Path-integral approach to the one-dimensional large- U Hubbard model

Z. Y. Weng, D. N. Sheng, C. S. Ting, and Z. B. Su*

Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204-5506

(Received 19 July 1991)

A path-integral formalism for the one-dimensional Hubbard model in the strong-coupling regime, which is equivalent to the t - J model in t/U expansion but without any explicit constraint, is developed. Based on this formalism, the zero-temperature properties of the Hubbard chain are systematically studied. In the infinite- U limit, the charge and spin degrees of freedom are shown to be completely separated. Such a separation at $U=\infty$ provides a controllable perturbative scheme to study the strong-coupling case. In the large- U regime, the spin degree of freedom is represented by a “squeezed” Heisenberg chain. We solve the (squeezed) Heisenberg chain by introducing a soliton representation. Both the charge and spin excitations are found to agree well with the exact solution. The bare electron (hole) is shown to be a composite particle of these basic excitations, i.e., holon and spinon, together with a nonlocal string field. This string field makes the electron behave like a “semion” and plays an important role in determining various correlation functions. We analytically derive the asymptotic forms of the spin-spin and density-density correlation functions as well as the single-electron and the pair-electron Green’s functions. The implications of the present work to the two-dimensional model are discussed.

I. INTRODUCTION

The Hubbard Hamiltonian is one of the simplest models for describing a strongly correlated electron system. In recent years, it has drawn intense attention because of its possible relation with high- T_c superconductivity¹ in the two-dimensional (2D) case.

In the strong-coupling regime of the Hubbard model, the on-site Coulomb repulsion U is quite large as compared with the electron hopping energy t . Electrons will become strongly correlated to avoid double occupancy which, otherwise, would very unfavorably cost energy U . A useful way of incorporating this non-double-occupancy condition is to introduce a representation for the electron operator with the charge and spin degrees of freedom being (formally) separated,² such as the slave-boson³ and slave-fermion⁴ methods, and the recent path-integral formalisms.^{5,6} It turns out that there is always a $U(1)$ phase uncertainty associated with such a separation, which results in a $U(1)$ gauge invariance in the corresponding actions.

This gauge invariance inspires one to construct a gauge theory for the large- U Hubbard method (or equivalently t - J model), as the $U(1)$ gauge theory has been well studied in the quantum field theory. A series of works^{4,7–10} have been done to develop such a gauge theory in 2D case. In all these approaches, the local spin state [e.g., local Néel state, resonating-valence-bond (RVB) state, etc.] has been properly handled such that the only important fluctuation is from the $U(1)$ phase of the $SU(2)$ spin. An extensive study of the metallic properties in the copper-oxide superconductors has been made based on the gauge theory.¹⁰

However, a $U(1)$ gauge description of the present lattice model may be an oversimplified theory. With the presence of holes, the local spiral fluctuations of spin could dominate over the phase fluctuations as shown by

Shraiman and Siggia,¹¹ and Weng¹² in the small-doping regime. The spiral field is related to the $SU(2)$ spin where the $U(1)$ phase is only a subgroup. The local spiral distortion favors the hopping energy of the holes, while the gauge aspects favor the local spin order. They are in a different limit and could lead to distinct long-wavelength behaviors. The possible oversimplified symmetry in the $U(1)$ gauge approach has been also pointed out by Anderson¹³ from a different point of view.

The one-dimensional (1D) Hubbard model provides a good test for the various approaches and theoretical considerations of the 2D case. The exact wave function and the ground-state energy of the 1D Hubbard Hamiltonian have been obtained about twenty years ago by Lieb and Wu.¹⁴ The basic excitations have been studied by Coll.¹⁵ However, the Green’s function and various correlation functions are hard to calculate directly by using the exact wave function. Recently, with renewing the interests in the 1D model in large- U limit, Ogata and Shiba¹⁶ have numerically calculated the spin-spin correlation function and the momentum distribution based on the Lieb and Wu solution. Their results suggest that the analysis¹⁷ of the weakly correlated regime may persist into the strong-coupling limit and the Luttinger liquid behavior holds through the whole finite- U regime. A series of works^{18–22} are devoted to deriving the various asymptotic correlation functions. Most of these approaches^{19–22} use the bosonization method, which originally is only justified in the small- U perturbative regime, to find the exponents of the correlations in the large- U limit by incorporating the exact solution. Although these methods are confined only to 1D models, the “phase-shift” analysis by Anderson and Ren²⁰ may be generalized to the 2D case.

In the present paper, we shall study the 1D Hubbard model directly from the strong-coupling regime. This is an extended work of our previous paper.²³ It will be a

first-principles calculation based on a path-integral formalism for the large- U Hubbard model, which has been previously^{6,12} used to investigate the 2D case. Such a formalism is equivalent to the t - J model to order t/U but without an explicit constraint imposed between the charge and spin degrees of freedom.

A peculiar property for the 1D model is the charge and spin separation in the limit of $U \rightarrow \infty$. This property has already shown up in the Lieb-Wu wave function.¹⁶ We shall demonstrate that such a decoupling of the holes from the spin background is realized by an SU(2) transformation, which cannot be derived from the usual U(1) gauge theory. As a result, each hole is found carrying a domain wall on the top of the spin background and contributes a nonlocal effect, which is responsible for getting the correct exponents of the Luttinger-liquid behavior.

This charge and spin separation will persist into the strong-coupling regime due to the existence of two distinct energy scales t and J ($t \gg J$, the superexchange energy defined by $J = 2t^2/U$). The spin part is represented by a “squeezed” Heisenberg chain with all the hole sites removed. To solve the (squeezed) Heisenberg chain, a soliton representation is developed to avoid the constraint problem. Then a BCS superconductinglike condensation of the solitons is found in the ground state of the (squeezed) Heisenberg model, which provides an alternative picture for the RVB state²⁴ in the 1D case.

The bare electron (hole) is found to be a composite particle of two basic excitations, holon and spinon, together with a nonlocal string field. Based on this formulation, various correlations are systematically derived which basically agree with the generally accepted results. For instance, the momentum distribution shows the power-law singularities at k_f and $3k_f$ with the exponents $\frac{1}{8}$ and $\frac{9}{8}$, respectively.

The remainder of this paper is organized as follows. In Sec. II, we formulate the large- U Hubbard model by a path-integral formalism, which will be the starting point of the present work. In Sec. III, we discuss the half-filling case where the Lagrangian is reduced to the Heisenberg model. We map it exactly into a soliton representation and treat the resulting Hamiltonian by the mean-field decoupling. We then find the ground-state energy and the excitation spectrum and calculate the spin correlation function. In Sec. IV, we first show the charge and spin separation at the $U \rightarrow \infty$ limit. We then demonstrate that such a peculiar property holds through the strong coupling regime. We then determine the electron operator by the fundamental charge and spin excitations: holon and spinon. Finally, in Sec. V, we calculate the various correlation functions based on the previous formulation and the bosonization technique.

II. PATH-INTEGRAL FORMALISM OF LARGE- U HUBBARD MODEL

The one-dimensional single-band Hubbard model is given by

$$H = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2.1)$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is electron annihilation (creation) operator with $\sigma = \uparrow$ or $\downarrow$ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the electron number.

The Hubbard interaction in the second term of (2.1) introduces the on-site electron correlations. In the strong-coupling regime where $U/t \gg 1$, a usual way to handle such a correlation is to projectively transform (2.1) into the t - J model²⁵ in the t/U expansion. The Hilbert space is then restricted in the low-energy sector, enforced by a non-double-occupancy constraint in the t - J Hamiltonian

$$\sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \leq 1.$$

This inequality constraint is replaced by some equality constraint in the slave-boson and slave-fermion methods.²⁻⁴ How to treat this constraint in a controllable approximation is still one of the main difficulties associated with the t - J model.

Recently, a new approach to the large- U Hubbard model has been developed.⁶ In this method, the spin quantization axis (originally in the z axis) is defined along the on-site spin polarization direction. In this new reference frame, each electron's spin will be polarized along its z axis by a strong fictitious magnetic field. Such a “symmetry-broken” fictitious field plays a similar role as that in the spin-density-wave (SDW) theory.²⁶ Then a SDW gap is found which is nothing but the Hubbard charge gap U . By keeping electrons in the lower band, the non-double-occupancy condition is automatically satisfied. The local spin polarization direction, serving as the reference axis, will be determined self-consistently through its coupling with the charge carrier in the lower Hubbard band. Thus, we obtain a representation with the separated charge and spin degrees of freedom in a natural way, which is quite similar to the slave fermion⁴ language but without an additional constraint. Similar results can be found in work by Schulz⁵ and some closely related ideas may be also found in Ref. 8 by Wen.

In the rest of the present section, we shall derive this formalism in a different way, without introducing the Hubbard-Stratonovich auxiliary fields as in Ref. 6. The basic result is given by the Lagrangian (2.32), which is accurate to t/U order.

The density product $n_{i\uparrow} n_{i\downarrow}$ in the Hubbard interaction can be expressed by the on-site electron number and spin operators as

$$n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} \rho_i - 2S_{iz}^2, \quad (2.2)$$

where ρ_i is the electron number at site i

$$\rho_i = n_{i\uparrow} + n_{i\downarrow}, \quad (2.3)$$

and $S_{iz} = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$ is the z component of the electron spin operator $\mathbf{S}_i$ which is defined by

$$\mathbf{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} (\hat{\sigma})_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}, \quad (2.4)$$

in which $\hat{\sigma}$ is the Pauli matrix and the index $\sigma = \pm 1$. Notice that $n_{i\uparrow} n_{i\downarrow}$ is SU(2) invariant (independent of the rotation in spin space), but the right-hand side of (2.2) is formally not. In general, the following relation holds for an arbitrary unit vector $\mathbf{n}_i$:

$$S_{ix}^2 = S_{iy}^2 = S_{iz}^2 = (\mathbf{S}_i \cdot \mathbf{n}_i)^2. \quad (2.5)$$

Then one may rewrite Eq. (2.2) as

$$n_{i\uparrow}n_{i\downarrow} = \frac{1}{2}\rho_i - 2(\mathbf{S}_i \cdot \mathbf{n}_i)^2. \quad (2.6)$$

We shall develop a path-integral formalism of the Hub-

bard model (2.1). Defining the partition function $Z = \text{Tr}(\exp(-\beta H))$, where $\beta = 1/k_B T$, one may write $Z = \text{Tr}[\cdots \exp(-\Delta\tau H) \exp(-\Delta\tau H) \cdots]$, where $\Delta\tau$ is an infinitesimal slice of β . According to the equality (2.6), we write down the following identity for the interaction:

$$\exp \left[-\Delta\tau U \sum_i n_{i\uparrow}n_{i\downarrow} \right] = \int \prod_i d^2\mathbf{n}_i W(\{\mathbf{n}_i\}) \exp \left[-\Delta\tau U \sum_i [\rho_i/2 - 2(\mathbf{S}_i \cdot \mathbf{n}_i)^2] \right], \quad (2.7)$$

where $W(\{\mathbf{n}_i\})$ is an arbitrary functions of $\mathbf{n}_i$ satisfying

$$\int \prod_i d^2\mathbf{n}_i W(\{\mathbf{n}_i\}) = 1. \quad (2.8)$$

Then by the standard procedure, Z could be formulated in the coherent state by the path-integral form

$$Z = \int \prod_{i\tau} dc_i^\dagger(\tau) dc_i(\tau) d^2\mathbf{n}_i(\tau) W(\{\mathbf{n}_i\}) \exp \left[-\int_0^\beta d\tau \mathcal{L}(\tau) \right], \quad (2.9)$$

with

$$\begin{aligned} \mathcal{L}(\tau) = & \sum_{i\sigma} c_{i\sigma}^\dagger \partial_\tau c_{i\sigma} - t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) \\ & + U \sum_i [\frac{1}{2}\rho_i - 2(\mathbf{S}_i \cdot \mathbf{n}_i)^2], \end{aligned} \quad (2.10)$$

where $c_i(\tau)$ and $c_i^\dagger(\tau)$ become the Grassmann variables and, in obtaining (2.10), the identity (2.7) has been used. $W(\{\mathbf{n}_i\})$ in (2.9) actually is a product of the weight functionals defined in (2.8) for all the imaginary time intervals.

So far we have not yet chosen the weight functional $W\{\mathbf{n}_i\}$, and $\mathbf{n}_i$ has no specific meaning except as an arbitrary unit vector. In the operator formalism, one finds

$$(\mathbf{S}_i \cdot \mathbf{n}_i)^2 = \frac{1}{4}\rho_i(2 - \rho_i). \quad (2.11)$$

That is, $(\mathbf{S}_i \cdot \mathbf{n}_i)^2 = 0$ when the site is vacant or doubly occupied, while $(\mathbf{S}_i \cdot \mathbf{n}_i)^2 = \frac{1}{4}$ if it is singly occupied. In general the operator $\mathbf{S}_i \cdot \mathbf{n}_i$ itself should not be replaced by a numerical number when there is an electron at site i . But if $\mathbf{n}_i$ is chosen always to coincide with the spin polarization axis of the electron, then one find $\mathbf{S}_i \cdot \mathbf{n}_i = \pm \frac{1}{2}$. Furthermore, including the vacancy and double-occupancy cases, one has

$$\mathbf{S}_i \cdot \mathbf{n}_i = \frac{(-1)^i}{2} \rho_i(2 - \rho_i), \quad (2.12)$$

where the staggered factor $(-1)^i$ is chosen for convenience of the later discussion. As we have a freedom in choosing $\mathbf{n}_i$, we may let (2.12) always hold in (2.10).

This could be realized by choosing the proper weight functional $W\{\mathbf{n}_i\}$ in (2.9). For example, we may define

$$\begin{aligned} W(\{\mathbf{n}_i\}) \\ = \mathcal{C} \exp \left[-\int_0^\beta d\tau \tilde{U} \sum_i \left[\mathbf{S}_i \cdot \mathbf{n}_i - \frac{(-1)^i}{2} \rho_i(2 - \rho_i) \right]^2 \right], \end{aligned} \quad (2.13)$$

where the parameter $\tilde{U} \rightarrow +\infty$ and $\mathcal{C}$ is the normalization factor such that the condition (2.8) holds. Thus the constraint (2.12) is enforced by the weight functional (2.13).

With the choice of $W(\{\mathbf{n}_i\})$ in (2.13), the Lagrangian in (2.10) can be simplified, as $(\mathbf{S}_i \cdot \mathbf{n}_i)^2$ could be replaced by the linear operator $\mathbf{S}_i \cdot \mathbf{n}_i$ by using (2.11) and (2.12). This gives

$$\begin{aligned} \mathcal{L}(\tau) = & \sum_{i\sigma} c_{i\sigma}^\dagger \partial_\tau c_{i\sigma} - t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) \\ & + U \sum_i \left[\frac{\rho_i}{2} - (-1)^i \mathbf{S}_i \cdot \mathbf{n}_i \right]. \end{aligned} \quad (2.14)$$

Only the quadratic terms of $c, c^\dagger$ are present in (2.14) which couple with the auxiliary field $\mathbf{n}_i$ through the $\mathbf{S}_i \cdot \mathbf{n}_i$ term. Notice that there is a prefactor U in front of $\mathbf{S}_i \cdot \mathbf{n}_i$ in (2.14). In the strong-coupling limit $U \gg t$, one may expect the suppression of the fluctuation in $\mathbf{S}_i \cdot \mathbf{n}_i$ such that $\mathbf{S}_i$ is always fully polarized along the $\mathbf{n}_i$ direction. Thus Eq. (2.12) may be automatically satisfied in the t/U expansion. In other words, Lagrangian (2.14) itself can enforce the constraint (2.12) after projecting out the high-energy sector ($\geq U$). This is indeed the case as will be shown below.

First of all, we define a new spin-quantization axis at site i along the $\mathbf{n}_i$ direction. The rotation from the z axis to $\mathbf{n}_i$ direction is given by

$$c_{i\sigma} = \sum_{\sigma'} U_{i\sigma\sigma'} a_{i\sigma'}, \quad (2.15)$$

where the SU(2) transformation U_i satisfies

$$U_i \hat{\sigma}_z U_i^\dagger = \mathbf{n}_i \cdot \hat{\boldsymbol{\sigma}}. \quad (2.16)$$

Correspondingly, Lagrangian (2.14) is transformed into the form

$$\begin{aligned}\mathcal{L}(\tau) = & \sum_i \hat{a}_i^\dagger \partial_\tau \hat{a}_i + \sum_i \hat{a}_i^\dagger (U_i^\dagger \partial_\tau U_i) \hat{a}_i \\ & - t \sum_i [\hat{a}_i^\dagger (U_i^\dagger U_{i+1}) \hat{a}_{i+1} + \text{H.c.}] \\ & + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i - \frac{U}{2} \sum_i (-1)^i \hat{a}_i^\dagger \hat{\sigma}_z \hat{a}_i, \quad (2.17)\end{aligned}$$

where the spinor $\hat{a}_i$ is defined by

$$\hat{a}_i = \begin{pmatrix} a_{i\uparrow} \\ a_{i\downarrow} \end{pmatrix}. \quad (2.18)$$

The path-integral measures for $a_{i\sigma}$ and $a_{i\sigma}^\dagger$ are not changed since U_i is a canonical transformation. The $\mathbf{n}_i$ field is represented by U_i field in (2.17). It is noted that U_i is determined by $\mathbf{n}_i$ only up to the U(1) subgroup through (2.16). For example, the transformation $U_i \rightarrow U_i \exp(i\phi_i \hat{\sigma}_z)$ does not change (2.16). Therefore, there is a local gauge freedom in Lagrangian (2.17) under $U_i \rightarrow U_i \exp(i\phi_i \hat{\sigma}_z)$ and $a_{i\sigma} \rightarrow a_{i\sigma} \exp(-i\phi_i \sigma)$.

On the other hand, the constraint (2.12) can be written as

$$\tilde{S}_{iz} = \frac{(-1)^i}{2} \rho_i (2 - \rho_i), \quad (2.19)$$

in which $\tilde{S}_{iz} = \frac{1}{2} (a_{i\uparrow}^\dagger a_{i\uparrow} - a_{i\downarrow}^\dagger a_{i\downarrow})$. (2.19) implies a Néel order along the z axis in the new spin reference frame, with a full staggered magnetization at the occupied sites and a zero magnetization at the vacant sites or doubly occupied sites.

The Lagrangian (2.17) is composed of two parts:

$$\mathcal{L}(\tau) = \mathcal{L}_0(\tau) + \mathcal{L}_n(\tau), \quad (2.20)$$

where

$$\begin{aligned}\mathcal{L}_0 = & \sum_i \hat{a}_i^\dagger \partial_\tau \hat{a}_i - t \sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + \text{H.c.}) \\ & + \frac{U}{2} \sum_i [\hat{a}_i^\dagger \hat{a}_i - (-1)^i \hat{a}_i^\dagger \hat{\sigma}_z \hat{a}_i] \quad (2.21)\end{aligned}$$

and

$$\begin{aligned}\mathcal{L}_n(\tau) = & \sum_i \hat{a}_i^\dagger (U_i^\dagger \partial_\tau U_i) \hat{a}_i \\ & - t \sum_i [\hat{a}_i^\dagger (U_i^\dagger U_{i+1} - 1) \hat{a}_{i+1} + \text{H.c.}] \quad (2.22)\end{aligned}$$

The Hubbard repulsion U only appears in $\mathcal{L}_0$, while the spin field U_i is present only in $\mathcal{L}_n(\tau)$. We note that $\mathcal{L}_0$ is similar to a spin-density-wave (SDW) mean-field Lagrangian and can be exactly diagonalized.²⁶ Consider the Hamiltonian corresponding to $\mathcal{L}_0$

$$\begin{aligned}H_0 = & -t \sum_{i\sigma} (a_{i\sigma}^\dagger a_{i+1\sigma} + \text{H.c.}) \\ & + \frac{U}{2} \sum_{i\sigma} [1 - (-1)^i \sigma] a_{i\sigma}^\dagger a_{i\sigma}, \quad (2.23)\end{aligned}$$

which is easily diagonalized by Fourier and Bogoliubov transformations as

$$H_0 = - \sum'_{k\sigma} \left[E_k - \frac{U}{2} \right] \alpha_{k\sigma}^\dagger \alpha_{k\sigma} + \sum'_{k\sigma} \left[E_k + \frac{U}{2} \right] \beta_{k\sigma}^\dagger \beta_{k\sigma}. \quad (2.24)$$

In (2.24), the summation only runs over the reduced (or magnetic) Brillouin zone with $|k| \leq \pi/2$ and

$$\begin{aligned}E_k = & \sqrt{U^2/4 + \varepsilon_k^2}, \\ \varepsilon_k = & -2t \cos ka, \quad (2.25)\end{aligned}$$

and the quasiparticle operators $\alpha_{k\sigma}$ and $\beta_{k\sigma}$ are related to $a_{k\sigma}$ through

$$a_{k\sigma} = \begin{cases} u_k \alpha_{k\sigma} - \sigma v_k \beta_{k\sigma}, & |k| \leq \pi/2 \\ \sigma v_k \alpha_{k\sigma} + u_k \beta_{k\sigma}, & \pi/2 < |k| < \pi \end{cases} \quad (2.26)$$

in which all the right-hand side quantities are understood to be a periodic function of $\pm\pi$, with

$$u_k = \left[\frac{1 + |\varepsilon_k|/E_k}{2} \right]^{1/2}, \quad (2.27a)$$

$$v_k = \left[\frac{1 - |\varepsilon_k|/E_k}{2} \right]^{1/2}. \quad (2.27b)$$

In the case of $U \gg t$, the localized picture will be more convenient for our discussion. We define two spinless fermions in the lattice representation as follows:

$$\alpha_i = \sum_\sigma \theta(p_i \sigma) \sqrt{2/N} \sum_k e^{ikx_i} \alpha_{k\sigma}, \quad (2.28a)$$

$$\beta_i = \sum_\sigma \theta(-p_i \sigma) \sqrt{2/N} \sum_k e^{ikx_i} \beta_{k\sigma}, \quad (2.28b)$$

where $\theta(x)$ is the step function and $p_i \equiv (-1)^i$. Expanded in powers of t/U , $a_{i\sigma}$ can be expressed by α_i and β_i in terms of (2.26), (2.27), (2.25), and the inverse transformation of (2.28) as follows:

$$\begin{aligned}a_{i\sigma} = & \theta(p_i \sigma) \alpha_i + \theta(-p_i \sigma) p_i \beta_i + \theta(-p_i \sigma) \frac{t}{U} (\alpha_{i+1} + \alpha_{i-1}) \\ & + \theta(p_i \sigma) p_i \frac{t}{U} (\beta_{i+1} + \beta_{i-1}) + O\left[\frac{t^2}{U^2}\right]. \quad (2.29)\end{aligned}$$

H_0 in (2.24) then becomes

$$\begin{aligned}H_0 = & -J \sum_i (\alpha_i^\dagger \alpha_i - \beta_i^\dagger \beta_i) + U \sum_i \beta_i^\dagger \beta_i \\ & - \frac{J}{2} \sum_i (\alpha_i^\dagger \alpha_{i+2} - \beta_i^\dagger \beta_{i+2} + \text{H.c.}), \quad (2.30)\end{aligned}$$

up to the order of $J (= 2t^2/U)$.

We see from (2.30) or (2.24) that a gap U is opened between α band and β band. The physical picture would be more clear if we let $U \rightarrow \infty$ in (2.29). In this case, at a given site i , one finds $a_{i\sigma} = \alpha_i$, while $a_{i-\sigma} = (-1)^i \beta_i$ with $\sigma = (-1)^i$. Therefore, in the half-filling, by keeping the lower α band being filled with upper β band empty, a Néel order is found in the spin reference frame with $\{\mathbf{n}_i\}$ as the quantization axis. In the hole (electron) doping case, the Néel order is still there but the staggered mag-

netization is zero at the vacancy (double occupancy) sites. This is in agreement with the constraint (2.19). In fact, the constraint (2.19) is reduced to the form

$$(1 - \alpha_i^\dagger \alpha_i) \beta_i^\dagger \beta_i = 0 \quad (2.31)$$

in $U \rightarrow \infty$, which projects out all those exciton states with one hole from the α band and one particle from the β band sitting at the same site simultaneously. In this way, $(-1)^{i \cdot \mathbf{n}_i}$ is guaranteed always to be in the spin polarization direction. Those projected exciton states correspond to the singly occupied states in which the spins go in the opposite direction of $(-1)^{i \cdot \mathbf{n}_i}$.

It is straightforward to check that the terms of t/U order in (2.19) still lead to the constraint (2.31). We do not need to go through all higher-order terms of t/U in Eq. (2.19) because we shall in fact consider the expansion in $\mathcal{L}$ to t/U order just as in the t - J model. Relaxation of the constraint of Eq. (2.19) at the t^2/U^2 order will lead to

a leading t^2/U correction to the Lagrangian $\mathcal{L}$ in (2.14). But such a correction is found only involving hole hopping in the sublattice and it is negligible as compared with the leading kinetic energy of the hole, which is of order of t as will be shown in Sec. IV. Thus, Eq. (2.31) is equivalent to the constraint (2.19) in the large- U limit, and by keeping the electron in the lower-energy sector of H_0 , such a constraint is automatically satisfied.

Now we consider the full Lagrangian (2.20). As the Hubbard coupling constant U only appears in $\mathcal{L}_0$, which has been diagonalized above, we express the total Lagrangian $\mathcal{L}$ using the representation (2.29). To the order of t/U , the expression of $\mathcal{L}_n$ in the representation of α_i and β_i is given by Eq. (A.2) in Appendix A.

In the hole-doping case, one is interested only in the low-energy sector, i.e., α band. Projecting out (integrating out) the high-energy sector β band, we show in Appendix A that, to the order of t/U , Lagrangian $\mathcal{L}$ in the lower-energy sector becomes

$$\begin{aligned} \mathcal{L} = & \sum_i h_i^\dagger \partial_\tau h_i + \sum_{i\sigma} \theta(p_i \sigma) (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} (1 - h_i^\dagger h_i) + t \sum_i \left[\sum_\sigma \theta(p_i \sigma) (U_i^\dagger U_{i+1})_{\sigma-\sigma} h_{i+1}^\dagger h_i + \text{H.c.} \right] \\ & - \frac{J}{2} \sum_{i\sigma} \theta(p_i \sigma) [|(U_i^\dagger U_{i+1})_{\sigma\sigma}|^2 + |(U_i^\dagger U_{i-1})_{\sigma\sigma}|^2] (1 - h_i^\dagger h_i) \\ & + \frac{J}{2} \sum_{i\sigma} \theta(-p_i \sigma) [(U_i^\dagger U_{i-1})_{\sigma\sigma} (U_{i+1}^\dagger U_i)_{\sigma\sigma} h_{i-1}^\dagger h_{i+1} + \text{H.c.}] \\ & - \frac{J}{2t} \sum_{i\sigma} (U_i^\dagger \partial_\tau U_i)_{\sigma-\sigma} [\theta(p_i \sigma) (h_{i+1}^\dagger + h_{i-1}^\dagger) h_i + \theta(-p_i \sigma) h_i^\dagger (h_{i+1} + h_{i-1})], \end{aligned} \quad (2.32)$$

where the hole operator $h_i^\dagger = \alpha_i$ is introduced.

Thus, the large- U Hubbard model has been formulated in the path-integral form with the Lagrangian (2.32). In the present formalism, the bare electron $c_{i\sigma}$ is described by an SU(2) spin field U_i and a fermion $a_{i\sigma}$ through (2.15) and (2.29). After projecting out the upper Hubbard band, $a_{i\sigma}$ becomes a spinless fermion $\alpha_i = h_i^\dagger$. Lagrangian (2.32) is peculiar in that there is no additional constraint imposed on the hole operator h_i and the SU(2) spin field U_i . With the expansion to the order of t/U , the present formalism is equivalent to the t - J model, which will be demonstrated in the following sections. We have included all the relevant processes of the order t/U in (2.32), which seems slightly more complicated than the t - J model, where all the pair-hopping terms are usually neglected. A formalism for 2D case could similarly be obtained.

III. HALF-FILLING: GAPLESS SPINON EXCITATION

In the half-filling case, the lower Hubbard band is filled by electrons. The degree of freedom for holes (described by h_i) is thus frozen, and only the spin degree of freedom is left (described by $\mathbf{n}_i$ or U_i). After making the trace over h_i , the Lagrangian $\mathcal{L}$ in (2.32) is reduced to $\mathcal{L}_s$:

$$\begin{aligned} \mathcal{L}_s = & \sum_i \left[\sum_\sigma \theta(p_i \sigma) (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} \right] \\ & - \frac{J}{2} \sum_{i\sigma} |(U_i^\dagger U_{i+1})_{\sigma\sigma}|^2. \end{aligned} \quad (3.1)$$

We shall first show that $\mathcal{L}_s$ is equivalent to the Heisenberg model (i.e., the t - J model at half-filling). Then, by introducing the soliton representation, an analytical solution for Heisenberg chain will be obtained.

A. Bosonic representation: Heisenberg model

First we shall demonstrate the equivalence between the Lagrangian (3.1) and the Heisenberg model. Introduce the following CP^1 representation for U_i

$$U_i = \theta(p_i) \begin{bmatrix} b_{i\uparrow} & -b_{i\downarrow}^* \\ b_{i\downarrow} & b_{i\uparrow}^* \end{bmatrix} + \theta(-p_i) \begin{bmatrix} b_{i\uparrow}^* & -b_{i\downarrow} \\ b_{i\downarrow}^* & b_{i\uparrow} \end{bmatrix}. \quad (3.2)$$

In terms of the definition of U_i in (2.16), the complex field $b_{i\sigma}$ and its complex conjugate $b_{i\sigma}^*$ are determined through

$$b_i^\dagger \hat{\sigma} b_i = \mathbf{n}_i, \quad (3.3)$$

where

$$b_i = \theta(p_i) \begin{pmatrix} b_{i\uparrow} \\ b_{i\downarrow} \end{pmatrix} + \theta(-p_i) \begin{pmatrix} b_{i\uparrow}^* \\ b_{i\downarrow}^* \end{pmatrix}. \quad (3.4)$$

U_i is subject to the unitary condition $U_i^\dagger U_i = 1$, which leads to the following constraint for b_i :

$$\sum_{\sigma} b_{i\sigma}^* b_{i\sigma} = 1. \quad (3.5)$$

As discussed in Sec. II, U_i is determined up to the gauge freedom $U_i \rightarrow U_i \exp(ip_i \theta_i \sigma_z)$. Correspondingly, $b_{i\sigma}$ has a $U(1)$ freedom $b_{i\sigma} \rightarrow b_{i\sigma} e^{i\theta_i}$. The invariance of $\mathcal{L}_s$ under such a gauge transformation is easy to verify with the boundary condition $\theta_i(\beta) = \theta_i(0)$.

According to the CP^1 representation of (3.2)–(3.5), the Lagrangian $\mathcal{L}_s$ in (3.1) could be rewritten in the form

$$\begin{aligned} \mathcal{L}_s = & \sum_{i\sigma} b_{i\sigma}^* \partial_\tau b_{i\sigma} - J \sum_{i\sigma\sigma'} b_{i\sigma}^* b_{i+1\sigma}^* b_{i+1\sigma'} b_{i\sigma'} \\ & + \sum_i i\lambda_i \left[\sum_{\sigma} b_{i\sigma}^* b_{i\sigma} - 1 \right]. \end{aligned} \quad (3.6)$$

We impose the constraint (3.5) by the last term in (3.6) with a Lagrangian multiplier λ_i . One immediately sees that the Lagrangian (3.6) is nothing but the Heisenberg model (t - J model at half-filling) in the Schwinger-boson representation.²⁷

One may also write down the Heisenberg-type Hamiltonian H_s corresponding to $\mathcal{L}_s$ as

$$H_s = -J \sum_{i\sigma\sigma'} b_{i\sigma}^\dagger b_{i+1\sigma}^\dagger b_{i+1\sigma'} b_{i\sigma'}, \quad (3.7)$$

where the boson $b_{i\sigma}$ is subjected to the constraint (3.5) in the operator formalism (where $b^\dagger, b$ should be written in normal order, i.e., $b^\dagger b$).

As U_i is intimately related to the spin polarization direction $\mathbf{n}_i$, one may also easily derive the nonlinear σ model²⁸ in the long-wavelength, low-energy regime. As shown in Appendix B, the action S in this limit is reduced to

$$S \equiv \int_0^\beta d\tau \mathcal{L}_s \simeq \frac{i}{2} \sum_i (-1)^i \omega_i + \frac{1}{2} \int_0^\beta d\tau \int dx \left[\frac{\rho}{c^2} (\partial_\tau \mathbf{\Omega})^2 + \rho (\partial_x \mathbf{\Omega})^2 \right] - \beta J N, \quad (3.8)$$

here $\mathbf{\Omega}_i \approx \mathbf{n}_i$, $\rho = J/2a$, and $c = 2Ja$. ω_i is the solid angle [see Eq. (B6)] subtended by the closed path on the sphere defined by the imaginary time evolution of $\mathbf{\Omega}_i(\tau)$.

The Berry phase $i/2 \sum_i (-1)^i \omega_i$ in (3.8) serves as a topological term which would be responsible for the gapless spin excitation in the spin- $\frac{1}{2}$ Heisenberg chain, as conjectured by Haldane.²⁸ However, the mean-field theory²⁷ of $\mathcal{L}_s$ in (3.6) predicts a gap appearing in the low-lying spin excitation, which is contradictory to the gapless results^{29,30} by the Bethe ansatz. This is in contrast to the two-dimensional case, where the mean-field theory²⁷ of $\mathcal{L}_s$ gives a good description of the spin-wave excitation. We note this is due to the improper treatment of the constraint (3.5) in $\mathcal{L}_s$ which becomes crucial in the one-dimensional case. In fact, in the mean-field approximation, the condition (3.5) is realized only at the global level (by replacing $\lambda_i \rightarrow \lambda$) in (3.6). In order to include the constraint effect properly, in a previous work²³ we introduced the Jordan-Wigner transformation, which changes the statistics of $b_{i\sigma}$ into that of a fermion. In this way, the “hard-core” condition of $b_{i\sigma}$ is automatically realized for the same spin σ and $b_{i\sigma}$ gets partially liberated. We then relaxed the constraint between different spins. A gapless excitation as well as the power-law behavior of the spin-spin correlation (for the transverse part $\langle S_i^+ S_j^- \rangle \sim 1/x_{ij}$ and $\sim 1/x_{ij}^2$ for $\langle S_i^z S_j^z \rangle$) have been obtained. [The mean-field decoupling is represented by neglecting the $|(U_i^\dagger U_{i+1})_{\sigma\sigma} - 1|^2$ term in (3.1), which is of order $\sim (\partial \mathbf{\Omega})^4$ with the proper choice of $U(1)$ gauge.]

Thus, we conclude this section by noting that, in the 1D case, the constraint that confines a spin at each site is so important that a conventional way of mobilizing the

spin may result in some serious problems. A better representation should be composed of some excited configurations of the spins that are truly mobile entities, instead of the localized spins themselves. This is the soliton representation, which will be discussed below.

B. The soliton representation

Before introducing the soliton representation, we need to be more familiar with the boson operator $b_{i\sigma}$. The real spin operator $\mathbf{S}_i$ defined in (2.4) is equal to $\frac{1}{2}(-1)^i \mathbf{n}_i$ in the large- U limit in terms of (2.15), (2.16), and (2.29). According to the operator formalism of (3.3), one finds

$$S_i^z = \frac{p_i}{2} n_i^z = \frac{p_i}{2} (b_{i\uparrow}^\dagger b_{i\uparrow} - b_{i\downarrow}^\dagger b_{i\downarrow}), \quad (3.9a)$$

$$S_i^+ = \theta(p_i) b_{i\uparrow}^\dagger b_{i\downarrow} - \theta(-p_i) b_{i\downarrow}^\dagger b_{i\uparrow}, \quad (3.9b)$$

and $S_i^- = (S_i^+)^+$. Thus a spin state defined by $|\sigma i\rangle \equiv b_{i\sigma}^\dagger |0\rangle$ is the eigenstate of S_i^z with the eigenvalue $1/2 p_i \sigma = 1/2 (-1)^i \sigma$. Hereafter, we shall discuss the spin states in terms of $|\sigma i\rangle$. According to this definition, a ferromagnetic spin array in the present context will in fact correspond to a Néel order of true spins as Fig. 1(a) shows.

A soliton state is defined as a 180° domain wall shown in Fig. 1(b). It is characterized by a pair of antiparallel spins at the shaded bond in Fig. 1(b). In the real spin space, this corresponds to a defect of the Néel order at the shaded bond with its right-hand-side Néel order exchanging the sublattices. For such a single soliton, one may notice that there exist twofold degeneracies (by exchanging spin-up domain and spin-down domain). But

FIG. 1. (a) A Néel order of spin chain: The dashed arrows represent the real spin array of $\{\mathbf{S}_i\}$. The solid arrows describe the spin polarization direction $\{\mathbf{n}_i\}$ defined in the context by reversing all the odd-site spins. That is, $\mathbf{S}_i = (-1)^i \mathbf{n}_i$ and $\mathbf{n}_i = \mathbf{n}$. (b) A soliton excitation defined at the shaded bond $(i, i+1)$.

for a series of solitons on the spin chain, there are obviously only twofold global degeneracies left, which could be lifted up by a fixed boundary condition.

If one lets H_s in (3.7) act on the Néel state shown in Fig. 1(a), one gets excitation states like that shown in Fig. 2(a), which could be regarded as a creation of two solitons according to the definition. By applying the same process to the soliton state in Fig. 1(b), one may find a new state in Fig. 2(b) which corresponds to the sublattice “hopping” of the soliton. These are the basic processes involved in H_s , which all occur in the same sublattice bonds. Now we can introduce a creation operator $d_{l\alpha}^\dagger$ describing the soliton, where l is restricted in a sublattice chain (say, odd-site chain A , with $l = \dots, i_A - 2, i_A, i_A + 2, \dots$). The index $\alpha = A, B$. $d_{lA}^\dagger |0\rangle$ describes a soliton at the bond $(l, l+1)$, while $d_{lB}^\dagger |0\rangle$ defines a soliton at the bond $(l+1, l+2)$. So the solitons A and B are distinguished in terms of whether the domain-wall bond ends up on its left-hand side at the A sublattice site or B sublattice site.

Accordingly, the Heisenberg Hamiltonian (3.7) with the constraint (3.5) can be exactly mapped into the following Hamiltonian

$$H_s = -J \sum_l (d_{lA}^\dagger d_{l+2A} + d_{lA}^\dagger d_{l+2A}^\dagger + \text{H.c.}) (1 - d_{lB}^\dagger d_{lB}) + J \sum_l (d_{lA}^\dagger d_{lA} - 1) + (A \leftrightarrow B), \quad (3.10)$$

where the summations run over only the odd sublattice as defined. The first term describes the sublattice hopping of the A soliton as well as the creation or annihilation of a pair of A solitons. If there already exists a B soliton, then by a simple graphical argument, as in Fig. 2, one find that a neighboring A soliton cannot hop across such

FIG. 2. (a) H_s acts on the Néel state in Fig. 1(a): Two solitons are excited from the Néel vacuum. (b) H_s acts on the soliton state Fig. 1(b): The sublattice hopping of the soliton from bond $(i, i+1)$ [Fig. 1(b)] to $(i+2, i+3)$. The procedures in (a) and (b) are all realized by flipping two spins at $i+1$ and $i+2$.

a B soliton nor can a pair of A solitons be created or annihilated with a B soliton in between. This is the meaning of the factor $1 - d_{lB}^\dagger d_{lB}$ appearing in the first term. The second term in H_s measures the energy cost of creating an A soliton from the Néel vacuum. The remaining terms describe the B solitons, which are obtained just by exchanging the index A with B . The only constraint associated with (3.10) is the hard-core condition $(d_{lA}^\dagger)^2 = (d_{lB}^\dagger)^2 = 0$. As we have a freedom to choose the statistics of $d_{l\alpha}$, we may define it as a fermion such that the hard-core condition is automatically satisfied. If one chooses $d_{l\alpha}$ as a boson operator at first, a Jordan-Wigner transformation³¹ could transfer its statistics into those of a fermion without changing the Hamiltonian (3.10), because it only involves the nearest-neighbor interaction in the sublattice.

Before we go one step further to discuss the Hamiltonian (3.10), we first write down the spin operators in the soliton representation. To avoid the subtle sign problem, it is convenient to assume d_{lA} and d_{lB} are bosons in the first place. As the hard-core condition $(d_{lA}^\dagger)^2 = (d_{lB}^\dagger)^2 = 0$, one may check that d_{lA} and d_{lB} satisfy the on-site anticommutation relation

$$\{d_{l\alpha}, d_{l\alpha}^\dagger\} = 1, \quad (3.11)$$

and otherwise satisfy the bosonic commutation. In accordance with the definition of the soliton, the lattice sites are classified in terms of the odd sites and even sites as $\{(lA); (lB)\}$, where l only runs over the odd sublattice. From Eq. (3.9a), the spin operator S_i^z may be written as

$$S_{lA}^z = \frac{1}{2} (-1)^{\sum_{m < l} d_{mA}^\dagger d_{mA}} (-1)^{\sum_{m < l} d_{mB}^\dagger d_{mB}}, \quad (3.12a)$$

$$S_{lB}^z = -S_{lA}^z (-1)^{d_{lA}^\dagger d_{lA}}, \quad (3.12b)$$

where the real spin at the left-hand side boundary has been fixed as up for simplicity. Each soliton will change its right-hand spins by 180° , which is what (3.12) implies. One may similarly write down $S_i^\pm$ by the soliton operator d . Noticing that $S_i^\pm$ flips a spin at one site, which always involves two solitons (either creation or annihilation), one can verify that

$$S_{iA}^\pm = -(d_{iA}^\dagger + d_{iA})(d_{i-2B}^\dagger + d_{i-2B}) \frac{1 \mp 2S_{iA}^z}{2}, \quad (3.13a)$$

$$S_{iB}^\pm = (d_{iA}^\dagger + d_{iA})(d_{iB}^\dagger + d_{iB}) \frac{1 \mp 2S_{iB}^z}{2}. \quad (3.13b)$$

According to Eqs. (3.12), (3.13), and (3.11), a straightforward calculation shows that $\mathbf{S}_i$ satisfies all the spin algebra and H_s in (3.10) is equivalent to

$$H_s = 2J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4}), \quad (3.14)$$

which is just the t - J model at half-filling. Now we have completed the demonstration for the exact mapping of the Heisenberg model into the soliton representation. Finally, as the soliton operator d is defined as the hard-boson, we introduce the Jordon-Wigner transformation³¹

$$d_{iA} \rightarrow d_{iA} (-1)^{\sum_{m < i} d_{mA}^\dagger d_{mA}}, \quad (3.15)$$

in which d_{iA} on the right-hand side satisfies the fermionic anticommutation. For compactness, we do not use different notations to distinguish the boson and fermion here. The B soliton has a similar transformation. As Eq. (3.15) does not involve the B soliton, the solitons A and B still commute with each other. This transformation will not change the form of H_s in (3.10), which may be verified readily.

Hence H_s in (3.10) describes two types of spinless fermions (i.e., A and B solitons) staying in the different sublattices. The only coupling between them comes from the fact that the existence of a soliton B may block the motion of the soliton A and vice versa. In Appendix C, we decouple such a coupling self-consistently in the mean-field level. Then through the Bogoliubov transformation,

$$d_k = u_k \bar{d}_k + i v_k \bar{d}_{-k}^\dagger, \quad (3.16)$$

with

$$u_k = \cos \left[\frac{\pi}{4} - \frac{|ka|}{2} \right], \quad (3.17a)$$

$$v_k = \cos \left[\frac{\pi}{4} + \frac{|ka|}{2} \right] \text{sgn}(k). \quad (3.17b)$$

H_s is diagonalized in Appendix C as

$$H_s = \sum_k \epsilon_k^s (\bar{d}_{kA}^\dagger \bar{d}_{kA} + \bar{d}_{kB}^\dagger \bar{d}_{kB}) + E_0, \quad (3.18)$$

where $-\pi/2 < k \leq \pi/2$ and the spectrum ϵ_k^s is given by

$$\epsilon_k^s = \left[1 + \frac{2}{\pi} \right] (2J) |\sin ka|. \quad (3.19)$$

We identify such a fermion-type gapless excitation with the spin $\frac{1}{2}$ spinon excitation, found by Faddeev and Takhtajan³⁰ many years ago. They derived this spin- $\frac{1}{2}$ excitation based on the Bethe ansatz solution³² of the Heisenberg chain, with the spectrum given by $\epsilon_k^s = \pi/2 (2J) |\sin ka|$. Notice that the numerical factor $1 + 2/\pi \approx 1.64$ is quite close to $\pi/2 \approx 1.57$; we find a very good agreement. Furthermore, the ground-state energy of (3.18) is given by (see Appendix C)

$$E_0 = -(\frac{1}{2} + 2/\pi + 2/\pi^2) JN \approx -0.670 (2J)N, \quad (3.20)$$

and it is also quite close to the exact solution $-0.693 (2J)N$.³²

Therefore, the ground state of the Heisenberg chain involves a lot of soliton excitations above the vacuum state (i.e., the Néel state), with an average soliton number $\langle d_i^\dagger d_i \rangle = \frac{1}{2} - 1/\pi \approx 0.182$ at each bond [Eq. (C15)]. These excited solitons form Cooper-like pairs and condense just like the BCS superconducting condensation. The pair wave function is found to be

$$\langle d_i^\dagger d_{i'}^\dagger \rangle \sim -\frac{a}{\pi} \frac{1}{x_i - x_{i'}}, \quad (3.21)$$

which is in power-law decay without a finite coherent length scale. As the solitons in a pair can be infinitely far apart, the pair-breaking excitations could cost infinitesimal energy, i.e., could be gapless, which may be also understood by noticing that if the superconducting gap Δ_k has nodes, the coherent length $\xi \sim v_s / \Delta_k$ becomes singular in the one-dimensional case. The excitation state is obtained by breaking the Cooper pair of solitons as in the BCS theory. As a spin-1 excitation is composed of a pair of solitons [see, e.g., Eq. (3.13)], one may attach spin $\frac{1}{2}$ to each soliton. The hidden spin degree of freedom for solitons is related to the twofold degeneracies of a single soliton mentioned at the beginning of this section. It will be further discussed in the next section in calculating the spin-spin correlation function.

C. The spin-spin correlation function

In terms of (3.12a) and (3.12b), the spin-spin correlations $\langle S_i^z(t) S_j^z(0) \rangle$ is given by

$$\begin{aligned} \langle S_i^z(t) S_j^z(0) \rangle &= \frac{(-1)^{i-j}}{4} \langle (-1)^{\sum_{m < i} d_{mA}^\dagger(t) d_{mA}(t)} (-1)^{\sum_{m < j} d_{mA}^\dagger(0) d_{mA}(0)} \rangle \\ &\quad \times \langle (-1)^{\sum_{m < i} d_{mB}^\dagger(t) d_{mB}(t)} (-1)^{\sum_{m < j} d_{mB}^\dagger(0) d_{mB}(0)} \rangle, \end{aligned} \quad (3.22)$$

where the fact that A and B solitons are decoupled has been used [d is the fermion now by the transformation (3.15), which in fact does not change the form of (3.22)]. One may write down the similar expression for the transverse spin correlation function $\langle S_i^+ S_j^- \rangle$ in terms of (3.13) and (3.15).

As the motions of d_A and d_B have been already determined in Sec. III B, in principle one could directly calculate the averages in (3.22). Equation (3.22) shows that each soliton will contribute a phase factor $(-1) = \exp(\pm i\pi)$ in the correlation function. Obviously, the choice of the sign in the exponent should not affect the final result, and it is related to the $U(1)$ freedom of the system. However, we note that the average in (3.22) is quite singular and any uncontrolled approximation may lead to a large error in its asymptotic behavior. Thus we need to choose properly the $U(1)$ gauge in the following calculation.

In Sec. III B, we have already noted that, for a given soliton, there exist two possible configurations: the spins on its left-hand side domain are either up or down (correspondingly the spins on its right-hand side are either down or up). We may explicitly distinguish this hidden degree of freedom by assigning a spin index σ to the d_i operator: i.e., $d_{i\sigma A}$ and $d_{i\sigma B}$ where $\sigma = \uparrow, \downarrow$. What is the relation of $d_{i\sigma A}, d_{i\sigma B}$ with the previously discussed spinless solitons d_{iA}, d_{iB} ? First we should emphasize that distinguishing two types of solitons with different “spins” does not mean that the real degree of freedom has been increased, because there is a constraint imposed on them: two nearest-neighboring solitons should always have the opposite “spins” on the spin chain. Such a constraint is in fact the basis for us to define the spinless solitons in Sec. III B. We reintroduce the pseudospin degree of freedom to the soliton just for the convenience of properly describing the $U(1)$ degree of freedom for the spin chain. We shall thus assume that the phase $\exp(i\pi)$ will be attached to a soliton with spin “ $\uparrow$ ”, whereas a phase $\exp(-i\pi)$ will be associated with the soliton with spin “ $\downarrow$.” Then a typical phase factor in (3.22) could be written as

$$(-1)^{\sum_{m < i} d_{m\sigma A}^\dagger d_{m\sigma A}} = \exp \left[\pm i\pi \sum_{m < i, \sigma} \sigma d_{m\sigma A}^\dagger d_{m\sigma A} \right]. \quad (3.23)$$

In this way one finds that two solitons with opposite spins will contribute a canceled phase in (3.23). For example, two spontaneously excited solitons from the Néel vacuum will always involve opposite spins so that their phases are canceled with each other instead of the contribution of $e^{2\pi i}$.

Now we need to determine the motion of $d_{i\sigma A}$ and $d_{i\sigma B}$. As the A and B solitons always stay at the different

sublattices and they have been decoupled in the mean-field approximation in Sec. III B, one needs only to consider, say, type- A solitons. It is easy to find that the Hamiltonian (3.10) includes two basic processes: One is the sublattice hopping of the A soliton in which the pseudospin is obviously conserved; another one is a creation or annihilation of a soliton pair which must involve the opposite spins according to the definition. Therefore, we find the correspondence in the single-particle Green's function as follows:

$$G_{\sigma\sigma'}^A(ij; t) = \delta_{\sigma, \sigma'} G^A(ij; t), \quad (3.24a)$$

$$F_{\sigma\sigma'}^A(ij; t) = \delta_{\sigma, -\sigma'} F^A(ij; t), \quad (3.24b)$$

where

$$G_{\sigma\sigma'}^A(ij; t) = -i \langle T d_{i\sigma A}(t) d_{j\sigma' A}^\dagger(0) \rangle, \quad (3.25a)$$

$$F_{\sigma\sigma'}^A(ij; t) = -i \langle T d_{i\sigma A}^\dagger(t) d_{j\sigma' A}^\dagger(0) \rangle, \quad (3.25b)$$

$$G^A(ij; t) = -i \langle T d_{iA}(t) d_{jA}^\dagger(0) \rangle, \quad (3.25c)$$

$$F^A(ij; t) = -i \langle T d_{iA}^\dagger(t) d_{jA}^\dagger(0) \rangle. \quad (3.25d)$$

Equations (3.24) and (3.25) uniquely determine the motion of the soliton $d_{i\sigma A}$. Similar to the Bogoliubov transformation (3.16), one may introduce

$$d_{k\sigma A} = u_k \bar{d}_{k\sigma A} + i v_k d_{-k-\sigma A}^\dagger, \quad (3.26)$$

and find, according to the k -space correspondence of Eqs. (3.24) and (3.25), that $\bar{d}_{k\sigma A}$ behaves just like the spinless soliton $\bar{d}_{kA}$ with the linear dispersion (3.19). In other words, it is equivalent to say that its dynamics is determined by the effective Hamiltonian

$$H_{\text{eff}}^A = \sum_{k\sigma} \epsilon_k^s \bar{d}_{k\sigma A}^\dagger \bar{d}_{k\sigma A}. \quad (3.27)$$

A similar conclusion holds for the B solitons. We then introduce the so-called right-moving and left-moving operators as follows:

$$\psi_R(x_i) = \frac{1}{\sqrt{aN}} \sum_{k>0} (e^{ikx_i} \bar{d}_{k\uparrow} - i e^{-ikx_i} \bar{d}_{k\downarrow}^\dagger), \quad (3.28a)$$

$$\psi_L(x_i) = \frac{1}{\sqrt{aN}} \sum_{k<0} (e^{ikx_i} \bar{d}_{k\uparrow} + i e^{-ikx_i} \bar{d}_{k\downarrow}^\dagger). \quad (3.28b)$$

For simplicity, we have neglected the superscript distinguishing A and B solitons. In terms of (3.26) and (3.28), we could write $d_{i\uparrow}$ as

$$d_{i\uparrow} = \sqrt{a/2} e^{i\pi/4} \psi_R \left[x_i - \frac{a}{2} \right] + \sqrt{a/2} e^{-i\pi/4} \psi_R \left[x_i + \frac{a}{2} \right] + \sqrt{a/2} e^{i\pi/4} \psi_L \left[x_i + \frac{a}{2} \right] + \sqrt{a/2} e^{-i\pi/4} \psi_L \left[x_i - \frac{a}{2} \right]. \quad (3.29)$$

A similar expression for $d_{i\downarrow}$ could also be obtained. Thus in the continuum limit (by taking $a \rightarrow 0$), Eq. (3.23) is reduced to the form

$$(-1)^{\sum'_{m < i} d_m^\dagger d_m} = \exp \left[\pm i\pi 2a \sum'_{l < i} : \psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L : \right], \quad (3.30)$$

where the normal order $:\psi^\dagger \psi: = \psi^\dagger \psi - \langle \psi^\dagger \psi \rangle$ and $\langle \psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L \rangle = 1/(2a)$. Recall that the motion of $\vec{d}_{k\sigma}$ is governed by H_{eff} in (3.27). In the continuum approximation we linearize the dispersion ϵ_k^σ in small $|k| \ll \pi/a$. H_{eff} then becomes a continuum Hamiltonian

$$H_{\text{eff}}^A = -iv_s \int dx \left[\psi_R^\dagger \frac{d}{dx} \psi_R - \psi_L^\dagger \frac{d}{dx} \psi_L \right] + \text{const.} \quad (3.31)$$

where the spinon velocity $v_s = (1 + 2/\pi)(2Ja)$.

Thus, by introducing the spin degree of freedom to properly describe the U(1) phase, the phase factor in (3.22) is expressed by (3.30) with ψ_R and ψ_L governed by (3.31). This is a standard form for the free spinless fermion system where the bosonization technique³³ could be directly employed to rigorously calculate the average in (3.22). So far the only approximation being made is the continuum approximation by letting $a \rightarrow 0$ in (3.29), as we are interested in the asymptotic behavior with $|x_i - x_j|, v_s |t| \gg a$.

The bosonization scheme has been briefly presented in Appendix D. With reference to (D12), one straightforwardly obtains the asymptotic form of $\langle S_i^z(t) S_j^z(0) \rangle$ from (3.22):

$$\frac{(-1)^{i-j}}{4} [\langle \exp[i\pi N_i(t)] \exp[-i\pi N_j(0)] \rangle]^2 \sim \frac{(-1)^{i-j}}{[(x_i - x_j)^2 - v_s^2 t^2]^{1/2}}, \quad (3.32)$$

where $N_i = \sum'_{m < i} d_m^\dagger d_m = 2a \sum'_{m < i} : \psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L :$ according to (3.30).

In terms of Eqs. (3.13) and (3.15), the leading term of $\langle S^+ S^- \rangle$ is found to have the forms like $|\langle d(t) e^{i\pi N(t)} e^{-i\pi N(0)} d^\dagger(0) \rangle|^2$ and $|\langle d^\dagger(t) e^{-i\pi N(t)} e^{-i\pi N(0)} d^\dagger(0) \rangle|^2$, etc. (those terms like $|\langle dd^\dagger \rangle|^2 \sim 1/x^2$ are of higher order and thus are neglected). Again, by introducing the pseudospins to properly determine the U(1) phase and by using the bosonization method in Appendix D, the leading term of $\langle S^+ S^- \rangle$ is found to be proportional to

$$(-1)^{i-j} |\langle \psi_{L,R} e^{i\pi N_i(t)} e^{-i\pi N_j(0)} \psi_{L,R}^\dagger \rangle|^2 \sim \frac{(-1)^{i-j}}{[(x_i - x_j)^2 - v_s^2 t^2]^{1/2}}. \quad (3.33)$$

Therefore, the asymptotic spin-spin correlation function for the Heisenberg chain is found to be

$$\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle \sim \frac{\cos \frac{\pi}{a}(x_i - x_j)}{[(x_i - x_j)^2 - v_s^2 t^2]^{1/2}}. \quad (3.34)$$

This $1/x$ behavior agrees with Luther and Peschel's result³⁴ obtained by the Jordan-Wigner transformation and bosonization approach to the XXZ model, where the isotropic Heisenberg case is realized by an extrapolation from $J_z = 0$.

IV. FINITE DOPING: CHARGE AND SPIN SEPARATION

In this section, we shall show how the charge and spin degrees of freedom are decoupled in the infinite- U limit for an arbitrary doping. Then we demonstrate that such a peculiar property will persist into the strong-coupling regime with $J \ll t$.

A. Infinite- U limit

We consider the $U \rightarrow \infty$ ($J=0$) limit. Lagrangian (2.32) is then reduced to

$$\mathcal{L}_\infty = \sum_i \sum_\sigma \theta(p_i \sigma) (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} (1 - h_i^\dagger h_i) + \sum_i h_i^\dagger \partial_\tau h_i + t \sum_i \left[\sum_\sigma \theta(p_i \sigma) (U_i^\dagger U_{i+1})_{\sigma-\sigma} h_{i+1}^\dagger h_i + \text{H.c.} \right]. \quad (4.1)$$

If one employs the CP^1 representation (3.2) and (3.5) for U_i in (4.1), the t - J model in the slave-fermion representation (with $J=0$) is recovered as follows:

$$\mathcal{L}_\infty = \sum_\sigma \tilde{b}_{i\sigma}^* \partial_\tau \tilde{b}_{i\sigma} + \sum_i h_i^\dagger \partial_\tau h_i + t \sum_{i\sigma} [h_{i+1}^\dagger (\tilde{b}_{i+1\sigma} \tilde{b}_{i\sigma}^*) h_i + \text{H.c.}] + i \sum_i \tilde{\lambda}_i \left[\sum_\sigma \tilde{b}_{i\sigma}^* \tilde{b}_{i\sigma} + h_i^\dagger h_i - 1 \right], \quad (4.2)$$

where the boson field $\tilde{b}_{i\sigma} = [\theta(p_i) b_{i\sigma} - \theta(-p_i) \sigma b_{i-\sigma}] (1 - h_i^\dagger h_i)^{1/2}$ has been introduced. But we shall not pursue such a method further because the constraint appearing in (4.2) is difficult to treat in a controllable approximation.

We shall start directly from (4.1). Lagrangian (4.1) shows that the hopping of the hole is greatly affected by the spin background as the hopping matrix element is re-

lated to $(U_i^\dagger U_{i+1})_{\sigma-\sigma}$. For a Néel order, the local spin orientation is along $(-1)^i \mathbf{n}_i = (-1)^i \mathbf{n}$, where $\mathbf{n}$ is a global direction. One finds $U_i^\dagger U_{i+1} = \hat{I}$ by using Eq. (B.1) and thus $(U_i^\dagger U_{i+1})_{\sigma-\sigma} = 0$. So the hole cannot hop in a rigid Néel background. This term is usually neglected in the U(1) gauge theory^{4,8,9} by assuming the existence of the short-range Néel order. However, this is the only hopping term appearing in (4.1). The sublattice hopping,

which is emphasized in U(1) gauge theory,^{4,8,9} vanishes at $U \rightarrow \infty$. Hence the hole has to distort the surrounding SU(2) spins to gain its kinetic energy.

The largest hopping matrix element ($=t$) could be found when the spin background is arranged such that

$$|(U_i^\dagger U_{i+1})_{\sigma-\sigma}|=1, \quad (4.3)$$

for all sites i . Such a state corresponds to a ferromagnetic spin background with $(-1)^i \mathbf{n}_i = \mathbf{n}$. This is the well-known Nagaoka state in which a hole behaves like a free spinless fermion and the total energy is optimized. A gauge theory in Ref. 35 is actually valid in the expansion around such a local ferromagnetic order. However, the hole could gain its greatest kinetic energy even in the generic spin states, which are degenerate at $U = \infty$ in the one-dimensional case. The singlet spin state will be of most interest, as it could survive in the large but finite U case. This is what we are going to discuss in the following.

First we notice that the quantum phase of spin is governed by the first term on the right-hand side of the Lagrangian (4.1), which describes the overlap of the coherent states in an infinitesimal imaginary time interval. But such a term disappears at the hole sites because of the factor $(1 - h_i^\dagger h_i)$. Thus the spin directions at hole sites could be arbitrary without any phase cost, which is equivalent to saying that the true spin is absent at these hole sites.

Now let us assume that a hole is hopping from site i to site $i+1$. As the “spin” direction at hole site i is not well defined, it could be arbitrary as noted above. In order to gain the greatest kinetic energy, the optimization path for U_i is to be arranged such that $|(U_i^\dagger U_{i+1})_{\sigma-\sigma}|=1$, which gives rise to the largest hopping matrix element ($=t$) from i to $i+1$ sites. Without a quantum phase, $\mathbf{n}_i$ or U_i at hole site could be regarded as a classic quantity, whose optimized path should be also the exact solution from the principle of the classic action. One may choose

$$U_i = U_{i+1}(-i\sigma_x), \quad (4.4)$$

which satisfies $|(U_i^\dagger U_{i+1})_{\sigma-\sigma}|=1$ without loss of any generality as the U(1) freedom of U_i . An example of such a procedure is diagrammatically shown in Figs. 3(a) and 3(b).

As Fig. 3(b) shows, after the hole hops into site $i+1$, a spin is produced at site i , given by U_i in (4.4), while the spin at $i+1$ becomes undetermined. Physically, it could be interpreted as the true spin (carried by electron) at site $i+1$ being transferred back to site i during the above hopping procedure. Such a process is more clearly shown in the real spin space by Figs. 4(a) and 4(b), which are obtained by reversing the odd-site spins in Figs. 3(a) and 3(b), in terms of the definition.

So we have seen that the hole could hop around just like a free fermion in the generic spin background. The question is how the motion of a hole can change the spin background. At a given moment, we may construct an effective spin chain by removing all the sites of the vacancies. For any site on this “squeezed” spin chain, one may define a new spin field $\tilde{U}_i$ which is related to U_i through

FIG. 3. The dashed arrow is the “spin” at the hole site which could be arbitrary without any phase cost. (a) The hole at site i is hopping to site $i+1$. In order to get the optimized hopping matrix with $|(U_i^\dagger U_{i+1})_{\sigma-\sigma}|=1$, the “spin” at site i is arranged to be antiparallel to the spin at site $i+1$. (b) After the hole hops to $i+1$, a spin is left at site i and the “spin” at hole site $i+1$ becomes undetermined.

$$U_i = \tilde{U}_i \exp \left[i \frac{\pi}{2} \sigma_x \sum_{l < i} h_l^\dagger h_l \right]. \quad (4.5)$$

$\{\tilde{U}_i\}$ determines the “spins” on the squeezed spin chain. Then one could check by (4.5) that the “squeezed” spin configuration which corresponds to Figs. 3(a) and 3(b) is the same as shown in Fig. 5. This implies $\{\tilde{U}_i\}$ is independent of the holes’ motion. In the following, we shall show that this conclusion is generally correct.

Suppose that a hole is hopping from site j to $j+1$. Before hopping, site $j+1$ belongs to the “squeezed” spin

FIG. 4. The real spin-hole configurations corresponding to Figs. 3(a) and 3(b). They are obtained by reversing all the odd-site spins according to the definition.

FIG. 5. The effective (squeezed) spin chain obtained by removing the hole site from Figs. 3(a) and 3(b). The “spins” configuration is determined by $\tilde{U}_i$ defined in (4.5).

chain, while site j does not, according to the definition. Recall that, at each step of hole hopping, there is always an accompanied spin transfer process (4.4). After the hopping, site j belongs to the “squeezed” spin chain, with $U_j = U_{j+1}(-i\sigma_x)$, whereas site $j+1$ now is occupied by the hole. By the definition of (4.5), one easily finds

$$\tilde{U}_j(\text{after hopping}) = \tilde{U}_{j+1}(\text{before hopping}). \quad (4.6)$$

So the effective (squeezed) spin chain, as described by the spin field $\{\tilde{U}_i\}$, is indeed independent of the motion of holes. Thus one finds the charge and spin separation.

Any real spin-hole configuration could be obtained just by inserting the vacancy sites into the squeezed chain to recover the original Hubbard chain. U_i at the spin site will be determined by $\tilde{U}_i$ according to (4.5). As Eq. (4.5) shows, each hole on the left-hand side of site i contributes a phase field $\exp(i\pi/2\sigma_x)$ to U_i . Such a phase factor is just a 180° rotation. Therefore, each mobile hole does affect the spin background by carrying a 180° domain wall on top of the spin field $\tilde{U}_i$. But such a domain-wall entity is decoupled from $\tilde{U}_i$. The domain-wall structure is clearly shown in Figs. 3(a) and 3(b), where $\tilde{U}_i$ simply describes a Néel order in Fig. 5. In the real spin space, the 180° domain wall represents an exchange of two sublattices on one side of the hole as shown by Figs. 4(a) and 4(b). One may generalize such a picture for the case of the generic spin field $\tilde{U}_i$.

In terms of (4.5), we find

$$\sum_{\sigma} \theta(p_i \sigma) (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} = \sum_{\sigma} \theta(\tilde{p}_i \sigma) (\tilde{U}_i^\dagger \partial_\tau \tilde{U}_i)_{\sigma\sigma}, \quad (4.7)$$

where

$$\tilde{p}_i = \exp \left[i\pi \left(\frac{x_i}{a} - \sum_{l < i} h_l^\dagger h_l \right) \right], \quad (4.8)$$

while $p_i = \exp(i\pi x_i/a) = (-1)^i$.

Finally, $\mathcal{L}_\infty$ is written in the following form according to the above discussions:

$$\mathcal{L}_\infty = \sum_i^s \sum_{\sigma} \theta(\tilde{p}_i \sigma) (\tilde{U}_i^\dagger \partial_\tau \tilde{U}_i)_{\sigma\sigma} + \mathcal{L}_h, \quad (4.9)$$

with

$$\mathcal{L}_h = \sum_i \tilde{h}_i^\dagger \partial_\tau \tilde{h}_i - t \sum_i (\tilde{h}_{i+1}^\dagger \tilde{h}_i + \tilde{h}_i^\dagger \tilde{h}_{i+1}), \quad (4.10)$$

where the summation $\sum^s$ is defined only on the squeezed spin chain. The function $\tilde{p}_i$ is a staggered factor on such an effective spin chain just like p_i on the original chain. $\tilde{h}_i = \exp[i\pi/(2a)x_i]h_i$ is introduced to write down $\mathcal{L}_h$ in a standard form. Lagrangian (4.9) clearly shows that the charge degree of freedom is decoupled from the spin part.

We call the charge excitation a holon. The holon behaves like a free spinless fermion and its excitation spectrum is found by

$$\epsilon_k^h = -2t \cos ka, \quad (4.11)$$

with the Fermi velocity

$$v_h = 2ta \sin(\pi\delta), \quad (4.12)$$

at the hole's Fermi momentum $\tilde{k}_f = \pi/a\delta$. δ is the doping concentration. The ground-state energy is given by $-2t/\pi \sin(\pi\delta)$, which agrees with the exact result.¹⁶

B. The strong-coupling regime: $0 < J \ll t$

Now let us turn on J , but still assume $J \ll t$. The finite- J contribution is given in the Lagrangian (2.32). We may classify two effects due to finite J . One is the correction to the hopping of the holon with a magnitude in order of J . This effect will be neglected because the hopping matrix of the holon is already of order of t , which is much larger than J . The second effect is to give rise to a nonzero spin stiffness in the squeezed spin chain, that will lift up the spin degeneracy and choose a spin singlet state.

With the presence of the nearest-neighbor superexchange coupling, however, the definition of the squeezed spin chain may cause problems. By removing a vacant site i , site $i-1$ and site $i+1$ now become the nearest-neighbor sites in the squeezed spin chain. But the superexchange coupling between $i-1$ and $i+1$ sites is obviously reduced (if not zero) and thus such a bond in the squeezed spin chain will be different from the other bonds originally without a hole in between. However, we notice that when the hole hops to the site $i+1$ from site i , the spin at $i+1$ will be transferred back to site i and then become truly a nearest neighbor to the site $i-1$. As $t \gg J$, the hole's hopping is very quick as compared with the spin dynamics. Thus we still expect that the spins in the squeezed spin chain connect with each other perfectly in the time scale $\sim J^{-1} \gg t^{-1}$, but the effective coupling constant will be reduced.

Based on the above consideration, in the Lagrangian (2.32), we may treat the holon part appearing in those terms involving J by the mean-field approximation, and neglect their effects to the holon's motion. That is, we substitute $\langle h_{i+1}^\dagger h_i \rangle = i/\pi \sin \pi\delta$ and $\langle h_{i+2}^\dagger h_i \rangle = -\sin(2\pi\delta)/(2\pi)$ into the corresponding J terms in Lagrangian (2.32). Correspondingly, U_i could be replaced by $\tilde{U}_i$ in these terms in terms of (4.5). But for the whole chain, there will be always δN sites where spins ($\tilde{U}_i$) are not well defined, as discussed in Sec. IV A. Thus we should remove these δN sites from the summation. That is consistent with the definition of the squeezed spin chain. The errors coming from these δN sites are of order of δJN ; they may be properly regarded as the polaron effects accompanying the holons and are negligible as compared to the leading holon energy δtN . This is actually the central approximation in the present paper. We always neglect the energy scale J whenever it is associated with the holes. In terms of Eqs. (4.9) and (4.10), Lagrangian (2.32) is then reduced to the form

$$\mathcal{L} = \mathcal{L}_h + \mathcal{L}_s, \quad (4.13)$$

with

$$\mathcal{L}_s = \sum_{i\sigma} \theta(\bar{p}_i\sigma) (\tilde{U}_i^\dagger \partial_\tau \tilde{U}_i) - \frac{\tilde{J}}{2} \sum_{i\sigma} |(\tilde{U}_i^\dagger \tilde{U}_{i+1})_{\sigma\sigma}|^2, \quad (4.14)$$

in which we have neglected a term $\sim J |(\tilde{U}_i^\dagger \tilde{U}_{i-1})_{\sigma\sigma} - (\tilde{U}_i^\dagger \tilde{U}_{i+1})_{\sigma\sigma}|^2$ as a higher order contribution ($\sim J |\mathbf{n} \cdot \partial_x^3 \mathbf{n}|^2$). The renormalized superexchange coupling $\tilde{J}$ is found to be

$$\tilde{J} = J(1-\delta) \left[1 - \frac{\sin 2\pi(1-\delta)}{2\pi(1-\delta)} \right]. \quad (4.15)$$

Compared to (3.1), $\mathcal{L}_s$ in (4.14) simply describes a (squeezed) Heisenberg chain with an enlarged lattice constant $\tilde{a} = a/(1-\delta)$ and a renormalized superexchange coupling $\tilde{J}$. So the results in the Sec. III could be directly used here.

In terms of (3.19) and (4.15), the spinon excitation spectrum becomes

$$\epsilon_k^s = (1 + 2/\pi) 2\tilde{J} |\sin(k\tilde{a})|. \quad (4.16)$$

The doping dependence of $\tilde{J}$ in (4.15) and ϵ_k^s in (4.16) is exactly in agreement with the results of Coll¹⁵ in discussing the spin excitation based on the solution of Lieb and Wu. The only difference is the factor $(1 + 2/\pi)$ in ϵ_k^s , which is slightly different from the $\pi/2$ factor appearing in Coll's result and it actually already exists in half-filling as discussed in Sec. III. Such an amazing agreement shows that the above mean-field decoupling of the spin and charge degrees of freedom is indeed a very good approximation in $J \ll t$ regime. The total ground-state energy can be directly obtained as follows:

$$E_0 = -\frac{2t}{\pi} \sin(\pi\delta)N - 0.670(2\tilde{J})(1-\delta)N,$$

which is found in good agreement with the exact solution¹⁶ up to the order of t/U within the whole doping regime.

C. Electron as a composite particle of holon and spinon

The decoupling of the charge and spin degrees of freedom has been shown to persist through the strong-coupling regime $J \ll t$. Two elementary charge and spin excitations are called the holon and spinon, respectively, following the general recognition. In order to calculate the physical quantities like the electron Green's function, we need to express the electron operator by these elementary excitations.

Recall that the bare electron operator $c_{i\sigma}$ is related to the spin field U_i and fermion $a_{i\sigma}$ by (2.15). At the occupied site, U_i is given by (4.5) and $a_{i\sigma} = \theta(p_i\sigma) h_i^\dagger$ in terms of (2.29) with the double-occupancy being projected out in the large U limit. Therefore one finds

$$c_{i\sigma} = h_i^\dagger \sum_{\sigma'\sigma''} \tilde{U}_{i\sigma\sigma'} \theta(p_i\sigma'') \left[\exp \left[i \frac{\pi}{2} \sigma_x \sum_{l < i} h_l^\dagger h_l \right] \right]_{\sigma'\sigma''}. \quad (4.17)$$

$\tilde{U}_i$ describes the spin defined on the squeezed spin chain composed by all the occupied sites. Its CP^1 representation is similar to (3.2) but with $p_i \rightarrow \bar{p}_i$ [Eq. (4.8)] which distinguishes two sublattices on the squeezed chain. In the operator formalism, $\tilde{U}_i$ is written as [in resemblance to (3.2)]

$$\tilde{U}_i = \theta(\bar{p}_i) \begin{bmatrix} b_{i\uparrow} & b_{i\downarrow}^\dagger \\ b_{i\downarrow} & b_{i\uparrow}^\dagger \end{bmatrix} + \theta(-\bar{p}_i) \begin{bmatrix} b_{i\uparrow}^\dagger & -b_{i\downarrow} \\ b_{i\downarrow}^\dagger & b_{i\uparrow} \end{bmatrix}. \quad (4.18)$$

We shall not directly use the boson $b_{i\sigma}$ description as in Ref. 23. Instead, we map $\tilde{U}_i$ into the soliton representation introduced in Sec. III. It is noted that $h_i^\dagger b_{i\sigma}^\dagger = 0$ due to the constraint $\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma} = 1$ at the occupied site. On the other hand, $h_i^\dagger b_{i\sigma}$ corresponds to simultaneously annihilating a spin and creating a hole at site i , or equivalently, removing an electron from the site i . Such a site then should be also removed from the effective spin chain by its definition. In the newly-squeezed chain (with the site i removed), the spin field $\tilde{U}_m$ on the right-hand side of the original i site will all be shifted by $\tilde{U}_m \rightarrow \tilde{U}_m \exp(i\pi/2\sigma_x)$ in terms of (4.5). Correspondingly, $\bar{p}_m \rightarrow -\bar{p}_m$ and

$$b_{m\sigma} \rightarrow i\sigma \bar{p}_m b_{m-\sigma}, \quad (4.19)$$

for $m > i$ according to (4.8) and (4.18). One sees that all the spins at $m > i$ have flipped once, as the phase factor $\exp(i\pi/2\sigma_x)$ is a 180° rotation. Then there is a 180° domain-wall (soliton) created in the new effective spin chain across the hole site i after its being removed. In the real spin space, it can be also understood in this way: After a hole is created at site i and then hops away, the spins originally staying at the same sublattice sites $i-1$, and $i+1$ now will be transferred to be the nearest neighbors, which will form a defect (parallel spins) of the Néel order, i.e., a soliton excitation. However, if there is already an excited soliton neighboring the site i , removing such a site could annihilate the aforementioned soliton, i.e., creating a hole soliton.

Since the total effective spin chain is squeezed by one bond with a spinon being produced, after a hole is added and then is turned into a mobile holon, how can we describe such a excitation state in the fermion representation of solitons? One may imagine that at first a pair of fermionic solitons is excited at the original ground state adjacent to site i . Then let one of the solitons go to the boundary. In this way, we can properly count the phase and write down the excitation. Therefore, $h_i^\dagger b_{i\sigma}$ has been written in the soliton representation as follows:

$$h_i^\dagger b_{i\sigma} = [\theta(\bar{p}_i)(d_{iA}^\dagger + d_{iA}) + \theta(-\bar{p}_i)(d_{iB}^\dagger + d_{iB})] \times (-1)^{N_{iA} + N_{iB}} \frac{1 + \sigma(-1)^{N_{iA} + N_{iB}}}{2} G_i h_i^\dagger, \quad (4.20)$$

where $\theta(\pm\bar{p}_i)$ determines the corresponding sublattice bond of the created soliton. $d_{i\alpha}$ is understood as the fermionic soliton operator corresponding to site $\tilde{i} = i - \sum_{l < i} h_l^\dagger h_l$ on the squeezed chain; also note $N_{i\alpha} = \sum_{m < i} d_{m\alpha}^\dagger d_{m\alpha}$, $\alpha = A, B$. The first factor before G_i is a projective operator, which ensures that $b_{i\sigma}$ annihi-

lates the spin σ (with no loss of generality, the spin at the left-side boundary is fixed as up). G_i in (4.20) is a nonlocal phase shift resulting from the transformation (4.19):

$$G_i = \prod_{m>i}' (-i\sigma_m \tilde{p}_m). \quad (4.21)$$

Rigorously speaking, (4.20) holds exactly in the Néel limit of the local environment. With the presence of the zero-point fluctuation (i.e., soliton excitations) nearby, adding a hole will not only create (annihilate) a soliton in the squeezed spin chain but also interrupt the correlation between solitons across the hole site (the removal of a spin will lead to the interchange of A and B solitons on the right-hand side). So (4.20) just represents the leading contribution since local spins are dominantly Néel ordered (see Sec. III). The neglected many-body effects would, in general, not affect the leading long-wavelength behavior.

We still need to evaluate the phase-shift G_i in (4.21) which is determined by the spin configuration at $m > i$ on the effective spin chain. A direct count results in

$$G_i = [\theta(\tilde{p}_i(-1)^{N-n_h}) + i\sigma_i(-1)^{d_i^\dagger d_i} \theta(-\tilde{p}_i(-1)^{N-n_h})] \\ \times (-1)^{\sum_{m>i}' d_m^\dagger d_m (x'_L - x'_m/a)}$$

where x'_L is the coordinate corresponding to the right-hand side boundary site on the effective spin chain. N is the total number of the lattice sites and n_h is the number of holes in the state that $c_{i\sigma}$ is acting on. Without loss of generality, we choose $N, n_h = \text{even}$. Then $(-1)^{N-n_h} = 1$

$$c_{i\sigma} \approx \frac{1}{4} [\tilde{d}_{iA}^\dagger + \tilde{d}_{iA} + i\sigma(\tilde{d}_{iB}^\dagger + \tilde{d}_{iB})] h_i^\dagger \exp \left[i \frac{\pi}{2} \sum_{l<i} h_l^\dagger h_l \right] + \frac{p_i}{4} [\tilde{d}_{iA}^\dagger + \tilde{d}_{iA} - i\sigma(\tilde{d}_{iB}^\dagger + \tilde{d}_{iB})] h_i^\dagger \exp \left[-i \frac{\pi}{2} \sum_{l<i} h_l^\dagger h_l \right], \quad (4.25)$$

which acts on the ground state. It shows that a bare electron (hole) could be regarded as a composite particle of holon and spinon, together with a nonlocal string field which is caused by the domain-wall effects carried by the other holes from its left-hand side. We see from (4.25) that each of the other holes contributes a $\pm\pi/2$ phase to such a string field. The effects of this string field will be discussed in the next section.

So one finds an analytical description of the charge and spin separation in the 1D strong-coupling Hubbard model. The physics in the strong-coupling regime $J \ll t$ is well established, based on the charge-spin separation at $U = \infty$, which suggests the existence of a $U = \infty$ ($J = +0$) fixed point of the Hubbard model. We note that the meaning of the decoupling of the charge and spin is different in the two limits: weak coupling and strong coupling. In the weak-coupling regime, the electron is usually written as the sum of the right-moving part and left-moving part.³³ For each part, one may define its charge and spin components. The renormalization group analysis¹⁷ in the weak-coupling regime shows the decoupling of these charge and spin components. However, on the whole, one still sees that the left-moving (right-moving) charge excitation is always accompanied by the

and

$$(-1)^{\sum_{m>i}' d_m^\dagger d_m (x'_L - x'_m/a)} = (-1)^{\sum_{m>i}' d_{mB}^\dagger d_{mB}}. \quad (4.22)$$

Notice that the total number of the $A(B)$ solitons is not conserved but it is either even or odd which is conserved. Thus one can replace $\sum_{m>i}' d_{mB}^\dagger d_{mB}$ in (4.22) by $\sum_{m\leq i}' d_{mB}^\dagger d_{mB}$. Finally $h_i^\dagger b_{i\sigma}$ in (4.20) is reduced to the form

$$h_i^\dagger b_{i\sigma} = h_i^\dagger [\theta(\tilde{p}_i)(\tilde{d}_{iA}^\dagger + \tilde{d}_{iA}) + i\theta(-\tilde{p}_i)(\tilde{d}_{iB}^\dagger + \tilde{d}_{iB})] \\ \times \frac{1 + \sigma(-1)^{N_{iA} + N_{iB}}}{2}. \quad (4.23)$$

Here $\tilde{d}_\alpha$ ($\alpha = A, B$) is defined as

$$\tilde{d}_\alpha = d_\alpha (-1)^{\sum_{m<i}' d_{m\alpha}^\dagger d_{m\alpha}}, \quad (4.24)$$

Recalling the Jordan-Wigner transformation (3.15), one finds that now $\tilde{d}_\alpha$ is formally a hard-core bosonic form of the fermion d_α . But one needs to be careful in taking it as an “operator” since d_α here just describes a local spinon excitation above the ground state, not a real operator in the whole Hilbert space. It is noted that the left phase factor $(-1)^{\sum_{d^<} d}$ appearing in (4.23) will contribute an additional power-law decay in calculating the asymptotic Green's function. Since we are interesting in the leading contribution in the present context, we may neglect this phase factor for simplicity. Therefore, in terms of (4.17), (4.18), and (4.23), we obtain

left-moving (right-moving) spin excitation with different velocities, even though there is a mixture of left- and right-moving parts in the charge channel due to the forward scattering.²² On the other hand, in the strong-coupling case, the charge and spin degrees of freedom are completely separated according to (4.25). The electron (hole) will then decay into two excitations, i.e., holon and spinon, which carry different quantum numbers and move independently.

V. CORRELATION FUNCTIONS

Based on the previous formulation of large- U Hubbard model, various correlation functions will be derived in this section.

A. The spin-spin correlation function

The spin operator S_i is found in the large- U limit by

$$S_i = (1 - h_i^\dagger h_i) \sum_{\sigma} \theta(p_i \sigma) \left[U_i^\dagger \frac{\hat{\sigma}}{2} U_i \right]_{\sigma\sigma}, \quad (5.1)$$

according to (2.15) and (2.29). The spin-spin correlation function is then given by

$$\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle = \frac{p_i p_j}{16} \langle \text{Tr}[\hat{\sigma}_z U_i^\dagger(t) \hat{\sigma} U_i(t)] \text{Tr}[\hat{\sigma}_z U_j^\dagger(0) \hat{\sigma} U_j(0)] h_i(t) h_i^\dagger(t) h_j(0) h_j^\dagger(0) \rangle. \quad (5.2)$$

In obtaining (5.2), the equality $\text{Tr}(U^\dagger \hat{\sigma} U) = \text{Tr}(\hat{\sigma}) = 0$ has been used. By employing the expression (4.5) for U_i and the charge-spin separation condition, the right-hand side of (5.2) can be rewritten as

$$\frac{1}{16} (-1)^{(x_i - x_j)/\tilde{a}} \langle \text{Tr}[\tilde{U}_i(t) \hat{\sigma}_z \tilde{U}_i^\dagger(t) \hat{\sigma}] \text{Tr}[U_j(0) \hat{\sigma}_z \tilde{U}_j^\dagger(0) \hat{\sigma}] \rangle \langle h_i(t) h_i^\dagger(t) (-1)^{\sum_{l < i} h_l^\dagger(t) h_l(t)} (-1)^{\sum_{l < j} h_l^\dagger(0) h_l(0)} h_j(0) h_j^\dagger(0) \rangle.$$

Notice that the first average just represents the spin-spin correlation on the effective (squeezed) Heisenberg chain with an enlarged lattice constant $\tilde{a} = a/(1-\delta)$. We shall denote it by $\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle_s$. In the second average, one may write $h_i h_i^\dagger = 1 - \delta_{\pm} h_i^\dagger h_i$: in which the fluctuation part $h_i^\dagger h_i$ could be shown to contribute to a higher-order term in the asymptotic behavior of $\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle$. Neglecting such a higher-order correction, the spin-spin correlation is simplified to

$$\begin{aligned} \langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle &= (1-\delta)^2 \langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle_s \\ &\times \langle (-1)^{\sum_{l < i} h_l^\dagger(t) h_l(t)} (-1)^{\sum_{l < j} h_l^\dagger(0) h_l(0)} \rangle. \end{aligned} \quad (5.3)$$

The spin-spin correlation $\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle_s$ on the squeezed Heisenberg chain has already been found by (3.34) with a replaced by $\tilde{a}$. Thus we shall only consider the average on the holon part in (5.3). As the holon is a free spinless fermion as discussed in Sec. IV, we may use the bosonization technique to calculate the asymptotic average in (5.3). According to the discussion in Appendix D, we first linearize the holon spectrum near the Fermi surface and write the holon operator h by the right- and left-moving operators ψ_R, ψ_L . Then by using the expression³³

$$\sum_{l < i} h_l^\dagger h_l \approx \int_{-\infty}^{x_i} dx : \psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L :$$

the following asymptotic behavior is obtained

$$\begin{aligned} \langle \delta \rho_i(t) \delta \rho_j(0) \rangle &= \langle h_i(t) h_j^\dagger(0) \rangle \langle h_i^\dagger(t) h_j(0) \rangle \\ &\sim -\frac{1}{4\pi^2} \left[\frac{1}{(x + v_h t)^2} + \frac{1}{(x - v_h t)^2} \right] + \frac{1}{2\pi^2} \frac{\cos 4k_f x}{x^2 - v_h^2 t^2} \end{aligned} \quad (5.7)$$

In (5.7), the absence of $2k_f$ oscillation is distinct from the bosonization approach of 1D Hubbard model where both holon and spinon will contribute to a leading $2k_f$ oscillation term.^{19,20}

C. Single-electron Green's function

Another important quantity is the electron Green's function $G_{\sigma\sigma'}^e(x, t) = -i \langle T c_{i\sigma}(t) c_{j\sigma'}^\dagger(0) \rangle$. The bare electron operator $c_{i\sigma}$ has been expressed through the holon and spinon operators by (4.25). The decoupling between the holon and spinon, G^e is simply a product of the charge and spin parts as follows:

$$G_{\sigma\sigma'}^e(x, t) = \frac{\delta_{\sigma, \sigma'}}{8} \langle T [\tilde{d}_i^\dagger(t) + \tilde{d}_i(t)] [\tilde{d}_j(0) + \tilde{d}_j^\dagger(0)] \rangle [e^{i(\pi/2a)x} G^{1/2}(x, t) + e^{-i(\pi/2a)x} G^{-1/2}(x, t)], \quad (5.8)$$

where in the spinon part, we have dropped the superscripts A and B since there is no difference between their averages. For $\sigma = -\sigma'$, the holon part will be found to be giving a vanishing contribution as the string field factors extend to the infinite boundary. Therefore, $G_{\sigma\sigma'}^e = \delta_{\sigma, \sigma'} G^e$ as shown in (5.8).

$$\langle (-1)^{\sum_{l < i} h_l^\dagger(t) h_l(t)} (-1)^{\sum_{l < j} h_l^\dagger(0) h_l(0)} \rangle \sim \frac{1}{(x^2 - v_h^2 t^2)^{1/4}}, \quad (5.4)$$

with $x = x_i - x_j$. Therefore, in terms of (5.3), (5.4), and (3.34), the spin-spin correlation function is finally found to be

$$\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(0) \rangle \sim \frac{\cos(2k_f x)}{(x^2 - v_h^2 t^2)^{1/4} (x^2 - v_s^2 t^2)^{1/2}}, \quad (5.5)$$

where the electron Fermi momentum k_f is defined by $k_f = \pi/2a(1-\delta)$. The incommensurate $2k_f$ oscillation is contributed by the squeezed spin chain. This $2k_f$ behavior of the spin-correlation function has also been obtained by other methods.^{16, 18-22}

B. The density-density correlation function

The density-density correlation is more easy to derive since the spinon makes no contribution. Notice that

$$\rho_i = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} = \sum_{\sigma} a_{i\sigma}^\dagger a_{i\sigma} = 1 - h_i^\dagger h_i \quad (U \rightarrow \infty). \quad (5.6)$$

The correlation function of $\delta \rho_i = \rho_i - \langle \rho_i \rangle$ is then found by

The holon's contribution is represented in (5.8) by the "semion" Green's function

$$G^\theta(x, t) = i \langle T \tilde{h}_j^\theta(0) \tilde{h}_i^{\theta\dagger}(t) \rangle, \quad (5.9)$$

with $\theta = \pm \frac{1}{2}$. We call G^θ as "semion" Green's function because $\tilde{h}_i^\theta$ is defined by

$$\tilde{h}_i^\theta = \tilde{h}_i \exp \left[-i\pi\theta \sum_{l < i} \tilde{h}_l^\dagger \tilde{h}_l \right], \quad (5.10)$$

where $\tilde{h}_i = h_i e^{i(\pi/2a)x_i}$ is introduced in Sec. IV. Equation (5.10) is formally similar to the Jordan-Wigner transformation³¹ [see, e.g., (3.15)] except now $\theta = \pm \frac{1}{2}$ instead of ± 1 . However, $\tilde{h}_i^\theta(t)$ and $\tilde{h}_j^\theta(0)$ in (5.9) should not be involved in each other's string fields, which keep the fermionic property of the electron. The nonlocal string field in (5.10) induced by the domain-wall effects from other holes will be crucial in determining the asymptotic exponents of the Green's function as well as the "Fermi surface" in the large- U limit. A straightforward bosonization calculation of G^θ in (5.9) gives (see Appendix D)

$$G^\theta(x, t) = \sum_{p=\pm 1} e^{-ix(p-\theta)\delta\pi/a} \frac{|x - pv_h t|^{p\theta}}{[p(x - pv_h t) + i0^+ \text{sgn}(t)](x^2 - v_h^2 t^2)^{1/6}}. \quad (5.11)$$

On the other hand, the spinon part $\langle T(\tilde{d}_i^\dagger + \tilde{d}_i)(\tilde{d}_j + \tilde{d}_j^\dagger) \rangle$ has already been discussed in Sec. III. By using the transformation (4.24) to go back to the fermion d , and by introducing the spin degree of freedom to d , its leading asymptotic form is found to be [similar to the procedure to get (3.33)]

$$\langle T[\tilde{d}_i^\dagger(t) + \tilde{d}_i(t)][\tilde{d}_j(0) + \tilde{d}_j^\dagger(0)] \rangle \propto \left[\frac{1}{x^2 - v_s^2 t^2} \right]^{1/4}. \quad (5.12)$$

Combining the above results, we obtain the electron Green's function

$$G_{\sigma\sigma'}^e(x, t) \propto \frac{\delta_{\sigma\sigma'}}{(x^2 - v_s^2 t^2)^{1/4} (x^2 - v_h^2 t^2)^{1/6}} \left[\frac{e^{ik_f x}}{(x - v_h t)^{1/2}} + \frac{e^{i3k_f x}}{(x - v_h t)^{3/2}} - (t \rightarrow -t; k_f \rightarrow -k_f) \right]. \quad (5.13)$$

G^e in (5.13) shows k_f and $3k_f$ oscillations which implies the singularities in the momentum space. The momentum distribution $n(k) = -i \int dx e^{-ikx} G(x, 0^-)$ could be obtained according to (5.13) [in order to determine the correct analytic properties of G^e , we need to keep G^θ in its original form (D16), taking the continuum limit $a \rightarrow 0$ at last]. The singular behavior of $n(k)$ near $k \sim k_f$ is found by

$$n(k) \sim n(k_f) - C |k - k_f|^{1/8} \text{sgn}(k - k_f), \quad (5.14)$$

and near $k \sim 3k_f$ the power-law singularity becomes $|k - 3k_f|^{9/8}$. Hence, the ground state of the 1D strong-coupling Hubbard model shows the Luttinger liquid behavior without a finite jump at k_f .

The asymptotic form (5.13) of the Green's function is basically in agreement with the result of Anderson and Ren's phase-shift analysis²⁰ based on Lieb and Wu solution and the bosonization description. In fact, we may identify the nonlocal string field appearing in (5.10) with the "phase shift" of Ref. 20. But in the present approach, such a $\pi/2$ phase shift field will be responsible to both the asymptotic exponents of the Green's function as well as the k_f and $3k_f$ singularities. And the spinon part is totally separated from the holon part. As a result, the spinon contributes a factor $(x^2 - v_s^2 t^2)^{-1/4}$ in (5.13) instead of $(x \pm v_s t)^{-1/2}$ as obtained in the bosonization method.^{20,21} The recent numerical calculation¹⁶ from the Lieb-Wu solution as well as the bosonization methods^{20,21} have reached essentially the same result of (5.14) for the momentum distribution of electrons.

D. Pair susceptibility

For simplicity, we shall assume that two holes are created at the neighboring sites, although the general case could be similarly discussed. Define the singlet pair operator

$$B_i^s = 1/\sqrt{2} (c_{i\uparrow} c_{i+1\downarrow} - c_{i\downarrow} c_{i+1\uparrow}), \quad (5.15)$$

and the triplet pairing

$$B_i^t = 1/\sqrt{2} (c_{i\uparrow} c_{i+1\downarrow} + c_{i\downarrow} c_{i+1\uparrow}). \quad (5.16)$$

First we note that one may not directly use $c_{i\sigma}$'s expression (4.25) to get B_i^s and B_i^t because c_i and c_{i+1} are not in the same Hilbert space for spinon. A simple way is to directly write down B_i^s and B_i^t in the holon and spinon representation just as we have done for single electron $c_{i\sigma}$ in Sec. IV. By using (4.17) and (4.18), we obtain

$$B_i^s = \tilde{h}_i^\dagger \tilde{h}_{i+1}^\dagger \frac{1}{\sqrt{2}} \left[\sum_{\sigma} b_{i\sigma} b_{i+1\sigma} \right], \quad (5.17a)$$

$$B_i^t = \tilde{h}_i^\dagger \tilde{h}_{i+1}^\dagger \frac{\tilde{p}_i}{\sqrt{2}} \left[\sum_{\sigma} \sigma b_{i\sigma} b_{i+1\sigma} \right], \quad (5.17b)$$

where $\tilde{p}_i$ is defined by (4.8).

Simultaneously annihilating two spins at sites i and $i+1$ in (5.17) by $b_{i\sigma} b_{i+1\sigma}$ will not produce soliton excitations in the resulting squeezed spin chain (two successive 180° rotations are just like the annihilation of a pair of solitons). But there is still a nonlocal phase shift induced by the creation of two holes as $\tilde{U}_j \rightarrow \tilde{U}_j(i\sigma_x)^2 = -\tilde{U}_j$ for

$j > i + 1$. This means $b_{j\sigma} \rightarrow -b_{j\sigma}$ at $j > i + 1$, which will contribute a phase factor

$$\prod'_{j>i+1} (-1) = (-1)^{[N-(i+1)-(n_h - \sum_{l<i} h_l^\dagger h_l)]} \\ = -(-1)^{N-n_h} \tilde{p}_i.$$

Again one may choose N and n_h as even for simplicity, as in Sec. IV C. Similar to (4.20), $b_{i\sigma}$ could be replaced by the projective operator $\frac{1}{2}[1 + \sigma(-1)^{N_{iA}+N_{iB}}]$ with $N_{i\alpha} = \sum'_{m<i} d_{m\alpha}^\dagger d_{m\alpha}$ and we find that the leading terms of (5.17) are given by

$$B_i^s \approx \frac{\tilde{p}_i}{\sqrt{2}} \tilde{h}_i^\dagger \tilde{h}_{i+1}^\dagger, \quad (5.18a)$$

$$B_i^t \approx \frac{1}{\sqrt{2}} \tilde{h}_i^\dagger \tilde{h}_{i+1}^\dagger (-1)^{N_{iA}+N_{iB}}. \quad (5.18b)$$

It is straightforward to calculate the asymptotic behaviors in the singlet channel

$$\langle B_i^{s\dagger} B_j^s \rangle \propto \frac{\cos(2k_f x)}{x^{2.5}}, \quad (5.19a)$$

and the triplet channel

$$\langle B_i^{t\dagger} B_j^t \rangle \propto \frac{1 - \cos(4k_f a)}{x^3}. \quad (5.19b)$$

Physically, a doped hole decays into a mobile holon and a spinon, as discussed in Sec. IV. For a singlet pair of doped holes, the two spinons accompanying the holons will annihilate each other, leaving only a pair of holons on the Hubbard chain as (5.18a) shows, while in the triplet channel, there is still a phase shift contributed by the spinon. According to (5.19a) and (5.19b), one could see that a pair of holes becomes easier to propagate in the singlet channel than in the triplet channel. A similar situation in the two-dimensional case has been discussed in Ref. 12 where it has been argued that a true singlet superconducting condensation will become possible after the interlayer coupling is introduced.

VI. SUMMARY AND CONCLUSIONS

We have systematically studied the 1D Hubbard model in the strong-coupling regime. Our formulation is equivalent to the t - J model to the order of t/U . But the non-double-occupancy condition is realized by keeping the electrons in the lower Hubbard band. There is no additional constraint appearing in the present method. To be specific, the electron operator is given by $c_i = U_i a_i$ where U_i is the SU(2) transformation describing the spin degree of freedom and a_i is actually a spinless fermion ($h_i^\dagger$) after the upper Hubbard band is projected out. Lack of an explicit constraint between U_i and a_i distinguishes our approach from the slave-fermion method in the t - J model.

In the infinite- U limit, there does exist a coupling between the bare hole and spin background. This coupling is the only available energy scale in this limit which dominates all the physics. As the result of such a coupling,

we found a “phase-shift” in the spin background: $U_i \rightarrow \tilde{U}_i e^{i\tilde{A}_i}$ where $e^{i\tilde{A}_i}$ is a SU(2) transformation induced by the holes with $\tilde{A}_i = (\pi/2) \hat{\sigma}_x \sum_{l<i} h_l^\dagger h_l$. $\tilde{U}_i$ describes the squeezed spin chain (with the removal of all the vacant sites) and is decoupled from the holon. Due to the SU(2) string field $e^{i\tilde{A}_i}$, each holon could be regarded as a “renormalized” hole carrying a domain wall of spins. Such a mobile entity is decoupled from the spin background and is as mobile as a spinless fermion in the Nagaoka ferromagnetic state. This is the meaning of the charge and spin separation in the infinite- U limit. On the other hand, the physical electron (hole), though described by the fermionic operator c_i , behaves like a “semion” due to the presence of the nonlocal string field $e^{i\tilde{A}_i}$, in resembling a generalized Jordan-Wigner transformation.

In the case of finite J , we have shown that the charge and spin separation is still a very good approximation as long as $J \ll t$. This suggests a $J = +0$ fixed point for the large- U Hubbard model. With the finite J , the degeneracy of the squeezed spin chain is lifted up and it behaves just like a Heisenberg chain with an enlarged lattice constant and a doping-dependent superexchange coupling. This doping dependence agrees with the exact solution in the whole doping regime.

We have solved the (squeezed) Heisenberg chain by introducing the soliton representation in which the usual constraint problem has been avoided. These solitons are the 180° domain walls which are the defects of the Néel order with a displacement of two sublattices on their right-hand (left-hand) side chain. The mean-field ground-state energy and excitation spectrum are found to be quite close to the exact results. The ground state is a BCS-like condensation of paired solitons excited from the Néel vacuum. These Cooper-like pairs of solitons could be far apart so that the pair-breaking excitations have a gapless spectrum. The x^{-1} behavior of the spin-correlation is also obtained for the Heisenberg chain.

Finally, we have analytically calculated the spin-spin, density-density correlations, the single-electron Green's function, as well as the pair susceptibility. Many of our results are in agreement with those obtained by the bosonization methods, such as the spin-correlation function and the power-law singularities of the momentum distribution at k_f and $3k_f$, etc. However, there are some remarkable distinctions. For example, we do not find any $2k_f$ oscillation in the density-density correlation function whereas it appears as the leading term in the bosonization solution. The time-dependent Green's function also shows some distinction. We note that these differences may be related to the spin and charge separation which have different meanings in the strong-coupling regime and the weak-coupling regime.

Although the present derivation may not be directly generalized to the 2D Hubbard model, we have learned some important lessons from the present study of the 1D model. In the strong-coupling regime $J \ll t$, the hopping energy t is crucial and should be fully respected, which actually dominates the long-wavelength behaviors in 1D case. $U(1)$ gauge theory⁹ is oversimplified in this case. In order to gain the hopping energy, the local spins

around the hole have to be twisted such that the amplitude part (spiral field), in contrast to the $U(1)$ phase, may play an important role in 2D, as it does in the 1D model. A theory of the dynamical spiral field has been proposed for 2D in Ref. 12. More efforts are needed to clarify whether there is still a charge and spin separation in 2D case. As in the 1D model, the existence of a $U=\infty$ ($J=+0$) fixed point for the 2D Hubbard model would make a perturbative approximation possible in the strong-coupling regime.

The present approach could be straightforwardly generalized to finite temperature.

ACKNOWLEDGMENTS

The authors would like to thank P. W. Anderson, L. Y. Chen, F. D. M. Haldane, G. Levine, T. K. Lee, J. R. Schrieffer, X. G. Wen, J. H. Xu and J. Yu for helpful discussions. The present work is supported by a grant from the Robert A. Welch Foundation and also by the Texas Center for Superconductivity at the University of Houston under the Prime Grant No. MDA-972-88-G-0002 from the Defense Advanced Research Project Agency.

APPENDIX A: DERIVATION OF EQ. (2.32)

We shall present a derivation of the Lagrangian (2.32) in a t/U expansion in this Appendix. The total Lagrangian $\mathcal{L}=\mathcal{L}_0+\mathcal{L}_n$. According to (2.30), $\mathcal{L}_0$ is given by

$$\mathcal{L}_0 = \sum_i (\alpha_i^\dagger \partial_\tau \alpha_i + \beta_i^\dagger \partial_\tau \beta_i) - \frac{J}{2} \sum_i (\alpha_i^\dagger \alpha_{i+2} - \beta_i^\dagger \beta_{i+2} + \text{H.c.}) - J \sum_i \alpha_i^\dagger \alpha_i + (U+J) \sum_i \beta_i^\dagger \beta_i. \quad (\text{A1})$$

In the representation of the spinless fermions α_i and β_i , $a_{i\sigma}$ is determined by Eq. (2.29) in the t/U expansion. $\mathcal{L}_n$ in (2.22) can be written by α_i and β_i to t/U order as follows:

$$\begin{aligned} \mathcal{L}_n = & \sum_{i\sigma} (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} [\theta(p_i\sigma) p h \alpha_i^\dagger \alpha_i + \theta(-p_i\sigma) \beta_i^\dagger \beta_i] + \sum_{i\sigma} p_i (U_i^\dagger \partial_\tau U_i)_{\sigma-\sigma} [\theta(p_i\sigma) \alpha_i^\dagger \beta_i + \theta(-p_i\sigma) \beta_i^\dagger \alpha_i] \\ & + \frac{t}{U} \sum_{i\sigma} (U_i^\dagger \partial_\tau U_i)_{\sigma-\sigma} \{ \theta(p_i\sigma) \alpha_i^\dagger (\alpha_{i+1} + \alpha_{i-1}) + \theta(-p_i\sigma) (\alpha_{i+1}^\dagger + \alpha_{i-1}^\dagger) \alpha_i \} \\ & - t \sum_{i\sigma} \{ (U_i^\dagger U_{i+1})_{\sigma-\sigma} [\theta(p_i\sigma) \alpha_i^\dagger \alpha_{i+1} - \theta(-p_i\sigma) \beta_i^\dagger \beta_{i+1}] + \text{H.c.} \} \\ & - \frac{t^2}{U} \sum_{i\sigma} \{ (U_i^\dagger U_{i+1} - 1)_{\sigma\sigma} [\theta(p_i\sigma) \alpha_i^\dagger (\alpha_{i+2} + \alpha_i) + \theta(-p_i\sigma) (\alpha_{i+1}^\dagger + \alpha_{i-1}^\dagger) \alpha_{i+1}] + \text{H.c.} \} \\ & - t \sum_{i\sigma} \{ p_i (U_i^\dagger U_{i+1} - 1)_{\sigma\sigma} [\theta(-p_i\sigma) \beta_i^\dagger \alpha_{i+1} - \theta(p_i\sigma) \alpha_i^\dagger \beta_{i+1}] + \text{H.c.} \} + O(t^2/U^2). \end{aligned} \quad (\text{A2})$$

The second term on the right-hand side of (A2) involves the interband transition, which give the order of t/U . In the long-wavelength limit, such a term is reduced to $\sim J/t^2(\partial_\tau \Omega)^2$, which will lead to a correction of order $\sim J^3$ to the spin-wave velocity in the nonlinear σ model (Appendix B). Thus it is neglected in our t/U expansion to the first order of t/U . The last term is also related to the interband transition. One needs to integrate out the upper- β band to get its contribution. As the β band has a dominant large energy scale U as shown by the last term of (A1), to the order of t/U it is easy to perform such a integration, and it gives

$$- \frac{t^2}{U} \sum_{i\sigma} \theta(-p_i\sigma) [(U_{i+1}^\dagger U_i - 1)_{\sigma\sigma} \alpha_{i+1}^\dagger + (U_{i-1}^\dagger U_i - 1)_{\sigma\sigma} \alpha_{i-1}^\dagger] [(U_i^\dagger U_{i+1} - 1)_{\sigma\sigma} \alpha_{i+1} + (U_i^\dagger U_{i-1} - 1)_{\sigma\sigma} \alpha_{i-1}]. \quad (\text{A3})$$

It is noted that the process of the interband transition may violate the constraint (2.31), i.e., $(1 - \alpha_i^\dagger \alpha_i) \beta_i^\dagger \beta_i = 0$. That is, when there is a hole at site i , the virtual process creating $\beta_i^\dagger \alpha_{i\pm 1}$ would be forbidden by Eq. (2.31). Such a constraint could be included in (A3) by adding (multiplying) a factor $\alpha_i^\dagger \alpha_i$ in (A3). We shall drop it for simplicity as it brings only negligible polaron effect associated with the hole in order of J .

Finally, the Lagrangian $\mathcal{L}=\mathcal{L}_0+\mathcal{L}_n$ is reduced to the following form after projecting out the high-energy β band:

$$\begin{aligned} \mathcal{L} = & \sum_i \alpha_i^\dagger \partial_\tau \alpha_i + \sum_{i\sigma} \theta(p_i\sigma) (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} \alpha_i^\dagger \alpha_i - t \sum_{i\sigma} [\theta(p_i\sigma) (U_i^\dagger U_{i+1})_{\sigma-\sigma} \alpha_i^\dagger \alpha_{i+1} + \text{H.c.}] \\ & - \frac{J}{2} \sum_{i\sigma} \theta(p_i\sigma) [|(U_i^\dagger U_{i+1})_{\sigma\sigma}|^2 + |(U_i^\dagger U_{i-1})_{\sigma\sigma}|^2] \alpha_i^\dagger \alpha_i - \frac{J}{2} \sum_{i\sigma} \theta(-p_i\sigma) [(U_{i+1}^\dagger U_i)_{\sigma\sigma} (U_i^\dagger U_{i-1})_{\sigma\sigma} \alpha_{i+1}^\dagger \alpha_{i-1} + \text{H.c.}] \\ & + \frac{J}{2t} \sum_{i\sigma} (U_i^\dagger \partial_\tau U_i)_{\sigma-\sigma} [\theta(p_i\sigma) \alpha_i^\dagger (\alpha_{i+1} + \alpha_{i-1}) + \theta(-p_i\sigma) (\alpha_{i+1}^\dagger + \alpha_{i-1}^\dagger) \alpha_i] + O(t^2/U^2). \end{aligned} \quad (\text{A4})$$

APPENDIX B: NONLINEAR σ MODEL WITH THE TOPOLOGICAL TERM

As U_i is related to the spin polarization direction $\mathbf{n}_i$, the derivation of the nonlinear σ model from the Lagrangian (3.1) is straightforward.

U_i is defined as a SU(2) rotation from the z axis to the spin $\mathbf{n}$ direction by Eq. (2.16). So far we have not yet given a specific form of U_i in terms of $\mathbf{n}_i$ because of its U(1) freedom. Here we may choose

$$U_i = \exp[-i\frac{1}{2}\hat{\sigma} \cdot (\mathbf{z} \wedge \mathbf{n}_i)\theta_i] \quad (\text{B1})$$

where $\mathbf{z} \wedge \mathbf{n}_i \equiv (\mathbf{z} \times \mathbf{n}_i)/|\mathbf{z} \times \mathbf{n}_i|$ and θ_i is the polar angle of $\mathbf{n}_i$. In terms of (B1), a direct calculation gives

$$(U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} = i\frac{1}{2}\sigma \mathbf{A}(\mathbf{n}_i) \cdot \partial_\tau \mathbf{n}_i \quad (\text{B2})$$

in which $\mathbf{A}(\mathbf{n}_i)$ is found to be

$$\mathbf{A}(\mathbf{n}_i) = \frac{1 - \cos\theta_i}{\sin\theta_i} (\mathbf{z} \wedge \mathbf{n}_i). \quad (\text{B3})$$

Substituting Eq. (B2) into the first term of (3.1), under the integral over the imaginary time, we get the familiar Berry phase which has been discussed by Haldane.²⁷ We follow Haldane²⁷ to separate the long-wavelength part and short-wavelength part of $\mathbf{n}_i$ by assuming

$$\mathbf{n}_i \approx \mathbf{\Omega}_i + (-1)^i \mathbf{L}_i, \quad (\text{B4})$$

where both $\mathbf{\Omega}_i$ and $\mathbf{L}_i$ are slowly varying fields on the lattice satisfying $\mathbf{L}_i \cdot \mathbf{\Omega}_i = 0$, $|\mathbf{L}_i| \ll 1$ and $|\mathbf{\Omega}_i| \approx 1$. According to the definition of $\mathbf{n}_i$, $\mathbf{\Omega}_i$ actually describes the staggered magnetization direction and $\mathbf{L}_i$ is a ferromagnetic component deviating from the local Néel state. To the lowest order of $\mathbf{L}_i$ and $\partial_\tau \mathbf{\Omega}_i$, we find

$$\begin{aligned} \int_0^\beta d\tau \sum_{i\sigma} \theta(p_i\sigma) (U_i^\dagger \partial_\tau U_i)_{\sigma\sigma} &= \frac{i}{2} \int_0^\beta d\tau \sum_i p_i \mathbf{A}(\mathbf{n}_i) \cdot \partial_\tau \mathbf{n}_i \\ &= \frac{i}{2} \sum_i p_i \omega_i - \frac{i}{2} \sum_i \int_0^\beta d\tau \mathbf{\Omega}_i \cdot (\partial_\tau \mathbf{\Omega}_i \times \mathbf{L}_i), \end{aligned} \quad (\text{B5})$$

where

$$\omega_i \equiv \int_0^\beta d\tau \mathbf{A}(\mathbf{\Omega}_i) \cdot \partial_\tau \mathbf{\Omega}_i \quad (\text{B6})$$

is the solid angle subtended by the closed path on the sphere defined by the time evolution of $\mathbf{\Omega}_i(\tau)$. The first term in Eq. (B5) is the topological term which in the continuum limit could be written as $(i/4) \int dx d\tau \mathbf{\Omega} \cdot \partial_x \mathbf{\Omega} \times \partial_\tau \mathbf{\Omega}$.⁹

In terms of Ref. 36, one has the identity

$$\begin{aligned} (U_i^\dagger U_{i+1})_{\sigma\sigma} &= \exp \left[i \frac{\sigma}{2} \int_{\mathbf{n}_i}^{\mathbf{n}_{i+1}} \mathbf{A}(\mathbf{n}) \cdot d\mathbf{n} \right] \\ &\times \left[\frac{1 + \mathbf{n}_i \cdot \mathbf{n}_{i+1}}{2} \right]^{1/2}. \end{aligned} \quad (\text{B7})$$

By the assumption followed in Eq. (B4), to the order of quadratic $\mathbf{L}_i$, the second term in the Lagrangian (3.1) is reduced to

$$\begin{aligned} -\frac{J}{2} \sum_{i\sigma} |(U_i^\dagger U_{i+1})_{\sigma\sigma}|^2 &= -\frac{J}{2} \sum_i (\mathbf{n}_i \cdot \mathbf{n}_{i+1} + 1) \\ &\approx \frac{J}{4} \sum_i [(a \partial_x \mathbf{\Omega}_i)^2 + 4\mathbf{L}_i^2] - JN. \end{aligned} \quad (\text{B8})$$

In obtaining the last line, the slowly varying condition for both $\mathbf{\Omega}_i$ and $\mathbf{L}_i$ fields has been used such that the cross

term $\sum_i (-1)^i \nabla \mathbf{\Omega}_i \cdot \mathbf{L}_i$ is neglected.

Finally, after integrating out $\mathbf{L}_i$, one gets the standard form

$$\begin{aligned} S &\equiv \int_0^\beta d\tau \mathcal{L}_s \\ &= \frac{i}{2} \sum_i p_i \omega_i + \frac{1}{2} \int_0^\beta d\tau \int dx \left[\frac{\rho}{c^2} (\partial_\tau \mathbf{\Omega})^2 \right. \\ &\quad \left. + \rho (\partial_x \mathbf{\Omega})^2 \right] - \beta JN, \end{aligned} \quad (\text{B9})$$

where $\rho = J/2a$ and $c = 2Ja$.

APPENDIX C: THE MEAN-FIELD DIAGONALIZATION OF H_s IN (3.10)

We decouple the coupling between A and B solitons in (3.10) by the mean-field approximation

$$\begin{aligned} d_{lA}^\dagger d_{l+2A} (1 - d_{lB}^\dagger d_{lB}) &\approx d_{lA}^\dagger d_{l+2A} (1 - \bar{n}_B) \\ &\quad - \Delta_A^1 d_{lB}^\dagger d_{lB} + \Delta_A^1 \bar{n}_B, \end{aligned} \quad (\text{C1a})$$

$$\begin{aligned} d_{lA}^\dagger d_{l+2A}^\dagger (1 - d_{lB}^\dagger d_{lB}) &\approx d_{lA}^\dagger d_{l+2A}^\dagger (1 - \bar{n}_B) \\ &\quad - \Delta_A^2 d_{lB}^\dagger d_{lB} + \Delta_A^2 \bar{n}_B, \end{aligned} \quad (\text{C1b})$$

where

$$n_B = \langle d_{lB}^\dagger d_{lB} \rangle, \quad (C2a)$$

$$\Delta_A^1 = \langle d_{lA}^\dagger d_{l+2A} \rangle, \quad (C2b)$$

$$\Delta_A^2 = \langle d_{lA}^\dagger d_{l+2A}^\dagger \rangle. \quad (C2c)$$

There are similar terms for $A \leftrightarrow B$. As the symmetry between A and B solitons, we assume $\bar{n}_A = \bar{n}_B = \bar{n}$, $\Delta_A^1 = \Delta_B^1 = \Delta_1$, $\Delta_A^2 = \Delta_B^2 = \Delta_2$. Then the Hamiltonian H_s is simplified as

$$H_s = -J_1 \sum_{l\alpha}' (d_{l\alpha}^\dagger d_{l+2\alpha} + d_{l\alpha}^\dagger d_{l+2\alpha}^\dagger + \text{H.c.}) + J_2 \sum_{l\alpha}' d_{l\alpha}^\dagger d_{l\alpha} - JN - 2J\bar{n}(\Delta_1 + \Delta_2)N, \quad (C3)$$

where

$$J_1 = J(1 - \bar{n}), \quad (C4a)$$

$$J_2 = J[1 + 2(\Delta_1 + \Delta_2)]. \quad (C4b)$$

We write (C3) in the momentum space

$$H_s = \sum_{k\alpha}' [(J_2 - 2J_1 \cos 2ka) d_{k\alpha}^\dagger d_{k\alpha} - iJ_1 \sin 2ka (d_{k\alpha}^\dagger d_{-k\alpha}^\dagger - d_{-k\alpha} d_{k\alpha})] - JN - 2J\bar{n}(\Delta_1 + \Delta_2)N, \quad (C5)$$

where $|k| \leq \pi/2a$. Equation (C5) is easily diagonalized through the Bogoliubov transformation

$$d_k = u_k \bar{d}_k + i v_k \bar{d}_{-k}^\dagger, \quad (C6)$$

where

$$u_k = \left[\frac{1}{2} \left(1 + \frac{J_2 - 2J_1 \cos 2ka}{\epsilon_k^s} \right) \right]^{1/2}, \quad (C7a)$$

$$v_k = \left[\frac{1}{2} \left(1 - \frac{J_2 - 2J_1 \cos 2ka}{\epsilon_k^s} \right) \right]^{1/2} \text{sgn}(k), \quad (C7b)$$

with

$$\epsilon_k^s = [(J_2 - 2J_1 \cos 2ka)^2 + 4J_1^2 \sin^2 2ka]^{1/2}. \quad (C8)$$

Finally, one arrives

$$H_s = \sum_{k\alpha}' \epsilon_k^s \bar{d}_{k\alpha}^\dagger \bar{d}_{k\alpha} + E_0, \quad (C9)$$

in which the ground state energy is given by

$$E_0 = - \sum_k' \epsilon_k^s + [J_2/2 - 2J\bar{n}(\Delta_1 + \Delta_2) - J]N. \quad (C10)$$

The parameters J_1 and J_2 are defined in Eq. (C4) through $\bar{n}$, Δ_1 , and Δ_2 which are determined by the self-consistent condition (C2). Using the canonical transformation (C6), one finds the equations

$$J_1 = \frac{J}{2} \left[1 + \frac{2}{N} \sum_k' \frac{J_2 - 2J_1 \cos 2ka}{\epsilon_k^s} \right], \quad (C11a)$$

$$J_2 = J \left[1 + \frac{2}{N} \sum_k' \frac{2J_1 - J_2 \cos 2ka}{\epsilon_k^s} \right]. \quad (C11b)$$

According to Eqs. (C11a) and (C11b), it is easy to find

$$2J_1 = J_2 \equiv \bar{J} \quad (C12)$$

and

$$\begin{aligned} \bar{J} &= J \left[1 + \frac{2}{N} \sum_k' \frac{1 - \cos 2ka}{\sqrt{(1 - \cos 2ka)^2 + \sin^2 2ka}} \right] \\ &= J \left[1 + \frac{2}{\pi} \right]. \end{aligned} \quad (C13)$$

The quasiparticle excitation spectrum becomes gapless as

$$\epsilon_k^s = \left[1 + \frac{2}{\pi} \right] (2J) |\sin ka|. \quad (C14)$$

The average excited soliton number at each bond is given by

$$\langle d_l^\dagger d_l \rangle = \bar{n} = \frac{1}{2} - \frac{1}{\pi}. \quad (C15)$$

APPENDIX D: BOSONIZATION FOR A FREE SPINLESS FERMION SYSTEM

As the spinon and holon excitations obtained in the context are described by some noninteraction fermions, the bosonization method provides an effective way to rigorously calculate their asymptotic correlations.

Consider the following noninteraction spinless fermion Hamiltonian:

$$H = -\tilde{t} \sum_i (\psi_i^\dagger \psi_{i+1} + \text{H.c.}) = -2\tilde{t} \sum_k \cos(ka) \psi_k^\dagger \psi_k. \quad (D1)$$

The most important low-energy excitations are the particle-hole excitations near the two Fermi points, which determine the long-range correlation of the system.

Following Ref. 33 we may write the spinless fermion operator ψ_i as the sum of the right-moving and left-moving fermion operators:

$$\frac{\psi_i}{\sqrt{a}} \approx e^{-ik_f x_i} \psi_L(x_i) + e^{ik_f x_i} \psi_R(x_i), \quad (D2)$$

where ψ_R and ψ_L are slowly varying on the lattice scale and mainly contain the Fourier modes near $\pm k_f$. ψ_R and ψ_L may be written as

$$\psi_R = \frac{1}{\sqrt{aN}} \sum_{k>0} (e^{ikx} \psi_{k+k_f} + e^{-ikx} \psi_{-k+k_f}), \quad (D3)$$

$$\psi_L = \frac{1}{\sqrt{aN}} \sum_{k<0} (e^{ikx} \psi_{k-k_f} + e^{-ikx} \psi_{-k-k_f}),$$

where ψ_k is defined through

$$\psi_i = \frac{1}{\sqrt{N}} \sum_k e^{ikx_i} \psi_k.$$

In the continuum approximation, the dispersion relation

is linearized near the Fermi points and one gets the continuum Hamiltonian

$$H = -iv \int dx \left[\psi_R^\dagger \frac{d}{dx} \psi_R - \psi_L^\dagger \frac{d}{dx} \psi_L \right], \quad (\text{D4})$$

where $v = 2\tilde{t}a \sin k_f a$ is the Fermi velocity.

It has been shown³³ that ψ_R and ψ_L could be expressed by some boson operators ϕ_R and ϕ_L :

$$\psi_p^\dagger(x) \propto \exp[i\phi_p^\dagger(x)] \exp[i\phi_p(x)], \quad (\text{D5})$$

in which $p = \pm 1$ represents R and L , respectively. The phase field $\phi_p(x)$ satisfies the commutations³³

$$[\phi_p(x), \phi_{p'}(x')] = [\phi_p^\dagger(x), \phi_{p'}^\dagger(x')] = 0, \quad (\text{D6})$$

$$[\phi_p(x), \phi_{p'}^\dagger(x')] = -\delta_{pp'} \lim_{\epsilon \rightarrow 0^+} \ln(1 - e^{-2\epsilon z^{2p}}),$$

where $z = e^{i\pi(x-x')/(aN)}$.

Then by using the relations (D5) and (D6) and the condition that $\phi_p(x)|G\rangle = 0$ in the zero-temperature case ($|G\rangle$ is the ground state), the various correlation functions can be calculated. One may find the following relation useful in the calculation³³

$$\nabla(\phi_p(x) + \phi_p^\dagger(x)) = -2\pi p \rho_p(x), \quad (\text{D7})$$

where $\rho_p(x)$ is the local density operator

$$\rho_p(x) = \psi_p^\dagger(x) \psi_p(x) - \langle \psi_p^\dagger(x) \psi_p(x) \rangle \equiv : \psi_p^\dagger(x) \psi_p(x) :. \quad (\text{D8})$$

As an example, we first calculate the average in (3.32):

$$\langle \exp[i\pi N_i(t)] \exp[-i\pi N_j(0)] \rangle, \quad (\text{D9})$$

where $N_i = \int_{-\infty}^{x_i} dx : \psi_R^\dagger \psi_R + \psi_L^\dagger \psi_L :$.

For the linear dispersion, one finds

$$\begin{aligned} \psi_R(x, t) &= \psi_R(x - v_s t, 0), \\ \psi_L(x, t) &= \psi_L(x + v_s t, 0), \end{aligned} \quad (\text{D10})$$

according to (3.31) or (D4). Therefore, the time-dependent Heisenberg operator $\psi_{R,L}(x, t)$ is expressed by the operator $\psi_p(x_p)$ in the Schrödinger representation with $x_p = x - pv_s t$. Then the relation (D5) and (D6) can be directly used. Thus $N_i(t)$ in (D9) can be rewritten as

$$\begin{aligned} N_i(t) &= \int_{-\infty}^{x_i - v_s t} dx : \psi_R^\dagger \psi_R : + \int_{-\infty}^{x_i + v_s t} dx : \psi_L^\dagger \psi_L : \\ &= -\frac{1}{2\pi} \sum_{p=\pm 1} p [\phi_p(x_i - pv_s t) - \phi_p(-\infty) + \text{H.c.}] \end{aligned} \quad (\text{D11})$$

In the second line, relation (D7) has been used. We then express the operator in (D9) in the normal order of ϕ_p by employing the identities

$$e^A e^B = e^B e^A e^{[A, B]}, \quad e^{A+B} = e^A e^B e^{-1/2[A, B]}$$

and (D6), where $[A, B]$ should commute with both A and B operators. Recalling that $\phi_p|G\rangle = 0$, the right-hand side of (D9) is thus reduced to

$$\propto \lim_{\epsilon \rightarrow 0} \left[\frac{1}{x^2 - [v_s t - i\epsilon \operatorname{sgn}(t)]^2} \right]^{1/4}, \quad (\text{D12})$$

where $x \equiv x_i - x_j$.

A second example is the calculation of the “semion” Green function of $G^\theta(x, t)$ in (5.9) and (5.10):

$$\begin{aligned} G^\theta(x, t) &= i \left\langle T \tilde{h}_j(0) \exp \left[-i\pi\theta \sum_{l < j} n_l^h(0) \right] \right. \\ &\quad \left. \times \exp \left[i\pi\theta \sum_{l < i} n_l^h(t) \right] \tilde{h}_i^\dagger(t) \right\rangle, \end{aligned} \quad (\text{D13})$$

where $n_l^h = \tilde{h}_l^\dagger \tilde{h}_l$.

As discussed in Sec. IV, $\tilde{h}$ describes the free spinless fermion with Fermi momentum $\tilde{k}_f = \pi\delta/a$. Then the $\tilde{h}$ operator could be written as a sum of left and right parts,

$$\tilde{h}_i = \sum_{p=\pm 1} e^{ip\tilde{k}_f x_i} \psi_p(x_i). \quad (\text{D14})$$

As $n_i^h(t) \approx \delta + a \sum_{p=\pm 1} : \psi_p^\dagger(x_i - pv_h t) \psi_p(x_i - pv_h t) :$,^{33,34} $\sum_{l < i} n_l^h(t)$ is expressed in terms of (D7) as follows

$$\sum_{l < i} n_l^h(t) = \delta \int_{-\infty}^{x_i - a} \frac{dx}{a} - \frac{1}{2\pi} \sum_{p=\pm 1} \left[\int_{-\infty}^{x_j - a} + \int_{x_j + a}^{x_i - pv_h t - a} \right] p (\nabla \phi_p + \nabla \phi_p^\dagger) dx, \quad (\text{D15})$$

where $\tilde{h}_j(0)$ has been excluded as noted in the context. Then by a procedure similar to that used in calculating (D9), one obtains

$$G^\theta(x, t) \propto e^{i\pi\theta x \delta / a} \left[\frac{\epsilon^2}{x^2 - [v_h t - i\epsilon \operatorname{sgn}(t)]^2} \right]^{\theta^2/4} \sum_{p=\pm 1} e^{-ip\tilde{k}_f x} \frac{(|x - pv_h t|/a + 1)^{p\theta}}{p(x - pv_h t) + i0^+ \operatorname{sgn}(t)}. \quad (\text{D16})$$

In the continuum limit $x/a \gg 1$, this expression is reduced to the formula (5.11).

*On leave from the Institute of Theoretical Physics, Academia Sinica, Beijing, China.

- ¹P. W. Anderson, *Science* **235**, 1196 (1987); in *Frontiers and Borderlines in Many Particle Physics*, Proceedings of the Enrico Fermi International School of Physics (North-Holland, Amsterdam, 1987).
- ²S. E. Barnes, *J. Phys. F* **6**, 1375 (1976); **7**, 2637 (1977); P. Coleman, *Phys. Rev. B* **29**, 3035 (1984); N. Read and D. Newns, *J. Phys. C* **16**, 3237 (1983).
- ³G. Kotliar and A. E. Ruckenstein, *Phys. Rev. Lett.* **57**, 1362 (1986).
- ⁴P. A. Lee, *Phys. Rev. Lett.* **63**, 680 (1989).
- ⁵H. J. Schulz, *Phys. Rev. Lett.* **65**, 2462 (1990).
- ⁶Z. Y. Weng, C. S. Ting, and T. K. Lee, *Phys. Rev. B* **43**, 3790 (1991).
- ⁷P. B. Wiegmann, *Phys. Rev. Lett.* **60**, 821 (1988).
- ⁸X. G. Wen, *Phys. Rev. B* **39**, 7223 (1989).
- ⁹R. Shankar, *Phys. Rev. Lett.* **63**, 203 (1988); *Nucl. Phys. B* **330**, 433 (1990).
- ¹⁰N. Nagaosa and P. A. Lee, *Phys. Rev. Lett.* **64**, 2450 (1990); L. B. Ioffe and P. B. Wiegmann, *ibid.* **65**, 653 (1990).
- ¹¹B. I. Shraiman and E. D. Siggia, *Phys. Rev. Lett.* **62**, 1564 (1989).
- ¹²Z. Y. Weng, *Phys. Rev. Lett.*, **66**, 2156 (1991).
- ¹³P. W. Anderson (unpublished).
- ¹⁴E. H. Lieb and F. Y. Wu, *Phys. Rev. Lett.* **20**, 1445 (1968).
- ¹⁵C. F. Coll III, *Phys. Rev. B* **9**, 2150 (1975).
- ¹⁶M. Ogata and H. Shiba, *Phys. Rev. B* **41**, 2326 (1990).
- ¹⁷J. Sólyom, *Adv. Phys.* **28**, 201 (1979).
- ¹⁸A. Parola and S. Sorella, *Phys. Rev. Lett.* **64**, 1831 (1990).
- ¹⁹H. J. Schulz, *Phys. Rev. Lett.* **64**, 2831 (1990).
- ²⁰P. W. Anderson and Y. Ren (unpublished).
- ²¹A. M. Tsvelik (unpublished).
- ²²X. G. Wen, *Phys. Rev. B* **42**, 6623 (1990).
- ²³Z. Y. Weng, D. N. Sheng, C. S. Ting, and Z. B. Su, *Phys. Rev. Lett.* **67**, 3318 (1991).
- ²⁴P. W. Anderson, *Int. J. Mod. Phys. B* **4**, 181 (1990).
- ²⁵C. Gros, R. Joynt, and T. M. Rice, *Phys. Rev. B* **36**, 8190 (1987).
- ²⁶See, Z. Y. Weng, T. K. Lee, and C. S. Ting, *Phys. Rev. B* **38**, 6561 (1988).
- ²⁷D. P. Arovas and A. Auerbach, *Phys. Rev. B* **38**, 316 (1988).
- ²⁸F. D. M. Haldane, *Phys. Lett.* **93A**, 464 (1983); *Phys. Rev. Lett.* **50**, 1153 (1983).
- ²⁹J. Des Cloizeaux and J. J. Pearson, *Phys. Rev.* **128**, 2131 (1962).
- ³⁰L. D. Faddeev and L. A. Takhtajan, *Phys. Lett.* **85A**, 375 (1981).
- ³¹E. H. Lieb, T. Schultz, and P. J. Mattis, *Ann. Phys. (N.Y.)* **16**, 407 (1961).
- ³²H. Bethe, *Z. Phys.* **71**, 205 (1931); L. Hulthén, *Arkiv. Mat. Astron. Fys.* **26A**, No. 11 (1938).
- ³³F. D. M. Haldane, *J. Phys. C* **14**, 2585 (1981); I. Affleck, in *Fields, Strings and Critical Phenomena*, edited by E. Bezin and J. Zinn-Justin (North-Holland, Amsterdam 1990).
- ³⁴A. Luther and I. Peschel, *Phys. Rev. B* **12**, 3908 (1975).
- ³⁵D. Schmeltzer, *Phys. Rev. B* **43**, 8650 (1991).
- ³⁶E. Fradkin and M. Stone, *Phys. Rev. B* **38**, 7215 (1988).