One-Dimensional Large-U Hubbard Model: An Analytical Approach

Z. Y. Weng, D. N. Sheng, C. S. Ting, and Z. B. Su [(a)]

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

(Received 5 March 1991)

The basic properties of the Hubbard chain are systematically studied in the large-U regime by a path-integral formalism. The bare electron (hole) is shown to be a composite particle of two basic excitations, holon and spinon, together with the nonlocal string fields. Both holon and spinon are described by fermions with gapless spectra. Based on these quasiparticles, various correlation functions are analytically derived.

PACS numbers: 71.45.−d, 71.30.+h, 75.10.Jm

The one-dimensional Hubbard model in the large-U limit has recently attracted extensive attentions [1–5]. This is primarily due to its possible important implication to the two-dimensional case where the Hubbard model is considered as a promising candidate [1] to describe the high-T_c oxide materials. In terms of the exact solution of Lieb and Wu [6] for the Hubbard chain, some fundamental physics in the large-U limit, e.g., the charge and spin separation, has been qualitatively clarified by Anderson and other authors [1,2]. However, many important properties like the correlation functions are still quite difficult to calculate by a systematic way. Some remarkable progress has been achieved recently by the bosonization method [4], but such an approach originally is only justified in the weak-coupling regime.

In this Letter, we shall present a systematic approach to the one-dimensional Hubbard chain in the strong-coupling regime. The elementary excitations of charge and spin together with all the important correlation functions will be analytically derived. The path-integral formalism used here has been developed previously to study the two-dimensional Hubbard model [7,8].

The Hubbard Hamiltonian is given by

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

By a SU(2) invariant Hubbard-Stratonovich transformation, the partition function $Z=\mathrm{Tr}(\exp-\beta H)$ could be expressed in the path-integral formalism as

$$Z=\int da^{\dagger}\,da\,d\phi\,d\Delta\,d^2n\exp\left(-\int d\tau L\right),$$

where [7]

$$L(\tau)=\sum_i\hat{a}_i^{\dagger}\partial_\tau\hat{a}_i+\sum_i\hat{a}_i^{\dagger}(U_i^{\dagger}\partial_\tau U_i)\hat{a}_i-t\sum_{\langle i,j\rangle}[\hat{a}_i^{\dagger}(U_i^{\dagger}U_j)\hat{a}_j+\text{H.c.}]+\sum_i\left(\frac{\phi_i^2}{U}+i\phi_i\hat{a}_i^{\dagger}\hat{a}_i+\frac{\Delta_i^2}{U}-\Delta_i\hat{a}_i^{\dagger}\sigma_z\hat{a}_i\right), \tag{2}$$

in which the spinor $\hat{a}_i$ is related to the electron operator $\hat{c}_i=(c_{i\uparrow},c_{i\downarrow})$ through

$$\hat{c}_i=U_i\hat{a}_i. \tag{3}$$

U_i is a SU(2) transformation such that $U_i\sigma_zU_i^{\dagger}=\mathbf{n}_i\cdot\boldsymbol{\sigma}$. U_i is determined up to U(1) which leaves a local U(1) gauge freedom of $L(\tau)$ in (2).

There are three auxiliary fields ϕ_i, Δ_i, and U_i (or equivalently $\mathbf{n}_i$) involved in the Lagrangian (2). If ϕ_i and Δ_i are replaced by some mean fields $\phi_i=\phi$ and $\Delta_i=(-1)^i\Delta$, then similar to the conventional spin-density-wave (SDW) theory, there will be an "antiferromagnetic" symmetry broken in the "z" direction, as seen by the fermion $a_{i\sigma}$ according to (2). But in the real space such a z axis will coincide with the $\mathbf{n}_i$ direction because of the definition (3) where U_i is a rotation from the true z axis to the $\mathbf{n}_i$ direction. Therefore $(-1)^i\mathbf{n}_i$ will represent the spin-polarization direction after the above mean-field replacement. In the strong-coupling regime, as the result of the suppression of the double occupancy, the spin at the occupied site becomes fully polarized and is determined by the direction $\mathbf{n}_i$. In this case, to the order of t/U, the charge and amplitude fluctuations at the occupied sites are negligible [7,9], and ϕ_i and Δ_i could be safely replaced by their mean-field values $\phi_i=\phi=-iU/2$ and $\Delta_i=(-1)^i\Delta=(-1)^iU/2$, with a full local (staggered) moment $m_i=2\Delta_i/U=(-1)^i$. The equivalence between the present formalism and the t-J model will be discussed elsewhere [7,9].

Now there is only one auxiliary $\mathbf{n}_i$ field left in Lagrangian (2), represented by U_i, which describes the spin-polarization direction. First we consider a simple Hamiltonian

$$H_0=-t\sum_{\langle i,j\rangle}(\hat{a}_i^{\dagger}\hat{a}_j+\text{H.c.})+\tfrac{1}{2}U\sum_i\hat{a}_i^{\dagger}\hat{a}_i-\tfrac{1}{2}U\sum_i(-1)^i\hat{a}_i^{\dagger}\sigma_z\hat{a}_i, \tag{4}$$

which is obtained after taking the mean-field values for ϕ_i and Δ_i as well as $U_i^{\dagger}U_j=1$ and $U_i^{\dagger}\partial_\tau U_i=0$ in (2). It could be used as an unperturbed Hamiltonian in studying the spin fluctuations of $U_i^{\dagger}U_j-1$ and $U_i^{\dagger}\partial_\tau U_i$. H_0 is easily diagonalized through a Bogoliubov transformation in k space [7]. In the case of $U\gg t$, the localized picture will be more convenient for our discussion and we could write down this transformation in the lattice representation as

follows:

$$a_{i\sigma}=\theta(p_i\sigma)\alpha_i+\theta(-p_i\sigma)p_i\beta_i+\theta(-p_i\sigma)\frac{t}{U}(\alpha_{i+1}+\alpha_{i-1})+\theta(p_i\sigma)p_i\frac{t}{U}(\beta_{i+1}+\beta_{i-1})+O\left(\frac{t^2}{U^2}\right), \tag{5}$$

where α_i and β_i are two spinless fermions, and $\theta(x)$ is the step function with $p_i\equiv(-1)^i$. According to the transformation (5), H_0 in (4) is expressed as

$$H_0=-J\sum_i(\alpha_i^\dagger\alpha_i-\beta_i^\dagger\beta_i)+U\sum_i\beta_i^\dagger\beta_i-\tfrac{1}{2}J\sum_i(\alpha_i^\dagger\alpha_{i+2}-\beta_i^\dagger\beta_{i+2}+\text{H.c.}), \tag{6}$$

where $J\equiv 2t^2/U$. We see that there is a large charge gap U between the α band and the β band. In the half-filling case the lower α band will be filled by electrons with the upper β band being empty; the hole will go to the lower band in the hole-doping case. Thus the nondouble occupancy constraint in the t-J model could be realized in a natural way here.

We shall discuss the Lagrangian (2) based on the representation (5) with H_0 as the unperturbed Hamiltonian. Now we consider the $U\to\infty$ limit where (2) can be simplified as

$$L_\infty=\sum_i\sum_\sigma\theta(p_i\sigma)(U_i^\dagger\partial_\tau U_i)_{\sigma\sigma}(1-h_i^\dagger h_i)+\sum_i h_i^\dagger\partial_\tau h_i+t\sum_i\left[\sum_\sigma\theta(p_i\sigma)(U_i^\dagger U_{i+1})_{\sigma-\sigma}h_{i+1}^\dagger h_i+\text{H.c.}\right], \tag{7}$$

in which only the lower band has been retained and the hole operator $h_i^\dagger\equiv\alpha_i$ is introduced for the convenience of discussion below.

The Lagrangian (7) shows that the hole could get the largest hopping matrix ($=t$) when $|(U_i^\dagger U_{i+1})_{\sigma-\sigma}|=1$ for all sites i. It corresponds to a ferromagnetic state with $\mathbf{n}_i=-\mathbf{n}_{i+1}$ [because the amplitude field $\Delta_i=(-1)^i\Delta$ changes sign between different sublattices]. It is the well-known Nagaoka ground state.

However, we shall show that the hole could gain its largest kinetic energy even in the generic spin states, which are all degenerate at $U=\infty$. Notice that the spin dynamics will be determined by the first term in Lagrangian (7). But such a term disappears at the hole sites because of the factor $1-h_i^\dagger h_i$ (which is more clear if we understand it from the operator formalism). The physical meaning here is very simple: There is no true spin (carried by the electron) at the hole site i and thus the "direction" of spin there could be arbitrary. Now suppose the hole is hopping from site i to site $i+1$. In order to get the largest hopping matrix element in (7), the direction of spin at site i needs to be arranged such that $|(U_i^\dagger U_{i+1})_{\sigma-\sigma}|=1$. Without loss of any generality one may choose $U_i^\dagger U_{i+1}=i\sigma_x$ as U_i has a U(1) gauge freedom. In this way, the hole can always get the best kinetic energy just like in the Nagaoka state.

On the other hand, after the hole hops to site $i+1$, a "spin" will be produced at site i which is determined by $U_i=U_{i+1}(-i\sigma_x)$. Physically, it could be interpreted as the spin (carried by the electron) at site $i+1$ being transferred to site i during the above hopping procedure. At a given moment, an effective spin chain can be obtained by removing all the sites occupied by holes. For any site on this effective spin chain, we may define $\tilde{U}_i$ through

$$U_i=\tilde{U}_i(i\sigma_x)^{\Sigma_{l<i}h_l^\dagger h_l}. \tag{8}$$

According to the discussion above, when the hole hops from site i_0 to i_0+1, one easily finds $\tilde{U}_{i_0}$(after hopping) $=\tilde{U}_{i_0+1}$(before hopping). Therefore, the effective spin chain, described by $\{\tilde{U}_i\}$, will be independent of the motion of holes. One could reproduce any real spin-hole configurations in the whole chain just by inserting the sites of holes into this effective spin chain and determine U_i at the spin site by $\tilde{U}_i$ according to (8).

In terms of the above discussions, L_∞ could be rewritten by

$$L_\infty=\sum_i{}^s\sum_\sigma\theta(\tilde{p}_i\sigma)(\tilde{U}_i^\dagger\partial_\tau\tilde{U}_i)_{\sigma\sigma}+L_h, \tag{9}$$

with

$$L_h=\sum_i\tilde{h}_i^\dagger\partial_\tau\tilde{h}_i-t\sum_i(\tilde{h}_{i+1}^\dagger\tilde{h}_i+\tilde{h}_i^\dagger\tilde{h}_{i+1}), \tag{10}$$

where the summation $\sum^s$ goes over the effective spin chain with hole sites removed.

$$\tilde{p}_i=(-1)^{i-\Sigma_{l<i}h_l^\dagger h_l}$$

is the staggered factor on the squeezed chain. $\tilde{h}_i=\exp[i(\pi/2a)x_i]h_i$ is also introduced in (10). Equations (9) and (10) show that the hole is decoupled from the spin background and behaves like a free spinless fermion. It is easy to obtain the holon's excitation spectrum as $\epsilon_k^h=-2t\cos(ka)$ with the Fermi velocity $v_h=2ta\times\sin(\pi\delta)$. δ is the doping concentration.

Then let us turn on $J=2t^2/U$, but still assume $J\ll t$. Using the representation of (5) to formulate Lagrangian (2) [with ϕ_i and Δ_i being substituted by ϕ and $(-1)^i\Delta$ as discussed before], one may classify two effects due to finite J. One is the correction to the hopping matrix of the holon with a magnitude in order of J, which includes the next-nearest-neighbor hopping [like those terms shown in (6)]. This effect will be neglected because the bare hopping matrix t is much larger than J. The second effect of finite J is to give a nonzero spin stiffness which will lift the spin degeneracy and choose a spin singlet state. To be precise, a finite-J contribution to the spin part could be found as the second term in the following Lagrangian:

$$L_s=\sum_i{}^s\sum_\sigma\theta(\tilde{p}_i\sigma)(\tilde{U}_i^\dagger\partial_\tau\tilde{U}_i)_{\sigma\sigma}+\tfrac{1}{2}\tilde{J}\sum_i{}^s\left[\sum_\sigma(1-\tilde{U}_i^\dagger U_{i+1})_{\sigma\sigma}+\text{H.c.}\right], \tag{11}$$

which is obtained after the holon part coupled with it has been treated by a mean-field approximation [9], with $\tilde{J}=J[(1-\delta)+\sin(2\pi\delta)/2\pi]$. The first term in L_s comes from L_∞ in (9). Then the total Lagrangian at small J is given by $L=L_s+L_h$.

The Lagrangian L_s determines the dynamics of the effective spin chain. One could show [7] that L_s can be reduced to a nonlinear σ model associated with a topological term in the long-wavelength, low-energy limit, which is equivalent to a Heisenberg chain with an enlarged lattice constant $\tilde{a}=a/(1-\delta)$ and a renormalized superexchange coupling $\tilde{J}$. But we shall pursue a different way to treat L_s in the following.

Introduce a CP^1 representation for $\tilde{U}_i$ as follows:

$$\tilde{U}_i=\begin{pmatrix} b_{i\uparrow} & -b_{i\downarrow}^\dagger \\ b_{i\downarrow} & b_{i\uparrow}^\dagger \end{pmatrix}. \tag{12}$$

The unitary condition $\tilde{U}_i^\dagger\tilde{U}_i=1$ requires $\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma}=1$. Then L_s in (11) can be expressed by

$$L_s=\sum_{i\sigma}{}^s b_{i\sigma}^\dagger\partial_\tau b_{i\sigma}-\tilde{J}\sum_{i\sigma}{}^s(b_{i\sigma}^\dagger b_{i+1\sigma}^\dagger+\text{H.c.}) +\sum_i{}^s\lambda_i\left(\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma}-1\right), \tag{13}$$

in which $b_{i\sigma}$ has been redefined by $b_{i\sigma}^\dagger$ at odd sublattice $\tilde{p}_i=-1$. The Lagrangian (13) actually describes a hard-core boson system. In the operator formalism, we introduce a Jordan-Wigner transformation [10],

$$b_{i\sigma}^\dagger=\exp\left(i\pi\sum_{j<i}n_{j\sigma}^f\right)[\theta(\tilde{p}_i)f_{i\sigma}^\dagger+\theta(-\tilde{p}_i)f_{i\sigma}], \tag{14}$$

where $f_{i\sigma}$ is a fermion operator and $n_{j\sigma}^f=f_{j\sigma}^\dagger f_{j\sigma}$. After this transformation we relax the constraint appearing in (13) by replacing λ_i with a constant λ and thus get the following Hamiltonian:

$$H_s=-\tilde{J}\sum_{i\sigma}{}^s(f_{i+1\sigma}^\dagger f_{i\sigma}+\text{H.c.}) +\lambda\sum_i{}^s\tilde{p}_i\left(\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}-1\right). \tag{15}$$

H_s is easy to diagonalize and we find the spectrum $\epsilon_k^s=-2\tilde{J}\cos(k\tilde{a})$. One can also verify that $\lambda=0$ and all states with $\epsilon_k^s<0$ are filled by the fermions. The Fermi surface is at $\epsilon_{k_f}=0$ with $k_f=\pi/2\tilde{a}=\pi(1-\delta)/2a$ and a Fermi velocity $v_s=2J\{1-\sin[2\pi(1-\delta)]/2\pi(1-\delta)\}a$. ϵ_k^s and v_s agree with Coll's results [11] based on the Lieb and Wu solution except a $\pi/2$ factor.

Therefore, we have obtained two elementary excitations described by the fermions $\tilde{h}_i$ and $f_{i\sigma}$, which will be called the holon and spinon, respectively, after Anderson [1]. The bare electron is composed by these two quasiparticles, together with some nonlocal string operators as shown by Eqs. (3), (5), and (8). One may write down an explicit expression for $c_{i\sigma}$ in the large-U limit:

$$c_{i\sigma}=\frac{1}{2}h_i^\dagger\left[\exp\left(i\frac{\pi}{2}\sum_{l<i}\tilde{h}_l^\dagger\tilde{h}_l\right)\sum_{\sigma'}\tilde{U}_{i\sigma\sigma'}+\exp\left(-i\frac{\pi}{2}\sum_{l<i}\tilde{h}_l^\dagger\tilde{h}_l\right)p_i\sum_{\sigma'}\sigma'\tilde{U}_{i\sigma\sigma'}\right],$$

where $\tilde{U}_i$ is related to the spinon f_i through (12) and (14). The charge and spin separation is mathematically determined through this relation.

Then various correlation functions can be calculated. An example is the spin-spin correlation whose leading contribution is given by $\frac{1}{4}\langle(-1)^i\mathbf{n}_i(t)\cdot(-1)^j\mathbf{n}_j(0)\rangle$. It could be written in the following form according to (8):

$$\langle\mathbf{S}_i(t)\cdot\mathbf{S}_j(0)\rangle=\tfrac{1}{8}p_ip_j\langle\mathrm{Tr}\tilde{U}_i(t)\sigma_z\tilde{U}_i^\dagger(t)\tilde{U}_j(0)\sigma_z\tilde{U}_j^\dagger(0)\rangle_s\langle\exp[-i\pi N_i(t)]\exp[i\pi N_j(0)]\rangle_h, \tag{16}$$

where $N_i=\sum_{l<i}\tilde{h}_l^\dagger\tilde{h}_l$. As the holon and spinon have linear spectra near their Fermi momenta, the averages of $\langle\cdots\rangle_s$ and $\langle\cdots\rangle_h$ in (16) could be systematically treated by the bosonization technique [10] in the long-wavelength limit. We then get the asymptotic behavior of

$$\langle\mathbf{S}_i(t)\cdot\mathbf{S}_j(0)\rangle\sim\frac{\cos(2k_fx)}{(x^2-v_h^2t^2)^{1/4}(x^2-v_s^2t^2)^{1/2}}, \tag{17}$$

with $x\equiv x_i-x_j$. This $2k_f$ behavior has also been obtained by different approaches [2–5].

The density-density correlation is readily derived as the spinon part makes no contribution,

$$\langle\delta n_i(t)\delta n_j(0)\rangle\propto-(x_+^{-2}+x_-^{-2})/4\pi^2+1/(2\pi^2x_+x_-)\cos(4k_fx), \tag{18}$$

with $x_\pm\equiv x\pm v_ht$.

Another important quantity is the electron Green's function $G_{\sigma\sigma'}^e(x,t)=-i\langle Tc_{i\sigma}(t)c_{j\sigma'}^\dagger(0)\rangle$. After some algebraic calculations, G^e is reduced to

$$G_{\sigma\sigma'}^e(x,t)=\tfrac{1}{4}\langle[\tilde{U}_i(t)\tilde{U}_j^\dagger(0)]_{\sigma\sigma'}\rangle_s\sum_{\theta=\pm1/2}\exp\left(i\frac{\theta\pi}{a}x\right)G^\theta(x,t), \tag{19}$$

where the "semion" Green's function $G^\theta(x,t)$ is defined as $-i\langle T\tilde{h}_i^{\theta\dagger}(t)\tilde{h}_j^\theta(0)\rangle_h$, with $\tilde{h}_i^\theta=\tilde{h}_i\exp(-i\pi\theta N_i)$. Again using

the bosonization technique, the asymptotic behavior of $G^e_{\sigma\sigma'}$ is found by

$$G^e_{\sigma\sigma'}(x,t) \propto \frac{\delta_{\sigma,\sigma'}}{(x^2-v_s^2t^2)^{1/4}(x^2-v_h^2t^2)^{1/16}}\left[\frac{e^{ik_fx}}{(x-v_ht)^{1/2}}+\frac{e^{i3k_fx}}{(x-v_ht)^{3/2}}-(t\to -t;\, k_f\to -k_f)\right]. \quad (20)$$

The momentum distribution near $k\sim k_f$ is determined according to (20),

$$n(k)\sim n(k_f)-C|k-k_f|^{1/8}\mathrm{sgn}(k-k_f)\,, \quad (21)$$

and near $k\sim 3k_f$, the power-law singularity becomes $|k-3k_f|^{9/8}$.

The asymptotic form (20) of the Green's function is basically in agreement with the results based on the bosonization approach [4]. But there is a difference in the spinon part. As shown in (20), the spinon contributes a factor $(x^2-v_s^2t^2)^{-1/4}$ instead of $(x\pm v_st)^{-1/2}$ as obtained in the usual bosonization method [4,5]. In the density-density correlation (18), the absence of $2k_f$ oscillation is also distinct from the bosonization approach where both the holon and spinon will contribute to such a leading oscillation term [4].

Finally, we consider the pair susceptibility. In the singlet channel, one can define $B_i^s=1/\sqrt{2}(c_{i\uparrow}c_{i+1\downarrow}-c_{i\downarrow}c_{i+1\uparrow})$ and find the leading part

$$\langle B_i^{s\dagger}B_j^s\rangle \propto \cos(2k_fx)/x^{2.5}\,. \quad (22)$$

In obtaining (22), a nonlocal phase shift in terms of (8) due to the creation of a pair of holes should be taken into account [9]. Similarly, the pair susceptibility in the triplet channel is found to be $\sim x^{-3}$ which has a higher power to decay as compared to the singlet pairing. Physically, a doped hole will decay into a spinon and a holon. In the case of a pair of holes doped into the system, the two spinons accompanying the holons may annihilate with each other in the singlet channel such that the singlet-pair propagator has a smaller power to decay than in the triplet case. A very similar situation in the two-dimensional case has been discussed in Ref. [8] where it has been argued that a true superconducting condensation will become possible after the interlayer coupling is introduced.

In conclusion, a first-principals calculation of the zero-temperature properties of the large-U Hubbard chain is presented. It is found that the electron (hole) will decay into two independent excitations, i.e., holon and spinon, in the large-U regime. The obtained energy spectra of the holon and spinon are in good agreement with the exact Lieb and Wu solution. A series of correlation functions have been explicitly calculated in asymptotic form, which, in some aspects, differ from the bosonization results.

The authors would like to thank P. W. Anderson, G. Levine, T. K. Lee, J. R. Schrieffer, X. G. Wen, 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 Defence Advanced Research Project Agency.

[a]On leave from the Institute of Theoretical Physics, Academia Sinica, Beijing, China.

[1] P. W. Anderson, in *Frontiers and Borderlines in Many Particle Physics,* International School of Physics "Enrico Fermi" Vol. 104, edited by R. A. Broglia and J. R. Schrieffer (North-Holland, Amsterdam, 1987); in *Current Trends in Condensed Matter, Particle Physics and Cosmology, Kathmandu, 1989* (World Scientific, Singapore, 1990); in *Proceedings of the Los Alamos Symposium on High Temperature Superconductivity,* edited by K. S. Bedell, D. Coffey, D. E. Meltzer, D. Pines, and J. R. Schrieffer (Addison-Wesley, Reading, MA, 1990).

[2] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990).

[3] A. Parola and S. Sorella, Phys. Rev. Lett. **64**, 1831 (1990); H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).

[4] P. W. Anderson and Y. Ren (to be published); A. M. Tsvelik (to be published).

[5] X. G. Wen, Phys. Rev. B **42**, 6623 (1990).

[6] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[7] Z. Y. Weng, C. S. Ting, and T. K. Lee, Phys. Rev. B **43**, 3790 (1991).

[8] Z. Y. Weng, Phys. Rev. Lett. **66**, 2156 (1991).

[9] Z. Y. Weng, D. N. Sheng, C. S. Ting, and Z. B. Su (unpublished).

[10] F. 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).

[11] C. F. Coll, III, Phys. Rev. B **9**, 2150 (1974).