Critical properties of a one-dimensional frustrated quantum magnetic model

P. Sen and B. K. Chakrabarti
Saha Institute of Nuclear Physics, Sector-1, Block-AF, Bidhannagar, Calcutta 700 064, India
(Received 1 October 1990)

The phase diagram and ground-state energy along the phase boundary are estimated for a one-dimensional spin-$\frac{1}{2}$ Ising model with competing nearest- and next-nearest-neighbor interactions in presence of a transverse field. We have used a self-consistent Hartree-Fock approximation and a real-space renormalization-group treatment. The phase diagram (of this one-dimensional quantum model) is compared to that of a two-dimensional classical axial next-nearest-neighbor model and the Lifshitz point is located. The estimated ground-state energy, along the critical line, is seen to reduce considerably (like the critical fields), with increasing competition, showing the effect of frustration.

I. INTRODUCTION

The study of quantum systems with frustration and competing interactions has been of much current interest. The question of stability of various modulated (commensurate and incommensurate) phases of classical magnetic systems with competing interactions, under the effect of quantum fluctuations, has been raised in several recent studies.[1-3] The model that has been especially studied is a one-dimensional Ising model with competing nearest- and next-nearest-neighbor interactions,[4] and the quantum fluctuation is brought about by putting the system in a (noncommuting) transverse field.[1-3] On the other hand, the investigations on the nature of the ground (and also excited) states of the quantum antiferromagnetic system also led to the study of the effects of frustration in quantum magnetic systems.[5-9] These studies have recently become quite important in the context of investigations of a possible magnetic origin of high-temperature superconductivity.[6,7] These investigations[1-3,5-9] are indeed complementary to each other. In fact, in the first group of models,[1-3] the cooperative interaction is between the (classical) Ising spins, while for the second group,[5-9] all the terms in the cooperative interaction are noncommuting. However, we believe that the simplest of such quantum frustrated systems should really be the first group of models[1-3] mentioned above, and we therefore consider such a system at zero temperature. The Hamiltonian of this system[1,2] is

$$H = H_{xx} + H_q \ , \tag{1}$$

where

$$H_{xx} = -J_1 \sum_i S_i^x S_{i+1}^x - J_2 \sum_i S_i^x S_{i+2}^x \ ,$$

$$H_q = -\Gamma \sum_i S_i^z$$

with $J_1 > 0$ and $J_2 < 0$ (to ensure competition or frustration). Without the transverse field ($\Gamma = 0$), the Hamiltonian describes the axial next-nearest-neighbor Ising (ANNNI) chain[4] which has exactly known ground state: the ferromagnetic phase for $\kappa \equiv |J_2|/J_1 < 0.5$ and the antiphase (two spins up and two spins down, respectively, phase denoted by $\langle 2 \rangle$) for $\kappa > 0.5$. $\kappa = 0.5$ is an infinitely degenerate point where the effect of frustration is most felt.

The zero-temperature phase diagram of a quantum spin-$\frac{1}{2}$ Ising system in d dimensions is usually related to the corresponding classical system in $d+1$ dimensions.[10] Thus, the phase diagram of (1) may be compared to that of the two-dimensional (2D) ANNNI model. The phase diagram of the 2D ANNNI model[4] consists of a ferromagnetic phase, an antiphase, and a paramagnetic phase which goes down to zero temperature at $\kappa = 0.5$. There are considerable indications for the existence of a floating (incommensurate) phase (where the correlation decays following a power law as in the XY model) just above the $\langle 2 \rangle$ phase,[11,12] although the existence is not yet established.[4] It is also debated whether there is a Lifshitz point at finite temperature. These questions about the phase diagram of our system described by (1) have already been addressed.[2,3] Here, however, we are interested, in particular, to see whether the zero-temperature quantum fluctuation is able to destroy the ordered state, especially at the fully frustrated point $\kappa = 0.5$, since this happens in the corresponding classical Hamiltonian due to thermal fluctuations. We have also estimated the ground-state energies near the order-disorder phase boundaries.

Frustrated antiferromagnetic Heisenberg models with anisotropy, in general [i.e., H_q also includes cooperative interaction in the y and z directions (and $\Gamma = 0$) with competition between nearest- and next-nearest-neighbor interactions], indeed exhibit[5-9] that the zero-point quantum fluctuation can destroy the Néel order, so that the quantum-spin-liquid phase is argued to be the ground state of that system. For a special model,[5] in which the second-neighbor interaction is exactly half of that of the first neighbor, the (twofold degenerate) dimer phase has been shown to be the exact ground state. It is therefore interesting to find out whether the effect of zero-point (transverse) quantum fluctuation in the frustrated Ising system (1) at $\kappa = 0.5$ can also destroy order, and to inves-

tigate the (spin liquid, dimer, or otherwise) nature of the ground state there.

The model (1) has already been studied with the use of some approximate methods. For the spin-$\frac{1}{2}$ ($S=\frac{1}{2}$) case using the Jordan-Wigner transformation, the Hamiltonian can be diagonalized[1] by approximating a four-fermion term (arising from the second-neighbor interaction) by a two-fermion one. Here we have a Lifshitz point at a finite value of Γ, and a first-order transition at $\kappa=0.5$. However, this method could not give a vanishing Γ value for the Lifshitz point because the approximation for the four-fermion term assumes $\Gamma\neq 0$. The $1/S$ corrections to the $S\rightarrow\infty$ limit also results[2] in a Lifshitz point at finite Γ and the phase diagram has some qualitative similarity with[4] that of the 3D (and not 2D) ANNNI model. In this paper, we improve upon the treatment used by Sen and Chakrabarti[1] (henceforth referred to as I) by treating the four-fermion term self-consistently, following the scheme used by Wolf and Zittarz[13] in the case of an antiferromagnetic Heisenberg chain. The same approximation gives an approximate value of the ground-state energy along the critical line. We also perform a real-space renormalization-group (RSRG) study (using the truncation method) to get a rough estimate of the critical field as well as the ground-state energy of the system and compare these values with those obtained from the previous self-consistent treatment. Our methods, as will be seen later, are, however, practically restricted to cases with $\kappa\leq 0.5$.

II. HARTREE-FOCK APPROXIMATION: CRITICAL FIELD AND GROUND-STATE ENERGY

In this section, we study the model (1) using a Hartree-Fock approximation of the corresponding fermion model. Using the Jordan-Wigner transformation,[14] the Hamiltonian (1) can be written in terms of fermion operators c_i and $c_i^\dagger$ as[1]

$$H_f=-\Gamma\sum_i (c_i^\dagger c_i-\tfrac{1}{2})-J_1\sum_i (c_i^\dagger-c_i)(c_{i+1}^\dagger+c_{i+1})/4 -J_2\sum_i (c_i^\dagger-c_i)(1-2c_{i+1}^\dagger c_{i+1})(c_{i+2}^\dagger+c_{i+2})/4 , \tag{2}$$

where

$$S_i^x=\left[c_i\exp\left[-i\pi\sum_{j<i}c_j^\dagger c_j\right]+c_i^\dagger\exp\left[i\pi\sum_{j<i}c_j^\dagger c_j\right]\right]\Big/2 ,$$

$$S_i^z=c_i^\dagger c_i-\tfrac{1}{2} .$$

The Hamiltonian in this form cannot be diagonalized because of the J_2 (four-fermion) term. In I, the quantity $(1-2c_i^\dagger c_i)$ appearing in the last term of (2) was approximately taken to be a constant. With this approximation, the resultant Hamiltonian H_0, thus obtained could be diagonalized. In general, H_0 is of the form

$$H_0=-\Gamma'\sum_i (c_i^\dagger c_i-\tfrac{1}{2}) + \left[-J_1'\sum_i c_i^\dagger c_{i+1}^\dagger - J_{11}'\sum_i c_i^\dagger c_{i+1}+J_2'\sum_i c_i^\dagger c_{i+2}^\dagger +J_{22}'\sum_i c_i^\dagger c_{i+2}+\text{H.c.}\right] . \tag{3}$$

When the Hamiltonian H_f in (2) is treated self-consistently and the Hamiltonian is effectively written in the form of H_0, the renormalized parameters are given by (see Appendix A)

$$\Gamma'=\Gamma-J_2(\langle c_i^\dagger c_{i+2}\rangle+\langle c_i^\dagger c_{i+2}^\dagger\rangle) , \tag{4a}$$

$$J_1'=J_1+4J_2(\langle c_i^\dagger c_{i+1}^\dagger\rangle+\langle c_i^\dagger c_{i+1}\rangle) , \tag{4b}$$

$$J_2'=J_2[2(\langle c_i^\dagger c_i\rangle-\tfrac{1}{2})] , \tag{4c}$$

$$J_{11}'=J_1' ,$$

and

$$J_{22}'=J_2' .$$

The above results can also be obtained alternatively by employing a random-phase approximation- (RPA) like approximation to the Hamiltonian (2) ($\langle ABC\rangle=\langle AB\rangle\langle C\rangle+\langle AC\rangle\langle B\rangle+\langle A\rangle\langle BC\rangle$ with proper signatures following fermion commutation rules) and collecting the equivalent terms.

With $\kappa'=|J_2'|/J_1'$ the phase boundaries, as obtained in I (for H_0), are given by

$$\Gamma'/J_1'=\kappa'/2 \tag{5a}$$

for the paramagnetic to modulated phase boundary ($\kappa'>0.5$) and for the paramagnetic to ferromagnetic phase boundary ($\kappa'<0.5$),

$$\Gamma'/J_1'=\tfrac{1}{2}-\kappa'/2 . \tag{5b}$$

Using relation (4), these surfaces map onto two corresponding surfaces in the (Γ,κ) plane. For $\kappa\leq 0.5$, the para- to ferromagnetic boundary is given by

$$\kappa=-2\pi\kappa'/(2\{\alpha[1-\tfrac{1}{2}(1-\kappa')]+[-4\kappa'(1-\kappa')+1]^{1/2}/(1-\kappa')\}+4\kappa'\alpha) , \tag{6}$$

$$\Gamma/J_1=\alpha(1-2\kappa')/(2\{\alpha[1-\tfrac{1}{2}(1-\kappa')]+[-4\kappa'(1-\kappa')+1]^{1/2}/(1-\kappa')\}+4\kappa'\alpha) \tag{7}$$

($\kappa\leq 0.5$ as $\kappa'\leq 0.5$ here). The expression for α and the details of calculations are given in Appendix B.

The other phase boundary (paramagnetic to modulated) cannot be mapped here because all values of κ corresponding to $\kappa'>0.5$ (where we get the paramagnetic to modulated phase boundary in I for H_0) give $\kappa=0.5$ and $\Gamma=0$ there (see Appendix B). This apparently signifies that the modulated to paramagnetic phase transition only

exists at $\kappa=0.5$ and the paramagnetic phase already exists at $\Gamma=0$ (i.e., the infinitely degenerate spin-flipped states at $\kappa=0.5$ immediately become unstable at the onset of a transverse field). What happens for $\kappa>0.5$ is not clear; it might be that the paramagnetic phase condenses into some phase other than any ordered phase which might be simply looked upon as a mode softened phase (from paramagnetic); it may be some floating phase as well. The known result that there should be a paramagnetic to modulated transition at $\kappa\rightarrow\infty$ cannot be obtained from this method since the ratio $\kappa\rightarrow\infty$ cannot be mapped from any ratio of κ'.

In fact, the existence of a floating phase can be easily justified for this model at zero temperature, although its location cannot be found as easily. Using Gaussian functional averages[15] (over the transverse field term) for the spin correlations, the effective Landau-Ginzburg Hamiltonian may be written as

$$H\sim\sum_m S[1+JG(\omega_m)]S+O(S^4)$$

with the spin Green's function

$$G(\omega_m)\sim\Gamma\tanh\beta\Gamma(4\Gamma^2+\omega_m^2)$$

and Matsubara frequencies $\omega_m=2\pi m/\beta$. Also, because of the competing interactions, we expect the fluctuations (with q_0 and $-q_0$) over some modulated structure (say with wave vector q_0) to be dominant in the critical region, thereby effectively driving[11] an n-component competing system equivalent to a $2n$-component system without competition (here $n=1$ for an Ising system):

$$H\sim\int d^dq\sum_{\alpha=1}^{2}\sum_m(r_m+q^2)S_\alpha(q)S_\alpha(-q)+O(S^4)\ ,$$

where $r_m=r+\omega_m^2$, r being the usual critical temperature interval. At $T=0$, the Matsubara frequencies come continuous and the sum over m gives an effective additional dimension ($d\rightarrow d+1$). The system therefore shows an effective $(d+1)$-dimensional classical behavior (due to integration over quantum fluctuations) for an effective two-component (XY-like) regular magnetic system (because of integrations over the competing fluctuations in the Ising system). For our one-dimensional ANNNI model in a transverse field, we thus expect effective two-dimensional XY-like (power-law) correlations (floating phase[12]) at zero temperature. At finite temperatures, of course, the lowest value of r_m for which the field remains finite after renormalization is that for $m=0$ and fields corresponding to other m values become irrelevant.[15] There is thus no dimensional increase for $T>0$ and no floating phase is expected. It may be mentioned that the phase diagram of the $S\rightarrow\infty$ limit of the dual Hamiltonian of (1) was also found to have a floating phase.[3]

Since the critical field Γ_c cannot be obtained from this method for $\kappa>0.5$, we restrict ourselves to the other region. In any case, it is observed that Γ_c approaches zero at the fully frustrated point.

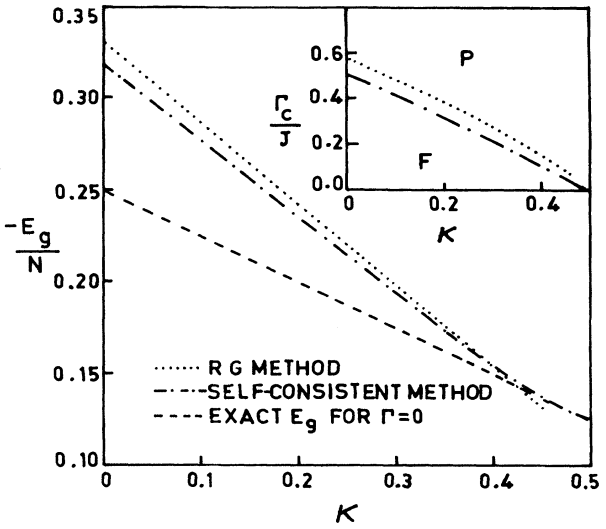

FIG. 1. The ground-state energy per site (E_g/N) along the critical line [$\Gamma=\Gamma_c(\kappa)$] is shown for $\kappa\leq0.5$. The exact E_g/N in the absence of any field is also shown. The inset shows the critical fields (Γ_c/J_1) separating the ferromagnetic (F) and paramagnetic (P) phases for $\kappa<0.5$.

The ground-state energy per site can be expressed as [from (A2)]

$$\begin{aligned}E_g/N=&-[\Gamma-J_2(\langle c_i^\dagger c_{i+2}^\dagger\rangle+\langle c_i^\dagger c_{i+2}\rangle)]\langle c_i^\dagger c_i-\tfrac{1}{2}\rangle\\&-J_1(\langle c_i^\dagger c_{i+1}\rangle+\langle c_i c_{i+1}\rangle)/2\\&+J_2(\langle c_i^\dagger c_{i+1}\rangle+\langle c_i c_{i+1}\rangle)\\&\times(\langle c_i c_{i+1}\rangle+\langle c_i^\dagger c_{i+1}\rangle)\ .\end{aligned}\tag{8}$$

Using Eqs. (B1) and (B2) (for $\kappa\leq0.5$),

$$E_g/N=I_1(J_2I_3/2\pi-\Gamma)/4\pi-J_1\alpha/4\pi-J_2\alpha^2/4\pi^2\ ,\tag{9}$$

where I_1, I_3, and α are as given in Appendix B.

The ground-state energy along the critical line is shown in Fig. 1. The phase diagram is shown in the inset.

III. CRITICAL FIELD AND GROUND-STATE ENERGY FROM REAL-SPACE RENORMALIZATION-GROUP APPROACH

The method followed here is the truncation method[16] in which a number (here, three) of spins are grouped in a cell and the Hamiltonian for a single cell is solved exactly. Only the two lowest-lying eigenstates, out of the possible states (here, eight), are retained to construct an effective Hamiltonian having the same form as that of the original one. The process is iterated until a fixed-point Hamiltonian is reached. It may be noted that, for finding out the fixed point for $\kappa>0.5$, cells with at least four spins should be constructed; otherwise, even the ground state (antiphase) for at least $\Gamma=0$ cannot be represented

by the cell. However, the problem then becomes difficult to tackle analytically and hence we restrict ourselves to cells with three spins, thus restricting ourselves again to studies for $\kappa < 0.5$ only.

With the above three-spin cell, the effective Hamiltonian reads (cf. Ref. 16)

$$H' = -\Gamma' \sum_i S_i^z - J_1' \sum_i S_i^x S_{i+1}^x - J_2' \sum_i S_i^x S_{i+2}^x + c \ , \quad (10)$$

where the renormalized quantities (denoted by primes) are as follows:

$$\Gamma' = -(x_0 - x_1)/2 \ , \quad (11a)$$

$$J_1' = J_1 a/b \ , \quad (11b)$$

$$J_2' = J_2 a/b \ , \quad (11c)$$

$$c = (x_0 + x_1)/2 \quad (11d)$$

with

$$a = \{ -2J_1(x_0+x_1)[(x_1-3\Gamma)(x_0+3\Gamma)+(x_1+\Gamma)(x_0-\Gamma)] + 4J_1 J_2^2 (x_0+x_1) - 8J_1 J_2^3 + 4J_1 J_2 [(x_1-3\Gamma)(x_1+\Gamma)+(x_0+3\Gamma)(x_0-\Gamma)] \}^2 \ ,$$

$$b = \{ 2[(x_0+3\Gamma)(x_0-\Gamma)-J_2^2]^2 + [-2J_1(x_0-\Gamma)+2J_1J_2]^2 + [-2J_1(x_0+3\Gamma)+2J_1J_2]^2 \} \times \{ 2[(x_1-3\Gamma)(x_1+\Gamma)-J_2^2]^2 + [-2J_1(x_1+\Gamma)+2J_1J_2]^2 + [-2J_1(x_1-3\Gamma)+2J_1J_2]^2 \} \ ,$$

and x_0 is the smallest root of the following equation:

$$x^3 + (\Gamma + J_2)x^2 + (-5\Gamma^2 - J_2^2 - 4J_1^2 + 2\Gamma J_2)x + 3\Gamma^3 + \Gamma J_2^2 - 4(\Gamma - J_2)J_1^2 - 3J_2\Gamma^2 - J_2^3 = 0 \ , \quad (12)$$

while x_1 is the smallest root of (12) with $\Gamma \to -\Gamma$. The ground-state energy per site is given by

$$E_g/N = \sum_n \left[\frac{f(J_1(n), J_2(n))}{3^n} \right] \Big/ 3 \ , \quad (13)$$

where

$$f(J_1(0), J_2(0)) = (x_1 + x_0)/2 \ .$$

Notice that, at the zeroth iteration, $J_2(0) = 2J_2$ as the contribution from the second neighbor appears twice in the intercell interaction when the cells consist of three spins. Also, the value of J_2/J_1 does not get renormalized at all. Thus, the fixed point is determined only by the fixed-point value of Γ/J_1. Above the critical value of Γ/J_1, any initial value of Γ approaches infinity, while below this value it iterates to zero; the resulting flow diagram gives the phase diagram.

The estimated values of the ground-state energies along the order-disorder phase boundary are shown in Fig. 1, the inset showing the phase diagram. Notice that this method does not produce the exact results $E_g/N = -1/\pi$ and $\Gamma_c = 0.5$ for $\kappa = 0$. The behavior of both E_g and Γ_c, however, agree well with the results of the self-consistent method.

IV. SUMMARY AND DISCUSSIONS

We have estimated the phase diagram and the ground-state energies along the critical line of a one-dimensional ANNNI model in the presence of a transverse field. The phase diagram of this (one-dimensional quantum-spin-$\frac{1}{2}$) model may be compared to that of the two-dimensional ANNNI model where the thermal fluctuations destroy order at $\kappa = 0.5$.[4,12] The results from both the self-consistent method and RSRG treatment (shown in Fig. 1) indicate that the quantum fluctuation due to the transverse field also destroys the order at the fully frustrated point $\kappa = 0.5$. This result contradicts some earlier findings;[1,2] the results obtained here indicate that there is no Lifshitz point at a nonvanishing value of Γ as was found in Refs. 1 and 2. In fact, this type of disappearance of order due to quantum fluctuation at the fully frustrated point ($\kappa = 0.5$) is also observed in frustrated Heisenberg antiferromagnets.[5-7,9]

For $\kappa > 0.5$, the two-dimensional ANNNI system is argued to have a floating phase with XY-like algebraic correlations.[4] Here, also, the existence of a floating phase is argued, using an effective Landau-Ginzburg free-energy functional, although its exact location could not be found out from such arguments. The absence of disorder-order transition beyond $\kappa > 0.5$, as seen in the self-consistent method, has been interpreted as a possible indication of an intervening floating[4] or algebraic[8] phase (which cannot be viewed as a mode-softened phase; see Sec. II). The possibility of the existence of a disorder line[4] (where the disordered phase has an oscillatory decay of correlation) for the one-dimensional quantum model cannot be examined by the self-consistent method as we can only calculate the order-disorder boundaries using this method.

The ground-state energies along the critical line have been obtained here for the model. The shape of the curve for the ground-state energy follows that of the critical field (see Fig. 1); the absolute value of E_g falls considerably with κ due to the effect of frustration. At $\kappa = 0$, we get the exact result $E_g/N = -1/\pi$ from the self-consistent method (H_f can be exactly diagonalized here). The RSRG treatment gives an overestimation. Since the self-consistent method gives $\Gamma_c = 0$ at $\kappa = 0.5$ (with similar

indication from the RSRG method), the exact result $E_g/N=-0.125$ at $\kappa=0.5$ is also reproduced here. The RSRG does not give very accurate results as κ approaches 0.5 (from below) because the effect of J_2 cannot be taken fully into account by using the cells (consisting of three spins) considered. However, the general variation of E_g/N and Γ_c, with κ, agrees well for the two different methods employed and clearly shows the effect of frustration.

ACKNOWLEDGMENTS

We express our gratitude to S. Dasgupta for valuable discussions and to D. Sen for sending us a copy of his work prior to publication.

APPENDIX A

The renormalized quantities J_1', J_{11}', etc., are obtained by minimizing the free-energy functional

$$F/N=F_0/N-(\langle H_0\rangle-\langle H_F\rangle)\ . \tag{A1}$$

Applying Wick's theorem, F is given by

$$\begin{aligned}F/N=&F_0/N-[-(\Gamma'-\Gamma)\langle c_i^\dagger c_i-\tfrac{1}{2}\rangle]-[J_{11}'-J_1-2J_2(\langle c_i^\dagger c_{i+1}^\dagger\rangle+\langle c_i^\dagger c_{i+1}\rangle)]\langle c_i^\dagger c_{i+1}\rangle/2\\&-[J_{11}-J_1+2J_2(\langle c_i c_{i+1}^\dagger\rangle+\langle c_i c_{i+1}\rangle)]\langle c_i^\dagger c_{i+1}^\dagger\rangle/2+[J_{22}'-2J_2(\langle c_i^\dagger c_i\rangle-\tfrac{1}{2})]\langle c_i^\dagger c_{i+2}^\dagger\rangle/2\\&+[J_{22}'-2J_2(\langle c_i^\dagger c_i\rangle-\tfrac{1}{2})]\langle c_i c_{i+2}\rangle/2\ .\end{aligned} \tag{A2}$$

Variation of F with respect to Γ', J_1', etc. (noting that $\partial F_0/\partial\beta'=\langle\partial H_0/\partial\beta'\rangle$, where β' is any parameter), yields, under stationary condition $\partial F/\partial\beta'=0$, the following equation given in matrix form:

$$M\times\begin{bmatrix}-(\Gamma'-\Gamma)-J_2(\langle c_i^\dagger c_{i+2}\rangle+\langle c_i c_{i+2}\rangle)\\[J_1'-J_1-4J_2(\langle c_i^\dagger c_{i+1}\rangle-\langle c_i c_{i+1}\rangle)]/2\\[J_{11}'-J_1+4J_2(\langle c_i c_{i+1}^\dagger\rangle+\langle c_i c_{i+1}\rangle)]/2\\[-J_2'+J_2(2\langle c_i^\dagger c_i\rangle-1)]/2\\[-J_{22}'+J_2(2\langle c_i^\dagger c_i\rangle-1)]/2\end{bmatrix}=0\ , \tag{A3}$$

where

$$M=\begin{bmatrix}\frac{\partial\langle c_i^\dagger c_i-\frac{1}{2}\rangle}{\partial\Gamma'} & \frac{\partial\langle c_i^\dagger c_{i+1}\rangle}{\partial\Gamma'} & \frac{\partial\langle c_i c_{i+1}\rangle}{\partial\Gamma'} & \frac{\partial\langle c_i^\dagger c_{i+2}\rangle}{\partial\Gamma'} & \frac{\partial\langle c_i c_{i+2}\rangle}{\partial\Gamma'}\\[2ex] \frac{\partial\langle c_i^\dagger c_i-\frac{1}{2}\rangle}{\partial J_1'} & \frac{\partial\langle c_i^\dagger c_{i+1}\rangle}{\partial J_1'} & \frac{\partial\langle c_i c_{i+1}\rangle}{\partial J_1'} & \frac{\partial\langle c_i^\dagger c_{i+2}\rangle}{\partial J_1'} & \frac{\partial\langle c_i c_{i+2}\rangle}{\partial J_1'}\\[2ex] \frac{\partial\langle c_i^\dagger c_i-\frac{1}{2}\rangle}{\partial J_{11}'} & \frac{\partial\langle c_i^\dagger c_{i+1}\rangle}{\partial J_{11}'} & \frac{\partial\langle c_i c_{i+1}\rangle}{\partial J_{11}'} & \frac{\partial\langle c_i^\dagger c_{i+2}\rangle}{\partial J_{11}'} & \frac{\partial\langle c_i c_{i+2}\rangle}{\partial J_{11}'}\\[2ex] \frac{\partial\langle c_i^\dagger c_i-\frac{1}{2}\rangle}{\partial J_2'} & \frac{\partial\langle c_i^\dagger c_{i+1}\rangle}{\partial J_2'} & \frac{\partial\langle c_i c_{i+1}\rangle}{\partial J_2'} & \frac{\partial\langle c_i^\dagger c_{i+2}\rangle}{\partial J_2'} & \frac{\partial\langle c_i c_{i+2}\rangle}{\partial J_2'}\\[2ex] \frac{\partial\langle c_i^\dagger c_i-\frac{1}{2}\rangle}{\partial J_{22}'} & \frac{\partial\langle c_i^\dagger c_{i+1}\rangle}{\partial J_{22}'} & \frac{\partial\langle c_i c_{i+1}\rangle}{\partial J_{22}'} & \frac{\partial\langle c_i^\dagger c_{i+2}\rangle}{\partial J_{22}'} & \frac{\partial\langle c_i c_{i+2}\rangle}{\partial J_{22}'}\end{bmatrix}\ .$$

Equation (A3) leads to the self-consistent equations given in Eq. (4).

APPENDIX B

The correlations $\langle c_i^\dagger c_j\rangle$ and $\langle c_i c_j\rangle$ at zero temperature are given by

$$\langle c_i^\dagger c_j\rangle=\sum(\phi_{ki}\phi_{kj}+\psi_{ki}\psi_{kj}-\phi_{ki}\psi_{kj}-\psi_{ki}\phi_{kj})\ ,$$

$$\langle c_i c_j\rangle=\sum(\phi_{ki}\phi_{kj}-\psi_{ki}\psi_{kj}-\phi_{ki}\psi_{kj}+\psi_{ki}\phi_{kj})\ ,$$

where ϕ_{ki}, ψ_{ki}, and λ_k are given by[1]

$$\phi_{ki}=\begin{cases}\cos ki, & k<0\ ,\\ \sin ki, & k>0\ ,\end{cases}$$

$$\psi_{ki}=[-\Gamma'\phi_{ki}-J_1'\phi_{ki}\cos k-J_1'\phi_{-ki}\sin k+J_2'\phi_{ki}\cos 2k+J_2'\phi_{-ki}\sin 2k]/\lambda_k\ ,$$

$$\lambda_k=\Gamma'^2+J_1'^2/4+J_2'^2/4+\Gamma'J_1'\cos k-\Gamma'J_2'\cos 2k-J_1'J_2'\cos k/2\ .$$

Hence,

$$\langle c_i^\dagger c_j\rangle=\delta_{ij}/2+(1/2\pi)\int_0^\pi dk(\Gamma'+J_1'\cos k/2-J_2'\cos 2k/2)\cos k(i-j)/\lambda_k \tag{B1}$$

and

$$\langle c_i c_j\rangle=1/2\pi\int_0^\pi dk(J_1'\sin k/2-J_2'\sin 2k/2)\sin k(i-j)/\lambda_k\ . \tag{B2}$$

In order to study $\Gamma(\kappa)$, we have to obtain $\Gamma(\kappa')$, $J_1(\kappa')$, and $J_2(\kappa')$. The two regions $\kappa'<0.5$ and $\kappa'>0.5$ will be investigated separately.

1. $\kappa'\leq 0.5$

Here $\Gamma'/J_1=(1-\kappa')/2$ and

$$\lambda_k(1)\equiv\lambda_k(\Gamma'/J_1'=(1-\kappa')/2)=J_1'^2[(1+\cos k)/2-\kappa'(1-\cos 2k)/2+\kappa'^2(1-\cos 2k)/2]\ .$$

$J_1(\kappa')$, $J_2(\kappa')$, and $\Gamma(\kappa')$ are now given by

$$J_1=J_1'(-4\kappa' I_2/I_1)\ ,$$

$$J_2=2\pi J_2'/I_1\ ,$$

$$\Gamma/J_1=[I_1(J_1'+J_2')+J_2'(I_3)]/(J_1'I_1-4J_2'I_2)\ ,$$

where I_1, I_2, and I_3 are the integrals given by

$$I_1=\int_0^\pi dk[(1+\cos k)-\kappa'(1-\cos k)]$$
$$=2\{\alpha[1-1/2(1-\kappa')]+[-4\kappa'(1-\kappa')+1]^{1/2}/(1-\kappa')\}\ ,$$

$$I_2=\int_0^\pi dk[(\cos k+1)/2\lambda_k(1)]$$
$$=\alpha\ ,$$

$$I_3=\int_0^\pi dk[-(\cos 2k-1)\kappa'+\cos k+\cos 2k]/2\lambda_k(1)$$
$$=[1-4\kappa'(1-\kappa')]^{1/2}/\kappa'+\alpha(1-1/2\kappa')$$

with

$$\alpha=\{-1/[\kappa'(1-\kappa')]^{1/2}\}\{\sin^{-1}2[-4\kappa'(1-\kappa')+\tfrac{1}{2}]-\pi/2\}/2\ . \tag{B3}$$

2. $\kappa'>0.5$

Here $\Gamma'/J_1'=|\kappa'|/2$ and

$$\lambda_k(2)\equiv\lambda_k(\Gamma'/J_1'=|\kappa'|/2)=\tfrac{1}{2}+\kappa'\cos k\ .$$

From Eq. (4) we get

$$J_2=2\pi J_2'/I_1'\ ,$$

$$J_1=J_1'-4J_2'I_2'/I_1'\ ,$$

$$J_2/J_1=-2\pi\kappa'/(I_1'+4I_2'\kappa')\ ,$$

where

$$I_1' = \int_0^{\pi} dk\,[\cos k - \kappa'(1+\cos 2k)]\lambda_k(2)^{-1}/2 = 0\ ,$$

$$I_2' = \int_0^{\pi} dk\,[(\tfrac{1}{2}+\kappa'\cos k)\cos^2 k + \sin^2 k + \kappa'\sin^2 k\,\cos k]/\lambda_k(2) = \pi\ .$$

Therefore, $J_2/J_1 = -\frac{1}{2}$ for all values of κ'. From Eq. (4a),

$$\Gamma/J_1 = I_1(\kappa'/2 - \kappa' I_3')/(I_1' + 4\kappa' I_2')\ ,$$

where

$$I_3' = \int_0^{\pi} dk\,\{\cos 2k\,[\cos k + \kappa'(1+\cos 2k)] + \sin 2k\,(\sin k + \kappa'\sin 2k)\}/2\lambda_k(2) = 0\ .$$

Hence, $\Gamma/J_1 = 0$ for all values of κ'.

---

[1] P. Sen and B. K. Chakrabarti, Phys. Rev. B **40**, 760 (1989).
[2] D. Sen and B. K. Chakrabarti, Phys. Rev. B **41**, 4713 (1990).
[3] D. Sen, Phys. Rev. B **43**, 5939 (1991).
[4] W. Selke, Phys. Rep. **170**, 213 (1988).
[5] C. K. Majumdar and D. Ghosh, J. Math. Phys. **10**, 1388 (1969); **10**, 1399 (1969).
[6] P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).
[7] P. Locher, Phys. Rev. B **41**, 2537 (1990).
[8] V. J. Emery and C. Noguera, Phys. Rev. Lett. **60**, 631 (1988).
[9] J. Igarashi and T. Tonegawa, Phys. Rev. B **40**, 756 (1989).
[10] M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976); R. J. Elliot, P. Pfeuty and C. Wood, Phys. Rev. Lett. **25**, 443 (1970).
[11] T. Garel and P. Pfeuty, J. Phys. C **9**, L245 (1976).
[12] J. Villain and P. Bak, J. Phys. (Paris) **42**, 657 (1981).
[13] D. Wolf and J. Zittarz, Z. Phys. B **43**, 173 (1981).
[14] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. **16**, 407 (1961).
[15] A. P. Young, J. Phys. C **8**, L309 (1975); J. A. Hertz, Phys. Rev. B **14**, 1163 (1976).
[16] B. Hu, Phys. Lett. **71A**, 83 (1982); P. Pfeuty, R. Jullien, and K. A. Penson, in *Real Space Renormalization,* Vol. 30 of *Topics in Current Physics,* edited by T. W. Burkhardt and J. M. van Leeuwen (Springer-Verlag, Berlin, 1982), p. 119.