Quantum-liquid regimes for spin chains coupled to phonons:
Phonon density wave versus magnetic order

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We consider a chain of localized spins, coupled to phonons. Recently this problem has been solved exactly for a ''basic model,'' a family of spin-phonon Hamiltonians $\mathcal{H}_{BM}$ characterized by one parameter (coupling constant K), and a zero-T first-order phase transition from the magnetic (ferro or antiferro) state at low couplings to the nonmagnetic state with a phonon density wave at high couplings was found. Here we probe the general case, constructing an effective Hamiltonian H for low-energy degrees of freedom by means of regular expansion in deviations $\delta\mathcal{H} = \mathcal{H} - \mathcal{H}_{BM}$ of the general Hamiltonian $\mathcal{H}$ from that of the basic model. In linear approximation in $\delta\mathcal{H}$ the problem appears to be exactly solvable as well, due to an infinite number of conservation laws. If K is far enough from the critical value K_c, then the character of the basic model solution is not altered. In the vicinity of K_c the magnetic state is dramatically reconstructed: Here the ground state is a gapless magnetic quantum liquid, consisting of mobile singlet spin-phonon complexes and unbound spins. The fraction of singlets increases gradually upon approaching K_c, and the magnetic order parameter gradually vanishes. Thus we have here a partial screening of spins by phonons without formation of a phonon density wave. The latter appears only at $K = K_c$ in the first-order phase transition. Corrections, quadratic in $\delta\mathcal{H}$, destroy the integrability of the system, but outside a narrow critical region around K_c they only lead to an opening of a small gap in the spectrum of the quantum liquid. The behavior of the system within the critical region is an open question. Most likely the continuous magnetic phase transition at $K = K_c$ becomes a first-order one, but close to second order. The relevance of our results for three-dimensional systems and possible applications to compounds with anomalously weak magnetism are briefly discussed. [S0163-1829(96)02222-9]

I. INTRODUCTION

In a previous paper[1] a model of a strongly interacting spin-phonon system was introduced, which aimed to give an alternative explanation for a peculiar magnetic behavior of certain materials (mostly the so-called heavy-fermion compounds, containing anomalous rare earths, e.g., Ce). These materials exhibit, at high temperatures, quite normal paramagnetic properties, while at lower temperatures they gradually ''become nonmagnetic.''[2] The freezing out of magnetism is usually not accompanied by any substantial change of the lattice symmetry. On the other hand, most of these compounds demonstrate gigantic magnetoelastic anomalies,[3] which implies that the relevant spin-phonon interactions might be strong. These facts have provided us with a motivation for a *nonperturbative* study of spin-phonon interactions mainly in order to answer the major question whether phonons can screen spins. It is also especially interesting whether it can happen without a lowering of lattice symmetry.

For the simple one-parameter family of spin-phonon Hamiltonians (''basic model''), with the realistic phonon modes being replaced by local isotropic three-component Einstein oscillators with frequency ω and the spin-phonon interaction posessing a special high symmetry, the authors of Ref. 1 were able to find the ground state of the system and its low-lying excitations in a nonperturbative way for an arbitrary coupling constant K and for arbitrary space dimensionality. It was shown that in a certain range of K,

$K_c < K < \omega$, the ground state of the model is indeed nonmagnetic. It consists of singlet complexes (clusters), each of which is constituted by one excited oscillator, coupled to adjacent spins. These complexes tile the entire lattice in such a way that each spin belongs to one and only one cluster (close packing). The low-lying excitations are packings with holes (free dangling spins). The excitation spectrum is separated from the ground state by the gap $\Delta_{BM}(K)$, which vanishes, when K tends either to K_c or to ω.

In Ref. 1 the authors also discussed briefly what happens to the properties of the system when its Hamiltonian $\mathcal{H}$ deviates slightly from the Hamiltonian $\mathcal{H}_{BM}$ of the basic model. An answer to this question is relatively simple, if $\delta\mathcal{H} \equiv \mathcal{H} - \mathcal{H}_{BM}$ is small compared to Δ_{BM}. Then $\delta\mathcal{H}$ is either irrelevant (for systems with nondegenerate or only globally degenerate ground states), or, for systems with a local degeneracy of the ground state, it mixes the different ground states (i.e., different close packings) and lifts, partially or fully, the ground state degeneracy.

A quite different (and much more interesting) situation must arise, however, if $\delta\mathcal{H}$ is comparable to Δ_{BM}. Then the excited states of $\mathcal{H}_{BM}$ can be admixed considerably to the ground state, and one can expect a mixture of singlet clusters and free spins to form already at $T = 0$ in the ground state. This mixture is most likely a quantum liquid of mobile clusters, but its properties, even the presence or absence of long-range magnetic order, is still an open question.

The problem of a quantum liquid and its properties seems to be intriguing not only from a purely theoretical, but also

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from a practical, point of view. Actually the nonmagnetic ground state of the basic model is characterized by *broken* translational symmetry. In Ref. 1 it was argued that this symmetry breaking is hard to observe because a modulation occurs only in zero-vibration amplitudes (a kind of ''phonon density wave''), but not in classic lattice displacements. Anyway, it seems more attractive to get rid of modulation whatsoever, and restore the full translational invariance, which is exactly what happens in a quantum-liquid regime. The possibility of partial spin screening at $T=0$ in a quantum-liquid regime is also attractive, since some substances reveal a long-range magnetic order, but with dramatically suppressed effective magnetic moment.[4] Note that the pure basic model provides only two possibilities: either full screening or no screening at all.

So far we have not been able to develop a reliable quantitative approach to the quantum-liquid state in any two-dimensional (2D) or three-dimensional (3D) version of our model. In this paper we undertake a special study of the quantum-liquid state in the 1D chain, where the problem turned out to be tractable. Some preliminary results were already presented in Ref. 5; here we give a full solution of the problem. We consider a class of one-dimensional systems with Hamiltonians $\mathcal{H}$, deviating from $\mathcal{H}_{\mathrm{BM}}$ in the vicinity of the threshold K_c. In Sec. II, in a form of series expansion in $\delta\mathcal{H}=\mathcal{H}-\mathcal{H}_{\mathrm{BM}}$, we derive an effective Hamiltonian H for low-energy degrees of freedom. In Sec. III we formulate a set of conservation laws, valid in linear approximation in $\delta\mathcal{H}$. These conservation laws make an exact solution of the problem possible. The effects of second order in $\delta\mathcal{H}$ break the internal symmetry of the effective Hamiltonian H and destroy the integrability of the problem, the most important consequence being an opening of a gap in the spectrum of the quantum liquid. In Sec. IV we discuss the ground state and thermodynamics of a chain with an inversion center, and in Sec. V we do the same for a chain without an inversion center. In both cases the solution describes a uniform quasi-gapless magnetic quantum liquid, but with somewhat different magnetic properties. In Sec. VI we discuss the character of the zero-T phase transition between magnetic and nonmagnetic phases. Finally, in Sec. VII we try to single out most general results and speculate about their possible generalization for higher dimensions.

II. EFFECTIVE HAMILTONIAN

Consider a 1D chain of alternating spins $\mathbf{s}_a$ ($s=1/2$) at sites a of sublattice A, and three-component oscillators at sites b of sublattice B (see Fig. 1), $\mathbf{Q}_b$, $\mathbf{P}_b$ being the displacements and momenta of an oscillator. A reasonably general Hamiltonian (see the detailed discussion in Ref. 1) for such a chain would be

$$\mathcal{H}_{\mathrm{tot}}=\mathcal{H}+\mathcal{H}_m, \quad \mathcal{H}_m=\sum_{aa'} J_{aa'}^{\alpha\alpha'} s_a^\alpha s_{a'}^{\alpha'}, \qquad (1)$$

$$\mathcal{H}=\sum_b \mathbf{P}_b^2/2+\sum_{bb'} U_{bb'}^{\beta\beta'} Q_b^\beta Q_{b'}^{\beta'}/2+\sum_{abb'} K_{abb'}^{\alpha\beta\beta'} s_a^\alpha Q_b^\beta P_{b'}^{\beta'}, \qquad (2)$$
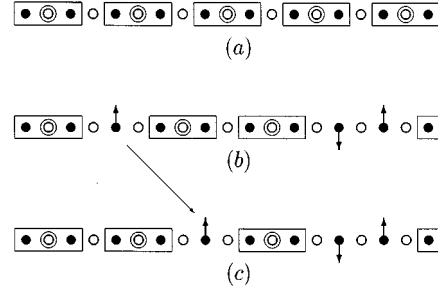

FIG. 1. Low-energy configurations for the chain of alternating spins and oscillators ($K>K_c$); solid circles, spins; single open circles, unexcited oscillators; doubled open circles, excited oscillators; rectangular boxes, singlet spin-phonon complexes (dimers). (a) The ground state: fully dimerized ''close packing.'' (b),(c) Excited states with holes in the packing; (c) is related to (b) by a first-order process, described by the hopping Hamiltonian $H^{(1)}$, and vice versa. The orientation of the free spin at its new position after the hop is unaltered.

where the units are chosen so that masses of the oscillators and $\hbar$ are unities. In this paper we adopt the following assumptions, concerning $\mathcal{H}$.

(i) The crucial assumption—the spin-phonon Hamiltonian $\mathcal{H}$ is in a sense close to the Hamiltonian $\mathcal{H}_{\mathrm{BM}}$ of the basic model. Namely, characteristic matrix elements of $\delta\mathcal{H}=\mathcal{H}-\mathcal{H}_{\mathrm{BM}}$ should be small, compared to characteristic phonon frequencies.

(ii) Only interactions of nearest neighbors $\langle aa'\rangle, \langle bb'\rangle, \langle bab\rangle, \langle bab'\rangle$ are assumed to be essential. Some effects of non-nearest-neighbor interactions are discussed only briefly: They actually play the same role as the higher corrections in $\delta\mathcal{H}$.

(iii) The ''direct'' spin-spin interaction $\mathcal{H}_m$, Eq. (2), is supposed to be the weakest interaction in the problem. It is considered only so far as it lifts some residual degeneracies, which other interactions fail to lift. If $\mathcal{H}_m$ were large, the system would be dominated by the magnetic interaction, which case is well known and is not our concern here.

A. Principal features of the basic model

We review here briefly the properties of the ground state and low-lying excitations in the basic model (for details see Ref. 1). This model, allowing for a nonperturbative solution, is characterized by the following three assumptions.

(1) The modes $\mathbf{Q}_b$ are isotropic and local (dispersionless): $U_{bb'}^{\beta\beta'}=\omega^2\delta_{\beta\beta'}\delta_{bb'}$.

(2) The spin-phonon interaction is local and spherically symmetric: $K_{abb'}^{\alpha\beta\beta'}=K\delta_{bb'}\delta_{\langle ab\rangle}\epsilon_{\alpha\beta\beta'}$.

(3) The direct spin-spin interaction is totally neglected: $J_{aa'}^{\alpha\alpha'}=0$.

Thus the Hamiltonian of the basic model is

$$\mathcal{H}_{\mathrm{BM}}=\sum_b \left(\frac{1}{2}\mathbf{P}_b^2+\frac{\omega^2}{2}\mathbf{Q}_b^2\right)+K\sum_{\langle ab\rangle}(\mathbf{s}_a\mathbf{L}_b), \qquad (3)$$

with $\mathbf{L}_b=[\mathbf{Q}_b\mathbf{P}_b]$ being the angular momentum of an oscillator. The properties of the system are actually governed by unique dimensionless parameter K/ω.

We note that the radial quantum number $N_b^{(r)}$ and the angular momentum L_b of each oscillator are good quantum numbers, the only nontrivial dynamics being associated with orientations of $\mathbf{L}_b$ and $\mathbf{s}_a$. In each sector, characterized by the set $\{N_b^{(r)}, L_b\}$, one can write

$$\mathcal{H}_{\mathrm{BM}}\{N^{(r)}, L\} = \sum_b \omega(N_b^{(r)} + L_b + 3/2) + K \sum_{\langle ab \rangle} (\mathbf{s}_a \mathbf{L}_b),$$

and at $T \ll \omega$ one can consider only the sectors with $N_b^{(r)} \equiv 0$. Thus the basic model is mapped to the Heisenberg chain of alternating spins 1/2 and momenta L_b, the latter ones varying from site to site in their sublattice. This model, of course, cannot be solved for a general set $\{L_b\}$, but, fortunately, it has been shown[1] that the ground state and the low-lying excitations correspond to very simple sets, allowing for an exact solution. Namely, (1) for $|K| > \omega$ the lattice is unstable (formally all $L_b \to \infty$ in the ground state and $E_G \to -\infty$); (2) for $-\omega < K < K_c^{(\mathrm{BM})} \equiv \omega/2$ all $L_b = 0$, the oscillators are unexcited, the spins are decoupled from them, and the ground state of the spin subsystem is governed by $\mathcal{H}_m$; and (3) for $K_c^{(\mathrm{BM})} < K < \omega$ the ground state is nonmagnetic and dimerized [Fig. 1(a)], and there is only a global twofold degeneracy: One-half of the oscillators is unexcited, while the other half is excited to the $L = 1$ state and each excited oscillator binds two adjacent spins, forming a dimer, a *singlet* spin-phonon complex, $E_G = N_0(K_c^{(\mathrm{BM})} - K)$, N_0 being the total number of spins in the chain.

For general $K \sim \omega$ the only natural energy scale for the system is ω. If, however, K is close to the dimerization threshold $K_c^{(\mathrm{BM})}$, then a lower scale arises. For $K < K_c^{(\mathrm{BM})}$ it is the energy of a dimer creation,

$$\Delta_d = 2(K_c^{(\mathrm{BM})} - K), \tag{4}$$

while for $K > K_c^{(\mathrm{BM})}$ it is the energy of a free spin creation, $\Delta_f = K - K_c^{(\mathrm{BM})}$. The low-energy excited states, relevant for $T, \Delta_{\mathrm{BM}} \ll \omega$, are partial tilings of the chain by dimers, where some spins remain free [Figs. 1(b), 1(c)]. All the configurations with overlapping dimers (i.e., with neighboring excited oscillators), or with dimers in internal states, different from the singlet one, have energies $\sim \omega$, and are ruled out. Each allowed configuration can be labeled by a sequence of positions of (nonoverlapping) dimers and of projections of the free spins [e.g., the configurations, shown in Figs. 1(a), 1(b), 1(c) are $|d_1 d_3 d_5 d_7 \cdots\rangle$, $|d_1(\uparrow)_3 d_4 d_6(\downarrow)_8(\uparrow)_9 \cdots\rangle$ and $|d_1 d_3(\uparrow)_5 d_6(\downarrow)_8(\uparrow)_9 \cdots\rangle$ correspondingly]. An energy of any allowed configuration $|\lambda\rangle$ depends only on the total number N_λ of dimers within it:

$$H_{\lambda\lambda'}^{(\mathrm{BM})} \equiv \langle \lambda | \mathcal{H}_{\mathrm{BM}} | \lambda' \rangle = \delta_{\lambda\lambda'} \Delta_d N_\lambda. \tag{5}$$

The arising statistical problem may be reduced to the problem of classic hard dimers, whose partition function in 1D can be calculated in the closed form.[6]

Our aim is the construction of an effective Hamiltonian H, equivalent to $\mathcal{H}$ so far as the low-energy scales ($\ll \omega$) are concerned. It acts in the subspace of eigenstates of $\mathcal{H}_{\mathrm{BM}}$, constituted by the ground state and the low-lying excited states, i.e., the allowed configurations $|\lambda\rangle$, mentioned above. Since according to our principal assumption (i) matrix ele-

ments of $\delta\mathcal{H}$ are small compared to ω (but not necessarily to Δ_{BM}), we will present H in a form of a series in powers of $\delta\mathcal{H}$:

$$H = H^{(0)} + H^{(1)} + H^{(2)} + \cdots, \tag{6}$$

$H^{(0)}$ we know already: It is given by Eq. (5); $H^{(1)}$ describes direct transitions within the low energy subspace; $H^{(2)}$ describes the second-order processes with both initial and final states having low energies, but with a high-energy intermediate state; etc.

B. First-order processes: Effective kinetic energy of dimers

The Hamiltonian $H^{(1)}$ can be found by means of direct projection of $\delta\mathcal{H}$ onto the low-energy space. A structure of relevant matrix elements can be found from the following considerations, based mainly on the symmetry arguments.

The part of $\delta\mathcal{H}$ describing the phonon dispersion and anisotropy, as well as a deviation of the spin-phonon interaction from the form prescribed by the basic model, is bilinear in the operators $\mathbf{Q}, \mathbf{P}$. There are two kinds of terms. The terms of the first kind contain two operators $\mathbf{Q}_b, \mathbf{P}_b$, corresponding to the same site b. They may have matrix elements either being diagonal in L_b, or describing transitions $L_b \to L_b \pm 2$. Since the only low-energy states for the dimers are those with $L_b = 0$ or $L_b = 1$, it is clear that the latter transitions cannot keep a configuration within the low-energy subspace, and thus they are irrelevant. The matrix elements diagonal in L_b lead to unimportant shifts of the configuration energies, resulting only in a shift of K_c.

This is not the case for terms of the second kind, containing two phononic operators at neighboring sites $\langle b, b+1 \rangle$. They have matrix elements corresponding to the transitions $(L_b, L_{b+1}) \to (L_b \pm 1, L_{b+1} \pm 1)$, which can keep a configuration within the low-energy subspace [e.g., the transition $(L_b = 1, L_{b'} = 0) \to (L_b = 0, L_{b'} = 1)$ describes the move of a cluster from site b to site $b+1$; see Figs. 1(b), 1(c)].

As a result, $H^{(1)}$ has a form of effective kinetic energy of dimers:

$$H^{(1)} = -\sum_{m\sigma\sigma'} t_{\sigma\sigma'} |\cdots (\sigma)_{m-1} d_m \cdots\rangle$$
$$\times \langle \cdots d_{m-1}(\sigma')_{m+1} \cdots | + \mathrm{H.c.} \tag{7}$$

It describes a process where a dimer hops to a neighboring position (if it is allowed by the constraint, the requirement, that the dimers do not overlap) while the neighboring free spin ''dives'' under the hopping dimer [Figs. 1(b), 1(c)]. The spin structure of the matrix element, $t_{\sigma\sigma'} = t\delta_{\sigma\sigma'} + i(\tau\sigma)_{\sigma\sigma'}$, with real t and τ, follows from the symmetry with respect to time reversal. It is convenient to treat t and τ as phenomenological parameters of the effective Hamiltonian, though they can be expressed through the constants $U_{bb'}^{\beta\beta'}$ and $K_{abb'}^{\alpha\beta\beta'}$, entering the expression (2).

If the spin-quantization axis is chosen to be parallel to τ, then the projection σ of the ''diving'' spin $\mathbf{s}$ is conserved in the hopping process, described by the Hamiltonian (7), namely, $\sigma = \sigma'$, and the Hamiltonian $H^{(1)}$ may be rewritten in a form

$$H^{(1)} = -\sum_{m;\sigma=\pm 1} (t+i\tau\sigma)|\cdots(\sigma)_{m-1}d_m\cdots\rangle$$
$$\times\langle\cdots d_{m-1}(\sigma)_{m+1}\cdots| + \text{H.c.}, \tag{8}$$

where the free spin emerges on the opposite side of the dimer without changing its orientation.

C. Second-order processes: Creation and annihilation of pairs of dimers

Second-order processes involve forbidden configurations (with high energies $\sim\omega$) as intermediate states. The most important second-order process is an effective annihilation of two neighboring dimers accompanied by creation of four free spins (or vice versa). One possible path $(L_b=1, L_{b+1}=0, L_{b+2}=1) \rightarrow (L_b=0, L_{b+1}=1, L_{b+2}=1) \rightarrow (L_b=0, L_{b+1}=0, L_{b+2}=0)$ for this process is shown in Fig. 2. The corresponding effective Hamiltonian has the form

$$H^{(2)} = \sum_{m\sigma\widetilde\sigma\sigma'\widetilde\sigma'} \widetilde\Delta_{\sigma\widetilde\sigma\sigma'\widetilde\sigma'}|\cdots d_m d_{m+2}\cdots\rangle$$
$$\times\langle\cdots(\sigma)_m(\widetilde\sigma)_{m+1}(\sigma')_{m+2}(\widetilde\sigma')_{m+3}\cdots| + \text{H.c.}, \tag{9}$$

where the magnitude of matrix elements $\widetilde\Delta$ is of order $t^2/\omega \ll t$. The spin structure of $\widetilde\Delta_{\sigma\widetilde\sigma\sigma'\widetilde\sigma'}$ depends on the symmetry of the Hamiltonian $\delta\mathcal{H}$.

We should mention that the very same ''pair processes'' would arise already in first order in $\delta\mathcal{H}$ if we took into account an interaction of next-nearest oscillators. Such an interaction leads to direct transitions $(L_b=L_{b+2}=1) \leftrightarrow (L_b=L_{b+2}=0)$, the result of those being equivalent to the second-order process, described above.

Besides the pair processes there are also other second-order processes. One leads to four-lattice-spacings-long hops of free spin, and the other leads to effective exchange of neighboring free spins. We will not, however, discuss them in detail, because the former only renormalizes the kinetic energy term $H^{(1)}$, and the latter renormalizes the effective magnetic interaction H_m, arising from $\mathcal{H}_m$.
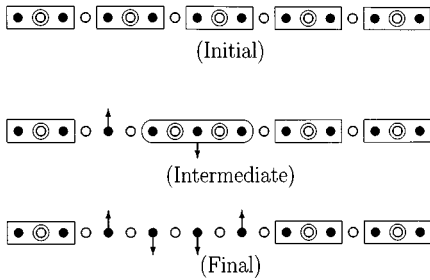

FIG. 2. An example of the process of second order in $\delta\mathcal{H}$, described by effective Hamiltonian $H^{(2)}$. Two neighboring dimers in the close packing annihilate, giving rise to a hole in a close packing, containing four free spins in the final state. In the intermediate state there is a forbidden configuration (oval box), involving two neighboring excited oscillators, coupled to three spins; this configuration has relatively high energy $\sim\omega$.

D. Effective magnetic interactions

The Hamiltonian $\mathcal{H}_m$, corresponding to direct spin-spin interactions, being projected onto the low-energy subspace, couples neighboring *free* spins, but does not affect the dimers. A corresponding effective Hamiltonian is then

$$H_m = \sum_{\langle aa'\rangle(f)} (\mathbf{s}_a\cdot\hat{J}\cdot\mathbf{s}_{a'}), \tag{10}$$

where the summation runs *only over the free spins*. The tensor of effective exchange constants $\hat{J}\equiv J^{\alpha\alpha'}$, entering H_m, consists of two parts: $\hat{J}_{\langle aa'\rangle}$ of the initial spin-spin Hamiltonian $\mathcal{H}_m$ and renormalization $\delta\hat{J}\sim t^2/\omega$, arising from the second-order processes, mentioned at the end of the previous section.

III. CONSERVATION LAWS

Following our basic assumptions, we imply that $J\ll t\ll\omega$, but Δ_d is not necessarily large, compared to t. Consequently, the Hamiltonians, obtained in the previous section, obey the following hierarchy:

$$H^{(2)}, H_m \ll H^{(0)}, H^{(1)}, \tag{11}$$

but $H^{(0)}$ and $H^{(1)}$ may be in arbitrary relation to each other, because $H^{(0)}$ vanishes, when $K\rightarrow K_c^{(BM)}$. So our first task should be to understand the properties of the Hamiltonian

$$H_{01} = H^{(0)} + H^{(1)}. \tag{12}$$

In this section we describe the internal symmetries inherent in this Hamiltonian, and also discuss how these symmetries are violated by additional terms $H^{(2)}$ and H_m.

A. Conservation of the number of dimers

A very important property is that both $H^{(0)}$ and $H^{(1)}$ commute with the total number of dimers, N. We will see that the conservation of the number of particles leads to the gapless spectrum of excitations. This conservation law is unaffected by magnetic interactions (because H_m also commutes with N), but it is broken by the particle-nonconserving $H^{(2)}$ interaction, which opens a small gap Δ in the excitation spectrum.

B. Conservation of ''floating spins'': Separation of variables

Since the total number of dimers, N, commutes with H_{01}, we can consider a state with any fixed $N<N_0/2$. Then the number of free spins, $M=N_0-2N$, is also fixed. Let us look at any particular configuration (with free spins, say, in positions $a_1<a_2<\cdots<a_M$) and renumber all the *free* spins from left to right: $\sigma_{a_1}\rightarrow\sigma'_1, \sigma_{a_2}\rightarrow\sigma'_2, \ldots, \sigma_{a_M}\rightarrow\sigma'_M$ [see Fig. 3(a)]. We will call $\{\sigma'_1, \ldots, \sigma'_M\}$ the *floating spin variables*. The crucial point is that these variables commute with the Hamiltonian H_{01}; i.e., the floating-spin configuration is conserved in time, although the identities (i.e., the physical positions) of the free spins may be changed. This property is a direct consequence of the symmetry of H_{01}: In any elementary process a free spin just hops over a neighboring dimer, without changing projection.
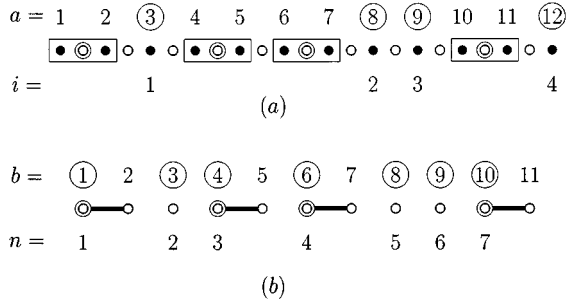
FIG. 3. The renumbering tricks (Ref. 8). (a) Renumbering of free spins introduces the ''floating spins'': Numbers a are physical positions for the spins $\mathbf{s}_a$, while numbers i are their ''floating'' labels, appearing when only the free spins are counted. This renumbering reveals a hidden symmetry of the system: The floating spins are conserved. (b) Renumbering of dimers by the squeezing transformation (spins are not shown). Solid bars (i.e., the rigid segments, mentioned in the text) realize the finite-size hard-core constraint, forbidding the dimers from occupying neighboring sites. Again numbers b are the natural physical positions of dimers (the positions of corresponding excited oscillators), while numbers n are their ''internal'' labels in the ''squeezed'' numeration, when the RHS neighbor of any cluster is not counted. This renumbering is equivalent to the nonlocal unitary transformation, Eq. (16), which resolves the constraint.

Conservation of floating-spin configurations is a characteristic feature for many of 1D models; for example, it is also present in the 1D large-U Hubbard model. The real source of it is in the absence of nontrivial closed loops in the 1D particle trajectories, which leads to the following basic property of the system: Suppose that someone looks at the system at some initial moment of time and memorizes the positions of particles and the configurations of spins at this moment. When he comes again, after some time, he may look only at the positions of particles. The point is that these data are sufficient to reconstruct the new spin configuration as well.

Thus the projections σ_i' of all the ''floating spins'' $\mathbf{s}_i'$ are good quantum numbers and one can, in principle, write down a reduced Hamiltonian $H_{\{\sigma_i'\}}$ acting only on N ''orbital'' degrees of freedom (i.e., the positions of dimers $\{b_j\}$), and depending on M parameters $\{\sigma_i'\}$. The orbital wave function $\psi_{(\sigma_1', \ldots, \sigma_M')}(b_1, \ldots, b_N)$ must be symmetric with respect to any permutation of its variables b_j.

For a general set $\{\sigma_i'\}$ and for a general Hamiltonian with $\tau \neq 0$ an expression for $H_{\{\sigma_i'\}}$ is, however, too complicated because of the necessity to express the physical spin σ_a (entering the matrix element of the $H^{(1)}$) through the floating-spins σ_i' and the orbital degrees of freedom b_j explicitly. So it is practically useless unless the floating-spin configuration is especially simple.

An important simplification arises, however, if the point of the unit cell, where the spin is situated, is the inversion center. In this case $\tau = 0$, the matrix elements of $H^{(1)}$ are spin independent, and the floating-spin degrees of freedom are completely split from the orbital ones. Then the total wave function of the system can be factorized:

$$\Psi = \Xi(\sigma_1', \ldots, \sigma_M') \psi(b_1, \ldots, b_N), \qquad (13)$$

where all 2^M possible floating-spin wave functions Ξ are degenerate.

The degeneracy of eigenenergies with respect to floating-spin configurations is not so general property, since it implies the spin independence of the matrix elements (but this property is still present for the large-U 1D Hubbard model). The degenerate case is a marginal one in the sense of the Nagaoka theorem[7] which states, roughly, that, if the system is dominated by the kinetic energy of the mobile particles, then the *ferromagnetic order* in the background spins is preferable, as the most homogeneous one. In the degenerate case, however, the ferromagnetic state has exactly the same energy, as any other one.

Thus, the internal symmetry of the system in the inversion-symmetrical case is much higher than in the inversion asymmetrical one. We will see that it leads to dramatic consequences: The inversion-symmetrical case occurs to be exactly solvable for all eigenstates, while in the asymmetrical case only the ground state and low-lying excitations of H_{01} may be found exactly.

The conservation of floating spins is violated by both $H^{(2)}$ and H_m interactions. Their role is, however, restricted: They just lift the residual degeneracy of the ground state of H_{01} (which is infinite in the symmetrical case, and only fourfold in the asymmetrical one). The exception is the close vicinity of the magnetic phase transition (critical region), where $H^{(2)}$ and H_m become of primary importance (see discussion in Sec. VI).

IV. CHAIN WITH INVERSION SYMMETRY: EXACT SOLUTION

In the linear approximation in $\delta\mathcal{H}$ a symmetric chain is described by the Hamiltonian $H_{\text{sym}} \equiv H_{01}|_{\tau=0}$, and, as was shown in Sec. III, the eigenfunctions of this Hamiltonian system can be factorized according to Eq. (13). Then our first step should be determination of the orbital part ψ. In this section we demonstrate that this problem can be solved *exactly*, with the aid of the trick, used previously[8] to solve the 1D Emery model[9] in the large-U limit. After that we will take into account the corrections $H^{(2)}$ and H_m, which lift the degeneracy with respect to floating-spin configurations and find the floating-spin part Ξ of the wave function. Finally, we discuss the thermodynamics of the system.

A. Orbital degrees of freedom

The finite-size hard-core constraint, following from the definition of low-energy states, forbids to have two dimers either at the same site or at neighboring sites. Thus we arrive at the problem of N spinless bosonic rigid segments on the chain with N_0 equivalent sites [see Fig. 3(b)]. The corresponding Hamiltonian has the form

$$H_{\text{sym}} = \Delta_d \sum_{b=1}^{N_0} d_b^\dagger d_b + \sum_{b=1}^{N_0-1} \{ -t(d_b^\dagger d_{b+1} + d_{b+1}^\dagger d_b)$$
$$+ U(d_b^\dagger d_b^\dagger d_b d_b + d_{b+1}^\dagger d_b^\dagger d_b d_{b+1}) \} \quad (U \to +\infty),$$
$$(14)$$

where $d_b^\dagger$ (d_b) are Bose operators creating (annihilating) a dimer at a site b.

The part of the constraint which forbids double occupancy of sites can be easily eliminated by a transformation to fermionic variables $\alpha_b^\dagger(\alpha_b)$, which is a standard trick for 1D hard-core bosons. Then the Hamiltonian H_{sym} takes the form

$$H_{sym} = \Delta_d \sum_{b=1}^{N_0} \alpha_b^\dagger \alpha_b + \sum_{b=1}^{N_0-1} \{ -t(\alpha_b^\dagger \alpha_{b+1} + \alpha_{b+1}^\dagger \alpha_b) + U(\alpha_{b+1}^\dagger \alpha_{b+1})(\alpha_b^\dagger \alpha_b) \}. \tag{15}$$

The corresponding antisymmetric wave functions (they vanish if coordinates of any two dimers coincide) should then be resymmetrized [see Eq. (18) below].

The remaining part of the constraint, which does not allow dimers to occupy neighboring sites, can be resolved by the nonlocal transformation, ''squeezing'' the segments (see Ref. 8),

$$a_n = \left\{ \prod_{b'=N_0}^{b+1} (\alpha_{b'-1}^\dagger \alpha_{b'} + \alpha_{b'} \alpha_{b'}^\dagger) \right\} \alpha_b,$$

$$n = b - \sum_{b'=1}^{b-1} \alpha_{b'}^\dagger \alpha_{b'}, \quad L = N_0 - N. \tag{16}$$

This transformation renumbers the sites of the chain *dynamically* in such a way that only one site is associated with any segment (dimer), the second one is excluded [see Fig. 3(b)], and therefore the chain is shortened by N sites. We will call the variables $n_1, \ldots, n_N$, the internal coordinates of dimers, $b_1, \ldots, b_N$ being their physical coordinates. It can be shown that the new operators a_n obey the standard Fermi-Dirac commutation rules in the subspace of allowed configurations.

Let us comment on the physical meaning of the operators $a, a^\dagger$. The operator a destroys a dimer at a certain place and then shifts one step to the left the entire string of dimers on the right-hand side of that place. As a result, only one of the two free spins, created when the dimer was destroyed, survives. In particular, being applied to the close packing configuration, the operator a creates exactly one single free spin (the soliton). Vice versa, the operator $a^\dagger$ creates a dimer out of *one* free spin in a following manner: First it shifts one step to the right the entire string of dimers on the right-hand side of that free spin, opening a second free spin to the right of the initial one. Then a dimer is made out of these two free spins. In particular, being applied to the configuration without dimers, the operator $a^\dagger$ just creates one isolated dimer. Thus the operators $a, a^\dagger$ correctly describe the true quasiparticles in both limiting cases: If the concentration of dimers is low, then a ($a^\dagger$) corresponds to annihilation (creation) of dimers; if there are only few solitons, then a ($a^\dagger$) corresponds to creation (annihilation) of solitons. The above observation gives an intuitive answer for the question why the transformation (16) diagonalizes the Hamiltonian (15).

Finally we have arrived at the Hamiltonian of N *free spinless fermions* on a chain of length $L = N_0 - N$:

$$H_{sym} = \Delta_d \sum_{n=1}^{L} a_n^\dagger a_n - t \sum_{n=1}^{L-1} (a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}). \tag{17}$$

The effective contraction of the chain length, occurring in the transformation (16), reflects the obvious effect of excluded volume, due to the finite length of rigid segments. The eigenfunctions ψ of the initial Hamiltonian, expressed in terms of internal coordinates $\{n\}$, are the symmetrized Slater determinants of plane waves:

$$\psi_{\{k_i\}}(n_1, \ldots, n_N) = (-1)^{P(n_1, \ldots, n_N)} \det\|\sin k_i n_j\|, \tag{18}$$

where ''internal momenta'' $k_i = \pi m_i/(L+1)$ and $0 < m_1 < \cdots < m_N$ are *different* integers. Generally, the internal momenta k are not identical to the physical momenta p of quasiparticles. The factor $(-1)^P$ provides a proper Bose-type symmetry to the wave function, $P(n_1, \ldots, n_N)$ being the parity of permutation from the initial order $n_1, n_2, \ldots, n_N$ to the ''normal'' one (numbered from left to right). The form of the orbital wave function in terms of the physical variables $b_1, \ldots, b_N$ can be obtained with the aid of the transformation (16), but the explicit expression is cumbersome and we will not present it here. The eigenenergies are

$$E_{\{k_i\}} = \sum_{i=1}^{N} \varepsilon(k_i), \quad \varepsilon(k) = \Delta_d - 2t\cos k. \tag{19}$$

As usual, the ground state corresponds to a filled Fermi segment ($m_1 = 1, m_2 = 2, \ldots, m_N = N$) with internal Fermi momentum $k_F = \pi N/(L+1)$, and in the thermodynamic limit the ground state energy is

$$E^{(G)} = N\Delta_d - \frac{2tL}{\pi} \int_0^{k_F} dk \cos k$$

$$= N_0 \left\{ n\Delta_d - \frac{2t}{\pi}(1-n)\sin\left(\frac{\pi n}{1-n}\right) \right\}. \tag{20}$$

Let us recall now that the concentration of dimers, $n = N/N_0$, is not an external parameter, but it has to be found from the condition of minimal energy ($\partial E_G/\partial n = 0$), which leads to the following equation for n:

$$\frac{1}{1-n}\cos\left(\frac{\pi n}{1-n}\right) - \frac{1}{\pi}\sin\left(\frac{\pi n}{1-n}\right) = \frac{\Delta_d}{2t} \equiv \frac{K_c^{(BM)} - K}{t}. \tag{21}$$

Its solution $n = n(K)$ is shown in Fig. 4(a) by a solid line. In the quantum-liquid range $\widetilde{K}_c < K < K_c$ (where $\widetilde{K}_c = K_c^{(BM)} - t$ and $K_c = K_c^{(BM)} + 2t$) the concentration n is neither zero nor 1/2. In this range the spectrum of the system is *gapless* and the excitations are fermionlike, while outside the range there is a gap: $\Delta(K) = 2(\widetilde{K}_c - K)$ for $K < \widetilde{K}_c$ and $\Delta(K) = K - K_c$ for $K > K_c$ [see Fig. 4(b)].

Let us discuss a physical interpretation of the above exact solution for two simple limiting cases.

(1) Close to the lower threshold $0 < K - \widetilde{K}_c \ll t$. In this case the Fermi level is close to the bottom of the band, Eq. (19), where internal momenta $k \ll 1$ of fermions asymptotically coincide with physical momenta p of dimers, and their energy $\epsilon(p) \approx \varepsilon(k)$ can be expanded:

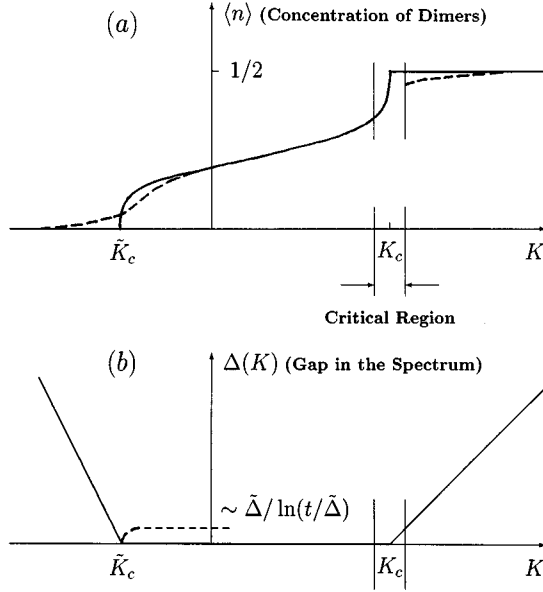$$\epsilon(p) = 2(\widetilde{K}_c - K) + \frac{p^2}{2m}, \tag{22}$$

FIG. 4. The K dependence of the average dimer concentration $\langle n \rangle$ at $T=0$ (a) and the gap Δ (b). Solid lines, the results in first order in $\delta \mathcal{H}$ (exact solution of the Hamiltonian H_{01}); dashed lines, the results corrected due to effects of second order in $\delta \mathcal{H}$. The true behavior of the gap in the critical region near the phase transition K_c is not clear (see Sec. VI).

where the effective mass of a dimer $m = 1/2t$. The concentration of fermions, $\rho \equiv \langle a_n^\dagger a_n \rangle$, and the concentration of dimers, $n = \rho/(1+\rho)$, are both small:

$$n \approx \rho \approx \frac{1}{\pi}\sqrt{2(K-\widetilde{K}_c)/t} \ll 1, \quad k_F = \pi\rho. \quad (23)$$

Thus, we have here a dilute gas of dimers; in this limit the low-energy quasiparticles are isolated dimers.

(2) Close to the upper threshold $0 < K_c - K \ll t$. In this case the Fermi level is close to the top of the band. Here each hop of a fermionic hole by one lattice spacing in the internal coordinates is equivalent to a hop of a soliton by two lattice spacings in the physical coordinates; hence internal momenta k and physical momenta p are connected by an asymptotic relation $k \approx 2p$. Similarly, the internal concentration of fermionic holes, $\rho^* = 1 - \rho = \langle a_n a_n^\dagger \rangle$, is related to the physical concentration of solitons, $\nu \equiv 1 - 2n$, by $\nu \approx \rho^*/2$, and both concentrations are small:

$$\rho^* \approx 2\nu \approx \frac{1}{\pi}\sqrt{(K_c-K)/t} \ll 1, \quad k_F = \pi(1-\rho^*). \quad (24)$$

We have here a dilute gas solitons, carrying one free spin.

Outside the quantum-liquid range the band for fermions is either totally empty (for $K < \widetilde{K}_c$) or totally filled (for $K > K_c$). The kinetic energy term $H^{(1)}$ is therefore effectively turned off, and H_{01} coincides with $H^{(0)}$. Note that the entire above scenario is analogous to the spontaneous quantum-vacancy production[10] and has none of the 1D specifics. It can be applied to the 3D case with small modifications.

B. Floating spins: Role of magnetic interactions

So far we have neglected the magnetic interaction, Eq. (10); thus the ground state was 2^M-fold degenerate with respect to all the floating-spin configurations. To study how this degeneracy is lifted by H_m and what is the true ground state, one can treat the magnetic interaction within the framework of the adiabatic approximation.

Two neighboring floating spins $\mathbf{s}_i'$ and $\mathbf{s}_{i+1}'$ are coupled to each other by the exchange $(\mathbf{s}_i' \cdot \hat{J} \cdot \mathbf{s}_{i'}')$ only in those moments of time when they are real physical neighbors (not only neighbors in their floating numeration), i.e., when there are no dimers between them. At all other times they are decoupled.

On the other hand, the dimer configurations are changing very rapidly. Namely, the characteristic time scale t^{-1} for the orbital motions within the quantum-liquid regime is much shorter than that for spin-flip processes (J^{-1}). Therefore we can introduce effective time-averaged exchanges $\hat{J}_{\text{eff}}(K)$, proportional to the fraction of time, when a given free spin has its *physical* right-hand-side neighbor being also free (but not coupled in a dimer):

$$\hat{J}_{\text{eff}}(K) = \frac{\langle a_{n+1}a_{n+1}^\dagger a_n a_n^\dagger \rangle}{\langle a_n a_n^\dagger \rangle}\hat{J} = \left(\rho^* - \frac{\sin^2(\pi\rho^*)}{\pi^2\rho^*}\right)\hat{J}. \quad (25)$$

For low dimer concentration ($K \rightarrow \widetilde{K}_c$) almost all the spins are free, and so $\hat{J}_{\text{eff}} \approx \{1 - (1/\pi)[2(K-\widetilde{K}_c)/t]^{1/2}\}\hat{J} \rightarrow \hat{J}$, while for low concentration of free spins (at $K \rightarrow K_c$) the probability to have free spins on two neighboring sites vanishes, and $\hat{J}_{\text{eff}} \approx (1/3\pi)[(K_c-K)/t]^{3/2}\hat{J} \rightarrow 0$.

Thus, in the adiabatic approximation, which is valid (with the exception of a very narrow critical region near the threshold K_c) if $t \gg J$, the total wave function of the system can still be factorized in the form of Eq. (13). The orbital part $\psi(n_1, \ldots, n_N)$ is the same, as before [see Eq. (18)], but the floating-spin part $\Xi(\sigma_1', \ldots, \sigma_M')$ is not an arbitrary one any more. It is an eigenfunction of the effective Heisenberg Hamiltonian

$$H_m^{(\text{eff})} = \sum_{i=1}^{M-1} (\mathbf{s}_i' \cdot \hat{J}_{\text{eff}} \cdot \mathbf{s}_{i+1}'). \quad (26)$$

The chain of spins $s = 1/2$ with Hamiltonian (26) is a well-known exactly solvable XYZ model (see, e.g., Ref. 11). Its ground state is either ferromagnetic, antiferromagnetic, or (in the case of isotropic antiferromagnetic exchange) singlet. We will not discuss here the well-known properties of these states, but only mention one peculiarity, specific to our problem.

The magnetism of the floating spins has rather an itinerant character, and a physical distance a-a' between two floating spins $\mathbf{s}_i'$ and $\mathbf{s}_{i'}'$ (with fixed separation i-i' in their floating notation) is not fixed, but is subject to Gaussian fluctuations with dispersion $\propto \ln|i-i'|$ (see Ref. 8). This leads to a faster decay of magnetic correlations in real physical space than for the conventional chain.[8] In particular, for the axially symmetric case (XXZ model) the transverse magnetic fluctuations decay as

$$\langle s_a^+ s_{a'}^- \rangle \propto (1-2n)^2 |a-a'|^{-\theta-1},$$

while $\langle s'^+_i s'^-_{i'} \rangle \propto |i-i'|^{-\theta}$,   (27)

where

$$\theta = \frac{1}{2}\sqrt{\frac{\pi - 2J_z/J_x}{\pi + 2J_z/J_x}}$$

is the standard index of the transverse correlation function for the *XXZ* model (see Ref. 11).

Note that in the above consideration we have taken into account only the H_m correction, but not the $H^{(2)}$ one. The latter does not conserve the number of dimers and, therefore, contributes to the ground-state energy only in second order. The corresponding correction $\sim t^4/\omega^3$ cannot compete with the contribition of H_m, which is $\sim J \gtrsim t^2/\omega$.

One should have in mind that the total wave function Ψ has a relatively simple factorized structure only in the above floating-spin (s'_i)–internal-coordinate (n) representation. In the initial physical representation the *physical* spin variables (s_a) are heavily mixed with the *physical* orbital ones (b), and the explicit form of Ψ in the initial representation is immense and practically useless.

C. Gap in the spectrum of the quantum liquid

Except certain highly symmetric cases (the isotropic Heisenberg chain or the easy-plane one) the spectrum of Hamiltonian $H_m^{(\mathrm{eff})}$, describing ''magnetic excitations'' in the system, has a finite gap $\Delta_{\mathrm{mag}} \sim J_{\mathrm{eff}}(K)$. It is not the case for the spectrum of the ''orbital excitations,'' described by the Hamiltonian H_{sym}: These excitations are gapless in the whole range $\widetilde{K}_c < K < K_c$, where the Fermi surface exists. The low-energy orbital excitations should, therefore, be renormalized by the weak residual interaction $H^{(2)}$. In what follows we demonstrate briefly that this interaction, violating the conservation of number of dimers, N, opens a gap in the spectrum of orbital excitations. For simplicity we consider here only the case when $\Delta_{\mathrm{mag}} \gg |\widetilde{\Delta}|$, so that the magnetic excitations are frozen and the spin dependence of $\widetilde{\Delta}_{\sigma \widetilde{\sigma} \sigma' \widetilde{\sigma}'}$ can be eliminated by means of projecting onto the ground state of $H_m^{(\mathrm{eff})}$. Then we arrive at the effective Hamiltonian for orbital degrees of freedom,

$$H = H_{\mathrm{sym}} + \sum \{\widetilde{\Delta} d_b^\dagger d_{b+2}^\dagger + \widetilde{\Delta}^* d_{b+2} d_b\},$$

$$\widetilde{\Delta} \equiv \langle \Xi | \widetilde{\Delta}_{\sigma_0 \sigma_1 \sigma_2 \sigma_3} | \Xi \rangle;   (28)$$

the indices $\sigma_0 \sigma_1 \sigma_2 \sigma_3$ in the last formula are to be convoluted with the arguments of the ground state Ξ functions, corresponding to four consequent floating spins $s'_i, s'_{i+1}, s'_{i+2}, s'_{i+3}$.

The transformation to the fermionic fields $\alpha_b^\dagger (\alpha_b)$, resolving the on-site constraint and used in the previous section, can be applied to the Hamiltonian (28) as well. Choosing an appropriate phase for operators α_b, we obtain the Hamiltonian

$$H = \sum_b \{\Delta_d \alpha_b^\dagger \alpha_b - t(\alpha_b^\dagger \alpha_{b+1} + \alpha_{b+1}^\dagger \alpha_b) + U(\alpha_{b+1}^\dagger \alpha_{b+1})$$

$$\times (\alpha_b^\dagger \alpha_b) - i|\widetilde{\Delta}|(\alpha_b^\dagger \alpha_{b+2}^\dagger - \alpha_{b+2}\alpha_b)\}   (29)$$

of interacting spinless fermions with repulsive constraint at neighboring sites and superconductinglike $\widetilde{\Delta}$ terms. The sqeezing transformation (16), used in the previous section for resolving the constraint at neighboring sites, is here, unfortunately, not very helpful, because it makes $\widetilde{\Delta}$ terms nonlocal.

Thus, we have to stay with the problem of interacting fermions, governed by the Hamiltonian (29). This problem is tractable, if the concentration of dimers is low: $\langle n \rangle \ll 1$. We give here only an outline of the solution and restrict ourselves to an evaluation of relevant quantities, without calculation of numerical factors. As a first step, we renormalize the interaction of fermions and introduce the vertex function Γ in a standard way (see, e.g., Ref. 12). For small momenta p we obtain $\Gamma \sim tp^2$ (with a positive coefficient of order unity). Then, proceeding in the spirit of BCS-like mean-field theory (see Ref. 12) we find quasiparticles with the spectrum

$$\widetilde{\epsilon}(p) = \mathrm{sgn}[\epsilon(p)]\sqrt{\Delta^2(p) + \epsilon^2(p)},$$

where $\Delta(p) \approx Dp$ for $p \ll 1$,   (30)

and $\epsilon(p)$ is described by Eq. (22). Note that $\Delta(p) \propto p$ is an odd function of p, because spinless fermions can only be paired in a tripletlike antisymmetric state. For the constant D we get the self-consistency ''gap equation'' in the form

$$D = 4|\widetilde{\Delta}| - gDt \int \frac{p\,dp}{\widetilde{\epsilon}(p)},   (31)$$

where the dimensionless ''coupling constant'' $g \sim 1$ is positive and related to the numerical coefficient in the Γ amplitude.

For $K < \widetilde{K}_c$ the second term on the right-hand side of Eq. (31) can be completely neglected; therefore $D \approx 4|\widetilde{\Delta}|$. Then, in the range $0 < \widetilde{K}_c - K < |\widetilde{\Delta}|^2/t$ we obtain for the average number of dimers in the ground state

$$\langle n \rangle = \left\langle \sum_b \alpha_b^\dagger \alpha_b \right\rangle \approx \int \left(\frac{\Delta(p)}{\epsilon(p)}\right)^2 dp \sim \frac{|\widetilde{\Delta}|^2}{t^{3/2}(\widetilde{K}_c - K)^{1/2}}.   (32)$$

Thus $\langle n \rangle$ does not vanish identically for $K < \widetilde{K}_c$ but decays smoothly. In general, $\langle n(K) \rangle$ is a continuous function, increasing monotonously, when K increases [see Fig. 4(a)].

For $K > \widetilde{K}_c$ there are two regions with different behavior of the spectrum. In the immediate vicinity of $\widetilde{K}_c$, where the concentration of dimers is so small that $\langle n \rangle \ln(t/|\widetilde{\Delta}|) \ll 1$, their interaction can be neglected and the gap function still coincides with the ''bare'' one: $D \approx 4|\widetilde{\Delta}|$. Thus in the range $K - \widetilde{K}_c \ll t/\ln^2(t/|\widetilde{\Delta}|)$ the gap in the spectrum of excitations is

$$\Delta(K) \approx \Delta(k_F) \sim |\widetilde{\Delta}| \sqrt{\frac{K - \widetilde{K}_c}{t}}.   (33)$$

The reason for the suppression of the gap near $\widetilde{K}_c$, where the Fermi momentum k_F vanishes, is as follows: Spinless fermions have a tendency to avoid each other and keep distances of the order of an average one ($\sim k_F^{-1} \gg 1$). On the other hand, the pairing interaction becomes active if the fermions approach each other as close as two lattice spacings, which happens only rarely. Note that there exists a point $K = \widetilde{K}_c'$ where the gap $\Delta(K)$ vanishes. The position of $\widetilde{K}_c'$ is a little bit shifted with respect to $\widetilde{K}_c$ by an interplay of the interaction of fermions and $\widetilde{\Delta}$ terms. Exactly at the point $K = \widetilde{K}_c'$ the low-energy excitations of the system are massless fermions with a spectrum $\epsilon(p) = 4|\widetilde{\Delta}||p|$. The average number of dimers at this point is $\langle n(\widetilde{K}_c') \rangle \sim |\widetilde{\Delta}|/t$.

For higher K [i.e., for $t/\ln^2(t/|\widetilde{\Delta}|) \ll K - \widetilde{K}_c \ll 1$] the gap function is heavily suppressed by the repulsive interaction of fermions. Solution of Eq. (31) in this range gives $D \approx 4|\widetilde{\Delta}|/g k_F \ln(t/|\widetilde{\Delta}|) \ll |\widetilde{\Delta}|$, and the gap in the excitation spectrum,

$$\Delta(K) \approx \frac{4|\widetilde{\Delta}|}{g \ln(t/|\widetilde{\Delta}|)}, \qquad (34)$$

ceases to depend on the coupling constant K [see Fig. 4(b)].

If $|\widetilde{\Delta}| \sim J_{\text{eff}}$, the low-energy orbital excitations are strongly mixed with the magnetic ones. There are no doubts, however, that the gap in their spectrum survives also in this case. The existence of the special point $\widetilde{K}_c'$, where the gap vanishes, is also likely to survive, though it is a more delicate question.

The behavior of the system in the vicinity of the other boundary of the quantum-liquid range, close to the phase-transition point $K = K_c$, is an open question. In this region all three factors, the kinetic energy of solitons, their magnetic interaction, and the $\widetilde{\Delta}$ terms, creating 4's of solitons, become equally important and interplay actively. We do not have a quantitative theory for this critical behavior; a qualitative discussion is given in Sec. VI.

D. Thermodynamics of the symmetric chain

We discuss now the thermodynamics of the model. First we have to note that there are four temperature ranges with different behavior of the system: (1) $T < \Delta(K)$, "frozen" regime; (2) $\Delta < T \sim T_{\text{mag}} \ll T_F$, spin-chain regime; (3) $T_{\text{mag}} \ll T \ll T_F$, Fermi-liquid regime; and (4) $T \gg T_F$, classic regime. Here $\Delta(K)$ is the gap in the spectrum of fermions [see Eqs. (33),(34)], $T_{\text{mag}}(K) \sim J_{\text{eff}}(K)$ is the freezing temperature for the spin degrees of freedom, and $T_F(K)$ is the Fermi temperature for the Fermi gas, discussed in Sec. III A. If K is not very close to any of the thresholds, then $T_F \sim t$, though it vanishes upon approaching a boundary of the quantum-liquid domain: $T_F(K) \approx 2(K - \widetilde{K}_c)$ for $K \to \widetilde{K}_c$ and $T_F(K) \approx (K_c - K)$ for $K \to K_c$. We discuss these four regimes below.

(1) Frozen regime. Here all the excitations in the system are frozen out, and the thermodynamics is dominated by those quasiparticles which have the lowest gap, i.e., by the fermions (in the case, when the magnetic excitations have a gap). The thermodynamics of the system in this low-temperature range is identical to that of a superconductor with a gap $\Delta(K)$: the specific heat $C(T) \propto \exp[-\Delta(K)/T]$, etc.

(2) Spin-chain regime. Here the thermodynamics is dominated by the magnetic excitations, excitations of the floating-spin variables, governed by the Hamiltonian (26). Therefore the properties of the model in this range are identical to those of the XYZ chain of $M = N_0[1 - 2n(K)]$ spins, coupled by the exchange $\hat{J}_{\text{eff}}(K)$. (For a discussion of the thermodynamics of the XYZ chain see Ref. 11.) The corresponding specific heat $C_{\text{mag}}(T)$ reaches the maximum value $C_{\text{mag}}^{(\max)} \sim [1 - 2n(K)]$ at $T \sim T_{\text{mag}}$. At high temperatures $T \gg T_{\text{mag}}$ all the spin configurations become equipopulated, the specific heat $C_{\text{mag}}(T) \to 0$, and the magnetic part of the entropy tends to a saturation: $S_{\text{mag}} \to M \ln 2$.

(3) In the Fermi-liquid regime (and, certainly, also in the classic one) the magnetic interactions can be altogether neglected, and one is left with the spinless-fermions problem, Eq. (17), supplemented with an additional entropy $S_{\text{mag}} = N_0(1 - 2n)\ln 2$, regarding the degeneracy with respect to the floating-spin variables. The "superconductinglike" $\widetilde{\Delta}$ terms are also negligible in this regime, since $T_{\text{mag}} \gg \Delta(K)$. The population of fermionic states with different internal momenta k is described by the Fermi-Dirac distribution function $f_k = (1 + \exp\{[\varepsilon(k) - \mu]/T\})^{-1}$, where the spectrum $\varepsilon(k)$ is defined by Eq. (19), while the chemical potential for the fermions, $\mu = \mu(T)$, is to be found. One should not mix this chemical potential with the chemical potential for dimers; the latter is, of course, zero. The total free energy (normalized to the unit cell) of the system with fixed concentration of dimers n is

$$F(n, \mu(n,T), T) = \mu n + (1-n)\Omega(\mu, T) - (1 - 2n)T \ln 2, \qquad (35)$$

where the last term is the contribution of the free spins, mentioned above, while

$$\Omega(\mu, T) = -T \int_{-\pi}^{\pi} \frac{dk}{2\pi} \ln(1 + \exp\{[\mu - \varepsilon(k)]/T\}) \quad (36)$$

is a standard thermodynamical potential of an ideal 1D Fermi gas. The relation

$$\rho \equiv \frac{n}{1-n} = -\frac{\partial \Omega}{\partial \mu} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} f_k \qquad (37)$$

follows from the condition $\partial F/\partial \mu = 0$ and determines the dependence $\mu(n,T)$. Its meaning is clear: It relates the chemical potential of the fermions to their total concentration ρ. The equilibrium concentration then should be found from the condition of the free-energy minimum: $\partial F/\partial n = 0$. This condition leads to the following equation, governing the chemical potential:

$$\Omega(\mu, T) = \mu + 2T \ln 2. \qquad (38)$$

Solving it and substituting $\mu(T)$ into Eq. (37), one can, in principle, find the temperature dependence of the dimer concentration $n(T)$. Substituting Eq. (38) into Eq. (35) we arrive at the simple relation

$$F = \mu + T \ln 2, \qquad (39)$$

which facilitates the further calculations substantially. For example, for the specific heat it gives

$$C(T) = -T\frac{d^2\mu(T)}{dT^2}. \tag{40}$$

At relatively low temperatures $T_{\mathrm{mag}}(K) \ll T \ll T_F(K)$, when the Fermi gas is degenerate, the thermodynamical potential can be expanded in T:

$$\Omega = \Omega_0 - \frac{\pi T^2}{6v_F}, \quad \Omega_0 = \frac{2t}{\pi}(k_F\cos k_F - \sin k_F), \tag{41}$$

where $v_F = 2t\sin k_F$, $\mu = \Delta_d - 2t\cos k_F$. After some algebra we find the specific heat:

$$C(T) = \gamma(K)T, \tag{42}$$

where $\gamma(K) \sim 1/t$ if K is not close to any threshold, but $\gamma(K) \to \infty$ upon approaching a boundary of the quantum-liquid domain: $\gamma(K) \approx (\pi/6)[2t(K - \widetilde{K}_c)]^{-1/2}$ for $K \to \widetilde{K}_c$, $\gamma(K) \approx (\pi/12)[t(K_c - K)]^{-1/2}$ for $K \to K_c$. The linear temperature dependence of the specific heat is quite natural for the fermionic system. The above divergence is due to the fact that the Fermi velocity v_F, appearing in Eq. (41), vanishes when the Fermi level approaches either the bottom or the top of the band.

(4) In the classic regime (for $T \gg T_F$) the kinetic energy can be altogether neglected, and the results of Ref. 1, obtained for the basic model, are applicable. Note, however, that for the present 1D version of the basic model, all the thermodynamical properties can be found explicitly for an arbitrary relation between Δ_d and T.

Indeed, neglecting the dispersion [i.e., substituting $\varepsilon(k) \equiv \Delta_d$ in Eqs. (37),(38)], we arrive at the following equations for μ and n:

$$2\ln 2 + \frac{\mu}{T} = -\ln\left\{1 + \exp\left(\frac{\mu - \Delta_d}{T}\right)\right\}, \tag{43}$$

$$n = \frac{\rho}{1+\rho} = \left\{2 + \exp\left(\frac{\Delta_d - \mu}{T}\right)\right\}^{-1}, \tag{44}$$

which can be solved analytically. Their solution gives

$$\mu = -T\ln\{2[1 + \sqrt{1 + \exp(-\Delta_d/T)}]\}, \tag{45}$$

$$n(T) = \frac{1}{2}\left\{1 + \exp\left(\frac{\Delta_d}{T}\right)\left[1 + \sqrt{1 + \exp\left(-\frac{\Delta_d}{T}\right)}\right]\right\}^{-1}. \tag{46}$$

The explicit expressions for the specific heat and magnetic susceptibility (the latter being simply proportional to the concentration $1 - 2n$ of free spins: $\chi(T) = \chi_{\mathrm{para}}[1 - 2n(T)]$, where $\chi_{\mathrm{para}} \propto 1/T$ is the paramagnetic susceptibility of free spins; see Ref. 1) can also be easily derived with the aid of Eqs. (40) and (46); see Ref. 5 and Figs. 6,7 of Ref. 1.

V. CHAIN WITHOUT INVERSION SYMMETRY

Without inversion symmetry there is no reason for τ to be zero. We have already mentioned that in this case the form of

the reduced Hamiltonian $H_{\{\sigma_i'\}}$ is rather complicated (for a general set of the floating-spin quantum numbers $\{\sigma_i'\}$). We did not succeed in finding a general expression for a "partial" ground state energy $E_G\{\sigma_i'\}$ in order to find the true ground state of the system rigorously, in a straightforward procedure of minimization of $E_G\{\sigma_i'\}$ with respect to different sets $\{\sigma_i'\}$. Nevertheless, we can try to guess what the ground-state set $\{\sigma_i'\}$ could be, based upon symmetry considerations.

A. Ground state of the asymmetric chain

Since the Hamiltonian of the problem is translationally invariant, the most obvious choice of $\{\sigma_i'\}$ would be the fully translation-invariant ferromagnetic set, where all σ_i' are the same: either up ($\sigma = 1$) or down ($\sigma = -1$). The ferromagnetic choice seems to be supported by qualitative Nagaoka-theorem-like arguments: The ferromagnetic background is likely to facilitate the energy lowering due to the mobile dimer kinetic energy. There is, however, one additional internal symmetry of the Hamiltonian H_{01}, which modifies the Nagaoka theorem for our case. Actually any hop shifts the physical position of a free spin always by two lattice spacings ($a \to a \pm 2$). Then, having in mind that the parity of position a of a free spin $\mathbf{s}_a$ coincides with the parity of the number i of the corresponding floating spin $\mathbf{s}_i'$, one can conclude that the Nagaoka theorem[7] actually requires here ferromagnetism not for the entire set $\{\sigma_i'\}$, but for two subsets with even and odd i separately. Thus, on the basis of the Nagaoka theorem, we can expect the antiferromagnetic set of alternating floating spins $[\sigma_i' = (-1)^i \sigma]$ to have the same energy as the ferromagnetic one. The antiferromagnetic set describes a "minimal" breaking of the translational symmetry, a doubling of the period. The Nagaoka theorem, being an exact one only for a single dimer, cannot be proved rigorously for a finite concentration of dimers. So, strictly speaking, we cannot exclude further lowering of the initial symmetry in the ground state (like tripling of period or other exotic possibilities), but we find it unlikely. Therefore we restrict our consideration to the two physically plausible options mentioned above.

In both ferromagnetic and antiferromagnetic cases the Hamiltonians $H_{\{\sigma_i'\}}$ for the orbital degrees of freedom can be written explicitly:

$$H_{01}^{(F)} = \Delta_d N + \sum_b \{-t(d_b^\dagger d_{b+1} + d_{b+1}^\dagger d_b) - i\tau\sigma(d_b^\dagger d_{b+1}$$
$$- d_{b+1}^\dagger d_b) + U(d_b^\dagger d_b^\dagger d_b d_b + d_{b+1}^\dagger d_b^\dagger d_b d_{b+1})\}, \tag{47}$$

$$H_{01}^{(AF)} = \Delta_d N + \sum_{b=1}^{N_0-1} \{-t(d_b^\dagger d_{b+1} + d_{b+1}^\dagger d_b)$$
$$- i(-1)^b \tau\sigma(d_b^\dagger d_{b+1} - d_{b+1}^\dagger d_b) + U(d_b^\dagger d_b^\dagger d_b d_b$$
$$+ d_{b+1}^\dagger d_b^\dagger d_b d_{b+1})\}, \tag{48}$$

with the same notations as in Eq. (14). The crucial point is that, by means of the phase transformations

$$d_b \rightarrow d_b^{(F)} \exp[-i\sigma b \arctan(\tau/t)], \qquad (49)$$

for ferromagnetic case, and

$$d_b \rightarrow d_b^{(AF)} \exp\left(-i\sigma \frac{(-1)^b}{2} \arctan(\tau/t)\right), \qquad (50)$$

for antiferromagnetic case, both $H_{01}^{(F)}$ and $H_{01}^{(AF)}$ may be reduced to the *same* form, coinciding with the Hamiltonian H_{sym} of the symmetrical chain [see Eq. (14)] up to a replacement

$$t \rightarrow t' = \sqrt{t^2 + \tau^2}. \qquad (51)$$

Thus the Hamiltonian H_{01} with $\tau \neq 0$ has a fourfold-degenerate ground state (two ferromagnetic and two antiferromagnetic components). All the results of Sec. IV A are applicable also to the case of the asymmetric chain [with a substitution (51)]. In particular, the zero-T concentration of dimers $n(K)$ is given by Eq. (21).

The role of the spin-spin interactions H_m is here somewhat different from that in the case of the symmetric chain, especially for antiferromagnetic exchange. For the symmetric chain the magnetic interactions had to lift the *infinite* degeneracy with respect to floating-spin configurations $\{\sigma_i'\}$, which resulted in the nontrivial Bethe-ansatz ground-state wave function $\Xi(\sigma_i')$. For the asymmetric chain the magnetic interactions have to take care of the fourfold global degeneracy, and may only choose between the ferromagnetic state $\Xi_F = |\uparrow\uparrow\uparrow\uparrow\cdots\rangle$ and a Néel-type antiferromagnetic one $\Xi_{AF} = |\uparrow\downarrow\uparrow\downarrow\cdots\rangle$. Both states are of the Ising type: the magnetization (or staggered magnetization in AF case) is parallel to τ and there are no quantum fluctuations (spin flips) in terms of the floating spins. In terms of physical spins $\mathbf{s}_a$, of course, *there are strong quantum fluctuations* in both the ferromagnetic and antiferromagnetic cases; it is due to these fluctuations that the effective magnetic moment is reduced by a factor $1 - 2n(K)$ and tends to zero when $K \rightarrow K_c$.

The discussion of the gap in the spectrum of orbital excitations (fermions), opened by the interaction $H^{(2)}$, given in Sec. IV C for the symmetric case, applies to the asymmetric case as well; the gap is described by expressions (33),(34). An assumption $\widetilde{\Delta} \ll \Delta_{\text{mag}}$, necessary for the reduction of the spin dependence of the $\widetilde{\Delta}$ operator, is fulfilled in the asymmetric case even easier, because the gap in the spectrum of magnetic excitations Δ_{mag} is here much higher than in the symmetric case (namely, $\Delta_{\text{mag}} \sim \tau$ instead of $\Delta_{\text{mag}} \sim J_{\text{eff}}$).

B. Thermodynamics of the asymmetric chain

As in the symmetric case, we have here two types of excitations.

(1) Purely orbital excitations, not affecting the floating-spin quantum numbers $\{\sigma_i'\}$. They have fermionic character, their energies are given by Eq. (19), and their contribution to the specific heat at temperatures $T \gg \Delta(K)$ is described by Eq. (42). At very low $T < \Delta(K)$ we have again the frozen regime with exponentially small specific heat, etc.

(2) "Magnetic" excitations, affecting the quantum numbers $\{\sigma_i'\}$. In the symmetric case these excitations were decoupled from the orbital degrees of freedom; they had a low-energy scale $\sim J_{\text{eff}} \ll t$ and dominated the thermodynamics in

the range $T \sim J_{\text{eff}}$. In the asymmetric case, however, the magnetic excitations involve orbital degrees of freedom heavily. Therefore there is no reason any longer for the magnetic excitations to have an energy scale different from that for the purely orbital excitations. Although we are not able to calculate the spectrum of magnetic excitations explicitly, we will adopt a natural assumption that there is a gap Δ_{mag} in this spectrum. "Deep" in the quantum liquid regime (i.e., when K is not especially close to $\widetilde{K}_c$ or K_c), this gap can be estimated as $\Delta_{\text{mag}} \sim \tau \sim t$; close to any of the boundaries the gap should be suppressed. The magnetic excitations can contribute to thermodynamics only at relatively high $T \sim t$, while for $T \ll t$ the thermodynamics is dominated by the quasigapless purely orbital excitations (hence linear specific heat, etc.).

Thus, the thermodynamics of the asymmetric chain is similar to that of the symmetric one: The frozen regime, the Fermi-liquid regime, and the classical regime are basically the same. The spin-chain regime is, however, absent, and there is no corresponding maximum of the specific heat at $T \sim T_{\text{mag}}$; moreover, there is no such temperature scale as T_{mag} whatsoever.

VI. CHARACTER OF THE PHASE TRANSITION

From the most general point of view our system is characterized by following two order parameters: The magnetic order parameter is a magnetization (staggered magnetization) in ferromagnetic (antiferromagnetic) cases:

$$M_{F,\text{AF}} = \sum_a (\pm 1)^a \langle \mathbf{s}_a \rangle. \qquad (52)$$

The amplitude of the phonon density wave is

$$\Lambda = \sum_b (-1)^b \langle (\mathbf{Q})_b^2 \rangle. \qquad (53)$$

In the low-K magnetic phase $M \neq 0$, $\Lambda = 0$, and the time-inversion symmetry is broken, while in the high-K nonmagnetic phase the time-inversion symmetry is restored, but the translational invariance is broken (due to the formation of the phonon density wave). From the point of view of symmetry alone this situation is identical to the spin-Peierls transition (see Ref. 13). There is, however, an important physical difference: In the spin-Peierls case the nonmagnetic phase is characterized by the order parameter $\Lambda_{\text{SP}} = \sum_b (-1)^b \langle \mathbf{Q}_b \rangle$ —i.e., there is a modulation of the classical displacement $\langle \mathbf{Q}_b \rangle \neq 0$—while in our case $\langle \mathbf{Q}_b \rangle \equiv 0$, $\Lambda_{\text{SP}} = 0$, and it is only the amplitude of zero vibrations $\langle (\mathbf{Q})_b^2 \rangle$ that is modulated.

What is very important is that neither of the symmetry groups $\mathbf{G}_M$, $\mathbf{G}_{\text{NM}}$ of the two above phases is a subgroup of another one. It means (if one implies a direct transition, without any intermediate phases) that the necessary condition for the second-order transition is not fulfilled and it can only be of first order.[14]

Let us discuss our results from the point of view of this requirement. For the pure basic model it is fulfilled, since both M and Λ change abruptly at $K = K_c^{(\text{BM})}$ [see Fig. 5(a)]. The situation becomes much more peculiar when one takes into account deviations $\delta\mathcal{H}$ from the basic model. In the first approximation in $\delta\mathcal{H}$ the magnetic order parameter M vanishes at the point $K = K_c$ continuously, in a second-order
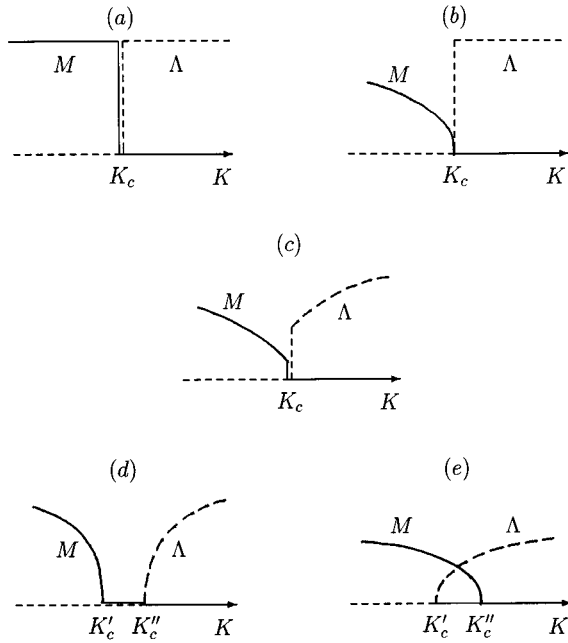
FIG. 5. The K dependence of the zero-T order parameters in the critical region; M, magnetic order parameter (solid lines); Λ, amplitude of phonon density wave (dashed lines): (a) for the basic model (zeroth approximation in $\delta\mathcal{H}$); (b) for the Hamiltonian H_{01} (first approximation in $\delta\mathcal{H}$). (c),(d),(e) Three types of possible true behavior in the immediate vicinity of the phase transition (second approximation in $\delta\mathcal{H}$): (c) the minimal scenario, a first-order phase transition, close to second order; (d) the transition is split into two subsequent second-order phase transitions with fully symmetric intermediate phase (neither magnetic order nor phonon density wave); (e) the same with the low-symmetry intermediate phase (both orders coexist).

manner, while the amplitude of the density wave Λ still undergoes a jump from zero to the saturation value at the same point [Fig. 5(b)]. Such an unusual behavior is pathological from the point of view of the Landau theory of phase transitions, and we can suspect that it is an artifact of the special symmetry of the effective Hamiltonian H_{01} in this approximation. It is likely to be unstable with respect to further corrections (H_m and $H^{(2)}$), violating this additional symmetry. These terms can only be essential in a narrow "critical" vicinity of the phase transition point, where the average concentration of the solitons (holes in the close packing), carrying free spins, is already very low. On the other hand, all the conservation laws which we have used (floating spins and the number of dimers N) are completely destroyed in this critical region. Therefore a description of the system behavior in the critical region (and thus the true character of the phase transition) is still a very tough problem, which is beyond the scope of the present paper. Here we will give only a qualitative discussion of certain possibilities.

Let us discuss what happens when one approaches the critical region from the nonmagnetic (high K) side. For K's which are far enough above the threshold K_c, the average concentration of solitons is very low. They are produced in 4's at random places in rare virtual processes, and disappear again almost immediately, without giving their free spins a chance to interact with each other. Therefore we do

not expect the magnetic order to exist in this region. On the other hand, from the point of view of the phonon density wave, the fact that virtual solitons are bound in 4's means that they are topologically neutral objects, containing two kinks and two antikinks. Hence the sign of the local order parameter Λ is the same in all the long segments, separating these virtual excitations, the long-range order is retained, and the average Λ is suppressed only slightly. Upon approaching K_c both the concentration and the radius of complexes increase and eventually, in the critical region, the complexes begin to overlap. Inside this region there are no well-defined four-soliton complexes any longer: Each soliton has a good chance to annihilate not with its three "brothers," with whom it was created together, but with partners, originating from different 4's. Eventually this will lead to the destruction of the phonon density wave. On the other hand, free spins, carried by unbound solitons, acquire a tendency to develop a magnetic long-range order.

It is *a priori* unclear whether the above two phase transformations must occur simultaneously, but this option seems to be the most likely "minimal scenario." In this case the phase transition is necessarily of first order, but close to second order. Although the magnetic order parameter does not vanish completely for $K \to K_c - 0$, it tends to a very small value. The order parameter Λ, in its turn, is not constant for all $K > K_c$ any longer, but decreases when approaching $K_c + 0$ [Fig. 5(c)].

The minimal scenario is, however, not the only possible one. The other option would be splitting of the phase transition in a sequence of 2, where in the intermediate phase either both orders coexist or both are absent (fully symmetric nonmagnetic quantum liquid). Then the two corresponding phase transitions could be of second order [Figs. 5(d), 5(e)].

The above arguments do not apply to one special case of chains with isotropic antiferromagnetic interactions, where the "magnetic" phase is actually nonmagnetic due to quantum fluctuations, inherent in a 1D Heisenberg antiferromagnet. This phase is fully symmetric and the necessary condition for the second-order phase transition is fulfilled.

VII. DISCUSSION

Here we will try to generalize the above results, and single out those features which seem to us model independent.

Both parts of the Hamiltonian $\mathcal{H}$, the purely lattice part and the spin-phonon interaction, are quadratic in lattice variables $\mathbf{Q}_b, \mathbf{P}_b$. While the former part is a positively determined quadratic form, the latter part is not, due to presence of spin variables $\mathbf{s}_a$ with an undetermined sign. Therefore, upon increasing the spin-phonon interaction, the lattice must sooner or later become unstable. In the basic model it happens at $|K| = \omega$; in the general case a certain instability surface $\mathcal{I}$ in the space of Hamiltonians must exist. What happens when $\mathcal{H}$ approaches this instability surface along a certain path $\mathcal{P}$ in the space of Hamiltonians?

The effective modes become softer and softer, and the level of quantum fluctuations in the system grows. These fluctuations involve both lattice and spin degrees of freedom, and one can expect the magnetic order to be suppressed (at least partly) near the instability surface. As was shown in

Ref. 1 for the path $\mathcal{P}_{\mathrm{BM}}$, constituted by the one-parameter family of basic model Hamiltonians $\mathcal{H}_{\mathrm{BM}}$, this suppression occurs at $K=K_c^{(\mathrm{BM})}$ abruptly, in such a way that for $K>K_c^{(\mathrm{BM})}$ the magnetization is totally suppressed (spins are fully screened), while for $K<K_c^{(\mathrm{BM})}$ there is no suppression at all (spins are free).

In the present paper we have studied paths $\mathcal{P}$, close to $\mathcal{P}_{\mathrm{BM}}$, in the sense that $\delta\mathcal{H}=\mathcal{H}-\mathcal{H}_{\mathrm{BM}}$ is small along a path $\mathcal{P}$. We have shown that for such a path the behavior of zero-T magnetic order is transformed in the following way: The point K_c of the phase transition to the nonmagnetic state is somewhat shifted towards the instability point, and the transition itself is smoothed in the sense that an ultimate vanishing of the magnetic order parameter M in a phase transition at $K=K_c$ is preceded by a continuous decrease of M already within the magnetic phase. In a narrow strip (its width being of the first order in $\delta\mathcal{H}$) the magnetism is gradually suppressed from the ''normal'' value to a very small one. In this strip a new quantum-liquid phase, which is a mixture of mobile singlet dimers and free spins, arises, and the fraction of singlets increases continuously upon approaching K_c. This phase is magnetic, homogeneous, and almost gapless (the gap in the excitations spectrum is $\Delta\propto\delta\mathcal{H}^2$). The behavior of the system in a very close vicinity of K_c (critical region) is not absolutely clear. The phase transition is most likely a first-order one, close to second order, but the possibility of its splitting in a sequence of two second-order phase transitions with the formation of an intermediate phase of new symmetry is also not excluded.

Let us speculate now about a general path $\mathcal{P}$, starting from the noninteracting point $K_{abb'}^{\alpha\beta\beta'}=0$ and going to large K's. Relying upon the experience obtained in the above perturbational (in $\delta\mathcal{H}$) study of the problem, we expect the following to be true.

(1) A general path $\mathcal{P}$ will necessarily meet the instability surface $\mathcal{I}$.

(2) Certain paths (not all, but at least those sufficiently close to $\mathcal{P}_{\mathrm{BM}}$) will cross the domain of nonmagnetic phase, adjacent to the surface $\mathcal{I}$. The surface $\mathcal{N}$, separating the nonmagnetic domain from the magnetic one, is the surface of zero-T phase transitions; it separates the phases of different symmetries. In the magnetic phase time-reversal symmetry is broken, and in the nonmagnetic one it is not. The translational symmetry in the nonmagnetic phase is most likely to be broken due to the formation of virtual-phonon density wave. A fully translationally symmetric nonmagnetic state is, in principle, also not excluded, but we could not build any example for such behavior (see Ref. 1 and references therein, concerning the ''Quantum dimer model'').

(3) For small spin-phonon couplings the magnetic order persists (if only it is not suppressed already by quantum fluctuations of magnetic Hamiltonian $\mathcal{H}_m$, like in isotropic antiferromagnetic Heisenberg chain). The order parameter, however, decreases gradually upon approaching the nonmagnetic domain boundary $\mathcal{N}$, due to the growth of the singlet spin-phonon fluctuations in the regime of magnetic quantum liquid.

(4) The phase transitions, occurring at the surface $\mathcal{N}$, are most likely of first order if the phonon density wave is present in the nonmagnetic phase. The second-order phase transition is, at least in principle, possible in a hypothetical case of a fully symmetrical phase of nonmagnetic quantum-liquid type.

We have deliberately mentioned here only those most general features of the ground state of the system which, we believe, persist in higher dimensions. In the one-dimensional model, considered in this paper, neither the magnetic order nor the phonon density wave can exist at any finite temperature. That is, of course, not the case for higher dimensions, where we can expect an order to persist up to some critical temperature T_c. However, since in this system we have to deal with the interplay of two different orders, its phase diagram may be complex and its description is beyond the scope of the present paper.

In conclusion, we have demonstrated the possibility of both complete and partial (though quite strong) suppression of magnetism due to quantum fluctuations, induced by strong spin-phonon coupling. While the complete screening of spins is almost inevitably accompanied by the formation of a phonon density wave, partial screening occurs in the translationally invariant system. The phenomenon exists in a finite domain of the space of spin-phonon Hamiltonians, and it is stable with respect to small variations of parameters. We believe that it may be relevant to those ''heavy-fermion'' compounds with a strong spin-phonon interaction, which exhibit either anomalously weak magnetism or no magnetism at all.

Note added. After this paper was submitted, G. Uimin drew my attention to a paper[15] by Villain and Bak, where the ''squeezing transformation'' for diagonalization of the Hamiltonian (15) [arising there from completely different physics, the anisotropic next-nearest-neighbor Ising (ANNNI) model] was introduced. We are sorry for not citing this paper in our work,[8] where we rediscovered the squeezing transformation independently, but 10 years later. Another important message, following from the discussions in Ref. 15, is that the spectrum of the Hamiltonian (28) may remain gapless in a certain range of K's adjacent to K_c, even despite the presence of symmetry-breaking $\widetilde{\Delta}$ terms.

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