Lightly doped dimerized spin chain in the one-dimensional *t-J-J′* model

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We study the one-dimensional *t-J-J′*-model in the limit of small hole doping x and small J/t, J'/t. Special emphasis is put on the regime $J'/J \approx 0.5$, where a spin gap is present at small doping and the undoped spin chain is strongly dimerized. Using a perturbative approach and Luttinger liquid arguments, we demonstrate for this nonintegrable class of models that the charge degrees of freedom behave as noninteracting spinless solitons in the dilute hole limit. Our approach is also used to evaluate the energy and mass renormalization of a single hole. Interestingly, the corrections of these quantities are in powers of $\sqrt{J/t}$. At $J'/J = 0.5$ we construct a variational spin-polaron wave function for the hole and find good agreement with our perturbative results.

I. INTRODUCTION

The discovery of high-T_c superconductors has generated great interest in models of strongly correlated insulators in low dimensions, both in the presence and absence of doped carriers. While in two dimensions the problem remains challenging even for the most elementary models that are believed to capture some of the physics of the cuprates, much can be learned from the study of one-dimensional counterparts of such models. Basic features that characterize the high-T_c materials, such as the absence of a quasiparticle pole near the Fermi surface and possibly spin-charge separation, are essential to one-dimensional systems and are well understood here.[1] The success of the theory in one dimension is due to the availability of powerful exact methods, such as numerical diagonalization and Bethe ansatz, in combination with the knowledge of a low-energy effective theory which has so far been found to describe all gapless degrees of freedom in one-dimensional systems, the Luttinger liquid.[2]

In the present work we study the effect of doping a small concentration of holes into a dimerized spin chain. This is motivated by the idea that in a dimerized system, there naturally exists an amplitude for pair formation. Upon introduction of carriers phase coherence may be established, resulting in superconductivity. This idea has been previously proposed in the literature.[3] We distinguish between two rough physical pictures of hole doping into a dimerized chain (Fig. 1). In the first scenario [Fig. 1(a)] the dimer order remains long ranged even after hole doping. The dimers tend to reside on every second link of the lattice as in the symmetry broken undoped state, and holes tend to pair on the empty sites in between.

We note that this case bears some resemblance to doped ladder models.[6] Indeed strong superconducting correlations have been proposed for dimer models with explicit symmetry breaking.[7,8]

A second possibility is that the holes enter as domain walls between different dimer phases [Fig. 1(b)]. Then the long-range order of dimers is destroyed, but the singlet gap remains. If the holes are mobile and become phase coherent, this leads to superconductivity in analogy with the original RVB scenario.[9] However, the pictures presented in Fig. 1 are based on the limit of large J/t. In physical systems, on the

other hand, J/t is usually a fraction of unity. In this regime, the hole kinetic energy is dominant and it is less clear intuitively if the dimer picture discussed above applies. In the present paper, we study this question in the context of the *t-J-J′* model in one dimension:

$$
\begin{aligned}
H = &-tP\sum_i \ (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \mathrm{H.c.})P \\
&+ J\sum_i \left(S_i \cdot S_{i+1} - \frac{1}{4} n_i n_{i+1} \right) \\
&+ J'\sum_i \left(S_i \cdot S_{i+2} - \frac{1}{4} n_i n_{i+2} \right) + V\sum_i \ n_i n_{i+1}. \quad (1)
\end{aligned}
$$

Here, P is a projection operator that enforces the constraint of no doubly occupied sites. The S_i are spin-1/2 operators, and the nearest- and next-nearest-neighbor couplings J and J' are assumed positive throughout this paper. In addition, we have included a nearest-neighbor interaction V for later convenience.

At finite doping, not much is known analytically about this model due to its nonintegrable nature. The phase diagram has been established numerically[4,5,10] (Fig. 2). However, in the regime around $\alpha \equiv J'/J \approx 0.5$ where the undoped spin chain is strongly dimerized and which is of particular interest to us, we feel that the numerics are somewhat inconclusive for small doping x and $J/t \lesssim 1$ as we will discuss below.

The purpose of this paper is twofold: First, in the case of strong frustration $\alpha \equiv J'/J \approx 0.5$ we wish to determine the fate of the various regions present in the phase diagram of
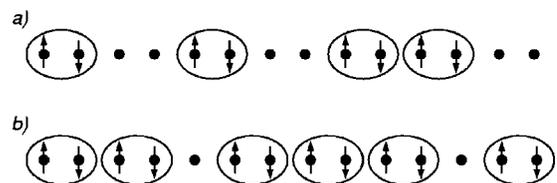

FIG. 1. (a) doping into frozen dimer state. Ovals represent singlet pairs. (b) mobile dimers with domain walls.
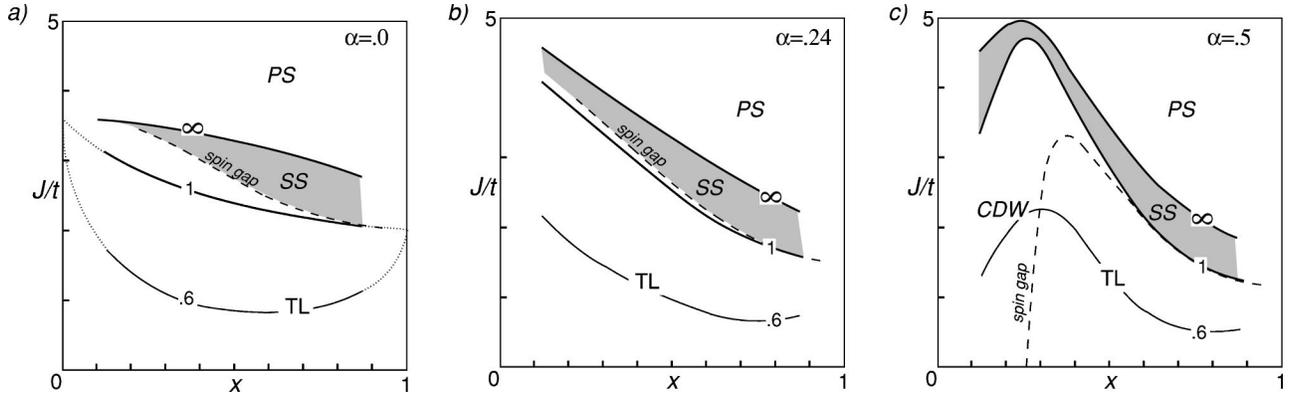
FIG. 2. Sketch of the zero temperature phase diagram of the t-J-J' model as determined numerically in Ref. 4 for $\alpha=0$ (a), $\alpha=0.24$ (b), and $\alpha=0.5$ (c). Contours are labeled by values of K_ρ. The shaded region marks the domain of dominant singlet superconducting correlations. The dotted lines in (a) were proposed in Ref. 5.

the t-J-J' model at small doping and small J/t [Fig. 2(c)]. In particular, we will answer the question whether a regime of dominant singlet superconducting correlations in the vicinity of an instability towards phase separation persists to values $J/t \leqslant 1$ and in the dilute hole limit. This would happen if all the contours in Fig. 2(c) extrapolate to the origin, which appears to be a possible interpretation of the numerics. To this end, we introduce a perturbative approach valid in this limit. We find that the scenario mentioned above does not occur, but instead the Luttinger liquid is stable for small J/t and small doping. Luttinger liquid arguments will then imply that strong superconducting correlations only exist above a finite critical value of J/t.

Second, below the critical value $(J/t)_c$ the liquid phase is stable in the limit $x \rightarrow 0$, and we will use our method to demonstrate certain properties that one expects to hold for one-dimensional lattice models based on general grounds. In particular, spin and charge are expected to correspond to separate degrees of freedom and any microscopic coupling between them should be irrelevant. As a consequence, dilute holes that are doped into a correlated spin chain should act as a gas of noninteracting spinless solitons,[11] where the coupling to the nontrivial spin background only gives rise to a renormalization of the effective hole mass. This phenomenon has been observed in integrable models such as the Hubbard model.[12] Our perturbative approach allows us to give a demonstration of the same behavior in the nonintegrable t-J-J' model, and to calculate the effective energy and mass renormalization of the hole for small J/t.

The remainder of this paper is organized as follows. In Sec. II we introduce the model, briefly discuss the numerical phase diagram, and cast the model into a language where holes are interpreted as domain walls. In Sec. III we treat the spin-charge couplings as a perturbation and derive expressions for the ground-state energy, compressibility and Kohn stiffness of the model for small J/t, J'/t, and small doping x. This will allow us to qualitatively continue the numerical phase diagram into the region of small doping. In Sec. IV we will explicitly evaluate these expressions as asymptotic series in powers of x and $\sqrt{J/t}$, demonstrating the convergence of our approach. In Sec. V we discuss the single polaron

energy and mass renormalization. We introduce a spin polaron type variational wave function where the hole is surrounded by a cloud of tightly bound triplet excitations and find good agreement with our perturbative results. We conclude in Sec. VI. Appendix A illustrates the behavior of our expansion at general order in various limits. An important technical issue is discussed in Appendix B.

II. FORMULATION OF THE PROBLEM

We wish to study the Hamiltonian (1) in the limit of vanishing exchange couplings and doping. For $V=0$ the phase zero temperature diagram of Eq. (1) has been obtained numerically[4,5,10] for various values of the parameter $\alpha \equiv J'/J$. The results are sketched in Fig. 2. These phase diagrams show a Tomonaga-Luttinger liquid (TL) region below the dashed line labeled spin gap, where both spin and charge degrees of freedom are gapless. Above the dashed line there is a spin gapped liquid phase which is subdivided into a regime of dominant singlet superconducting (SS) correlations (shaded gray) and, where present, a regime of dominant charge-density-wave (CDW) correlations. Also shown are contours of constant values of the Luttinger parameter K_ρ. Above the K_ρ line labeled ∞, there is a region of phase separation (PS), where the ground state has a phase boundary between a hole-rich and an electron-rich phase. The parameter K_ρ is directly related to the large distance behavior of the various correlation functions of a Luttinger liquid: For $K_\rho>1$ pairing correlations dominate over density-wave correlations, otherwise density-wave correlations dominate. Furthermore, in the presence of a spin gap, triplet pairing correlations and spin-density-wave correlations are exponentially suppressed. In this region, the main competition is therefore between CDW and SS correlations, which in the presence of a spin gap decay as r^{-K_ρ} and r^{-1/K_ρ}, respectively.[1,13]

At zero doping ($x=0$) it is well known that the spin chain undergoes a phase transition at a critical value of $\alpha_c \approx 0.24$ (Ref. 14) above which the ground state is dimerized with a gap in the spin excitation spectrum.[15] For $\alpha>\alpha_c$ this spin gap remains present over a finite range of doping for any value of J/t, as was shown in Ref. 10. Figure 2 shows that at
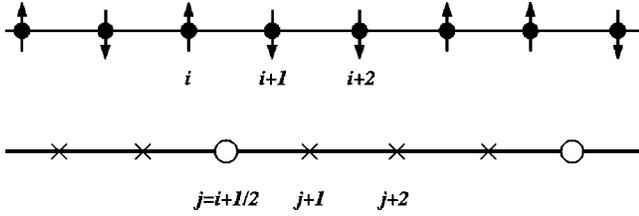
FIG. 3. Domain wall representation of the Hilbert space. The upper chain represents the spin sector with sites labeled by i. The holes live on a lattice of interstitial sites labeled by j. Crosses represent "empty" interstitial sites, circles represent holes between two spins.

$\alpha = 0.5$ the spin gapped region has considerable overlap with the pairing region $K_\rho > 1$ even at small values of doping x. Furthermore, it appears from the numerics as if all K_ρ contours, including the phase separation boundary $K_\rho = \infty$, flow to small values of J/t at small x (cf. Refs. 10,4). One expects that these contours will focus on a critical point $[x = 0, (J/t)_c]$, as was proposed in Ref. 5 for the t-J model $[J' = 0$, Fig. 2(a)]. A possibility that seems consistent with the numerics at $\alpha = 0.5$ is that $(J/t)_c = 0$, i.e., all contours flow into the origin of the phase diagram. In this case, a sufficiently small amount of doping would always lead to phase separation, and upon further doping one would enter a region of dominant SS correlations. Alternatively, $(J/t)_c$ could be finite but possibly smaller than its value at $\alpha = 0$, which is between 3 and 4 [Fig. 2(a)]. This would imply that the above phenomenology of phase separation and superconductivity at small doping occurs only for $J/t > (J/t)_c$, while for $J/t < (J/t)_c$ the liquid phase is stable at any doping x. In the latter case, one would expect the Luttinger parameter K_ρ to approach the value $1/2$ in the dilute hole limit $x \to 0$, which is the value corresponding to noninteracting spinless degrees of freedom. This behavior is clearly exemplified by the numerical phase diagram of the t-J model [Fig. 2(a)]. The primary goal of this paper is to determine which of these two scenarios applies to the t-J-J' model at $\alpha > \alpha_c$.

We begin our analysis by casting the Hamiltonian (1) into a language where the holes play the role of domain walls between broken segments of an infinite spin chain[16] (Fig. 3). We consider a lattice of L sites with a number of N_e electrons and $N_h = L - N_e$ holes. Denoting the ith spin on the lattice by S_i we may regard the spins as residing on a "squeezed" lattice where the hole sites have been dropped from the system and the label i of the spin S_i is a site label in this squeezed space, as in Fig. 3. We also introduce interstitial sites for the squeezed spin lattice whose labels $j = i + 1/2$ differ from those of the spin sites by $1/2$. Each interstitial site may accommodate a number $n_j = 0, 1, \ldots$ of holes. A faithful representation of the Hilbert space of Eq. (1) is given by states labeled by

$$| \ldots, \sigma_i, n_{i+1/2}, \sigma_{i+1}, \ldots \rangle \equiv | \ldots \sigma_i \ldots \rangle | \ldots n_j \ldots \rangle$$

$$\sum_j n_j = N_h, \quad i = 1 \ldots N_e, \quad j = \tfrac{1}{2} \cdots N_e + \tfrac{1}{2}, \quad (2)$$

where $\sigma_i = \pm \tfrac{1}{2}$ denotes the z component of the spin S_i. This language turns out to be particularly convenient when one introduces a large nearest-neighbor hole repulsion, i.e., if we let $V = \infty$ in Eq. (1), such that, it is forbidden for two holes to occupy neighboring sites. In the present language this means that the occupancy of the hole cluster labeled by j is now restricted to be $n_j = 0, 1$. This modification of the model will be irrelevant in the dilute hole limit which we are interested in.[17] We may now choose to formulate the hole dynamics either in terms of hard-core boson operators or spinless fermion operators. For convenience, we introduce fermion ladder operators c_j, $c_j^\dagger$, where the action of $c_j^\dagger$ can be described by cutting the spin chain open at the interstitial site j, introducing a hole at this position and multiplying the state by an appropriate fermion phase. The hole kinetic energy is then simply given by

$$H_c = - \sum_j (t c_j^\dagger c_{j+1} + \text{H.c.}). \quad (3)$$

Equation (3) can be thought of as the $J = J' = 0$ limit of the Hamiltonian. In the other limit of interest, namely, the limit of zero doping $x = N_h/L$, the Hamiltonian becomes that of a pure spin chain:

$$H_s = J \sum_i (X_{i,i+1} + \alpha X_{i,i+2}),$$

$$\text{where} \quad X_{i,i'} = S_i \cdot S_{i'} - \tfrac{1}{4}, \quad (4)$$

where we work at constant $\alpha = J'/J$ from now on, and assume that $\alpha > \alpha_c$, such that the small doping regime is spin gapped. The combined Hamiltonian

$$H_0 = H_s + H_c, \quad (5)$$

where the spin and charge part are still completely decoupled, will serve as a starting point for the perturbation theory we propose. In order to correctly reproduce matrix elements of the Hamiltonian (1), couplings between the spin sector and the charge sector must be introduced:

$$H = H_0 + H_{sc} + H'_{sc}, \quad (6)$$

$$H_{sc} = - J \sum_j n_j \gamma_j, \quad (7)$$

$$H'_{sc} = J \alpha \sum_i X_{i-1, i+1} n_{i-1/2} n_{i+1/2}, \quad (8)$$

where

$$\gamma_{i+1/2} = (1 - \alpha) X_{i,i+1} + \alpha (X_{i-1, i+1} + X_{i, i+2}). \quad (9)$$

Here, H_{sc} is a correction which couples spin and charge by adjusting nearest-neighbor bonds and removing next-nearest-neighbor bonds in the squeezed spin space in the vicinity of a hole. Certain corrections of the latter sort are redundant

whenever two holes are next-nearest neighbors in real space—or nearest neighbors in the present formalism—and this is corrected by H'_{sc}. Formally, H_{sc} and H'_{sc} are suppressed by powers of both *J/t and x*, and hence can be regarded as small compared to H_0. Our strategy is thus to treat the spin-charge coupling terms $H_{sc}+H'_{sc}$ as a perturbation. We must caution, however, that the hole kinetic energy H_c is very small, or order tx^2, and the small energy denominators that appear in perturbation theory must be treated with care. We apply this method to the spin gapped regime $\alpha > \alpha_c$ and find it to be a valid procedure in second-order perturbation theory, in the sense that corrections are indeed small in the limit we consider. The general systematics of this at higher-order perturbation theory are elucidated in Appendix A.

In the following section we will show that our approach gives rise to a perturbative expansion of the ground-state energy which may be used to analyze the phase diagram of Eq. (1) in the vicinity of the origin, where the fate of the various phases is uncertain from numerics for $\alpha > \alpha_c$ [Fig. 2(c)]. We note that the procedure proposed here bears some resemblance to that used by Xiang *et al.* to study the *t-J* model in a first-order perturbative approach.[18]

III. PERTURBATIVE ANALYSIS OF THE MODEL

In gapless one-dimensional systems it is generally possible to derive basic features of the phase diagram from spectral properties by means of Luttinger liquid theory.[2] The low-energy properties of a Luttinger liquid are completely defined in terms of three parameters which have the dimension of a velocity: A sound velocity v_s, a "compressibility" parameter v_N related to elementary charge excitations, and a "stiffness" parameter v_J related to elementary current excitations. These are not independent, but are related by the following universal relations identified by Haldane:[2]

$$v_N = v_s/K_\rho, \quad v_J = v_s K_\rho \tag{10}$$

The parameters v_N and v_J can be calculated from the dependence of the ground-state energy E_0 on the carrier density x and on a phase twist ϕ, respectively,[1] where ϕ is associated with a flux $L\phi$ penetrating the system when it is imposed on a ring with periodic boundary conditions:

$$v_N = \frac{2}{\pi L} \frac{\partial^2 E_0}{\partial x^2}, \tag{11}$$

$$v_J = \frac{\pi}{2L} \left.\frac{\partial^2 E_0}{\partial \phi^2}\right|_{\phi=0}. \tag{12}$$

By Eqs. (11) and (12), v_N is proportional to the inverse compressibility of the system, while v_J is proportional to the Kohn stiffness,[19] which is related to the Drude weight of the conductivity. Equations (10)–(12) allow the determination of K_ρ via

$$K_\rho = \sqrt{\frac{v_J}{v_N}} \tag{13}$$

from the ground-state energy of the system alone. The strategy in now to evaluate both the numerator and the denominator in Eq. (13) perturbatively.

We now proceed by imposing periodic boundary conditions on the charge sector and the spin sector of the system, Eqs. (6)–(8), separately. This is apparently not the same as imposing periodic boundary conditions in real space, since momenta are now quantized in units of $2\pi/N_e$ rather than $2\pi/L$. Note that there is a unique and well defined map between the state space introduced in Eq. (2) and the Hilbert space of the *t-J-J'* model only for a finite system with *open* boundary conditions. Indeed, imposing open boundary in real space *is* equivalent to imposing them in the spin sector and the charge sector separately. However, going from open to periodic boundary conditions is not expected to matter for large system sizes. The unperturbed Hamiltonian H_0 then has two separately conserved momenta, and we denote its ground state by

$$|\sigma_0, \psi_0\rangle \equiv |\sigma_0\rangle|\psi_0\rangle, \tag{14}$$

where $|\sigma_0\rangle$ is the ground state of the spin Hamiltonian H_s on a ring of N_e spin sites. Although for $\alpha > \alpha_c$ the ground state of H_s has a broken translational symmetry and is doubly degenerate, we will assume that $|\sigma_0\rangle$ is a symmetric superposition of the two symmetry broken ground states and thus has zero lattice momentum. Likewise $|\psi_0\rangle$ is a noninteracting Fermi sea of N_h spinless Fermions hopping on N_e sites with periodic boundary conditions. The unperturbed ground-state energy we write as

$$E_0 = E_{\sigma_0} + E_{\psi_0} = E_{\sigma_0} - N_e \frac{2t}{\pi}\sin(k_f), \tag{15}$$

where

$$k_f = \pi \frac{N_h}{N_e} = \frac{\pi x}{1-x} \tag{16}$$

and E_{σ_0}, E_{ψ_0} are the ground-state energy of H_s and the spinless fermion kinetic energy, respectively. We will focus our analysis on the limit $x \to 0$ where J/t is small but fixed. In this limit we argue that the ground-state energy of Eq. (6) has an asymptotic expansion of the form

$$E = E_{\sigma_0} + L(Ax + Bx^2 + Cx^3 + \cdots) \tag{17}$$

The coefficients $A, B, \ldots$ will depend on J/t. At the leading order, they can in principle be inferred from the spinless fermion kinetic energy in Eq. (15). Formally, however it will be more convenient to work with an expansion of the form

$$E = E_{\sigma_0} + N_e\left[\tilde{A}\left(\frac{k_f}{\pi}\right) + \tilde{B}\left(\frac{k_f}{\pi}\right)^2 + \tilde{C}\left(\frac{k_f}{\pi}\right)^3 + \cdots\right]. \tag{18}$$

The coefficients in Eqs. (17) and (18) will in general not be the same, due to the nonlinear dependence of k_f on x in Eq. (16). However, since $N_e = L(1-x)$, the $\tilde{A}$ term in Eq. (18) is linear in x, and hence

$$A = \tilde{A}, \quad B = \tilde{B}. \tag{19}$$

We will now proceed by evaluating the above series order by order in perturbation theory, treating the spin-charge coupling terms $H_{sc} + H'_{sc}$ perturbatively as we have outlined above. We write

$$E = E_0 + E_1 + E_2 + \cdots + E_k + \cdots$$

$$A = A_0 + A_1 + A_2 + \cdots + A_k + \cdots$$

$$\vdots \qquad (20)$$

and similarly for all other coefficients, where the label k denotes a term arising at kth order perturbation theory. We have

$$A_0 = -2t, \quad B_0 = 0, \quad C_0 = \frac{\pi^2}{3} t. \qquad (21)$$

From Eqs. (11)–(13), (17) it follows that at small J/t

$$K_\rho = \frac{\pi}{2} \sqrt{\frac{A_{\phi\phi} x}{2B + 6Cx}} \approx \frac{1}{2} \sqrt{\frac{tx}{B/\pi^2 + tx}}, \qquad (22)$$

where $A_{\phi\phi}$ denotes the second derivative with respect to the phase ϕ introduced above, and $A_0(\phi) = -2t \cos(\phi)$ was used. Equation (22) shows that if B acquires a finite negative value due to the spin-charge couplings, K_ρ will diverge as $x \to 0$ even at small J/t. This would imply strong superconducting fluctuations and phase separation at the divergence. On the other hand, if B is zero or positive, the liquid phase will be stable for small x and J/t, and dominant superconducting correlations will be absent in the vicinity of the origin of the phase diagram. In this case, one would expect that $B = 0$ to all orders in perturbation theory, since for $B > 0$ one would have $K_\rho \to 0$ as $x \to 0$, which seems inconsistent with the numerical phase diagram. Also, $K_\rho = 0$ is a somewhat unlikely pathological limit of Luttinger liquid theory, where the coefficient of the conjugate momentum of the charge field vanishes and the charges freeze into a classical state. This again seems unlikely in the absence of long-rage interactions, which one may assume especially in the presence of a spin gap. As we have argued initially, one would rather expect the charges to behave as noninteracting spinless solitons in the dilute limit, and Luttinger liquid physics then implies that K_ρ assumes the value $\frac{1}{2}$ in this limit, provided that no instability intervenes. This then requires that the coefficient $A_{\phi\phi}$ and C in Eq. (22) are not independent, but have a constant ratio independent of J.

Hence, we distinguish only two cases which we feel are the only ones consistent with the numerical phase diagram

for $\alpha > \alpha_c$, Luttinger liquid theory and general expectations from the study of integrable models:[2,12] 1. $B < 0$, leading to a phase separation instability in the dilute hole limit for any value of J/t, and 2. $B \equiv 0$, $6C \equiv \pi^2 A_{\phi\phi}$ for any J, corresponding to a stable liquid as $x \to 0$ and small J/t, where the charges act as a dilute gas of noninteracting spinless solitons. We will now show that the second case applies.

At first order perturbation theory the energy corrections factorize into mean-field like products, since spin and charge are not correlated in the ground state wave function (14). We have

$$
\begin{aligned}
E_1 &= \langle \sigma_0, \psi_0 | H_{sc} + H'_{sc} | \sigma_0, \psi_0 \rangle \\
&= -N_e J \langle n_j \rangle_0 \langle \gamma_j \rangle_0 + N_e J \alpha \langle X_{i-1,i+1} \rangle_0 \langle n_j n_{j+1} \rangle_0 \\
&= -L \langle \gamma_j \rangle_0 Jx + LJO(x^4),
\end{aligned}
\qquad (23)
$$

hence

$$A_1 = -\langle \gamma_j \rangle_0 J, \qquad (24)$$

where $\langle \ \rangle_0$ denotes the expectation value with respect to $|\sigma_0\rangle$ or $|\psi_0\rangle$ when no ambiguity is possible. Note that the contribution of H'_{sc} is of order x^4. The smallness of this term as $x \to 0$ reflects the fact that the holes obey the Pauli principle which suppresses the probability of two holes being near each other. We see that already at this order, H'_{sc} does not renormalize any of the coefficients in Eq. (17) that we are interested in. We will thus drop it from the subsequent discussion. To determine leading corrections to B and C, we will need to go to second order:

$$E_2 = -\sum_{|\sigma,\psi\rangle}' \frac{\langle \sigma_0, \psi_0 | H_{sc} | \sigma, \psi \rangle \langle \sigma, \psi | H_{sc} | \sigma_0, \psi_0 \rangle}{E_\psi - E_{\psi_0} + E_\sigma - E_{\sigma_0}}, \qquad (25)$$

where the sum goes over a complete set of unperturbed eigenstates and the prime excludes the ground state (14) from the sum. We now rewrite H_{sc} as

$$H_{sc} = -\frac{J}{N_e} \sum_q n_q \gamma_{-q}, \qquad (26)$$

where Fourier transforms

$$n_q \equiv \sum_j e^{iqj} n_j = \sum_k c_{k+q}^\dagger c_k$$

$$\gamma_q \equiv \sum_j e^{iqj} \gamma_j \qquad (27)$$

have been introduced. Using the fact that the intermediate states in Eq. (25) can be chosen to be momentum eigenstates, we have

$$E_2 = -\frac{J^2}{N_e^2} \sum_q \sum_{|\sigma,\psi\rangle}' \frac{\langle \psi_0 | n_{-q} | \psi \rangle \langle \psi | n_q | \psi_0 \rangle \langle \sigma_0 | \gamma_q | \sigma \rangle \langle \sigma | \gamma_{-q} | \sigma_0 \rangle}{E_\psi - E_{\psi_0} + E_\sigma - E_{\sigma_0}}. \qquad (28)$$

It is necessary to distinguish between terms with zero momentum exchange between spin and charge and those with $q \neq 0$. We write

$$E_2 = E_2^0 + E_2', \tag{29}$$

where E_2^0 contains all $q=0$ terms and E_2' contains all the rest. At $q=0$, $n_q = \Sigma n_j = N_h$ commutes with the Hamiltonian, hence there can be no virtual charge excitation and the charge matrix element is diagonal, $|\psi\rangle = |\psi_0\rangle$:

$$E_2^0 = -\left(\frac{k_f}{\pi}\right)^2 J^2 \sum_\sigma' \frac{\langle\sigma_0|\gamma_{q=0}|\sigma\rangle\langle\sigma|\gamma_{q=0}|\sigma_0\rangle}{E_\sigma - E_{\sigma_0}}. \tag{30}$$

Note that virtual states without spin excitations do not enter Eq. (28), since $|\sigma\rangle = |\sigma_0\rangle$ would imply $q=0$ and again the charge part vanishes unless also $|\psi\rangle = |\psi_0\rangle$, which is excluded from the sum. Thus for $\alpha > \alpha_c$ the energy denominator in Eq. (28) is bounded from below by the spin gap Δ which will dominate over charge excitation energies of order tx^2 very close to the Fermi surface. This assures that the perturbative expansion is well behaved in the limit $x \to 0$ (see Appendix A).

For $q \neq 0$ we note that n_q excites only single-particle-hole excitations. We can thus convert the sum over these terms into a double integral over a hole momentum k_1 and a particle momentum k_2:

$$E_2' = -N_e \int_{-k_f}^{k_f} \frac{dk_1}{2\pi} \int_{k_f}^{2\pi-k_f} \frac{dk_2}{2\pi} f(k_1, k_2), \tag{31}$$

where

$$f(k_1, k_2) = \frac{J^2}{N_e} \sum_{|\sigma\rangle}' \frac{\langle\sigma_0|\gamma_{k_2-k_1}|\sigma\rangle\langle\sigma|\gamma_{k_1-k_2}|\sigma_0\rangle}{\epsilon(k_2) - \epsilon(k_1) + E_\sigma - E_{\sigma_0}} \tag{32}$$

and $\epsilon(k) = -2t\cos(k)$ is the free-fermion dispersion. For later convenience, we also introduce the function

$$F(q) = \frac{1}{2}\left[f\left(\frac{q}{2}, -\frac{q}{2}\right) + f\left(-\frac{q}{2}, \frac{q}{2}\right)\right]$$
$$= \frac{J^2}{2N_e}\left(\sum_{|\sigma\rangle}' \frac{\langle\sigma_0|\gamma_{-q}|\sigma\rangle\langle\sigma|\gamma_q|\sigma_0\rangle}{E_\sigma - E_{\sigma_0}} + (q \to -q)\right), \tag{33}$$

where the symmetry of $\epsilon(k)$ was used.

The leading correction to the energy at second order perturbation theory is a contribution to the A coefficient in Eq. (17):

$$A_2 = \frac{\pi}{N_e} \frac{\partial}{\partial k_f} E_2' \Big|_{k_f=0}$$
$$= -\int_0^{2\pi} \frac{dk}{2\pi} f(0, k). \tag{34}$$

To leading order in J/t the integral over momenta may be carried out to give a quantity defined in terms of the pure

spin chain H_s. This will demonstrate that the present expansion is well behaved, but we defer the evaluation to the following section in order to continue with the analysis of the crucial B coefficient. Its correction at this order reads

$$B_2 = \frac{\pi^2}{2N_e}\left|\left(\frac{\partial^2}{\partial k_f^2} E_2^0 + \frac{\partial^2}{\partial k_f^2} E_2'\right)\right|_{k_f=0}$$
$$= -F(0) + \frac{\pi^2}{2N_e} \frac{\partial^2}{\partial k_f^2} E_2' \Big|_{k_f=0}. \tag{35}$$

Again, the contribution from E_2' is evaluated by straightforward differentiation of Eq. (31). Only boundary terms survive, as all derivatives of the integrand vanish by symmetry when the limit $k_f \to 0$ is taken, using the 2π periodicity of f in the second argument. We find

$$B_2 = -F(0) + \frac{1}{2}[F(2k_f) + F(2\eta)]|_{k_f \to 0}. \tag{36}$$

At this point we have introduced an infinitesimal η since terms with zero momentum transfer are really excluded in the sum defining E_2'. However, we argue that the function $F(q)$ will be continuous at $q=0$ and hence B_2 vanishes. We note that this is the effect of a nontrivial cancellation between $q=0$ processes and processes with $q \to 0$. Physically, the continuity of $F(q)$ can be seen by interpreting $F(q)$ as the second-order energy response of a pure spin chain due to a periodic perturbation, as we explain in detail in Appendix B. Hence, by Eq. (36)

$$B_2 = 0. \tag{37}$$

We have convinced ourselves that a similar cancellation in the B coefficient takes place at third order perturbation theory.[20] We therefore propose that

$$B = 0 \tag{38}$$

to all orders in perturbation theory, and thus for small J/t the liquid remains stable in the limit $x \to 0$ even in the case $\alpha \approx 0.5$ [Fig. 2(c)]. The physical implication of Eq. (38) is that indeed the holes act as spinless fermions whose interaction is short ranged, and is irrelevant in the dilute limit. The Pauli principle severely suppresses the wave function when two holes approach each other. The range of this suppression is larger in one dimension than for dimensions greater than one, since in higher dimensions a curvature of the wave function is less costly at small distances. Therefore, in one dimension this effect is strong enough in order to prevent a short-range interaction from generating a term of order x^2 in the energy.

As we have argued above, the noninteracting nature of the charge degrees of freedom in combination with Luttinger liquid arguments also imposes constraints on the linear and cubic terms in x when a magnetic flux is imposed. We now move on to verify these relations perturbatively. Note that $B=0$ leads to $C = \tilde{C}$ in Eqs. (17) and (18), such that

$$C_2 = \frac{\pi^3}{6N_e} \frac{\partial^3}{\partial k_f^3} E_2' \bigg|_{k_f=0}. \tag{39}$$

In this case boundary terms such as those displayed in Eq. (36) do not contribute, since they vanish by symmetry as $k_f \to 0$ when another derivative is acting on them. Instead, we have now again a "bulk" contribution analogous to that in Eq. (34):

$$C_2 = -\frac{1}{6} \frac{\pi}{2} \int_0^{2\pi} dk \frac{\partial^2}{\partial k_f^2} f(k_f, k) \bigg|_{k_f=0}. \tag{40}$$

As explained above, this is to be compared to the coefficient $A_{2,\phi\phi}$. The phase twist ϕ will modify all hopping matrix elements via $t \to te^{i\phi}$ in Eq. (3) and leads to the following replacement of the free hole dispersion in the function $f(k_1, k_2)$ in Eq. (32):

$$\epsilon(k) \to \epsilon_\phi(k) = -2t\cos(k+\phi),$$

$$f(k_1, k_2) \to f_\phi(k_1, k_2). \tag{41}$$

Hence from Eq. (34)

$$A_{2,\phi,\phi} = \frac{\partial^2}{\partial\phi^2} A_2 \bigg|_{\phi=0} = -\int_0^{2\pi} \frac{dk}{2\pi} \frac{\partial^2}{\partial\phi^2} f_\phi(0,k) \bigg|_{\phi=0}. \tag{42}$$

However, using the fact that

$$f_\phi(0,k) = f(\phi, k+\phi) \tag{43}$$

holds, it follows by shifting the integration variable and comparison with Eq. (40) that

$$6C_2 = \pi^2 A_{2,\phi\phi} \tag{44}$$

is satisfied. Again, we have confirmed an identical relation at third order perturbation theory,[20] and this suggests that indeed

$$6C = \pi^2 A_{\phi\phi} \tag{45}$$

to all orders. Hence, although the parameters v_N and v_J in Eq. (13) each receive nontrivial corrections, their ratio is fixed to leading order in x such that K_ρ always approaches $\frac{1}{2}$ in the limit $x \to 0$. Luttinger liquid theory then implies that the dilute holes share all the universal properties of a gas of noninteracting spinless particles. Presumably, this picture will hold in the entire regime $J/t < (J/t)_c$, where for $J/t > (J/t)_c$ small doping will give rise to phase separation.

IV. EXPLICIT EVALUATION OF COEFFICIENTS

In the preceding section we have shown that our perturbative approach is consistent in all details with a picture where the charge degrees of freedom behave as noninteracting spinless solitons in the dilute limit, and are effectively decoupled from the spin dynamics. The second-order expressions we derived involve complicated sums over both spin and charge degrees of freedom. We will now show that the

expressions for A_2 and C_2 can be evaluated more explicitly, to leading order in J/t, in terms of quantities that are derived from a pure spin chain problem. In this way we obtain explicit asymptotic expansions for the ground-state energy and the compressibility parameter v_N, showing that second-order corrections are suppressed by nontrivial powers of J/t compared to the leading orders. Also, these quantities are related to the single-hole energy and mass renormalization, which will be clarified in the following section.

We stress once more that the results we present here are valid in the limit $x^2 \ll J/t$. In this limit the low-lying charge excitations are dominated by the curvature near the band bottom of the bare dispersion $\epsilon(k)$ and their contribution to the energy denominator in Eq. (31) is dominated by that of the gapped spin excitations. In the opposite limit $J/t \ll x^2$ the perturbation theory presented here is still valid, yet a crossover will take place and the asymptotic expansion (17) will not hold (see Appendix A).

With this in mind, the first- and second-order energy corrections are dominated by the following terms:

$$E_1/L \simeq A_1 x = -\langle \gamma_j \rangle_0 Jx$$

$$E_2/L \simeq A_2 x. \tag{46}$$

We will now show that the second-order term is indeed suppressed by powers of J/t compared to the first-order term, which is of order Jx. To achieve a systematic expansion of A_2 in J/t we rewrite Eq. (34) in the form

$$A_2 = -\int_0^{2\pi} \frac{dk}{2\pi} \int dE \frac{A(k,E)}{\epsilon(k) - \epsilon(0) + E - E_{\sigma_0}}, \tag{47}$$

where we have introduced a spectral function

$$A(k,E) = \frac{J^2}{N_e} \sum_\sigma' |\langle \sigma_0 | \gamma_k | \sigma \rangle|^2 \delta(E_\sigma - E)$$

$$\equiv \sum_n K_n(E) e^{ikn} \tag{48}$$

and its energy dependent Fourier coefficients $K_n(E)$. In terms of the latter we may write

$$A_2 = -\frac{1}{2t} \int dE \sum_n K_n(E) \int_0^{2\pi} \frac{dk}{2\pi} \frac{e^{ikn}}{1 + \frac{E - E_{\sigma_0}}{2t} - \cos(k)}. \tag{49}$$

The k integral is readily performed to give

$$A_2 = -\frac{1}{2t} \int dE \sum_n K_n(E) \frac{(1 + \Delta - \sqrt{(1+\Delta)^2 - 1})^{|n|}}{\sqrt{(1+\Delta)^2 - 1}},$$

where

$$\Delta \equiv \frac{E - E_{\sigma_0}}{2t}. \tag{50}$$

The matrix elements defining $K_n(E)$ will decay rapidly when E is a few times J and hence we may expand Eq. (50) in powers of Δ. Keeping only the leading term this yields

$$A_2 \simeq -\frac{1}{2t}\int dE\sum_n K_n(E)\frac{1}{\sqrt{\dfrac{E-E_{\sigma_0}}{t}}}$$

$$\simeq -\frac{t}{2}\Gamma_{1/2}\left(\frac{J}{t}\right)^{3/2}, \tag{51}$$

where the coefficient $\Gamma_{1/2}$ is a quantity defined only in terms of eigenstates of the doped spin chain. For later convenience we define the more general function

$$\Gamma_p = J^{p-2}\int dE\,\frac{A(q=0,E)}{(E-E_{\sigma_0})^p}$$

$$=\frac{1}{N_e}\sum_{|\sigma\rangle}'\frac{\langle\sigma_0|\gamma_{q=0}|\sigma\rangle\langle\sigma|\gamma_{q=0}|\sigma_0\rangle}{\left(\dfrac{E_\sigma-E_{\sigma_0}}{J}\right)^p}. \tag{52}$$

Hence, it is apparent from Eqs. (46) and (51) that

$$\frac{E_2}{E_1}\sim\left(\frac{J}{t}\right)^{1/2} \tag{53}$$

indicating the convergence of our perturbative approach for small J/t. In Appendix A, we will further comment on convergence and expansion parameters of this series in various limits. Note that the nonanalytic nature of the expansion originates from the gaplessness of the charge degrees of freedom and the existence of a regime where the spin gap dominates the energy denominator in Eq. (47). Similarly, in second-order perturbation theory the compressibility parameter v_N reads to leading order in x:

$$v_N\simeq\left(4\pi t+\frac{12}{\pi}C_2\right)x. \tag{54}$$

By means of Eq. (40) the evaluation of C_2 goes analogous to that of A_2 and we get

$$C_2\simeq-\frac{\pi^2}{12}\Gamma_{3/2}\sqrt{Jt}$$

$$v_N\simeq\pi t\left(4-\Gamma_{3/2}\sqrt{\frac{J}{t}}\right)x. \tag{55}$$

Numerically, we found $\Gamma_{1/2}=0.2502(2)$ and $\Gamma_{3/2}=0.474(3)$ at $\alpha=0.5$ (Fig. 4). Hence, although the compressibility $\kappa\sim v_N^{-1}$ increases with J, no unstable value of J can be inferred that lies within the validity of our perturbation theory.
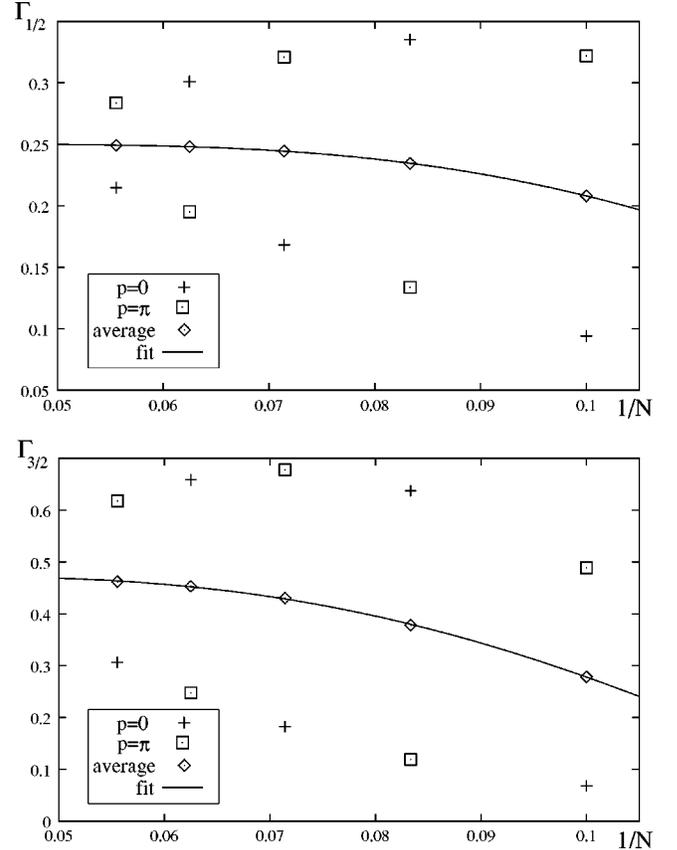

FIG. 4. Numerical determination of $\Gamma_{1/2}$ and $\Gamma_{3/2}$ by exact diagonalization of H_s for $\alpha=\frac{1}{2}$. System sizes of up to $N=18$ have been diagonalized. Results are plotted for the two degenerate ground states with momenta $p=0$ (crosses) and $p=\pi$ (squares). The extrapolated values have been determined by fitting their averages (diamonds) to the function $f(N)=a+b\,\exp(-cN)$.

V. SINGLE SPIN-POLARON PICTURE

We will now develop a variational picture of the polaronic effects of a single hole on its spin environment at small J/t in the special case $\alpha=0.5$. The perturbation theory presented in the preceding section for a finite carrier concentration may be applied to the problem of doping a single hole into the infinite spin chain as well, such that we will be able to compare variational and perturbative results. In second-order perturbation theory, the energy of a single hole at momentum k reads:

$$E_p(k)=-2t\cos(k)-\langle\gamma_j\rangle_0 J-\int_0^{2\pi}\frac{dk_2}{2\pi}f(k,k_2)+\cdots, \tag{56}$$

where we have not included the contribution E_{σ_0} from the spin background. At $k=0$ we immediately see by comparison with Eqs. (21), (24), and (34) that

$$E_p\equiv E_p(k=0)=A_0+A_1+A_2+\cdots\equiv A \tag{57}$$

holds for the single polaron energy in second-order perturbation theory. Likewise, for the renormalized mass of the spin polaron we have, comparing to Eqs. (21) and (40)

$$m^{-1} \equiv \frac{\partial^2}{\partial k^2} E_p|_{k=0} = \frac{6}{\pi^2}(C_0 + C_2 + \cdots) \equiv \frac{6}{\pi^2}C \quad (58)$$

at this order. We may therefore rewrite the ground-state energy of the system at finite doping (17) as

$$E = E_{\sigma_0} + L\left(E_p x + \frac{\pi^2}{6m}x^3 + \cdots\right)$$

$$= E_{\sigma_0} + N_e \int_{-k_f}^{k_f} \frac{dk}{2\pi} E_p(k) + O(k_f^4). \quad (59)$$

Hence up to third order in x the ground-state energy of the system is apparently given by the energy of noninteracting spinless particles with a dispersion $E_p(k)$, where interaction effects enter only beyond this order. This further confirms the picture established in the preceding sections.

We now focus on the Majumdar-Gosh point $\alpha = 0.5$, where the ground state of the spin Hamiltonian H_s is known exactly.[21] It consists of a direct product of uncorrelated singlet pairs:

$$|MG\rangle = \prod_i \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)_{2i,2i+1}. \quad (60)$$

Note that we use $|MG\rangle$ to denote one of the two doubly degenerate symmetry broken ground states, whereas $|\sigma_0\rangle$ has been used to denote their symmetric superposition. At $\alpha = 0.5$, our results for the single polaron energy and mass Eqs. (57) and (58) take the concrete form

$$E_p = -t\left(2 - \frac{9}{16}\frac{J}{t} + 0.125\left(\frac{J}{t}\right)^{3/2} + \cdots\right)$$

$$m^{-1} = t\left(2 - 0.237\sqrt{\frac{J}{t}} + \cdots\right). \quad (61)$$

We may write the ground state of the unperturbed Hamiltonian H_0 as a superposition of states depicted in Figs. 5(a) and 5(b):

$$|\Omega_0\rangle = \frac{1}{\sqrt{N_e}}\sum_j |j\rangle_c |MG\rangle_s, \quad (62)$$

where $|j\rangle_c$ denotes a state with a hole at the interstitial site j and "c" and "s" refer to the spin sector and the charge sector of the state. When the interaction H_{sc} is taken into account, a hole in the state $|2j\rangle_c$ will excite a spin configuration where the two dimers adjacent to the hole are in triplet states, and the two triplets form a singlet [Fig. 5(c)]. More precisely, the oval in Fig. 5(c) denotes the following spin state:

$$\left|\bullet_i \overbrace{\bullet_j \ \bullet_k} \bullet_l\right\rangle = \frac{1}{\sqrt{3}}\Bigg((|\uparrow\uparrow\rangle)_{ij}\otimes|\downarrow\downarrow\rangle_{kl} + |\downarrow\downarrow\rangle_{ij}\otimes|\uparrow\uparrow\rangle_{kl}$$

$$-\frac{1}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)_{ij}\otimes(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)_{kl}\Bigg). \quad (63)$$
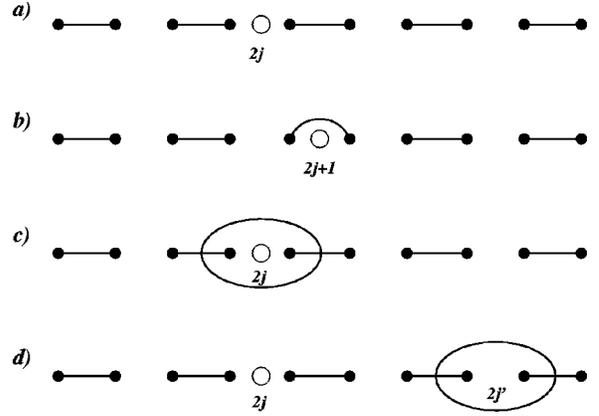

FIG. 5. (a) and (b) Single hole basis states forming the ground state of the noninteracting Hamiltonian H_0 [Eq. (62)]. Lines denote the singlet pairs in Eq. (60). (c) A pair of triplets excited by the presence of the hole. The oval denotes a singlet formed by two triplet states on the links adjacent to the hole, as displayed in Eq. (63). (d) States used to form the variational wave function (64).

We may now denote such a triplet pair excitation which is centered around the hole site $2j$ by $|2j\rangle_s$. Similarly, the hole state $|2j+1\rangle_c$ will excite the spin states $|2j\rangle_s$ and $|2j+2\rangle_s$. Clearly, a variational wave function will need admixtures of states such as shown in Fig. 5(c). However, in the vicinity of the hole the kinetic energy H_c is the dominant part of the Hamiltonian, and it will allow the hole to move away from the excited triplet states as shown in Fig. 5(d). To optimize the kinetic energy, it is hence necessary to include the more general states of Fig. 5(d) into the wave function. We therefore write down the following trial wave function for a state with one hole at momentum k:

$$|t_k\rangle = \frac{1}{\sqrt{N_e}}\sum_j e^{ikj}|j\rangle_c \otimes \Big(|MG\rangle_s$$

$$+ a\sum_{2j'} e^{-|j-2j'|\beta + i(j-2j')\delta}|2j'\rangle_s. \quad (64)$$

Hence $|t_k\rangle$ lives in the subspace of all states that can be reached by acting once with the perturbation H_{sc} on the zeroth order wave function (62) and then acting an arbitrary number of times with the hopping operator H_c. We also note that indeed certain exact excited states of a Majumdar-Gosh spin chain are given in terms of the tightly bound triplet excitations shown in Eq. (63) and Fig. 5 (Ref. 22). The following matrix elements are needed to evaluate the energy of the state (64):

$$_s\langle MG| -J\gamma_j |2j'\rangle_s = \frac{\sqrt{3}}{8}J(\delta_{j,2j'} + \delta_{j-1,2j'} + \delta_{j+1,2j'}), \quad (65)$$

$$_s\langle 2j'| -J\gamma_j |2j'\rangle_s = \frac{9}{16}J - (-1)^j \frac{3}{16}J$$

$$+ \frac{1}{4}J(3\delta_{j,2j'} - \delta_{j-1,2j'} - \delta_{j+1,2j'}), \quad (66)$$

$$_s\langle 2j'|H_s|2j'\rangle_s = {}_s\langle MG|H_s|MG\rangle_s + J = -\frac{3}{4}JN_e + J. \tag{67}$$

In addition, both γ_j and H_s do not have off-diagonal matrix elements among the states $|2j\rangle_s$. This leads to the following expectation values:

$$\langle t_k|H_c|t_k\rangle = -2t\cos(k) - 4t|a|^2\xi_3\cos(k+\delta), \tag{68a}$$

$$\langle t_k|H_s|t_k\rangle = -\frac{3}{4}JN_e\langle t_k|t_k\rangle + J|a|^2(\xi_1+\xi_2), \tag{68b}$$

$$\langle t_k|H_{sc}|t_k\rangle = \frac{9}{16}J\langle t_k|t_k\rangle + \frac{\sqrt{3}}{16}J[1+2e^{-\beta}\cos(\delta)](a+a^*)$$
$$+O(J|a|^2), \tag{68c}$$

$$\langle t_k|t_k\rangle = 1 + |a|^2(\xi_1+\xi_2), \tag{68d}$$

where the constants ξ_1 and ξ_2 are proportional to the weight of spin excited states with the hole on even positions and odd positions, respectively, and ξ_3 arises from hopping between even and odd sites in the presence of a spin excitation:

$$\xi_1 = \frac{1}{2}\sum_{j'}e^{-2\beta|2j'|} = \frac{1}{4\beta} + \frac{1}{3}\beta + \cdots,$$

$$\xi_2 = \frac{1}{2}\sum_{j'}e^{-2\beta|2j'-1|} = \frac{1}{4\beta} - \frac{1}{6}\beta + \cdots,$$

$$\xi_3 = \frac{1}{4}\sum_{j'}e^{-\beta|2j'|}(e^{-\beta|2j'-1|} + e^{-\beta|2j'+1|})$$
$$= \frac{1}{4\beta} - \frac{1}{24}\beta + \cdots. \tag{69}$$

Terms of order $J|a|^2$ were only kept in Eq. (68) when they are multiplied by $\xi_i \sim 1/\beta$. It is apparent from Eq. (68a) that $\delta = -k$ has to be chosen, and from Eq. (68c) that a is real and negative. Keeping only leading terms, this leads to the variational energy function

$$E_p^{var}(k;a,\beta) \equiv \langle t_k|H_c+H_s+H_{sc}|t_k\rangle/\langle t_k|t_k\rangle$$
$$= -2t\cos(k) + \frac{9}{16}J + \frac{1}{2}ta^2\beta - t\frac{a^2}{\beta}[1-\cos(k)]$$
$$+ J\frac{a^2}{2\beta} + \frac{\sqrt{3}}{8}Ja[1+2\cos(k)], \tag{70}$$

where again the bulk contribution of the spin chain was not included. We first minimize this function for $k=0$ and find for the variational parameters at the stationary point

$$\beta_0 = \sqrt{\frac{J}{t}}, \tag{71a}$$

$$a_0 = -\frac{3\sqrt{3}}{16}\sqrt{\frac{J}{t}}. \tag{71b}$$

By Eq. (71a), the size of the spin polaron cloud is proportional to $(J/t)^{-1/2}$ in agreement with Eq. (56), where the dominant contributions to the integral come from the region where k_2^2 is of the order of the spin gap. The variational energy of the spin polaron at $k=0$ is thus

$$E_p^{var} \equiv E_p^{var}(k=0;a_0,\beta_0) = -t\left[2 - \frac{9}{16}\frac{J}{t} + \frac{27}{256}\left(\frac{J}{t}\right)^{3/2}\right]. \tag{72}$$

This is indeed of the same form as Eq. (61), where the first two terms are reproduced exactly, as they are mean-field like in character. Moreover, the coefficient of the last term is about 0.105 and hence matches the one obtained by perturbative and numerical methods in Eq. (61) within roughly 15%.

The appearance of a mass term proportional to $\sqrt{J/t}$ as in Eq. (61) may also be understood from this variational approach. It is seen in Eq. (70) that a term of order $a^2/\beta \sim \sqrt{J}$ is no longer precisely canceled at finite k. The reason for this is that at finite k time reversal symmetry is absent and a nonzero value of the parameter δ introduced in Eq. (64) is generally allowed. We have tuned δ such that the polaronic corrections in the kinetic energy (68a) do not have the same k dependence as the leading term. This is giving rise to a a^2/β term at finite k. It leads to the variational mass

$$(m^{var})^{-1} = \frac{\partial^2}{\partial k^2}E_p^{var}(k;a_0,\beta_0)|_{k=0}$$
$$= t\left(2 - \frac{27}{256}\sqrt{\frac{J}{t}} + \cdots\right). \tag{73}$$

Here, the dependence of a and β on k^2 need not be taken into account because of stationarity. The coefficient of the second term happens to be the same as the one showing up in Eq. (72) which is now off by about a factor of 2 when compared to the mass shown in Eq. (61). This may be attributed to the variational character of the state (64), since the mass comes from a subdominant term proportional to k^2. However, the correct dependence on J as well as the right order of magnitude are again obtained. We therefore conclude that the wave function (64) provides a quite accurate picture of the large polaronic cloud in the limit of small J/t, especially at $k=0$.

In view of our original motivation to examine the stability of the liquid phase of the t-J-J' model as $x\to 0$ at small J/t, it is interesting to think about the possibility of the formation of bound hole states. It is generally expected that either at the critical value for the onset of phase separation, $(J/t)_c$, or at an even smaller critical value $(J/t)_{c_1} < (J/t)_c$ bound states of two holes will exist[11] (see also Ref. 5). The existence of such bound states can be discussed on a qualitative level based on the variational spin polaron picture proposed in this section. To form a bound state, the single polaron wave functions must significantly overlap, hence the size of a bound state will be of order $r\sim(J/t)^{-1/2}$. The potential energy gain will be of order $(J/t)^{3/2}$ since the mean-field term of order J in Eq. (72) will not be affected by pair formation. However, the

kinetic-energy cost of such a state is of order $1/r^2 \sim J/t$ and is dominant. We conclude that bound states of holes will require finite J/t of order 1 or greater, in agreement with the picture of free single-hole-like charge degrees of freedom established in the preceding sections.

VI. CONCLUSION

We have examined the t-J-J' model in one dimension, in the regime of small x and J/t by perturbative and variational approaches. This parameter regime is most challenging to numerical methods, and earlier numerical studies did not allow a firm conclusion whether a phase separation instability and a phase of dominant singlet superconducting fluctuations extend down to values of $J/t < 1$ in the case $\alpha = J'/J \approx 0.5$, where a spin gap is present at small doping.

Using an approach where couplings between spin and charge degrees of freedom are treated as a perturbation, we have presented a detailed analysis of the model in second-order perturbation theory, showing that no instability is present at small J/t. Instead, using Luttinger-liquid arguments and by studying the dispersion of a single hole immersed into the correlated spin system, we have demonstrated that the hole degrees of freedom precisely behave as free spinless solitons in the dilute limit, despite their microscopic coupling to the nontrivial spin background. This behavior conforms to Luttinger liquid physics, where spin and charge are separate degrees of freedom, and couplings between them are regarded as irrelevant in a renormalization group sense. While this point of view is generally accepted for one-dimensional systems, in microscopic one-dimensional lattice models it usually may be firmly demonstrated only at special integrable points.[2,12] The method we established in Sec. III provides a perturbative framework for such a demonstration in a nonintegrable model over a range of parameters. Moreover, it allows the calculation of nontrivial quantities such as the leading corrections to the single-hole energy and mass renormalization, which depend on nonanalytic powers of J/t. The numerical calculation of the coefficients in this expansion still requires an exact diagonalization of a pure spin problem. We used these results for a comparison to a variational approach. Proposing a variational wave function where the hole is surrounded by a polaronic cloud of tightly bound pairs of triplet excitations we were able to confirm the perturbative results for the dependence of the single polaron energy and mass on J/t, as well as the order of magnitude of the coefficients. In particular, the second-order perturbative energy corrections are in close quantitative agreement with the variational result. Based on these findings, we argue that for the parameter $\alpha = 0.5$ the onset of phase separation at small doping as well as the formation of bound states require J/t to be at least of order 1.

To conclude, the theory of the t-J-J' model presented here is limited to small values of J/t and cannot access a region of dominant superconducting correlations, which at $\alpha = 0.5$ might exists at moderate values of J/t and small doping from numerics. In a real system, additional interchain effects must be taken into account, that can either favor dimer locking, or a superconducting dimer liquid when dimer locking is frustrated (cf. Ref. 23). This calls for further investigations.

APPENDIX A: CONVERGENCE AND CROSSOVER BEHAVIOR OF THE PERTURBATIVE EXPANSION

Here we briefly illustrate the behavior of our expansion at kth order perturbation theory, where one will encounter terms analogous to Eq. (31):

$$E_k \sim \int_{-k_f}^{k_f} dh_1 \ldots \int_{-k_f}^{k_f} dh_m \int_{k_f}^{2\pi - k_f} dp_1 \ldots \int_{k_f}^{2\pi - k_f} dp_n$$

$$\times \sum_{\sigma_1 \ldots \sigma_{k-1}} \underbrace{\frac{J^k M(h_1 \ldots h_m; p_1 \ldots p_n; \sigma_1 \ldots \sigma_{k-1})}{(\epsilon(p_1) - \epsilon(h_1) + E_{\sigma_1} - E_{\sigma_0})(\ \ ) \ldots (\ \ )}}_{k-1 \text{ factors}}$$

$$+ \ldots \ . \tag{A1}$$

The phase space consists of m-hole momenta and n-particle momenta. It is enough to consider the case $m + n = k$. There will be terms with fewer integrals also, but they are multiplied by additional powers of x such as in Eq. (30).

We focus on the regime $k_f^2 \ll J/t$ first. Since $\epsilon(k) \approx \text{const} + tk^2$, the integrand does not significantly depend on the hole momenta such that each of the hole integrals will give rise to a factor of x. The integral over particle momenta p_i will be dominated by the region where all momenta are within a range of $\sqrt{\Delta/t}$ of the Fermi points, where $\Delta \sim J$ is the spin gap. In this regime, all of the $k-1$ factors in the denominator are dominated by the spin gap and are of order Δ. Hence we obtain the following estimate for the term displayed in Eq. (A1):

$$(A1) \sim x^m (\Delta/t)^{n/2} \frac{J^k}{\Delta^{k-1}} \sim x^m (\sqrt{J/t})^n J. \tag{A2}$$

The leading contribution to E_k in the limit $x^2 \ll J/t$ will thus be a term of order

$$E_k \sim x (\sqrt{J/t})^{k-1} J. \tag{A3}$$

Equation (A3) shows that subsequent orders in perturbation theory are always suppressed by powers of $\sqrt{J/t}$, as we verified explicitly up to second order [cf. Eq. (53)]. Note that relations (A2) and (A3) are valid asymptotically in a given limit, they do not imply the existence of a systematic expansion in powers of x and $\sqrt{J/t}$. Rather, the E_k's are quite complicated functions of x and J. Relation (A3) will hold until $x^2/J \sim 1/t$, and upon further increase of this ratio a crossover will take place. We may however write down an asymptotic expansion in x:

$$E_k = L[A_k(J)x + B_k(J)x^2 + C_k(J)x^3 + D_k(J)x^4 + \cdots]$$

$$E = \text{const} + E_1 + E_2 + \cdots \qquad (A4)$$

as we did in second-order perturbation theory. Recall from Eqs. (51) and (55) that $A_2 \sim (J/t)^{3/2}$, $C_2 \sim (J/t)^{1/2}$ while $B_2 = 0$. Formally, however, B_2 is of order J. This implies that in general $\sqrt{tx^2/J}$ is the expansion parameter of the series (A4).

In the opposite limit $J \ll tx^2$ it is easily seen from Eq. (A1) that now $E_k \sim J^k$ holds. In this limit it is not necessary, though still permissible, to include the spin chain part H_s in the unperturbed Hamiltonian H_0. Instead one may apply degenerate perturbation theory in the spin couplings, which gives rise to an asymptotic expansion in J:

$$E = \text{const} + L[a(x)J + b(x)J^2 + c(x)J^3 + d(x)J^4 + \cdots] \qquad (A5)$$

This method has been applied in Ref. 10 to calculate the intersection of the spin gap phase boundary with the x axis. Note that in Eq. (A5) x need not be small, whereas in Eq. (A4) both J/t and x^2t/J have to be small. However, due to the limitation $J \ll tx^2$, Eq. (A5) cannot be used to address the nature of the phase diagram in the dilute hole limit.

APPENDIX B: THE CONTINUITY OF THE FUNCTION $F(q)$

We will now give an argument for the continuity of the function $F(q)$ which leads to the crucial cancellation in Eq. (36). This question is more subtle than it may seem, and the following argument would require more scrutiny in the gapless case $\alpha < \alpha_c$. We restrict ourselves to the spin gapped case, as we have done throughout the paper. Recall the definition of $F(q)$ from Eq. (33):

$$F(q) = \frac{J^2}{2N_e}\left(\sideset{}{'}\sum_{|\sigma\rangle}\frac{\langle\sigma_0|\gamma_{-q}|\sigma\rangle\langle\sigma|\gamma_q|\sigma_0\rangle}{E_\sigma - E_{\sigma_0}} + (q \rightarrow -q)\right). \qquad (B1)$$

Physically, the continuity of $F(q)$ can be seen by interpreting $F(q)$ as the second-order energy response of a pure spin chain due to a periodic perturbation. More precisely, we consider the following auxiliary spin chain problem:

$$H_q(\lambda) = H_s + \lambda J \sum_j \cos(qj)\gamma_j$$

$$= H_s + \frac{\lambda}{2}J(\gamma_q + \gamma_{-q}), \qquad (B2)$$

where H_s is as defined in Eq. (4). Let $\mathcal{E}_q(\lambda)$ denote the ground-state energy per site of this problem. Then it is easily seen from second-order perturbation theory and the definition (B1) that at $q=0$

$$F(0) = -\tfrac{1}{2}\mathcal{E}''_{q=0} \qquad (B3)$$

holds, where the prime denotes a derivative with respect to λ taken at $\lambda = 0$. On the other hand, at $q \neq 0$ the same argument gives

$$F(q \neq 0) = -\mathcal{E}''_q. \qquad (B4)$$

Note the factor of 2 difference between Eqs. (B3) and (B4). Despite this apparent difference between the cases $q=0$ and $q \neq 0$, it is $\mathcal{E}''_q$ which is discontinuous at $q=0$, not $F(q)$, as the following argument shows: In the vicinity of a site j the ground state of $H_q(\lambda)$ will have great overlap with the ground state of $H_{q=0}[\lambda(j)]$ as $q \rightarrow 0$, where $\lambda(j) \equiv \lambda\cos(qj)$. In other words, as $q \rightarrow 0$ it should be justified to replace the oscillating perturbation in $H_q(\lambda)$ by a flat perturbation in a sufficiently large local region around each site j. The size of this region can still be chosen to be $\ll 1/q$. One can thus argue that up to powers of q the ground-state energy will be given by a sum over local contributions $\mathcal{E}_{q=0}[\lambda(j)]$:

$$\mathcal{E}_{q\rightarrow 0}(\lambda) = \frac{1}{N_e}\sum_j \mathcal{E}_{q=0}[\lambda(j)]$$

$$\approx \frac{1}{N_e}\int_0^{N_e}dx\,\mathcal{E}_{q=0}[\lambda\cos(qx)]$$

$$= \frac{1}{N_e}\int_0^{N_e}dx\bigg(\mathcal{E}_{q=0} + \lambda\cos(qx)\mathcal{E}'_{q=0}$$

$$+ \frac{1}{2}\lambda^2\cos^2(qx)\mathcal{E}''_{q=0} + \cdots\bigg)$$

$$\approx \mathcal{E}_{q=0} + \tfrac{1}{4}\lambda^2\mathcal{E}''_{q=0}. \qquad (B5)$$

From Eqs. (B4) and (B3) it then follows that

$$F(q \rightarrow 0) = -\tfrac{1}{2}\mathcal{E}''_{q=0} = F(0). \qquad (B6)$$

Note that the local point of view taken here is better justified in the gapped case, where any local perturbation decays exponentially in space.

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[16] We thank F.D.M. Haldane for pointing out to us this possibility.

[17] Note that for small doping and J/t the PS region consists of an insulating $x=0$ phase (no holes) and a liquid phase with $x = x_c$, where x_c is the critical doping at which phase separation just occurs. Since x_c is small in the region of interest, it is justified to consider the holes as dilute even in the PS regime.

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