The Hubbard Quantum Wire

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By introducing a boundary condition for the quantum wire, the Hubbard model is solved exactly by means of the Bethe ansatz. The wave function for the bounded state is clearly defined, and the secular equation for the spectrum is exactly obtained. The ground state and low-lying excited states are studied in the thermodynamic limit. The ground-state energy in the strong coupling limit is obtained explicitly, and compared with the results of a periodic boundary condition. [S0031-9007(97)05202-2]

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It is known that the behavior of a one-dimensional electronic system differs in many aspects from that of two-dimensional and three-dimensional systems [1]. The one-dimensional Hubbard model provides the opportunity to study correlation effects. There have been many discussions on the Hubbard model since the Lieb-Wu solution was found [2]. This solution is an exact result with a periodic boundary condition which can be thought of as on a ring. Because of the dramatic achievement in nanotechnology in recent years, the boundary effects of a sample will become more important. The Hubbard model on an open chain with completely confined ends was considered [3]. By adding some boundary field at the ends, the model was considered [4] and discussed [5]. The models [3–5] were easier and simpler as the wave function outside the wire is null. In the present Letter we study a more realistic model for quantum wires where the possibility of a nonvanishing wave function outside is taken into account. Using the Bethe ansatz and some other methods in the literature of integrable models, we obtain an exact result for the model Hamiltonian. The ground state and the low-lying excitations are studied in the thermodynamic limit. The ground-state energy in the strong coupling is shifted from the one for a periodic boundary condition in a small amount. Both the spinon excitation and the holon-antiholon excitation are gapless.

We consider a quantum wire of length L described by the Hamiltonian

$$H = \sum_{i=-\infty}^{\infty}\sum_{a}\left[-t(C_{ia}^{+}C_{i+1a} + C_{i+1a}^{+}C_{ia}) + \frac{U}{2}n_{ia}n_{i-a}\right] + \sum_{i=-\infty}^{-L/2-1}\sum_{a} V_L n_{ia} + \sum_{i=L/2+1}^{\infty}\sum_{a} V_R n_{ia}\,, \quad (1)$$

where C_{ia} is the operator annihilating an electron with spin component a on site i, and $n_{ia} \coloneqq C_{ia}^{+}C_{ia}$ the local-number operator of electrons. Clearly, it is a Hubbard Hamiltonian added with some terms which are defined outside of the wire. So the present model is different from either Hubbard ring [2] or the Hubbard chain with reflection ends [3] or with boundary fields [4,5]. The V_L and V_R in (1) represent the kinetic energies which an electron must lose if it escapes out of the wire from the left end or the right end, respectively. Instead of a periodic or completely confined boundary condition, we will treat this model with a more physical boundary condition. It is convenient to consider the states that span a Hilbert space of N particles

$$|\psi\rangle = \sum_{\{a_i\},\{x_i\}} \psi_{a_i,\cdots a_N}(x_1,\cdots,x_N)C_{x_1a_1}^{+}\cdots C_{x_Na_N}^{+}|0\rangle\,.$$

The eigenvalue problem $H|\psi\rangle = E|\psi\rangle$ becomes an N-particle quantum mechanical problem with the first quantized Hamiltonian,

$$H = \sum_{j=1}^{N}[-t\Delta_j + V(x_j)] + U\sum_{i<j}\delta(x_i, x_j)\,, \quad (2)$$

where $\Delta_j\psi \coloneqq \psi(\ldots, x_j + 1, \ldots) + \psi(\ldots, x_j - 1, \ldots)$, $V(x_j) = V_L\theta(-x_j - L/2 - 1) + V_R\theta(x_j - L/2 - 1)$, $\theta(x)$ the step function. The continuity limit of Eq. (2) concerns an equation in Ref. [6].

The number operator of electrons in the wire is defined as $\hat{N} = \sum_{i=-L/2}^{L/2} C_{ia}^{+}C_{ia}$, and that in the left side or the right side is given by $\hat{N}_L = \sum_{i=-\infty}^{-L/2-1} C_{ia}^{+}C_{ia}$ or $\hat{N}_R = \sum_{i=L/2+1}^{\infty} C_{ia}^{+}C_{ia}$, respectively (summation also runs over spins $a = 1/2, -1/2$). The total number operator $\hat{N}_t = \hat{N}_L + \hat{N}_R + \hat{N}$ always gives $\hat{N}_t|\psi\rangle = N|\psi\rangle$ in the Hilbert space of N particles. The boundary condition which will be used to determine the spectrum reads

$$\lim_{i\to\pm\infty} C_{ia}^{+}C_{ia}|\psi\rangle = 0\,. \quad (3)$$

The Schrödinger operator (2) is invariant under any permutation of S_N, but is not invariant under translation. Thus the total momentum of the system is not conserved, and the reflective waves must be taken into account. The wave function of the Bethe ansatz forms in the region $x \in C(Q) \coloneqq \{x \mid -L/2 < x_{Q1} < \cdots < x_{QN} < L/2\}$ reads

$$\psi_a(x) = \sum_{P\in\mathcal{W}_B} A_a(P, Q)e^{i(Pk\,|\,Qx)}, \quad (4)$$

where $x \coloneqq (x_1, x_2, \ldots, x_N)$ with $x_j \in \mathbb{Z}$; $a \coloneqq (a_{Q1}, a_{Q2}, \ldots, a_{QN})$, a_j stands for the spin component of

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the jth particle; Pk (or Qx) is the image of a given $k \coloneqq (k_1, k_2, \ldots, k_N)$ (or x) by a mapping $P \in \mathcal{W}_B$ (or $Q \in \mathcal{W}_A$); $(Pk \,|\, Qx) = \sum_{j=1}^{N} (Pk)_j (Qx)_j$. The coefficients $A(P, Q)$ are functionals on $\mathcal{W}_B \otimes \mathcal{W}_A$. One may notice that the sum runs over the Weyl group [7] of the Lie algebra B_N (denoted by $\mathcal{W}_B$) but the wave function is defined on various Weyl chambers corresponding to the Weyl group of the Lie algebra A_{N-1} (denoted by $\mathcal{W}_A$).

Any element of the Weyl group $\mathcal{W}_B$ can be expressed as a product of the neighboring interchanges, $\sigma^j : (\ldots, z_j, z_{j+1}, \ldots) \mapsto (\ldots, z_{j+1}, z_j, \ldots)$ and mirror reflection $\tau^1 : (z_1, z_2, \ldots) \mapsto (-z_1, z_2, \ldots)$, where z_j denotes either x_j, a_j, k_j or their image by a mapping. The requirement of antisymmetry is $(\sigma^j \psi)_a(x) = -\psi_a(x)$, which gives

$$A(P; \sigma^j Q) = -\mathcal{P}^{Qj,Q(j+1)} A(\sigma^j P; Q),$$

where the spin labels are omitted and $\mathcal{P}^{Qj,Q(j+1)}$ is the spinor representation of the permutation σ^j. The scattering matrix (S matrix) which relates the coefficients A's between distinct regions in the configuration space of N electrons reads

$$S^{Qj,Q(j+1)} = \frac{\sin(Pk)_j - \sin(Pk)_{j+1} + ic\mathcal{P}^{Qj,Q(j+1)}}{\sin(Pk)_j - \sin(Pk)_{j+1} + ic}, \tag{5}$$

where $2c = U/t$. Equation (5) is the same as that in the Lieb-Wu solution [2]. The coefficients A's in any region are determined up to an overall factor by the $\check{S}^{Qj,Q(j+1)} \coloneqq -\mathcal{P}^{Qj,Q(j+1)} S^{Qj,Q(j+1)}$ and the R_L (or R_R), i.e., $A(\sigma^j P; Q) = \check{S}^{Qj,Q(j+1)} A(P; Q)$, $A(\tau^1 P; Q) = R_L[(Pk)_1] A(P; Q)$, $A(\tau^N P; Q) = R_R[(Pk)_N] A(P; Q)$. The reflection matrices R_L and R_R are solved from the Schrödinger equation near the ends of the wire by taking into account the boundary condition (3); consequently,

$$\begin{aligned} R_L(k) &= -e^{-ikL - i\theta_L(k)}, \\ R_R(k) &= -e^{ikL + i\theta_R(k)}, \end{aligned} \tag{6}$$

where $i\theta(k) = \ln[(e^{\kappa + ik} - 1)/(e^{\kappa - ik} - 1)]$ with $2t \times (\cosh\kappa - \cos k) = V_L$ or V_R in θ_L or θ_R.

One may notice that the condition (3) does not give any constraints directly on ψ but gives that on ψ^L and ψ^R. In deriving (6) we have considered the wave functions outside of the wire, which actually vanishes in [3] but does not in the present case. The wave function in the region $x_{Q1} < -L/2 \le x_{Q2} < \cdots < x_{QN} \le L/2$ takes

$$\psi_a^L(x) = \sum_{j=1}^{N} \sum_{\sigma' \in \mathcal{W}'} A_a^L(\sigma' q_j', Q) e^{\kappa_j x_{Q1}} e^{i(\sigma' q_j' k \,|\, Q'x)}$$

where $Q'x = (0, x_{Q2}, \ldots, x_{QN})$ and $\kappa_j > 0$ with $2t(\cosh\kappa_j - \cos k_j) = V_L$; in the region $-L/2 < x_{Q1} < x_{Q2} < \cdots < x_{Q(N-1)} \le L/2 < x_{QN}$,

$$\psi_a^R(x) = \sum_{j=1}^{N} \sum_{\sigma'' \in \mathcal{W}''} A_a^R(\sigma'' q_j'', Q) e^{-\kappa_j x_{QN}} e^{i(\sigma'' q_j'' k \,|\, Q''x)}.$$

Here $Q''x = (x_{Q1}, \ldots, x_{Q(N-1)}, 0)$ and $\kappa_j > 0$ with $2t(\cosh\kappa_j - \cos k_j) = V_R$. In the above, some notation conventions are adopted, i.e., two subgroups of the Weyl group of B_N, $\mathcal{W}' \coloneqq \{\sigma^2, \sigma^3, \ldots, \sigma^{N-1}, \tau^N\}$ and $\mathcal{W}'' \coloneqq \{\sigma^1, \sigma^2, \ldots, \sigma^{N-2}, \sigma^{N-1}\tau^N\sigma^{N-1}\}$; two particular cycles q_j'': $(x_1, \ldots, x_j, \ldots, x_N) \mapsto (x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N, x_j)$ and q_j': $(x_1, \ldots, x_j, \ldots, x_N) \mapsto (x_j, x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N)$.

As there are several identities in the Weyl groups, several consistency relations must be checked for the above solution. The Yang-Baxter equations [8] arising from both $A(\sigma^j\sigma^{j+1}\sigma^j P; Q) = A(\sigma^{j+1}\sigma^j\sigma^{j+1} P; Q)$ and $A(P; \sigma^j\sigma^{j+1}\sigma^j Q) = A(P; \sigma^{j+1}\sigma^j\sigma^{j+1} Q)$ are fulfilled identically. The Yang-Baxter equations with reflections arising from $A(\tau^1\sigma^1\tau^1\sigma^1 P; Q) = A(\sigma^1\tau^1\sigma^1\tau^1 P; Q)$ and $A(\tau^N\sigma^{N-1}\tau^N\sigma^{N-1} P; Q) = A(\sigma^{N-1}\tau^N\sigma^{N-1}\tau^N P; Q)$ are satisfied identically because the reflection matrices are just scalar factors.

As either $\{\sigma^1, \ldots, \sigma^{N-1}, \tau^1\}$ or $\{\sigma^1, \ldots, \sigma^{N-1}, \tau^N\}$ can be chosen as the basic elements of Weyl group $\mathcal{W}_B$, we must consider another consistency condition for R_L and R_R. Using $\tau^1 = \sigma^1\sigma^2\cdots\sigma^{N-1}\tau^N\sigma^{N-1}\cdots\sigma^2\sigma^1$ and applying the $\check{S}$ matrices successively, we obtain an eigenvalue equation in the spinor space: $\check{S}^{1,2}(\eta_1 + \eta_2)\check{S}^{2,3}(\eta_1 + \eta_3)\cdots\check{S}^{N-1,N}(\eta_1 + \eta_N)\check{S}^{N-1,N}(\eta_1 - \eta_N)\cdots\check{S}^{2,3}(\eta_1 - \eta_3)\check{S}^{1,2}(\eta_1 - \eta_2) \times A(P; Q) = R_L[(Pk)_1] R_R^{-1}[(Pk)_1] A(P; Q)$, which is equivalent to

$$\begin{aligned} &S^{1,2}(\eta_1 + \eta_2) S^{1,3}(\eta_1 + \eta_3)\cdots S^{1,N}(\eta_1 + \eta_N) \\ &\quad S^{1,N}(\eta_1 - \eta_N)\cdots S^{1,2}(\eta_1 - \eta_2) A(P; Q) \\ &\qquad = R_L[(Pk)_1] R_R^{-1}[(Pk)_1] A(P; Q), \end{aligned} \tag{7}$$

where $\eta_j = \sin(Pk)_j$. This relation guarantees the consistency for any reflection $(k_1, \ldots, k_j, \ldots) \to (k_1, \ldots, -k_j, \ldots)$.

The eigenvalue problem (7) can be diagonalized by means of the Sklyanin approach [9], in which the transfer matrix is defined as $t(\alpha) = \operatorname{tr} R_L^{-1}(\alpha) T_+(\alpha) R_R(\alpha) T_-(\alpha)$, where $T_\mp(\alpha) = T_{AN}(\alpha \mp \alpha_N)\cdots T_{A2}(\alpha \mp \alpha_2) T_{A1}(\alpha \mp \alpha_1)$, and $T_{Aj}(\alpha) \coloneqq S^{Aj}(\alpha) \in \mathrm{End}(V^A \otimes V^j)$; End means endomorphism. The Bethe ansatz equations are obtained as follows:

$$e^{-i2k_j L} = e^{-i\theta_L(k_j) - i\theta_R(k_j)} \prod_{\nu=1}^{M} \Xi_{\frac{1}{2}}(\eta_j - \lambda_\nu) \Xi_{\frac{1}{2}}(\eta_j + \lambda_\nu),$$

$$\prod_{\substack{\nu=1 \\ \nu \neq \mu}}^{M} \Xi_1(\lambda_\mu - \lambda_\nu) \Xi_1^{-1}(\lambda_\mu + \lambda_\nu) = \prod_{l=1}^{N} \Xi_{\frac{1}{2}}(\lambda_\mu - \eta_l) \Xi_{\frac{1}{2}}(\lambda_\mu + \eta_l),$$

where $\Xi_\beta(x) = (x - i\beta c)/(x + i\beta c)$. A set of coupled transcendental equations is derived by taking the logarithm

$$k_j = \left(\frac{\pi}{L}\right) I_j - \frac{1}{2L}[\theta_L(k_j) + \theta_R(k_j)] + \frac{1}{2L}\sum_{\nu=1}^{M}[\Theta_{\frac{1}{2}}(\eta_j - \lambda_\nu) + \Theta_{\frac{1}{2}}(\eta_j + \lambda_\nu)],$$
$$\sum_{\nu=1}^{M}[\Theta_1(\lambda_\mu - \lambda_\nu) + \Theta_1(\lambda_\mu + \lambda_\nu)] = -2\pi J_\mu + \sum_{l=1}^{N}[\Theta_{\frac{1}{2}}(\lambda_\mu - \eta_l) + \Theta_{\frac{1}{2}}(\lambda_\mu + \eta_l)], \tag{8}$$

where $\Theta_\beta(x) \coloneqq 2\tan^{-1}(x/\beta c)$, $-\pi < \tan^{-1}(x) \le \pi$. The quantum numbers of both the quasicharge and quasispin, I_j and J_μ, take integer values regardless of $N - M$ being even or odd. Equation (8) becomes the result of Ref. [3] in the limit $V_{L,R} \to \infty$.

We consider the thermodynamic limit by introducing the densities (distribution function) of roots, $\rho(k)$ and $\sigma(\lambda)$, and that of holes $\rho_h(k)$ and $\sigma_h(\lambda)$. Then the secular equations (8) become the following coupled integral equations:

$$\rho(k) + \rho_h(k) = \frac{1}{2\pi}\left[2 + \frac{1}{L}\frac{d}{dk}[\theta_L(k) + \theta_R(k)]\right] + \cos k \int_{-B}^{B} d\lambda' K_{\frac{1}{2}}(\sin k \mid \lambda')\sigma(\lambda'),$$
$$\sigma(\lambda) + \sigma_h(\lambda) = \int_{-D}^{D} dk' K_{\frac{1}{2}}(\lambda \mid \sin k')\rho(k') - \int_{-B}^{B} d\lambda' K_1(\lambda \mid \lambda')\sigma(\lambda'), \tag{9}$$

where $K_\beta(x) \coloneqq \pi^{-1}\beta c/(\beta^2 c^2 + x^2)$ and a notation $F(x \mid y) \coloneqq [F(x - y) + F(x + y)]/2$ is used here and from now on. The B and D are determined from the conditions

$$\frac{1}{2}\int_{-B}^{B} d\lambda' \sigma(\lambda') = \frac{M}{L}, \qquad \frac{1}{2}\int_{-D}^{D} dk' \rho(k') = \frac{N}{L}, \tag{10}$$

where the factor $1/2$ is necessary [10].

The ground state of the present model is a Fermi sea described by $\rho_0(k)$ and $\sigma_0(\lambda)$, where $\rho_0(k)$ is the distribution function of charge with momentum k and $\sigma_0(\lambda)$ that of down spins with respect to the rapidity λ. The distributions of the roots satisfy (9) with $\rho_h = \delta(0)/L$, $\sigma_h = 0$, and $B = \infty$. The energy of the ground state can be calculated once $\rho_0(k)$ is known. In this case, the distribution functions are solved in a closed form by Fourier transform,

$$2\pi\rho_0(k) = 2 + \frac{1}{L}\frac{d}{dk}[\theta_L(k) + \theta_R(k)] - \frac{2\pi}{L}\delta(0) + \frac{2\pi}{c}\cos k \int_{-D_0}^{D_0} dk' \rho_0(k')\mathcal{R}_1\left(\frac{\sin k'}{c} \;\middle|\; \frac{\sin k}{c}\right),$$
$$\sigma_0(\lambda) = \frac{1}{8c}\int_{-D_0}^{D_0} dk\, \rho_0(k) S_1\left(\frac{\pi}{c}\lambda \;\middle|\; \frac{\pi}{c}\sin k\right), \tag{11}$$

where we have used the following definitions:

$$\mathcal{R}_n(x) = \frac{1}{\pi}\sum_{l=1}^{\infty}(-n)^{l-1}\frac{l}{x^2 + l^2},$$
$$S_n\left(\frac{\pi}{2}x\right) = \frac{4}{\pi}\sum_{l=1}^{\infty}(-n)^{l+1}\frac{2l - 1}{x^2 + (2l - 1)^2}.$$

Obviously, $S_1(x)$ is the conventional hyperbolic function $\mathrm{sech}(x)$ which occurs in Lieb-Wu solution.

Equations (11) can be solved explicitly in some special cases. In the strong coupling limit $c \gg 1$, it is simplified to

$$2\pi\rho_{\mathrm{str}}(k) = 2 + \frac{2\pi}{L}\rho_b(k) - \frac{2\pi}{L}\delta(0) + \frac{4\pi}{c}\left(\frac{N}{L}\right)\ln 2\cos k, \tag{12}$$

where $2\pi\rho_b(k) = d[\theta_L(k) + \theta_R(k)]/dk$ arises from the boundary contribution at the ends of the wire. The D_0 is completely determined from the explicit form (12); hence the energy density of the ground state is obtained

$$\frac{E_0}{L} = -2t\left[\frac{1}{\pi}\sin\left(\frac{N\pi}{L}\right) + \frac{\ln 2}{2c}\left(\frac{N}{L}\right)^2 \times \left(1 + \frac{\sin(2N\pi/L)}{2N\pi/L}\right)\right] + \frac{1}{L}(E_b + t), \tag{13}$$

where

$$E_b = -\frac{t}{\pi}\left[\theta_L\left(\frac{N\pi}{2L}\right) + \theta_R\left(\frac{N\pi}{2L}\right)\right]\cos\left(\frac{N\pi}{2L}\right) - \frac{t}{2\pi}\int_{-N\pi/2L}^{N\pi/2L}[\theta_L(k) + \theta_R(k)]\sin k\, dk,$$

which vanishes when $V_{L,R} \to \infty$. It is worthwhile to compare (13) with the result in the case of periodic boundary condition. The difference is calculated,

$$\frac{E_0 - E_0^{\mathrm{per}}}{L} = \frac{1}{L}(E_b + t),$$

where E_0^{per} stands for the ground-state energy with periodic boundary condition. Clearly, the difference is relatively small for a large system which agrees with the common understanding about the effects of a boundary condition.

It is convenient to study the excitations by introducing $\rho(k) = \rho_0(k) + \rho_1(k)/L$ and $\sigma(\lambda) = \sigma_0(\lambda) + \sigma_1(\lambda)/L$, where $\rho_0(k)$ and $\sigma_0(\lambda)$ satisfy (9) with $\rho_h(k) = \delta(0)/L$ and $\sigma_h(\lambda) = 0$. The excited energy up to the order $O(1/L)$ is

$$\Delta E = -\int_{-D}^{D} dk\,(2t\cos k + \mu)\rho_1(k)\,, \qquad (14)$$

where μ stands for the chemical potential [11]. Equation (14) is related to $\rho_1(k)$ only and is valid for both the spin excitation and the charge excitation. For a large system the D can be replaced by D_0.

The simplest spin excitation is a triplet, i.e., two-hole state with $\sigma_h(\lambda) = [\delta(\lambda\,|\,\bar{\lambda}_1) + \delta(\lambda\,|\,\bar{\lambda}_2)]/L$. The excitation energy is composed of two terms $\Delta E_{\rm trip} = \varepsilon_s(\bar{\lambda}_1) + \varepsilon_s(\bar{\lambda}_2)$; each of them can be identified as a spinon excitation energy

$$\varepsilon_s(\bar{\lambda}) = -\int_{-D_0}^{D_0} dk\,(2t\cos k + \mu)\rho_1^s(k,\bar{\lambda})\,, \qquad (15)$$

where $\rho_1^s(k,\bar{\lambda})$ solves the following integral equation:

$$\rho_1^s(k;\,\bar{\lambda}) = -\frac{\cos k}{8c}\,S_1\Big(\frac{\pi}{c}\bar{\lambda}\;\Big|\;\frac{\pi}{c}\sin k\Big) + \frac{2\cos k}{c}\int_{-D_0}^{D_0} dk'\mathcal{R}_1\Big(\frac{\sin k}{c}\;\Big|\;\frac{\sin k'}{c}\Big) \times \rho_1^s(k',\,\bar{\lambda})\,. \qquad (16)$$

From the asymptotic behavior of the S_1 one can find that the spinon excitation is gapless.

The excitation in charge configuration is a variation from the ground state in the sequence of charge quantum numbers $\{I_j\}$. The simplest case is the holon-antiholon excitation, i.e., one hole $k_h \in [-D_0, D_0]$ and one "particle" $k_p \notin [-D_0, D_0]$ state. In this case $\rho_h = \delta(k\,|\,k_h)/L$, the integral equations (9) give

$$\rho_1^c(k) = -\delta(k\,|\,k_h) + \cos k\int_{-\infty}^{\infty} d\lambda'\,K_{\frac{1}{2}}(\sin k\,|\,\lambda')\sigma_1^c(\lambda')\,,$$
$$\sigma_1^c(\lambda) = K_{\frac{1}{2}}(\lambda\,|\,\sin k_p) + \int_{-D_0}^{D_0} dk'\,K_{\frac{1}{2}}(\lambda\,|\,\sin k')\rho_1^c(k') - \int_{-\infty}^{\infty} d\lambda'\,K_1(\lambda\,|\,\lambda')\sigma_1^c(\lambda')\,. \qquad (17)$$

The excitation energy is composed of two terms $\Delta E = \varepsilon_c(k_h) - \varepsilon_c(k_p)$. They can be identified as a holon excitation energy $\varepsilon_c(k_h)$ and an antiholon (particle state) excitation energy $\bar{\varepsilon}_c = -\varepsilon_c(k_p)$, respectively, namely,

$$\varepsilon_c(\bar{k}) = 2t\cos\bar{k} - \int_{-D_0}^{D_0} dk\,(2t\cos k + \mu)\rho_1^c(k,\,\bar{k})\,, \qquad (18)$$

where the $\rho_1^c(k,\,\bar{k})$ is determined by

$$\rho_1^c(k;\,\bar{k}) = \frac{2\cos k}{c}\Big[\mathcal{R}_1\Big(\frac{\sin k}{c}\;\Big|\;\frac{\sin\bar{k}}{c}\Big) + \int_{-D_0}^{D_0} dk'\,\mathcal{R}_1\Big(\frac{\sin k}{c}\;\Big|\;\frac{\sin k'}{c}\Big) \times \rho_1^c(k';\,\bar{k})\Big]\,.$$

Since both k_h and k_p can tend to D_0, the holon-antiholon excitation is of no gap. A further case is the holon-holon excitation which involves complex k pairs and is gapful.

The excitation in spin configuration is allowed to form a singlet, i.e., two holes and a two-string $\bar{\lambda}^{\pm} = (\bar{\lambda}_1 + \bar{\lambda}_2)/2 \pm ic/2$. The excitation energy is composed of two terms

$$\Delta E_{\rm sing} = \varepsilon_s(\bar{\lambda}_1) + \varepsilon_s(\bar{\lambda}_2)\,. \qquad (19)$$

These two terms are free spinon excitation energies given by (15) and (16).

In summary, we obtained an exact solution for the Hubbard model with the realistic quantum-wire boundary condition that the possibility of a nonvanishing wave function outside is taken into account. The ground state and some low-lying excitations are studied in the thermodynamic limit.

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