Magnetization plateau in the $S=\frac{1}{2}$ Heinsenberg spin chain with next-nearest-neighbor and alternating nearest-neighbor interactions

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(Received 24 June 1997)

The magnetization process of the $S=1/2$ Heisenberg chain with next-nearest-neighbor (NNN) and alternating nearest-neighbor interactions is investigated using the bosonization technique. The existence of the NNN interaction is shown to stabilize a ''diluted'' dimer order at magnetization $m^z=1/4$, leading to a plateau, where two degenerate ground states appear. Effective Hamiltonians describing the low-energy physics in the vicinity of the $m^z=1/4$ plateau are also presented. The analogy to metal-insulator transitions is discussed briefly. [S0163-1829(98)02705-2]

I. INTRODUCTION

In the last decade, our understanding of low-dimensional quantum spin systems has been greatly deepened; strong quantum fluctuations play an important role and classical pictures valid in higher dimensions are known to break down in many cases. For example, an excitation gap exists for one-dimensional Heisenberg antiferromagnets with integral spin quantum numbers,[1,2] although a gapless spin-wave-like excitation is expected from the classical theory.

Quite recently, a new member has joined a family of nontrivial quantum phenomena in one-dimensional spin systems—intermediate plateaus in magnetization processes.[3–6] Namely, for some range of a magnetic field, the system ceases responding to it and a plateau is formed in the field (H) vs magnetization (m^z) curve. The value of m^z, at which the plateau appears, neither seems sensitive to a small change in the model parameters nor is restricted to half-integers; for example, the $m^z=1/6$ plateau appears in a trimerized $S=1/2$ model.[3] However, irrational values have not been found at least so far. Such *exactness* and *rationality* of the values are reminiscent of those occurring in the one-dimensional Mott transitions.[7,8] In fact, we can explain[6] the appearance of the $m^z=1/2$ plateau for bond-alternating $S=1$ chains[4] in such a way as in metal-insulator (MI) transitions.

An attempt at obtaining criteria for plateaus from a general viewpoint has been made recently by Oshikawa *et al.*[9] Guided by a soft argument in the manner of Lieb, Schultz, and Mattis[10] (LSM) and a heuristic reasoning based on bosonization, they concluded that plateaus in spin-S chains are possible only at values of m^z allowed by the condition

$$Q(S-m^z)\in\mathbb{Z}. \tag{1}$$

The above integer Q denotes the spatial period of the (infinite-volume) ground state. If the above condition is not satisfied for the spatial period Q_{Ham} of the *Hamiltonians*, the ground state with m^z is either (i) gapless (the word ''gap'' needs some remarks; we give the meaning in the next section) or (ii) degenerate. This is a finite-m^z generalization of the well-known LSM dichotomy.[10,11] In all the models mentioned above, Q equals Q_{Ham} (e.g., $Q=Q_{\mathrm{Ham}}=2$ for the bond-alternating $S=1$ chains), although they can be different from each other, by definition.

Quite recently, however, an $m^z=1/4$ plateau has been found in numerical calculations[12] carried out for the familiar $S=1/2$ Heisenberg chain with the next-nearest-neighbor (NNN) and alternating nearest-neighbor interactions (see below for the definition of the model). In Fig. 1, we show a typical magnetization curve exhibiting the plateau at $m^z=1/4$.

This model has been extensively studied[13–16] as a simple model showing a quantum phase transition caused by frustration and now attracts a renewed interest since it is considered[17] to be an (adiabatic) effective Hamiltonian for the spin-Peierls compound $CuGeO_3$.[18]

From the facts known for the magnetization process of $S=1/2$ chains,[16,19–21] such a plateau is quite unexpected. In fact, it is known[6,21] that there is *no* plateau if the NNN interaction is absent. In light of the LSM argument of Ref. 9, the first possibility (i) of the dichotomy is realized in this case. If the condition (1) is correct, the integer Q should be an integer multiple of 4, while the model has a period $Q_{\mathrm{Ham}}=2$; this is the first example where the ground state breaks the symmetry of the original model. Namely, the second possibility (ii) occurs and Q/Q_{Ham} ground states appear.

Furthermore, $S=1/2$ chains are known to have a fermionic description and can be considered to be most suitable to demonstrate the above-mentioned analogy to the Mott transitions.

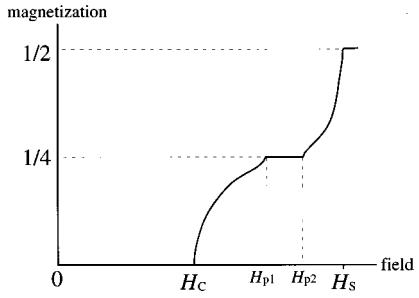

FIG. 1. Schematic drawing of the magnetization curve exhibiting a plateau. For $H_{p1}\leqslant H\leqslant H_{p2}$, magnetization takes a constant value 1/4. H_c and H_s denote the critical and saturation fields, respectively.

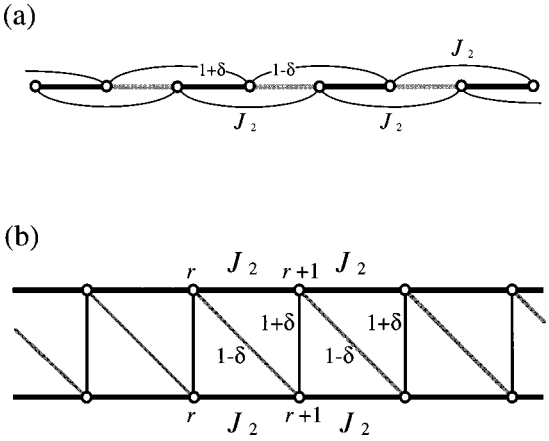

FIG. 2. Two models considered in the text: (a) chainlike Hamiltonian $\mathcal{H}_1$ and (b) ladderlike one $\mathcal{H}_2$. Note that the physical contents are the same.

The model we consider in the following is given by [Fig. 2(a)].

$$\mathcal{H}_1=\sum_{i:\text{chain}}[1-(-1)^i\delta]\mathbf{S}_i\cdot\mathbf{S}_{i+1}+J_2\sum_{j:\text{chain}}\mathbf{S}_j\cdot\mathbf{S}_{j+2}, \quad (2)$$

where $\mathbf{S}_i$ denote the spin-1/2 operator on the ith site. For the nonzero value of δ ($\geqslant 0$), the nearest-neighbor interaction alternates in strength. The next-nearest-neighbor interaction is controlled by the parameter J_2. Coupling to an external magnetic field is incorporated by adding the Zeeman term:

$$\mathcal{H}_{1,\text{Zeeman}}=-H\sum_{i:\text{chain}}S_i^z. \quad (3)$$

The point $\delta=0$, $J_2=1/2$ was rigorously shown[13] to have simple product-form ground states (Shastry and Sutherland[14] extended the region to a line $2J_2+\delta=1$); the spin correlations are extremely short ranged and an excitation gap actually exists above two degenerate ground states.[22] Haldane[15] discussed the ground-state phase diagram of the model with $\delta=0$ using the method developed by Luther and Peschel[23] and predicted that the system becomes spontaneously dimerized for $J_2>J_2^c$ ($J_2^c<1/2$). Subsequent numerical calculations[16,24] fixed the critical value $J_2^c=0.2411...$. Furthermore, the (δ-J_2) phase diagram for $H=0$ has been obtained by using the density-matrix renormalization-group method.[25] Finally, Hammar and Reich pointed out[26] that $\mathcal{H}_1$ will be a model Hamiltonian for a zigzag-chain compound Cu_2(1,4-diazacycloheptane)$_2Cl_4$(CHpC).

Apparently, the same model can be written in a slightly different form [Fig. 2(b)]:

$$\mathcal{H}_2=J_2\sum_r(\mathbf{S}_r^{(u)}\cdot\mathbf{S}_{r+1}^{(u)}+\mathbf{S}_r^{(l)}\cdot\mathbf{S}_{r+1}^{(l)})+(1+\delta)\sum_r\mathbf{S}_r^{(u)}\cdot\mathbf{S}_r^{(l)}$$
$$+(1-\delta)\sum_r\mathbf{S}_r^{(u)}\cdot\mathbf{S}_{r+1}^{(l)}. \quad (4)$$

In this expression, we regard the system as two (uniform) $S=1/2$ chains coupled via the vertical $(1+\delta)$ and the diagonal $(1-\delta)$ interactions or a frustrated ladder. Hereafter, we call the vertical coupling a ''rung'' as is usual in the business of ladder systems. The upper indices (u) and (l) denote the upper and lower chains, respectively. Of course, the Zeeman term is written as

$$\mathcal{H}_{2,\text{Zeeman}}=-H\sum_r(S_r^{(u),z}+S_r^{(l),z}). \quad (5)$$

It is important to note that the system is translationally invariant in the ladder (not chain) direction. This representation is convenient in discussing the cases with $\delta\sim 1$, $J_2\sim 0$ and $|1+\delta|$, $|1-\delta|\ll J_2$.

The setup of the present paper is as follows. In the next section (Sec. II), we map the system onto the field theory of interacting spinless fermions in the spirit of Luther and Peschel.[23,15] With the help of the bosonization technique and the renormalization-group theory, we investigate the low-energy behavior in the weak-coupling limit $|\delta|$, $|J_2|\ll 1$. It is shown that at $m^z=1/4$ the system becomes gapped for some region of the (J_2,δ) plane. When the plateau is formed, the elementary excitations are given by $S^z=\pm 1/2$ kink (1/2) and antikink ($-1/2$).

In the opposite limit $J_2\gg|1+\delta|$, $|1-\delta|$, the system can be viewed as two Heisenberg chains coupled via the *zigzag* interaction ($\mathcal{H}_2$);[27] in this case another weak-coupling treatment is possible. Again, using the continuum-theory method, we argue that the system is gapless for generic m^z; that is, no magnetization plateau appears for $0<m^z<1/2$ in this limit. Readers who are not interested in the details of bosonization can skip this section and proceed directly to Sec. III.

Then, in Sec. III, we present a simple explanation for the ground-state degeneracy occurring at $m^z=1/4$ using the strong-coupling expansion around the limit of $|1+\delta|\gg J_2$, $|1-\delta|$. In the lowest order, the system is described by the $S=1/2$ XXZ chain with z-axis anisotropy depending upon δ and J_2. For a certain range of parameters, it exhibits antiferromagnetic order; the ground state is twofold degenerate at $m^z=1/4$ and a kind of ''diluted'' dimer order is stabilized. Using the effective Hamiltonian, we can clearly see how the interplay between bond alternation and the NNN interaction yields a nontrivial plateau.

In Sec. IV, we summarize the main results of the analyses and obtain the phase diagram for $m^z=1/4$.

An analogy to metal-insulator transitions is described using a few examples in the final section. We can regard the appearance of the plateau in our model as a metal-insulator transition occurring at low densities.

II. CONTINUUM-THEORY APPROACH

Before embarking on the detailed discussions, we consider how the magnetization curve is determined from a general viewpoint. Since our system is invariant under rotation about the z axis, the z component of the total spin $S_{\text{tot}}^z=\Sigma_i S_i^z$ is a good quantum number. As a function of the field H, the energy levels of $\mathcal{H}_1+\mathcal{H}_{1,\text{Zeeman}}$ (or $\mathcal{H}_2+\mathcal{H}_{2,\text{Zeeman}}$) decompose into groups of straight lines with slopes $-M^z=-S_{\text{tot}}^z$. Among the lines with a given slope (i.e., M^z), only the lowest one is important in considering the magnetization process.

As has been well-known since the classical work of Bonner and Fisher,[20] the magnetization curve (precisely speak-

ing, steps for finite systems) is determined by

$$H=H_M\equiv E(M,0)-E(M-1,0), \tag{6}$$

where $E(M,0)$ denotes the lowest energy of $\mathcal{H}_1$ with a given M. For M^z of the order of the system size L, H_{M^z} will remain finite even in the thermodynamic limit. Therefore, a finite gap between $E(M,0)$ and $E(M+1,0)$ does not necessarily imply the existence of a plateau. This is in contrast to the fact that the critical field appearing in magnetically gapped systems actually corresponds to a gap.[2]

There are several ways to define a plateau. One is to characterize it as a nonanalytic point in the energy density as a function of m^z.[4,12]

Though this is quite general, it is not so useful for our purpose. Instead, we focus on the physical excitations. Following the standard method[28] in fermion systems, we use

$$E(M^z,0)-HM^z \tag{7}$$

as energy eigenvalues.

First we change the origin of the field H to H_0, at which the magnetization is given by $M^z=M$ $[\sim O(L)]$:

$$H=H_0+H'. \tag{8}$$

Typically, we may take

$$H_0=H_M=E(M,0)-E(M-1,0). \tag{9}$$

In general, for the purpose of considering how the magnetization curve behaves in the vicinity of the point (H_0,M), it is convenient to use the following reduced energy levels:

$$E_M(M^z-M)\equiv E(M^z,0)-E(M,0)-H_0(M^z-M). \tag{10}$$

Then the energy difference

$$\begin{aligned}&[E(M^z,0)-HM^z]-[E(M,0)-HM]\\&\quad=E_M(M^z-M)-H'(M^z-M)\end{aligned} \tag{11}$$

involves only finite quantities even for $L\gg 1$ as long as we consider finite excitations satisfying $(M^z-M)/L\ll 1$.

For generic cases, the reduced energy $E_M(M^z-M)$ can take arbitrarily small values as the system size becomes large, that is, the system is magnetically *gapless*.

However, if the gap to the ''one-particle'' excitation

$$E_M(1)\equiv E(M+1,0)-E(M,0)-H_0 \tag{12}$$

remains finite even in the thermodynamic limit, then there exists a magnetization plateau around $H=H_0$. In the following, we use the word ''gap'' in this sense.[29]

One way to determine whether such an excitation gap exists or not would be to investigate one in the corresponding continuum model. Taking the continuum limit around ''Fermi points'' to obtain a well-defined field theory for physical excitations with finite energies corresponds to the procedure described above; all physical quantities such as magnetization and energy are measured from infinitely large bulk values. This fact is implicit in earlier papers.[9,6]

A. Small-J_2 case

It is well known that one-dimensional $S=1/2$ systems can be described in terms of interacting spinless fermions by using the Jordan-Wigner transformation, and this fact enables us to use powerful tools developed in the study of one-dimensional electron systems.[30] Although most work in the field of quantum spin chains has been devoted to studying the ground-state property with $m^z=0$ since the pioneering work by Luther and Peschel,[23] the methods used there can in principle be extended to nonzero m^z. Some results have been already reported in Ref. 6. Below, we derive a continuum effective theory for the Hamiltonian $\mathcal{H}_1$.

The bosonization method was successfully applied for the model $\mathcal{H}_1$ with $\delta=0$ and $m^z=0$ first by Haldane.[15] Later, Kuboki and Fukuyama[31] generalized the model to include bond alternation δ caused by the spin-Peierls distortion and discussed the properties near $m^z=0$. However, probably because it was believed that nothing unusual happens for finite m^z, the effect of the magnetization m^z (or the fermion filling, in fermionic language) has been less investigated so far in spin systems than it has been in electron systems.

The derivation of the effective Hamiltonian for $m^z\neq 0$ is almost parallel to the one for $m^z=0$, and we give only the outline. In order to facilitate the procedure, it is convenient to introduce the z-axis anisotropy Δ:

$$\begin{aligned}\mathcal{H}_3=&\sum_{i:\text{chain}}[1-(-1)^i\delta](S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z)\\&+J_2\sum_{j:\text{chain}}\mathbf{S}_j\cdot\mathbf{S}_{j+2}.\end{aligned} \tag{13}$$

The first step is to consider the model with $\Delta=0$, $\delta=0$, and $J_2=0$ as a free part and to linearize the spectrum near the Fermi points determined by the magnetization m^z:

$$q=\pm k_F=\pm\frac{\pi}{2}(1-2m^z)\quad(0\leqslant m^z\leqslant 1/2). \tag{14}$$

When we introduce the interactions, we regard the magnetization m^z as a fundamental quantity rather than the magnetic field H (note that the interactions modify the relationship between m^z and H). In other words, we investigate how the system changes by the interactions with the magnetization m^z fixed.

In investigating the properties of $\mathcal{H}_1$ in the presence of a strong magnetic field, it is important to treat the effect of the (fermion) filling carefully. It affects the effective Hamiltonian in two ways: One is to change the marginal couplings. The other is—and this is essential for the quantization of the value of the plateau (1/4 in the present case)—to determine which interactions are commensurate.

After some careful calculations, we obtain the following Hamiltonian:

$$\mathcal{H}=\mathcal{H}_{\text{TL}}+\mathcal{V}_1+\mathcal{V}_2+\mathcal{V}_3, \tag{15}$$

where

$$\mathcal{H}_{\rm TL}=\int_0^L \frac{dx}{2\pi}\, v_0\{\pi^2{:}\Pi(x)^2{:}+{:}[\partial_x\phi(x)]^2{:}\}$$
$$+g_1\int dx[{:}J_L^2{:}+{:}J_R^2{:}]+g_2\int dx J_L J_R \qquad (16)$$

and

$$\mathcal{V}_1=\lambda_1\int dx{:}\cos[(G-4k_F)x+4R\tilde{\phi}]{:}\quad \text{(umklapp)}, \qquad (17)$$

$$\mathcal{V}_2=\lambda_2\int dx{:}\cos[(\pi-2k_F)x+2R\tilde{\phi}-k_F a]{:}, \qquad (18)$$

$$\mathcal{V}_3=\lambda_3\int dx{:}\cos[(\pi-4k_F)x+4R\tilde{\phi}-2k_F a]{:}. \qquad (19)$$

The first one denotes the Tomonaga-Luttinger Hamiltonian characterized by the Fermi velocity $v_0=\sin k_F$ and two kinds (g_1 and g_2) of forward scattering. The value of the reciprocal lattice vector G is given by 2π or π according to whether $\delta=0$ or not. The Tomonaga boson ϕ and its dual $\tilde{\phi}$ obey the following canonical commutation relation:

$$[\phi(x,t),\Pi(y,t)]=\left[\phi(x,t),\frac{1}{\pi}\partial_y\tilde{\phi}(y,t)\right]=i\delta(x-y). \qquad (20)$$

The meaning of them is clarified below.

The first interaction $\mathcal{H}_1$ is called the umklapp term and allowed for lattice systems. The normal-ordered ($:\cdots:$) interactions $\mathcal{H}_2$ and $\mathcal{H}_3$ come from bond alternation; the latter has been neglected in the literature because it does not affect the long-distance physics at $m^z=0$.

In obtaining them, we have bosonized the free spinless fermions Ψ_L and Ψ_R as[32]

$$\Psi_L\sim{:}e^{-2i\phi_L}{:},\quad \Psi_R\sim{:}e^{-2i\phi_R}{:}, \qquad (21)$$

where the chiral bosons are defined by

$$\phi=\phi_L+\phi_R,\quad \tilde{\phi}=\phi_L-\phi_R. \qquad (22)$$

For low energies, the original Jordan-Wigner fermion c is expressed as

$$c\sim e^{-ik_F x}\Psi_R(x)+e^{+ik_F x}\Psi_L(x). \qquad (23)$$

The left and right currents $J_{L/R}$ are given by

$$J_L=\frac{1}{\pi}\partial_+\phi_L(x^+),\quad J_R=\frac{1}{\pi}\partial_-\phi_R(x^-). \qquad (24)$$

Roughly speaking, the boson ϕ represents the gapless fluctuation around the in-plane (short-range) Néel order, whereas its dual $\tilde{\phi}$ is related to the so-called ''current excitations'' [note that the current operator $i(c_{j+1}^\dagger c_j-c_j^\dagger c_{j+1})$ defined on a lattice reduces to $\partial_0\tilde{\phi}$ in the continuum limit]. As is obvious from the above physical meaning of ϕ, it is a periodic variable:

$$\phi\sim\phi+2\pi R. \qquad (25)$$

The quantity R absorbs the effects of interactions and determines critical exponents, scaling dimensions, etc., in the gapless phase.[23,33]

With these expressions, we can write down continuum expressions of the spin operators[6]

$$s^z\sim m^z+\frac{R_*}{\pi}\partial_x\tilde{\phi}+\text{const}{:}\cos(2k_F x-2R_*\tilde{\phi}){:}, \qquad (26)$$

$$s^+\sim\cos(\pi x){:}e^{i(1/R_*)\phi}{:}+\text{const}{:}e^{i\pi x+i(1/R_*)\phi}\times\cos(2k_F x-2R_*\tilde{\phi}){:}. \qquad (27)$$

The first two terms of Eq. (26) and the first one of Eq. (27) have classical meanings; the former is related to a uniform spin density, and a $\cos(\pi x)$ factor of the latter reflects the in-plane (short-range) staggered order mentioned above. The canonical commutation relation (20) is a quantum analog of the classical Poisson bracket:

$$\{\phi(x),S\cos\,\theta(y)\}_{\rm PB}=\delta_{x,y}\quad (S^z=S\cos\,\theta).$$

On the other hand, the term $:\cos(2k_F x-2R_*\phi):$ stands for the charge-density wave (CDW) with a wave vector $2k_F$ around the average magnetization m^z.

The coupling constants are given in terms of Δ, J_2, and δ as

$$v_0=\sin\,k_F, \qquad (28)$$

$$g_1=2(\Delta-2J_2)\sin^2\,k_F+2J_2\,\sin 2k_F(\pi+\sin 2k_F), \qquad (29)$$

$$g_2=4(\Delta-2J_2)\sin^2\,k_F+4J_2\,\sin^2 2k_F, \qquad (30)$$

$$\lambda_1\sim(J_2-J_2^c),\quad \lambda_2\sim\delta,\quad \lambda_3\sim\delta. \qquad (31)$$

Of course, setting $k_F=\pi/2$ ($m^z=0$), we reproduce the results obtained in Ref. 15.

After the marginal couplings g_1 and g_2 are fully taken into account, the compactification radius R is given by

$$R(\Delta,J_2,m^z)=\left[\frac{1-(8/\pi)J_2\,\sin^2\,k_F+4J_2\,\cos\,k_F}{1+(4/\pi)\Delta\,\sin k_F+4J_2\,\cos k_F[1+(2/\pi)\sin 2k_F]}\right]^{1/4}. \qquad (32)$$

It determines the scaling dimensions of the cosine interactions as a function of k_F (or m^z). From Eq. (32), it follows that $R\to 1$ in the limit $m^z\to 1/2$ ($k_F\to 0$); the system becomes noninteracting near saturation. This is typical for spin chains approaching the saturation point.[34,35]

Since interactions containing quickly oscillating factors cannot enter the continuum theory, which operators contribute to the low-energy theory strongly depends on the value of $k_F=\pi(1-2m^z)/2$. Namely, we only keep interactions satisfying the following condition:

$$K_i\equiv 0\begin{cases}(\text{mod}\ 2\pi) & \text{for}\ \delta=0,\\ (\text{mod}\ \pi) & \text{for}\ \delta\neq 0\end{cases}, \qquad (33)$$

where the momenta K_i are defined as

$$K_1 = G - 4k_F \quad (G = 2\pi \quad \text{for} \quad \delta = 0,\ G = \pi \quad \text{for} \quad \delta \neq 0),$$

$$K_2 = \pi - 2k_F, \quad K_3 = \pi - 4k_F. \tag{34}$$

For generic values of m^z except 0 and 1/4, λ_1, λ_2, and λ_3 do not play any essential role in the low-energy physics; the fixed-point effective Hamiltonian is given by the Tomonaga-Luttinger model $\mathcal{H}_{\mathrm{TL}}$, and magnetic excitations are gapless, leading to a smooth increase of the magnetization.

At $m^z = 0$ ($k_F = \pi/2$), the λ_1 interaction, coming both from Δ and from J_2, together with λ_2 from bond alternation contribute:

$$\mathcal{H} = \mathcal{H}_{\mathrm{TL}} + \mathcal{V}_1 + \mathcal{V}_2 = \mathcal{H}_{\mathrm{TL}} + \lambda_1 \int dx :\cos[4R\tilde{\phi}]: + \lambda_2 \int dx :\sin[2R\tilde{\phi}]:. \tag{35}$$

According to the values of (Δ, J_2, δ), various phases appear.[15,25,31,36] The resulting phase diagram for $m^z = 0$ can be found in Refs. 25 and 36.

At $m^z = 1/4$, on the other hand, the umklapp term (λ_1) as well as the λ_3 term corresponding to bond alternation satisfies the commensurability condition $\pi - 4k_F \equiv 0 \pmod{2\pi/2}$ and becomes important. The appearance of the reciprocal vector π instead of 2π is understood by noticing that the spatial period is doubled due to alternation. The resulting model

$$\mathcal{H} = \mathcal{H}_{\mathrm{TL}} + \lambda_1 \int dx :\cos[4R\tilde{\phi}]: + \lambda_3 \int dx :\cos[4R\tilde{\phi} - 2k_F a]: = \mathcal{H}_{\mathrm{TL}} + \lambda_1 \int dx :\cos[4R\tilde{\phi}]: + \lambda_3 \int dx :\sin[4R\tilde{\phi}]: \tag{36}$$

is the so-called quantum sine-Gordon model. Note that the umklapp term λ_1 is permitted *only when* $\lambda_3 \neq 0$ (i.e., $\delta \neq 0$); if bond alternation δ is absent, $\mathcal{H} = \mathcal{H}_{\mathrm{TL}}$ and the magnetization curve is smooth as has been observed in numerical calculations.[16]

The appearance of a sine in Eq. (36) is natural because the system already breaks site parity [cf. Eq. (35)]. Hereafter, we combine the sine and cosine into a single sine whose coupling constant is proportional to δ. In considering the phase diagram, it is convenient to use the renormalization-group (RG) argument.[37]

The RG β function is computed using the operator-product expansion.[38] The result is the well-known Kosterlitz-Thouless-type β function:

$$\frac{dR}{d\ \ln L} = -2\pi^2 R^3 (\lambda_3)^2,$$

$$\frac{d\lambda_3}{d\ \ln L} = (2 - 4R^2)\lambda_3. \tag{37}$$

The RG flow is shown in Fig. 3.

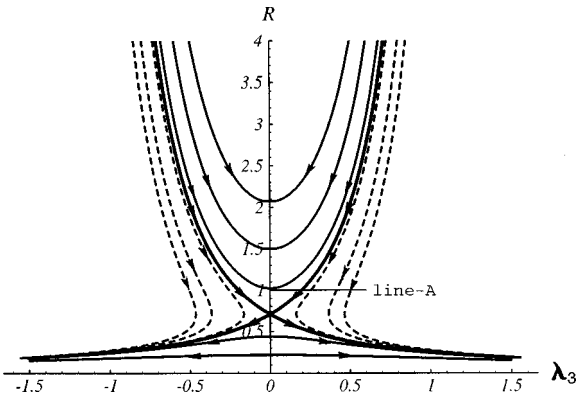

FIG. 3. Renormalization-group flow derived from the β function (37). The semi-infinite line $\lambda_3 = 0$, $R \geqslant 1/\sqrt{2}$ is the Gaussian fixed line, on which the system is described by $\mathcal{H}_{\mathrm{TL}}$ with the renormalized R_*. When we increase δ along the line A, a KT transition occurs on the bold line.

The scaling dimension of λ_3 is given by

$$x_3 = 4R^2, \tag{38}$$

and hence it becomes relevant to produce a gap if $R < 1/\sqrt{2}$.

In the region of interest, $0 < J_2 < 1$, $0 \leqslant \Delta \leqslant 1$, the radius R given by Eq. (32) is slightly larger than $1/\sqrt{2}$ and hence λ_3 is irrelevant. The RG flow shows that massive flows exist only outside the curve (the thick curve in Fig. 3)

$$\lambda_3 = \frac{\sqrt{3}}{\pi} \sqrt{\left(\frac{1}{2R^2} + 2 \ln R\right) - (1 - \ln 2)} \tag{39}$$

when the initial value of R is larger than $1/\sqrt{2}$. This implies that a *finite* value of alternation δ is necessary for the λ_3 interaction to produce a gap. In other words, the appearance of the plateau is *conditional* at least for small J_2; it appears if and only if the alternation δ exceeds a certain critical value $\delta_c(\Delta, J_2)$ (recall that for $m^z = 0$ a gap appears as soon as the alternation is switched on). At the critical point $\delta = \delta_c$, the system undergoes a Kosterlitz-Thouless (KT) transition.[39] Numerical results of Tonegawa *et al.*[12] actually show a tip-like phase boundary, which is characteristic of the KT transition, in $(H\text{-}\delta)$ diagrams. In Sec. IV, we show that the transition is of the second order for larger values of J_2.

If δ takes such a large value as the initial point $(\lambda_3^{(0)}, R_0)$ lies outside the curve (39), the system flows to the strong-coupling fixed point characterized by $|\delta| \nearrow \infty$ and $R \searrow 0$; the static susceptibility $\chi = R_*^2/(\pi v_*)$ actually vanishes and an incompressible (''insulating'') state is realized. At $\delta = \delta_c - 0$, the susceptibility takes a finite value $\chi = 1/(2\pi v_*)$, while it vanishes for $\delta = \delta_c + 0$. That is, χ is *discontinuous* at the transition point $\delta = \delta_c$ [and so is the spin stiffness $D_{\mathrm{spin}} = v_* R_*^2/(2\pi)$]. If we replace χ and D_{spin} with the compressibility and the Drude weight (=charge stiffness), respectively, this is just what happens in the Mott transitions.[8] Furthermore, our result (32) suggests that the critical value δ_c becomes larger if the anisotropy Δ gets smaller.

All these are in contrast with the case of the bond-alternating $S = 1$ chain discussed in Refs. 4 and 6, where an *arbitrarily* small value of alternation produces an excitation gap at $m^z = 1/2$. From the point of view of experiments, it is

fortunate that the plateau is *unconditional* for the alternating $S=1$ chain; the $m^z=1/2$ plateau has been actually observed[5] in Ni compounds.

Next, we consider what happens when we vary the external field H with $\delta\ (>\delta_c)$ fixed. If we approach the critical fields H_{p1} and H_{p2} (see Fig. 1) from the incommensurate sides (i.e., $H\to H_{p1}-0$ or $H\to H_{p2}+0$), application of the well-known method[40] predicts that the system is asymptotically described by free spinless fermions and that physical quantities behave like ($H_p=H_{p1}$ or H_{p2})

$$v_*\sim\sqrt{|H-H_p|}\searrow 0,\quad R\to 1/2,\quad D_{\rm spin}\sim\sqrt{|H-H_p|}\searrow 0,$$

$$m^z-1/4\sim\sqrt{|H-H_p|}\searrow 0,\quad \chi\sim\frac{1}{\sqrt{|H-H_p|}}\nearrow\infty. \quad (40)$$

From the fact $R\to 1/2$, it follows that the spin correlation exponents $\eta_{xx}=\eta_{yy}=1/\eta_{zz}$ approach 2 in the limit $H\to H_{p1}-0$ or $H\to H_{p2}+0$ (recall that $\eta_{xx}\to 1/2$ for the $S=1$ bond-alternating chain[6]).

Then let us discuss the property of the plateau state from the viewpoint of our continuum model (36). In our bosonization treatment, the plateau state is characterized by a strong-coupling fixed point $R_*\searrow 0$. Since the limit $R_*\searrow 0$ corresponds to the classical limit of the $\tilde{\phi}$ field, we can expect that the value of $\tilde{\phi}$ is pinned at one of the minima of $:\cos 4R\tilde{\phi}:$.

The low-energy effective Hamiltonian $\mathcal{H}_{\rm TL}$ possesses several internal symmetries; the translation $\phi\mapsto\phi+R\phi_0$ implies $S_j^{\pm}\mapsto e^{\pm i\phi_0}S_j^{\pm}$, while $\tilde{\phi}\mapsto\tilde{\phi}+\tilde{\phi}_0$ corresponds to translation in the spatial direction. The latter will be most easily understood in the density-wave picture [see Eq. (26)]. As has been derived in Ref. 6, the one-site translation is actually realized as

$$\phi\mapsto\phi+R\pi,\quad \tilde{\phi}\mapsto\tilde{\phi}-\frac{k_F}{R} \quad (41)$$

(the former is reminiscent of the classical antiferromagnetic order in the xy plane).

At $m^z=1/4$ ($k_F=\pi/4$), the period $\pi/2R$ of the cosine interaction $:\cos 4R\tilde{\phi}:$ fits with the two-site translation (note that the system is only invariant under two-site translation for $\delta\neq 0$). Since the circumference of the circle, on which the $\tilde{\phi}$ field resides, is given by π/R, $:\cos 4R\tilde{\phi}:$ may *spontaneously* break the two-site translation symmetry down to the four-site one, leading to two degenerate ground states (recall that $\cos 4R\tilde{\phi}$ takes its minima at $\phi=\pi/4R$ and $\phi=3\pi/4R$, which are related to each other by the two-site translation $\tilde{\phi}\mapsto\tilde{\phi}-\pi/2R$). A situation like this is known to occur in the commensurate CDW state.

This is analogous to the fact that the same type of operators coming from the umklapp process spontaneously breaks the translational invariance down to the two-site translation and brings about two dimerized ground states for $m^z=0$ and $\delta=0$.[13,15] The occurrence of this ground-state degeneracy in our case ($\delta\neq 0, m^z=1/4$) is explained naturally in the next section.

Now that we have obtained the effective Hamiltonian (36), some predictions about elementary excitations can be made. The sine-Gordon soliton (antisoliton) associated with Eq. (36) corresponds to a shift $\tilde{\phi}\mapsto\tilde{\phi}\pm 2\pi/(4R)$ (or, equivalently, two-site translation). On the other hand, the (bulk-subtracted) z component of the total spin is given by

$$S^z_{\rm tot}=\int_0^L dx\,\frac{R}{\pi}\,\partial_x\tilde{\phi}(x)=\frac{R}{\pi}\,[\,\tilde{\phi}(L)-\tilde{\phi}(0)\,]. \quad (42)$$

Thus we can conclude that the solitons (antisolitons) connecting two different ground states carry the S^z quantum number 1/2 ($-1/2$) and that they appear only in pairs as a consequence of their ''kinky'' character. They are nothing but the fractionally charged solitons well known in the theory of polyacetylene.[41] These solitonic excitations are clearly visualized in the next section.

For $\delta-\delta_c(J_2)\ll 1$, the low-energy (or low-temperature) physics is described by the (massive) soliton field theory; the width of the plateau is twice as large as the soliton mass. At finite temperatures (T), the plateau is not strictly flat; neglecting the temperature dependence of the soliton mass (this becomes exact in the limit $R\to 1/2$), we can write down the magnetization in the plateau region as

$$m^z(H,T)=\frac{1}{4}+\frac{\Delta_{\rm sol}}{\pi}\sum_{n=1}^{\infty}(-1)^{n-1}K_1(n\Delta_{\rm sol}/T)\times\sinh[n\mu(H)/T], \quad (43)$$

where K_1 is the modified Bessel function, which can be approximated by $K_1(n\Delta_{\rm sol}/T)\sim\sqrt{T/(n\Delta_{\rm sol})}e^{-n\Delta_{\rm sol}/T}$ for low enough temperatures. The soliton mass $\Delta_{\rm sol}$ and the ''chemical potential'' $\mu(H)$ are given by $\Delta_{\rm sol}=(H_{p2}-H_{p1})/2$ and $\mu(H)=H-(H_{p1}+H_{p2})/2$, respectively.

B. Large-J_2 case

There is one more region where a field-theory calculation based on weak-coupling perturbation is allowed: $J_2\gg|1+\delta|, |1-\delta|$. That is, we consider the problem of a double chain coupled via the zigzag interaction. Since the calculation is similar to that given in Refs. 6 and 42, we only give the final result. We are left with the following five important interactions:

$$\text{(i)}\begin{cases}\cos k_F:\cos[(G-4k_F)x+2\sqrt{2}R_{\rm sym}\tilde{\phi}_{\rm sym}-k_F]:,\\ -\delta\,\sin k_F:\sin[(G-4k_F)x+2\sqrt{2}R_{\rm sym}\tilde{\phi}_{\rm sym}-k_F]:,\end{cases}$$

$$\text{(ii)}\begin{cases}\cos k_F:\cos[2\sqrt{2}R_{\rm diff}\tilde{\phi}_{\rm diff}+k_F]:,\\ \delta\,\sin k_F:\sin[2\sqrt{2}R_{\rm diff}\tilde{\phi}_{\rm diff}+k_F]:,\end{cases}$$

$$\text{(iii)}\ \delta:\cos\left[\frac{\sqrt{2}}{R_{\rm diff}}\,\phi_{\rm diff}\right]:. \quad (44)$$

The Fermi wave vector k_F is the same as before. The above bosons $\phi_{\rm sym}$ and $\phi_{\rm diff}$ are obtained by recombining the two bosons ϕ_u and ϕ_l corresponding to the upper and lower chains, respectively:

$$\phi_{\rm sym}=\frac{1}{\sqrt{2}}\,(\phi_u+\phi_l),\quad \phi_{\rm diff}=\frac{1}{\sqrt{2}}\,(\phi_u-\phi_l). \quad (45)$$

The interactions (i) and (ii) are reminiscent of umklapp and backward scattering in g-ology,[30] respectively. Note that

only the $\phi_{\rm sym}$ sector is important for the magnetization process; if the sector is gapless, we may conclude that the H-m^z curve is smooth around $m^z=\frac{1}{2}-k_F/\pi$.

Within the weak-coupling approximation, the parameters $R_{\rm sym}$ and $R_{\rm diff}$ are given by

$$R_{\rm sym}=\left[1+\frac{2}{\pi J_2\ \sin\ k_F}+\frac{4\Delta_2}{\pi}\ \sin\ k_F\right]^{-1/4},$$

$$R_{\rm diff}=\left[1-\frac{2}{\pi J_2\ \sin\ k_F}+\frac{4\Delta_2}{\pi}\ \sin\ k_F\right]^{-1/4}, \qquad (46)$$

where we have introduced the z-axis anisotropy $J_2\Delta_2$ into the NNN interaction.

At $m^z=0$ ($k_F=\pi/2$), all five interactions vanish if $\delta=0$. Hence the remaining interactions are marginal and irrelevant ones as pointed out by White and Affleck using the non-Abelian bosonization.[27] If both J_2 and Δ_2 are positive, nonzero values of δ causes a gap to the $\phi_{\rm sym}$ sector only at $m^z=0$.

For $m^z\neq 0$, the type-(i) interactions never contribute and the $\phi_{\rm sym}$ sector remains gapless regardless of the value of δ, while the $\phi_{\rm diff}$ sector becomes gapped by the ''backscattering'' term.

A remark is in order here about higher-order interactions. A little calculation shows that an interaction

$$:\cos[8k_Fx-4\sqrt{2}R_{\rm sym}\widetilde{\phi}_{\rm sym}]: \qquad (47)$$

comes from the xy part of the interchain coupling. It is commensurate at $m^z=1/4$ and will generate a gap to the $\phi_{\rm sym}$ sector if the radius satisfies $R_{\rm sym}<1/2$. For sufficiently large J_2, where our weak-coupling approximation is valid, $R_{\rm sym}$ is larger than the critical value 1/2. However, it is highly nontrivial whether the condition $R_{\rm sym}>1/2$ is satisfied down to $J_2\approx 0$ or not.

It is interesting to see what happens when the above interaction is relevant. As has been shown in Ref. 6, the one-site translation in the leg direction is realized as a discrete symmetry of the $\phi_{\rm sym}$ field:

$$\widetilde{\phi}_{\rm sym}\mapsto\widetilde{\phi}_{\rm sym}-\frac{\sqrt{2}\pi}{4R_{\rm sym}}. \qquad (48)$$

It is not surprising that $\sqrt{2}\pi/4R_{\rm sym}$ is equal to the period of the cosine $:\cos[4\sqrt{2}R_{\rm sym}\widetilde{\phi}_{\rm sym}]:$ since the system is invariant under the translation in the leg direction.

On the other hand, the period of the $\widetilde{\phi}_{\rm sym}$ itself is twice as large as that of the above pinning potential. Hence the translational symmetry in the leg direction may be spontaneously broken down to the two-site (in the chain picture, this corresponds to the four-site translation) one; as a result, two degenerate ground states appear.

Thus we have reached the same conclusion as in the previous subsection starting from a completely different limit. In Sec. IV, we present an argument supporting the existence of a transition line below which the $\phi_{\rm sym}$ sector becomes gapped.

To summarize, at least for sufficiently large (positive) J_2, the spin excitation is gapless unless $m^z=0$ and the magnetization curve is smooth.

III. SIMPLE PICTURE OF THE GROUND STATE AT $m^z=1/4$

In the preceding sections, we have seen that a higher-order interaction generated by bond alternation becomes commensurate at $m^z=1/4$ ($k_F=\pi/4$) and generates a gap to magnetic excitations. In the framework of the continuum field theory, the bond alternation δ plays a main role; the NNN interaction J_2 only lowers the value of R and makes the λ_3 interaction relevant [note that $\frac{1}{2}+m^z\leqslant R(m^z)\leqslant 1 (0\leqslant\Delta<\infty)$ for $J_2=0$ (Ref. 6)].

In this section, we clarify how the interplay between J_2 and δ stabilizes the plateau state at $m^z=1/4$ and discuss the difference between the case with $J_2=0$ (Refs. 6 and 21) and that with $J_2\neq 0$. We also investigate the physical properties of the ground state realized for a certain region of the (J_2,δ) plane.

To this end, we consider a slightly extreme case $|1-\delta|$, $J_2\ll 1+\delta$. In this case, it is convenient to use the ''ladder'' representation $\mathcal{H}_2$ where the system is treated as a sum of decoupled ''rung'' dimers perturbed by NNN and diagonal interactions [see Fig. 2(b)]. To be concrete, we regard the second term of $\mathcal{H}_2$ as the unperturbed Hamiltonian and others as perturbations. Throughout this section, we assume that the length L of the chain $\mathcal{H}_1$ is twice as large as the total number $(2N)$ of rungs contained in the ladder $\mathcal{H}_2$: $L=4N$. Then the ground states at $m^z=1/4$ are easily found; N of the $2N$ rungs are occupied by singlet bonds and the others by triplet bonds with $S^z=1$. They apparently $\binom{2N}{N}$-fold degenerate in position. In order to consider the degenerate perturbation for these ground states, we introduce the so-called bond-operator formalism: namely, we use the tensor products of the states [singlet (s) or triplet (t)] on rungs (i.e., strong bonds),

$$\bigotimes_{r:\text{rungs}}|\phi_r\rangle:|\phi_r\rangle\in\left\{\begin{array}{l}|s\rangle=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad |t(1)\rangle=\begin{pmatrix}0\\1\\0\\0\end{pmatrix},\\ |t(0)\rangle=\begin{pmatrix}0\\0\\1\\0\end{pmatrix},\quad |t(-1)\rangle=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\end{array}\right\},$$

as a basis of the whole Hilbert space. For example, $|s\rangle$ can be written as

$$|s\rangle=\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{u,r}\otimes|\downarrow\rangle_{1,r}-|\downarrow\rangle_{u,r}\otimes|\uparrow\rangle_{1,r}\right). \qquad (49)$$

The others will be self-explanatory. With these $4^{2N}(=2^L)$ bases, any local spin operators are expressed by 4×4 matrices; the perturbation Hamiltonian in the new basis can also be written down by replacing the ordinary spin operators with

$$S_r^{(u)+}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&0&0&1\\-1&0&1&0\\0&0&0&1\\0&0&0&0\end{pmatrix},$$

$$S_r^{(l)z}=\frac{1}{2}\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

etc.

Up to now, no approximation has been made and the resulting Hamiltonian can be viewed as a certain one-dimensional model consisting of $2N$ sites, on each of which four states $|s\rangle$, $|t(1)\rangle$, $|t(0)\rangle$, and $|t(-1)\rangle$ are possible. Using the number $N(a)$ of sites taking the state $|a\rangle$, the total energy and the z component of the total spin are given by

$$E=(1+\delta)[2N-N(s)], \quad M^z=N(t(1))-N(t(-1)), \tag{50}$$

respectively.

Although the full Hamiltonian is slightly complicated, the situation becomes drastically simple when we restrict ourselves to the first-order (degenerate) perturbation for the lowest states with a given value of M^z.[43] That is, we can truncate the 4×4 matrices by 2×2 ones and the perturbation Hamiltonian can be written as

$$\mathcal{H}_{\rm eff}=\frac{1}{4}[2J_2-(1-\delta)]\sum_{r:\text{rungs}}^{2N}(d_r^\dagger d_{r+1}+d_{r+1}^\dagger d_r) + \frac{1}{4}[2J_2+(1-\delta)]\sum_{r:\text{rungs}}^{2N} n_r n_{r+1}, \tag{51}$$

where we have introduced the fermion operator $d_r^\dagger(d_r)$, which creates a triplet $|t(1)\rangle$ (singlet $|s\rangle$) on the rth rung, and the corresponding number operator n_r. For the lowest states, the total fermion number $\Sigma_{r=1}^{2N}d_r^\dagger d_r$ is related to M^z by

$$M^z=\sum_{r=1}^{2N} d_r^\dagger d_r. \tag{52}$$

A constant M^z implies a constant fermion number.

It is worth mentioning that singlet dimers become static along the line $2J_2+\delta=1$, on which a static (or solidlike) dimer configuration becomes the exact ground state for $H=0$.[14] Below we consider the effective Hamiltonian $\mathcal{H}_{\rm eff}$ within a sector with a fixed fermion number $N_F=\Sigma_r d_r^\dagger d_r=L/4$.

Let us consider an extreme case $|2J_2-(1-\delta)|\ll 2J_2+(1-\delta)$ first. Obviously, the ground state (g.s.) is given either by

$$|\text{g.s. A}\rangle=\prod_{r=\text{odd}} d_r^\dagger|0\rangle_F \tag{53}$$

or by

$$|\text{g.s. B}\rangle=\prod_{r=\text{even}} d_r^\dagger|0\rangle_F. \tag{54}$$

This implies that the symmetry-breaking ground state occurs in the infinite-volume limit. In (spinless) fermionic language, this situation can be viewed as the occurrence of the so-called $2k_F$-CDW ordering.[44] If we translate it back into the language of the original Hamiltonian $\mathcal{H}_1$, N dimer singlets occupy every other strong $(1+\delta)$ bond (the number of strong bonds is $2N$); the two degenerate ground states (A and B) corresponds to the two possible ways of assigning N singlets onto $2N$ strong bonds (see Fig. 4). Apparently, exciting another fermion (i.e., triplet with $S^z=1$) over the $N_F=N=L/4$ ground state costs extra energy $[2J_2+(1-\delta)]/2$ in addition to the increase $(1+\delta)$ on a strong bond. The first one is responsible for the plateau.

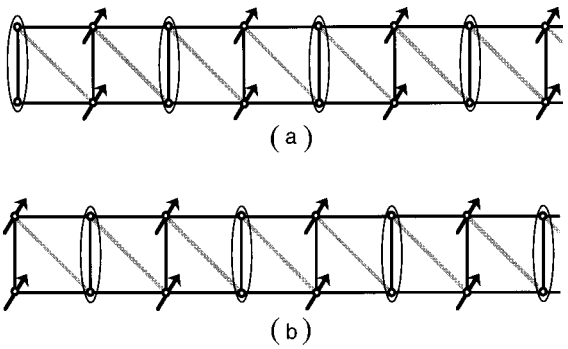

FIG. 4. Two degenerate ground states realized in the extreme case $|2J_2-(1-\delta)|\ll 2J_2+(1-\delta)$: $|$g.s. A$\rangle$ (a) and $|$g.s. B$\rangle$ (b). Ovals denote dimer singlets. Note that the dimer order is in a sense ''diluted.''

When $|2J_2-(1-\delta)|$ is not so small compared with $2J_2+(1-\delta)$, the energy gain due to the hopping of triplets and the repulsive interaction which favors the CDW compete with each other. The region of stability of the ordered states is obtained by noticing that the effective Hamiltonian is nothing but the one of the $S=1/2$ XXZ chain,

$$\mathcal{H}_{XXZ}=J_{\rm eff}\sum_{r=1}^{2N}(S_r^xS_{r+1}^x+S_r^yS_{r+1}^y+\Delta_{\rm eff}S_r^zS_{r+1}^z), \tag{55}$$

with the exchange coupling and the z-axis anisotropy given by

$$J_{\rm eff}=\frac{1}{2}[2J_2-(1-\delta)] \tag{56}$$

and

$$\Delta_{\rm eff}=\frac{1}{2}\left(\frac{2J_2+(1-\delta)}{|2J_2-(1-\delta)|}\right), \tag{57}$$

respectively. Of course, in order for the interaction between singlet dimers to be repulsive, a condition $2J_2+(1-\delta)>0$ is necessary. The magnetization of the above XXZ chain is given by $M_{XXZ}^z=\Sigma_{r=1}^{2N}(d_r^\dagger d_r-1/2)$ and hence the sector with $N_F=N$ fermions corresponds to the one with $M_{XXZ}^z=0$. It is well known from the exact solution[45] that the ground state is antiferromagnetically ordered and is gapped for $\Delta_{\rm eff}>1$; the antiferromagnetic order corresponds to the CDW order in the fermion model. Therefore, we may conclude that the symmetry-breaking ground state is stable in the region between two lines $J_2=(1-\delta)/6$ and $J_2=3(1-\delta)/2$. Since this region includes the perturbative regime $\delta\sim1$, $J_2\sim0$, our argument is self-consistent.

To summarize, at least in the perturbative regime the two-site translation symmetry can be spontaneously broken down

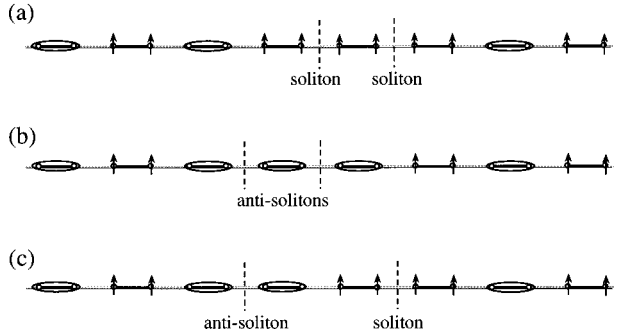

FIG. 5. Typical soliton configurations. The change in the quantum number $S^z_{\rm tot}$ is given by 1 (a), -1 (b), and 0 (c).

to the four-site one; two (not four) ground states degenerate and magnetic excitations have a gap leading to the $m^z=1/4$ plateau. Using the exact results,[45] the width of the plateau in the present regime is given by twice the soliton mass:

$$H_{p2}-H_{p1}\approx|2J_2-(1-\delta)|\,\frac{1}{\pi}\,K(k)\sqrt{(\Delta_{\rm eff}^2-1)(1-k^2)}$$

$$\left(\Delta_{\rm eff}=\cosh\frac{\pi K'(k)}{K(k)}\right), \tag{58}$$

where $K(k)$ and k denote the complete elliptic integral of the first kind and its modulus, respectively.

In fact, the above argument for symmetry breaking can be extended to the case of a small δ with the help of the bosonization method developed in Sec. II. The most suitable choice of an order parameter probing the above density wave would be

$$\langle\mathcal{O}_i\rangle=\langle\mathbf{S}_{4i}\cdot\mathbf{S}_{4i+1}\rangle-\langle\mathbf{S}_{4i+2}\cdot\mathbf{S}_{4i+3}\rangle. \tag{59}$$

Taking the continuum limit, we obtain, for $m^z=1/4$,

$$\mathcal{O}(x)=:\sin[2R_*\tilde{\phi}(x)-8k_Fx-3k_F]:, \tag{60}$$

whose correlation function is readily computed as

$$\langle\mathcal{O}(x)\mathcal{O}(0)\rangle\sim\frac{1}{x^{2R_*^2}}\cos(8k_Fx)=\frac{1}{x^{2R_*^2}}. \tag{61}$$

In the plateau phase, we have $R_*=0$ as has been shown in Sec. II using the RG argument. Hence, in the presence of the $m^z=1/4$ plateau, a ''dimer-density wave'' with a wave vector $q=\pi/2$ is formed. This shows that both the perturbative region $(J_2,1-\delta\ll1+\delta)$ and the weak-coupling region $(J_2,|\delta|\ll1)$ belong to the same unique density-wave phase.

The elementary excitations are expected to be given by massive kinks and antikinks, which have $S^z=\pm1/2$. Typical configurations with spin quantum number $S^z=1$, -1, and 0 are shown in Figs. 5(a), 5(b), and 5(c), respectively. These are consistent with the conclusion of the bosonization argument presented in the previous section. It would be interesting to compare such soliton configurations with those appearing for $m^z=0$, $\delta=0$, and $J_2>0.2411...$.[14]

In a recent paper,[6] we pointed out that although the cosine interaction $:\cos4R\tilde{\phi}:$ coming from bond alternation becomes commensurate at $m^z=1/4$, an expected ordered state such as in Fig. 4 is not realized because of strong fluctuations and

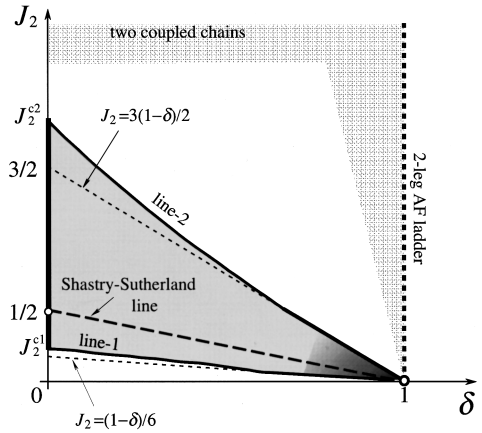

FIG. 6. $m^z=1/4$ phase diagram predicted by the analyses using the bosonized Hamiltonians and $\mathcal{H}_{\rm eff}$. Obviously, it is symmetric under $\delta\leftrightarrow-\delta$. The $m^z=1/4$ plateau appears in the shaded triangular region between two boundaries, line 1 and line 2, on which a KT transition occurs. Line 2 is shown only schematically. For $J_2^{c1}<J_2<J_2^{c2}$ (bold line), a second-order transition in δ occurs.

explained why the $m^z=1/4$ plateau is absent[21] from the Hamiltonian with $J_2=0$. In the present case, however, the NNN interaction stabilizes the dimerized order (note that the stability condition $\Delta_{\rm eff}>1$ cannot be met by δ or J_2 alone) and produces the plateau.

IV. PHASE DIAGRAM

In the present section, we summarize the results obtained in the preceding sections and discuss the (J_2,δ) phase diagram. The final results are summarized as a phase diagram for $m^z=1/4$ in Fig. 6 (see Ref. 25 for the $m^z=0$ phase diagram).

We have performed the bosonization analyses in two limits: (i) $|J_2|$, $|\delta|\ll1$ and (ii) $J_2\gg|1\pm\delta|$. In the first case, we have treated the NNN interaction (J_2) and the alternation (δ) as small perturbations to the ordinary uniform $S=1/2$ Heisenberg chain.

For $m^z=0$, there is a strongly relevant operator $:\cos2R\tilde{\phi}:$ in addition to the well-known umklapp one $:\cos4R\tilde{\phi}:$ when bond alternation is present; the system is gapless only in a restricted region $\delta=0$ and $J_2<0.2411...$.[24,25] A symmetry consideration predicts that the low-energy physics is described by the sine-Gordon model with $\beta=\sqrt{2\pi}$; the elementary excitation is given by a magnon triplet composed of the soliton, the antisoliton, and the breather together with a Raman-active singlet excitation corresponding to another breather.[15,46]

Away from half filling $(m^z>0)$, the well-known umklapp operator becomes negligible in the low-energy limit; the only nontrivial operator comes from the bond alternation δ. Exactly at $m^z=1/4$, it satisfies the commensurability condition and contributes to the low-energy physics. The result of our bosonization suggests that the cosine operator $:\cos[4R\tilde{\phi}-2k_Fa]:$ is slightly irrelevant at least for small J_2 [see Eq. (32)] and that a finite amount of alternation is necessary for the $m^z=1/4$ plateau to appear. On the transition line $\delta=\delta_c^{(1)}(J_2)$ (line 1 of Fig. 6), the Kosterlitz-Thouless transition occurs.

On the other hand, when J_2 is not small, our perturbative result (32) is not reliable and whether the bond alternation is relevant or not is nontrivial. Quite recently, correlation exponents of $\mathcal{H}_1$ along the line $\delta=0$ were investigated numerically.[47] According to their results, the radius R becomes smaller than $1/\sqrt{2}$ for $J_2>J_2^{c1}$ ($J_2^{c1}\approx 0.2$; we must not confuse it with the ''spin-fluid–to–dimer'' critical point J_2^c appearing for $m^z=0$) and hence becomes relevant [note that the authors of Ref. 47 evaluated a correlation exponent $\eta_3(J_2, m^z=1/4)$, which is expressed as $2R^2$ by our R]. Thus we may conclude that the plateau transition is of the KT type for $J_2<J_2^{c1}$, while it is an ordinary second-order one for $J_2>J_2^{c1}$; the transition point $\delta_c(J_2)$ is given by $\delta_c=0$ for $J_2>J_2^{c1}$ and the plateau appears as $H_{p2}-H_{p1}\sim\delta^{1/(2-4R^2)}$.

The second approach (ii) from the large-J_2 limit shows that the alternation δ does not play any essential role in the magnetization process except for $m^z=0$ and hence the plateau is absent. Therefore, it is natural that we assume the existence of another transition line $\delta_c^{(2)}(J_2)$ (line 2 of Fig. 6) beyond which the plateau is absent. Furthermore, we also show that two massive degenerate ground states appear if a possible higher-order interaction becomes relevant. Therefore, two completely different approaches give the same result.

Unfortunately, the determination of the second transition line is far beyond our bosonization calculation.[48] However, at least for small J_2, we can obtain some insight into the line using the effective Hamiltonian of Sec. III. In Sec. III, we have obtained the $S=1/2$ XXZ model as an effective Hamiltonian describing the low-energy physics at $m^z=1/4$. In the region between two lines $J_2=3(1-\delta)/2$ and $J_2=(1-\delta)/6$ (indicated by dark gray in Fig. 6), the system is in the gapped phase with the translation symmetry by two sites (spontaneously) broken. In the XXZ language, the z-axis anisotropy $\Delta_{\rm eff}$ is unity along these lines, beyond which the system becomes gapless (the XY region of the XXZ chain). Hence we may expect that the transition occurring on the line $J_2=3(1-\delta)/2$ is of the KT type too; we further expect that this line continues to the point $J_2=J_2^{c2}$ on the J_2 axis. In Fig. 6, we show the second line (line 2) only *qualitatively* except for $\delta\approx 1$.

On the portion of the J_2 axis between J_2^{c1} and J_2^{c2} (shown by a bold line in Fig. 6), the transition from the gapless phase to the plateau phase is of second order. The $m^z=1/4$ plateau appears in an area surrounded by line 1, line 2, and the J_2 axis (shaded triangular region in Fig. 6 except on the J_2 axis itself). In that region, such a ''diluted'' dimer order as in Figs. 4(a) and 4(b) is realized. Since singlet dimers become static on the Shastry-Sutherland line $2J_2+\delta=1$ as pointed out in Sec. III, we expect that the width of the plateau is largest around this line.

The resulting phase diagram is quite different from that obtained for $m^z=0$ in Ref. 25.

V. ANALOGY TO METAL-INSULATOR TRANSITIONS

In this section, we briefly discuss the aforementioned analogy to the metal-insulator (MI) transition[8] and roughly classify the plateaus found so far from the viewpoint of their origin.

There are several ways to see the analogy between the MI transitions and the plateau transition. First, there is a formal analogy between them; if we identify the spin stiffness and the (dc) susceptibility with the Drude weight and the compressibility, respectively, transitions to the plateau phase can be regarded as those from metallic states to insulating states. This has been already pointed out in Sec. II. Furthermore, we can characterize[49] the plateau state in the same manner as Kohn[50] did for the insulator.

Of course, these transitions are similar in a physical way as well. Although much wider classes of interactions are possible in spin systems than in electron systems, we restrict ourselves to the following two simple cases in demonstrating the similarity. The first category is the spin-S Heisenberg chain with the single-ion type anisotropy (D):

$$\mathcal{H}_D=J\sum_j \mathbf{S}_j\cdot\mathbf{S}_{j+1}+D\sum_j (S_j^z)^2. \tag{62}$$

The effect of an external magnetic field H is incorporated by adding the Zeeman term

$$\mathcal{H}_{\rm Zeeman}=-H\sum_j S_j^z. \tag{63}$$

When the nearest-neighbor exchange J vanishes, the problem reduces to a local one, for $S\geqslant 3/2$, there are intermediate $[S-1/2]$ (the brackets $[\cdots]$ denote the Gauss symbol) plateaus.

The second one is the spin-S Heisenberg model with bond alternation:

$$\mathcal{H}_{\rm alt}=\sum_j \mathbf{S}_{2j}\cdot\mathbf{S}_{2j+1}+J'\sum_j \mathbf{S}_{2j-1}\cdot\mathbf{S}_{2j}. \tag{64}$$

In the ground state with $m^z=0$, it shows a rich phase diagram according to S and J'.[51] For clarity of the argument, we only consider the case $0\leqslant J'\leqslant 1$. In this case, the model becomes local when $J'=0$; there appear $2S-1$ plateaus in the interval $0<m^z<S$.

In both cases, the spacings of the lowest-energy levels $E(M^z,0)$ are almost the same, i.e., $E(M^z,0)-E(M^z-1,0)=\text{const}$. As a result, the magnetization $M^z=\Sigma_j S_j^z$ can vary without loss of the total energy $\mathcal{H}-H\Sigma_j S_j^z$ when the field H equals to the level spacings. For example, consider the model $\mathcal{H}_D$ with $S=2$. When $J=0$, the spacing between energy levels $E(M^z,0)$ is equal to D for $0\leqslant M^z\leqslant L$. If M^z exceeds the system size L, the level spacing abruptly changes to $3D$; a level jump occurs at $M^z=L$. These equidistant levels become highly degenerate for $H=D$ and $H=3D$, and the magnetization curve is vertical (or metamagnetic) there. Plateaus occur between these equidistant regions as a consequence of the above level jumps. The $m^z=1/6$ plateau in a spin-1/2 chain[3] and in the (antiferromagnetic) three-leg ladder[52] can also be explained in the same manner.

When a small interaction between local sites (or dimerized bonds) is switched on, energy bands are formed by the hopping and vertical parts of the curve will have large but finite slopes; the widths of plateaus may be reduced, but they will remain finite provided that the interactions J and J' are small enough.

To compare the situation with those occurring in interacting fermion (or boson) systems, it is convenient to consider the increment of S_j^z (for $\mathcal{H}_D$) or $S_{2j}^z+S_{2j+1}^z$ (for $\mathcal{H}_{\rm alt}$) as adding a particle. Of course, an external magnetic field coupled to $S_{\rm tot}^z$ is replaced by a chemical potential. Then the roles played by

$$D\sum_j (S_j^z)^2 \quad \text{or} \quad \sum_j \mathbf{S}_{2j}\cdot\mathbf{S}_{2j+1} \quad \text{(strong bonds)} \tag{65}$$

are quite similar to those played by the on-site Coulomb repulsion. Here we use the word ''site'' in a generalized sense to include a strong bond as well.

The situation occurring for the Hamiltonian $\mathcal{H}_D$ with $S=3/2$ is reminiscent of that in the single-band Hubbard model; when the ''hopping'' J is absent, all lowest states with $S_{\rm tot}^z=M^z$ $(-L/2\leqslant M^z\leqslant L/2)$ degenerate and a finite ''charge gap'' $(2D)$ opens to the lowest state with one more particle $M^z=L/2+1$. On the other hand, when $D=0$ $(J>0)$, the system is ''metallic''; the transition to the ''insulating'' phase should take place in between. The critical value of D/J is obtained in Refs. 9 and 53. For S larger than 2, the situation is rather like the one in the interacting boson model discussed by Batrouni *et al.*[7]

In a sense, plateaus are consequences of ''MI transitions'' occurring for high densities (i.e., more than one particle per ''site'') in all cases treated above; finite level jumps responsible for plateaus exist already in the local limits $J=0$ and $J'=0$. The interaction between local sites (hopping, in the language of electron systems) plays only a secondary role in the formation of plateaus in such systems.

However, the $m^z=1/4$ plateau discussed in the preceding sections occurs at a low density (1/2 particle per site); there is no such simple local picture as exists for $\mathcal{H}_D$ and $\mathcal{H}_{\rm alt}$. No level jump exists as long as the interactions $1-\delta$ and J_2 are absent. That is, the $m^z=1/4$ plateau is purely a many-body effect. This situation is similar to the MI transition taking place in the extended Hubbard model at quarter filling.[54] The fact that longer-ranged density-density interactions (the NNN interaction here) are necessary for an ordered state to be stabilized is reminiscent of the fact that we need long- (but finite) range interactions to have the Mott transitions at low densities.[8,54,55]

ACKNOWLEDGMENTS

The author thanks Professor M. Kaburagi and Professor T. Tonegawa for showing their unpublished results and discussions. He is also grateful to Dr. M. Hagiwara and Dr. M. Hase for explaining the experimental realization of the frustrated spin chain discussed in the text and to Dr. C. Gerhardt for sending his numerical data. This work has been supported by the Special Researchers' Basic Science Program from RIKEN.

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