$

where $\sup(-\pi-k,k'-\pi)\le t\le\inf(\pi-k,k'+\pi)$.

The noninteracting ($\Delta=0$) ground-state $|\Phi\rangle$ is the Fermi-sea wave function of free Jordan-Wigner fermions. The effect of S_1 in (1) being only to change the single-particle orbitals of the Slater determinant, and since in view of further applications of the method we want here to test its simplest version, we do not attempt to optimize our starting point and thus directly consider an S_2-type contribution to S.

As two-particle-hole excitations, we consider in S_2 particle and hole momenta within an interval of width Λ (ranging from 0 to $\pi/2$) near the Fermi surface (at $k_F=\pm\pi/2$). There are *normal* terms, with one particle on each side of the Fermi surface:

$$\text{(N1)}\quad \psi_{p_1+\theta}^\dagger\psi_{p_2-\theta}^\dagger\psi_{p_2}\psi_{p_1} \ ,$$
$$\frac{\pi}{2}-\Lambda<p_1\le\frac{\pi}{2} \ , \quad -\frac{\pi}{2}\le p_2<-\frac{\pi}{2}+\Lambda \ , \tag{16}$$
$$\text{(N2)}\quad \psi_{p_1+\theta}^\dagger\psi_{p_1'-\theta}^\dagger\psi_{p_1'}\psi_{p_1} \ , \quad \Lambda>\pi/3 \ ,$$
$$\frac{\pi}{2}-\Lambda<p_1'<p_1\le\frac{\pi}{2} \ , \tag{17}$$

together with *umklapp* terms, with both particles on the same side of the Fermi surface, and large momentum transfer:

$$\text{(U1)}\quad \psi_{p_1-\theta}^\dagger\psi_{p_1'-(2\pi-\theta)}^\dagger\psi_{p_1'}\psi_{p_1} \ ,$$
$$\frac{\pi}{2}-\Lambda<p_1'<p_1\le\frac{\pi}{2} \ , \tag{18}$$
$$\text{(U2)}\quad \psi_{p_1+\theta}^\dagger\psi_{p_2+(2\pi-\theta)}^\dagger\psi_{p_2}\psi_{p_1} \ , \quad \Lambda>\pi/3 \ ,$$
$$\frac{\pi}{2}-\Lambda<p_1\le\frac{\pi}{2} \ , \quad -\frac{\pi}{2}\le p_2<-\frac{\pi}{2}+\Lambda \ , \tag{19}$$

(including in U1 and U2 the term symmetric with respect to zero momentum).

In the CCA in x space, the criterion to select relevant terms in S was the size of the hopping on the chain. In the case of k space, let us compare the various normal and umklapp terms with respect to the size of Λ and of momentum transfer. Only the N1-type terms allow small momentum transfers, since one has for these terms $0<\theta<2\Lambda$, while one has $\pi-\Lambda<\theta<\pi+\Lambda$ for U1-type terms and $\pi-\Lambda<\theta<2\Lambda$ for N2- and U2-type terms. If Λ is bigger than $(\pi/3)$ all types of terms are nevertheless to be considered together since they all allow momentum transfers of the same order. However, if Λ is smaller than $(\pi/3)$ the N1-type terms give momentum transfers always smaller than those of the U1-type terms.

In the spirit of the method in x space, we do not take the most general S_2, but we only retain in S the two-particle-two-hole excitations of the N1 type with $\Lambda \leq \pi/3$, allowing consistently the smallest momentum transfers, and with a constant coefficient α:

$$S=\alpha\frac{1}{N}\sum_{p_1,p_2}\sum_{\theta}\psi^{\dagger}_{p_1+\theta}\psi^{\dagger}_{p_2-\theta}\psi_{p_2}\psi_{p_1}\ , \tag{20}$$

where

$$\frac{\pi}{2}-\Lambda<p_1\leq\frac{\pi}{2}\ ,\quad -\frac{\pi}{2}\leq p_2<-\frac{\pi}{2}+\Lambda\ ,$$

$$\sup\left[\frac{\pi}{2}-p_1\ ,\ \frac{\pi}{2}+p_2\right]<\theta\leq\inf\left[\frac{\pi}{2}+\Lambda-p_1\ ,\ \frac{\pi}{2}+\Lambda+p_2\right]\ .$$

With the same transformation as in Eq. (2) and using Eq. (20) one then gets with hole momentum p and particle momentum q:

$$\tilde{\psi}_p=\psi_p\ , \tag{21}$$

$$\tilde{\psi}^{\dagger}_p=\psi^{\dagger}_p+\alpha\delta_p^{-\Lambda}\frac{1}{N}\sum_{p_1,\theta_1}\psi^{\dagger}_{p_1+\theta_1}\psi^{\dagger}_{p-\theta_1}\psi_{p_1}-\alpha\delta_p^{+\Lambda}\frac{1}{N}\sum_{p_2,\theta_2}\psi^{\dagger}_{p+\theta_2}\psi^{\dagger}_{p_2-\theta_2}\psi_{p_2}\ , \tag{22}$$

where

$$\delta_p^{-\Lambda}=\theta\left[p+\frac{\pi}{2}\right]\theta\left[-\frac{\pi}{2}+\Lambda-p\right]\ ,$$

$$\sup\left[\frac{\pi}{2}-p_1\ ,\ \frac{\pi}{2}+p\right]<\theta_1\leq\inf\left[\frac{\pi}{2}+\Lambda-p_1\ ,\ \frac{\pi}{2}+\Lambda+p\right]\ ,$$

$$\delta_p^{+\Lambda}=\theta\left[\frac{\pi}{2}-p\right]\theta\left[p+\Lambda-\frac{\pi}{2}\right]\ ,$$

$$\sup\left[\frac{\pi}{2}-p\ ,\ \frac{\pi}{2}+p_2\right]<\theta_2\leq\inf\left[\frac{\pi}{2}+\Lambda-p\ ,\ \frac{\pi}{2}+\Lambda+p_2\right]\ ;$$

$$\tilde{\psi}^{\dagger}_q=\psi^{\dagger}_q\ , \tag{23}$$

$$\tilde{\psi}_q=\psi_q+\alpha\delta_q^{+\Lambda}\frac{1}{N}\sum_{p_2,\tau_2}\psi^{\dagger}_{p_2-\tau_2}\psi_{p_2}\psi_{q-\tau_2}-\alpha\delta_q^{-\Lambda}\frac{1}{N}\sum_{p_1,\tau_1}\psi^{\dagger}_{p_1+\tau_1}\psi_{q+\tau_1}\psi_{p_1}\ , \tag{24}$$

where

$$\delta_q^{+\Lambda}=\theta\left[q-\frac{\pi}{2}\right]\theta\left[\frac{\pi}{2}+\Lambda-q\right]\ ,$$

$$\sup\left[-\frac{\pi}{2}+q\ ,\ \frac{\pi}{2}+p_2\right]\leq\tau_2\leq\inf\left[-\frac{\pi}{2}+\Lambda+q\ ,\ \frac{\pi}{2}+\Lambda+p_2\right]\ ,$$

$$\delta_q^{-\Lambda}=\theta\left[-\frac{\pi}{2}-q\right]\theta\left[q+\Lambda+\frac{\pi}{2}\right]\ ,$$

$$\sup\left[\frac{\pi}{2}-p_1\ ,\ -\frac{\pi}{2}-q\right]\leq\tau_1\leq\inf\left[\frac{\pi}{2}+\Lambda-p_1\ ,\ -\frac{\pi}{2}+\Lambda-q\right]\ .$$

One can then simplify $\tilde{H}|\Phi\rangle$. The ground-state energy by site in units of J is given by

$$\frac{E}{NJ}=-\frac{1}{\pi}-\frac{\Delta}{\pi^2}+\frac{\Delta}{4\pi^2}\Lambda^2F(\Lambda,\Delta)\ , \tag{25}$$

where

$$F(\Lambda,\Delta)=\bar{\alpha}(\Lambda,\Delta)\frac{32}{\Lambda^3}\left[\cos\frac{\Lambda}{2}\right]^2(\Lambda-\sin\Lambda)\ , \tag{26}$$

with $\bar{\alpha}(\Lambda,\Delta)\equiv(\Lambda/4\pi)\alpha$. As in the case of x space, one tries to determine $\bar{\alpha}(\Lambda,\Delta)$ by canceling a contribution to $\tilde{H}|\Phi\rangle$ of the type $S|\Phi\rangle$. However, contrary to what

happens in x space, the numerous contributions to $\tilde{H}|\Phi\rangle$ of the type $\psi^{\dagger}_{p_1+\theta}\psi^{\dagger}_{p_2-\theta}\psi_{p_2}\psi_{p_1}|\Phi\rangle$ appear summed over the momenta with momentum-dependent weights and thus do not give a term proportional to $S|\Phi\rangle$ with our S given by Eq. (20). But what we can do is to determine the limiting value $\bar{\alpha}(0,\Delta)$.

To show this point, let us illustrate the procedure on a typical contribution appearing in $\tilde{H}|\Phi\rangle$:

$$-2J\Delta\alpha\frac{1}{N^2}\sum_{p_1,p,q',\tau_1}[\cos(q'+\tau_1-p)-\cos\tau_1]\psi^{\dagger}_{p_1+\tau_1}\psi^{\dagger}_{p-\tau_1}\psi_p\psi_{p_1}|\Phi\rangle\ , \tag{27}$$

where

$$\frac{\pi}{2}-\Lambda<p_1<\frac{\pi}{2}\ ,\quad -\frac{\pi}{2}<p<-\frac{\pi}{2}+\Lambda\ ,\quad -\frac{\pi}{2}-\Lambda<q'<-\frac{\pi}{2}\ ,$$

$$\sup\left[\frac{\pi}{2}-p_1\ ,\ -q'-\frac{\pi}{2}\ ,\ \frac{\pi}{2}+p\right]<\tau_1<\inf\left[\frac{\pi}{2}-p_1+\Lambda\ ,\ -q'-\frac{\pi}{2}+\Lambda\ ,\ \frac{\pi}{2}+p+\Lambda\right]\ .$$

When Λ is small one can approximate (27) by:

$$-2J\Delta\alpha\left[\frac{1}{N^2}\sum_{p_1,p,q',\tau_1}[\cos(q'+\tau_1-p)-\cos\tau_1]\right]\psi^{\dagger}_{\pi/2+\Lambda/2}\psi^{\dagger}_{-\pi/2-\Lambda/2}\psi_{-\pi/2+\Lambda/2}\Psi_{\pi/2-\Lambda/2}|\Phi\rangle$$

$$=-2J\Delta\frac{1}{\pi}(-1+\Lambda^2+4\cos\Lambda-3\Lambda^2\cos\Lambda-3\cos2\Lambda-2\Lambda\sin\Lambda)$$

$$\times\alpha\frac{N^2}{(2\pi)^3}\psi^{\dagger}_{\pi/2+\Lambda/2}\psi^{\dagger}_{-\pi/2-\Lambda/2}\psi_{-\pi/2+\Lambda/2}\psi_{\pi/2-\Lambda/2}|\Phi\rangle\ , \tag{28}$$

which is proportional to $S|\Phi\rangle$ given in the same approximation by

$$\alpha\frac{2}{3}\frac{N^2\Lambda^3}{(2\pi)^3}\psi^{\dagger}_{\pi/2+\Lambda/2}\psi^{\dagger}_{-\pi/2-\Lambda/2}\psi_{-\pi/2+\Lambda/2}\psi_{\pi/2-\Lambda/2}|\Phi\rangle\ . \tag{29}$$

When Λ is small, we use the same procedure for all the contributions to $\tilde{H}|\Phi\rangle$ of the type $\psi^{\dagger}_{p_1+\theta}\psi^{\dagger}_{p_2-\theta}\psi_{p_2}\psi_{p_1}|\Phi\rangle$ and we thus obtain by summing up these contributions a term proportional to $S|\Phi\rangle$. Following the same method as in the CCA in x space, we cancel this term and thus obtain a second-order equation for $\bar{\alpha}(\Lambda,\Delta)$ whose solution is:

$$\bar{\alpha}(\Lambda,\Delta)=[-B+\mathrm{sgn}(\Delta)\sqrt{B^2-4AC}\,]/2A\ , \tag{30}$$

with

$$A\equiv\frac{128}{3\Lambda^5}\left[\cos\frac{\Lambda}{2}\right]^2(-66\Lambda+\Lambda^3-30\Lambda\cos\Lambda+96\sin\Lambda)\ ,$$

$$B\equiv-\frac{8}{\Lambda^4}[-40+12\Lambda^2+48\cos\Lambda-12\Lambda^2\cos\Lambda$$

$$-8\cos2\Lambda+4\Lambda\sin2\Lambda]$$

$$+\frac{4\pi}{\Delta}\frac{8}{\Lambda^4}\left[(4+\Lambda^2)\left[\sin\frac{\Lambda}{2}\right]^2-\Lambda\sin\Lambda\right]\ ,$$

$$C\equiv\frac{32}{\Lambda^3}\left[\cos\frac{\Lambda}{2}\right]^2(\Lambda-\sin\Lambda)\ .$$

This gives an approximation for $\bar{\alpha}(\Lambda,\Delta)$ when Λ is small. If we use this value (30) in Eq. (26), we obtain an expression for the ground-state energy, and it is reasonable to determine Λ by minimization of this energy for each value of Δ. However, the corresponding values of Λ are between $\pi/3$ and $\pi/2$. Thus Λ is not small and furthermore outside the range $0-\pi/3$ of our choice (20) of S, and the method fails.

Nevertheless, the above procedure exactly determines $\bar{\alpha}$ in the limit where Λ goes to zero, and we obtain from Eq. (30) the value:

TABLE I. Ground-state energy per spin for the anisotropic quantum antiferromagnet model in one dimension as a function of Δ: the exact results of Ref. 10, our results from Eq. (33) using our coupled-cluster approximation in k space on the fermionic version of the model, and the corresponding percentages of error.

Δ	Exact energy	Energy from (33)	Error (%)
−1.	−0.25	−0.261 1	−4.5
−0.75	−0.258 8	−0.264 2	−2.1
−0.5	−0.274 5	−0.275 9	−0.51
−0.25	−0.294 62	−0.294 72	−0.034
−0.1	−0.308 434	−0.308 429	0.001 6
0.1	−0.328 692	−0.328 663	0.008 7
0.25	−0.345 18	−0.344 91	0.079
0.5	−0.375	−0.373 4	0.43
0.75	−0.407 7	−0.403 1	1.1
1.	−0.443 1	−0.433 6	2.2
1.25	−0.481 6	−0.464 6	3.5
1.5	−0.523 4	−0.496 1	5.2

$$\bar{\alpha}(0,\Delta)=\frac{5}{18}\left\{\left[2+\frac{\pi}{\Delta}\right]-\mathrm{sgn}(\Delta)\left[\left[2+\frac{\pi}{\Delta}\right]^2+\frac{18}{5}\right]^{1/2}\right\}. \quad (31)$$

From Eq. (26) we are led to the following formula:

$$\Lambda^2 F(\Lambda,\Delta)=\Lambda^2\bar{\alpha}(0,\Delta)^{\frac{16}{3}} + (\text{unknown terms of order } \Lambda^4) . \quad (32)$$

Since $\Lambda\le\pi/3$ and $\Delta\bar{\alpha}(0,\Delta)$ is negative, the energy (25) with the Λ^2 term of Eq. (32) is minimum at $\Lambda=\pi/3$. Thus we fix Λ by minimization of this energy and finally obtain the approximation:

$$\frac{E}{NJ}=-\frac{1}{\pi}-\frac{\Delta}{\pi^2}+\frac{10}{243}\Delta\left\{\left[2+\frac{\pi}{\Delta}\right]-\mathrm{sgn}(\Delta)\left[\left[2+\frac{\pi}{\Delta}\right]^2+\frac{18}{5}\right]^{1/2}\right\}. \quad (33)$$

As shown in Table I and Figs. 2 and 3, this is a quite good approximation to the exact result in the whole range $-1\le\Delta\le+1$, much better than the corresponding results LSUB4 and SUB2 of CCA-type approximations in x space[6] for the spin version of the model. Our result is even much better for $-1\le\Delta\le 0$ than the elaborated LSUB8 of Ref. 7. Let us also note the important improvement to the Hartree-Fock energy $-(1/\pi)-(\Delta/\pi^2)$ in this model. The factor $(2\Delta+\pi)$ that appears in Eq. (33) is the Fermi-velocity renormalization factor that is seen also in the Hartree-Fock treatment[12] of the *XXZ* chain. It now appears in a manner signaling a partial summation of perturbation theory.

Above $\Delta=1$ our result for the ground-state energy slowly worsens, and its asymptotic behavior, though having the correct $-\Delta$ dependence, is only -0.1325Δ, to be compared with the exact[13] -0.25Δ large-Δ Ising limit. This can be traced to the absence in our procedure of the umklapp terms, which are known[11] to drive the transition occurring at $\Delta=1$.

On the other hand, it is interesting to write the $\Delta\to 0$ expansion of Eq. (33):

$$\frac{E}{NJ}=-\frac{1}{\pi}-\frac{\Delta}{\pi^2}-\frac{2}{27}\frac{\Delta^2}{\pi}+\cdots = -\frac{1}{\pi}-\frac{\Delta}{\pi^2}-0.0236\Delta^2+\cdots , \quad (34)$$

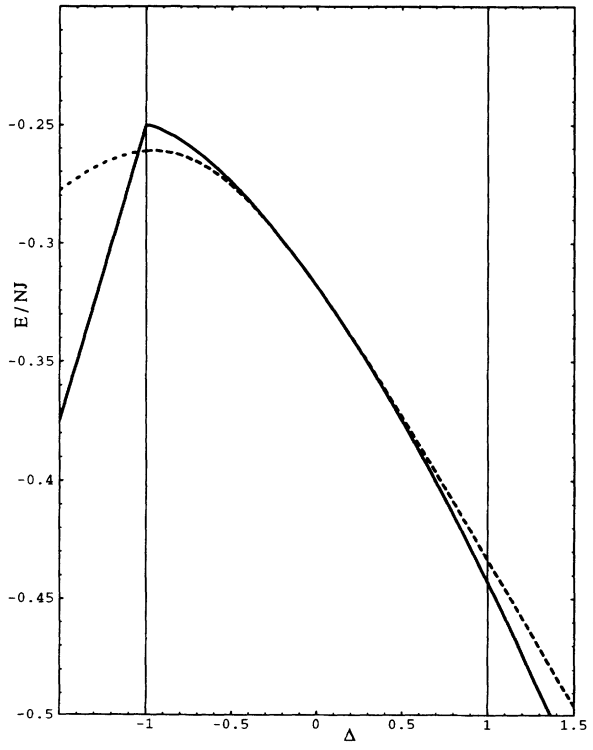

FIG. 2. Ground-state energy per spin for the anisotropic quantum antiferromagnet model in one dimension as a function of Δ: the solid curves are the exact results of Ref. 10; dashed curves are from our result (33) using our coupled-cluster approximation in k space on the fermionic version of the model.

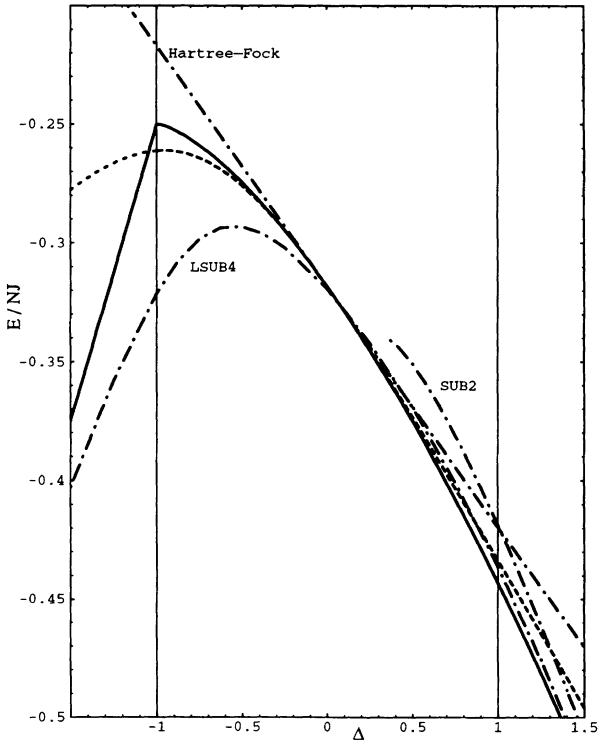

FIG. 3. Ground-state energy per spin for the anisotropic quantum antiferromagnet model in one dimension as a function of Δ: the solid curves are the exact results of Ref. 10; dashed curves are from our result (33) using our coupled-cluster approximation in k space on the fermionic version of the model; dot-dashed curves are the Hartree-Fock result and the best results LSUB4 and SUB2 of Ref. 6 from CCA-type approximations in x space for the spin version of the model.

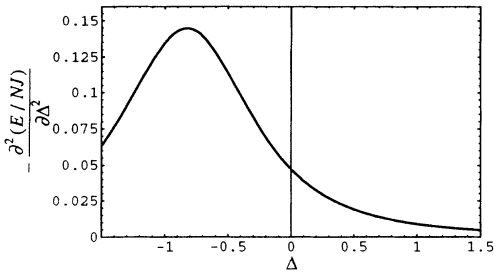

FIG. 4. Second derivative of the ground-state energy given by Eq. (33) as a function of Δ.

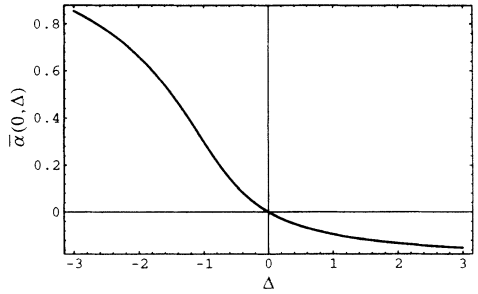

FIG. 5. Curve of $\bar{\alpha}(0,\Delta)$ given by Eq. (31) as a function of Δ.

which compares quite remarkably with the same limit of the exact result:

$$\frac{E}{NJ} = -\frac{1}{\pi} - \frac{\Delta}{\pi^2} - \left[\frac{4}{3\pi^2} - \frac{1}{18}\right]\frac{\Delta^2}{\pi} + \cdots$$
$$= -\frac{1}{\pi} - \frac{\Delta}{\pi^2} - 0.0253\Delta^2 + \cdots . \quad (35)$$

Another remarkable feature of Eq. (33) is the change of regime when Δ decreases towards -1: our approximation for the ground-state energy has a maximum at $\Delta = -0.96\ldots$, very near $\Delta = -1$, where the exact solution also has a maximum when it undergoes a phase transition from the antiferromagnetic to the ferromagnetic regime. More precisely, we present in Fig. 4 the second derivative $-\partial^2(E/NJ)/\partial\Delta^2$ of the ground-state energy with respect to the coupling Δ. This quantity corresponds to the specific heat in $T \neq 0$ phase transitions. It has a maximum at $\Delta = -0.83\ldots$. This signature of a transition is to be compared with the behavior of the exact corresponding quantity, which is zero for $\Delta < -1$ (the ferromagnetic phase) and rapidly decreases from infinity when Δ increases from -1.

Let us note that Eq. (33) cannot be compared with the exact solution of the spin model when $\Delta < -1$, since in the fermionic formulation we stay in the sector of total S_z equal to zero (mean site occupancy equals $\frac{1}{2}$).

The above change of regime of the ground-state energy, which thus can be related to the true phase transition, corresponds to the behavior of $\bar{\alpha}(0,\Delta)$ which, as shown in Fig. 5, presents an inflection point near $\Delta = -1$. Let us also note that the ground-state wave function is given in our approximation by:

$$|\Psi\rangle = \exp\left[12\,\bar{\alpha}(0,\Delta) \times \frac{1}{N}\sum_{p_1,p_2,\theta} \psi^\dagger_{p_1+\theta}\psi^\dagger_{p_2-\theta}\psi_{p_2}\psi_{p_1}\left(\Lambda = \frac{\pi}{3}\right)\right]|\Phi\rangle \quad (36)$$

which coherently reduces to $|\Phi\rangle$ for $\Delta = 0$.

In conclusion, our new and simple coupled-cluster approximation in k space successfully passes the test of the exactly solvable XXZ quantum spin-$\frac{1}{2}$ chain, both quantitatively and qualitatively. Applications to other situations can thus be considered and some are under investigation.

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