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Elementary excitations for the one-dimensional Hubbard model at finite temperatures

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Abstract. The elementary excitations for the one-dimensional Hubbard model at finite temperatures are studied with the use of the Bethe ansatz solution. The formulation is based on the method of Yang and Yang, which was developed for the one-dimensional boson systems with the δ-function type interaction. The dispersion relations and the excitation spectrums are obtained numerically for the charge and the spin degrees of freedom.

1. Introduction

Low-dimensional correlated electron systems have been studied intensively in recent years. In particular, metallic states close to the Mott insulator have attracted much interest. The one-dimensional (1D) Hubbard model is considered to be one of the fundamental models to describe both the quantum fluctuation and the metal–insulator transition in low-dimensional correlated electron systems, and is exactly solvable by means of the Bethe ansatz [1]. Various properties of the model, such as the ground-state properties, elementary excitations at zero temperature and thermodynamics have been investigated with the use of the Bethe ansatz solution [2]. Moreover, recent studies based on the conformal field theory [3, 4] and the bosonization method [5] have made it possible to calculate critical exponents for various correlation functions of the 1D Hubbard model precisely, and have clarified the universality class of the system as the Tomonaga–Luttinger liquid.

In the Hubbard model, physical quantities concerning the charge degrees of freedom, as well as the spin degrees of freedom, exhibit characteristic features. For example, in the 1D case, it has been shown that the charge susceptibility exhibits a divergence behaviour in the vicinity of the Mott insulating phase, and this behaviour is considered to be brought about by the Coulomb repulsion combined with the lattice structure [6]. In fact, the divergence behaviour of the charge susceptibility near the Mott insulating phase is also seen in the two-dimensional (2D) Hubbard model on a square lattice [7]. In this paper, we calculate the elementary excitations for the 1D Hubbard model at finite temperatures, laying stress on the charge excitation in the half-filled and near the half-filled cases. The formulation for the elementary excitations at finite temperatures is based on the method of Yang and Yang [8]. It is worth noting that in the Kondo problem, the elementary excitation spectrums at finite temperatures show behaviours characteristic of the local correlation effect in the system [9]. In section 2, we summarize the thermodynamic Bethe ansatz method for the 1D Hubbard model developed by Takahashi [10]. In section 3, we formulate the elementary excitations

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for the charge and the spin degrees of freedom. Numerical results for the dispersion curves and the excitation spectrums are presented in this section. Section 4 is devoted to the summary of this paper.

2. Bethe ansatz equations at finite temperatures

We consider the 1D Hubbard Hamiltonian,

$$H = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + 4U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu_0 H \sum_{i} (n_{i\uparrow} - n_{i\downarrow}) \tag{1}$$

where $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. In the following, we use t as a unit of the energy. In the Bethe ansatz method, the wavefunction for the many-body state is obtained as a superposition of the plane wave. On applying the periodic boundary condition, the basic algebraic equations of this model are obtained with the use of rapidities k_j and Λ_α concerning the charge and the spin degrees of freedom, respectively [1],

$$\exp(\mathrm{i}k_j N_a) = \prod_{\alpha=1}^{M} \frac{\sin k_j - \Lambda_\alpha + \mathrm{i}U}{\sin k_j - \Lambda_\alpha - \mathrm{i}U} \tag{2}$$

$$\prod_{j=1}^{N} \frac{\Lambda_\alpha - \sin k_j + \mathrm{i}U}{\Lambda_\alpha - \sin k_j - \mathrm{i}U} = -\prod_{\beta=1}^{M} \frac{\Lambda_\alpha - \Lambda_\beta + \mathrm{i}2U}{\Lambda_\alpha - \Lambda_\beta - \mathrm{i}2U} \tag{3}$$

where N_a, N and M are the numbers of sites, electrons and down spins, respectively. While rapidities are all real in the ground state [1], complex rapidities are introduced in order to describe excited states at finite temperatures [10]. The complex spin rapidities are given by two sets of the series which are called string solutions:

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \mathrm{i}(n+1-2j)U \qquad (n = 1, 2, \ldots; \ j = 1, 2, \ldots, n) \qquad (\alpha = 1, 2, \ldots, M'_n) \tag{4}$$

$$\Lambda_\alpha^{n,j} = \Lambda_\alpha^n + \mathrm{i}(n+1-2j)U \qquad (n = 1, 2, \ldots; \ j = 1, 2, \ldots, n) \qquad (\alpha = 1, 2, \ldots, M_n). \tag{5}$$

Here $M'_n(M_n)$ is the number of $\lambda_\alpha^n(\Lambda_\alpha^n)$. The complex charge rapidities $\{k_\alpha^{n,l}\}(l = 1, \ldots, 2n)$ are related to one of the sets of the complex spin rapidities as

$$k_\alpha^{n,1} = \pi - \sin^{-1}(\lambda_\alpha^n + \mathrm{i}nU) \tag{6}$$

$$k_\alpha^{n,2j} = \sin^{-1}[\lambda_\alpha^n + \mathrm{i}(n-2j)U] \qquad k_\alpha^{n,2j+1} = \pi - k_\alpha^{n,2j} \qquad (j = 1, 2, \ldots, n-1) \tag{7}$$

$$k_\alpha^{n,2n} = \pi - \sin^{-1}(\lambda_\alpha^n - \mathrm{i}nU). \tag{8}$$

In the description of the complex rapidities the corrections of $\mathrm{O}(\exp(-\delta N_a))$ or $\mathrm{O}(\exp(-\delta N))$ (δ a positive number) are included, but they vanish in the thermodynamic limit. The real parts of these rapidities and the real charge rapidities $k_j (j = 1, 2, \ldots, N - 2M')$ satisfy the following equations:

$$k_j N_a = 2\pi I_j - \sum_{n=1}^{\infty} \left[\sum_{\alpha=1}^{M_n} \theta\left(\frac{\sin k_j - \Lambda_\alpha^n}{nU}\right) + \sum_{\alpha=1}^{M'_n} \theta\left(\frac{\sin k_j - \lambda_\alpha^n}{nU}\right) \right] \tag{9}$$

$$N_a[\sin^{-1}(\lambda_\alpha^n + \mathrm{i}nU) + \sin^{-1}(\lambda_\alpha^n - \mathrm{i}nU)] = 2\pi K_\alpha^n + \sum_{j=1}^{N-2M'} \theta\left(\frac{\lambda_\alpha^n - \sin k_j}{nU}\right)$$

$$+\sum_{m=1}^{\infty}\sum_{\beta=1}^{M'_m}\Theta_{nm}\left(\frac{\lambda_\alpha^n-\lambda_\beta^m}{U}\right) \tag{10}$$

$$\sum_{j=1}^{N-2M'}\theta\left(\frac{\Lambda_\alpha^n-\sin k_j}{nU}\right)=2\pi J_\alpha^n+\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m}\Theta_{nm}\left(\frac{\Lambda_\alpha^n-\Lambda_\beta^m}{U}\right) \tag{11}$$

where $M'=\sum_{n=1}^{\infty}nM'_n$ and

$$\theta(x)=2\tan^{-1}x \tag{12}$$

$$\Theta_{nm}(x)=\begin{cases}\theta\left(\dfrac{x}{n+m}\right)+2\theta\left(\dfrac{x}{n+m-2}\right)+\cdots \\ \quad\cdots+2\theta\left(\dfrac{x}{|n-m|+2}\right)+\theta\left(\dfrac{x}{|n-m|}\right) & (n\neq m) \\ \theta\left(\dfrac{x}{2n}\right)+2\theta\left(\dfrac{x}{2n-2}\right)+\cdots+2\theta\left(\dfrac{x}{2}\right) & (n=m).\end{cases} \tag{13}$$

Quantum numbers I_j, K_α^n and J_α^n specify k_j, λ_α^n and Λ_α^n, respectively. The total energy and the total momentum of the system are given by

$$E=\sum_{j=1}^{N-2M'}(-2\cos k_j-\mu_0H)+\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M'_n}4\mathrm{Re}\sqrt{1-(\lambda_\alpha^n-\mathrm{i}nU)^2}+2\mu_0H\sum_{n=1}^{\infty}nM_n \tag{14}$$

$$P=\frac{2\pi}{N_a}\left(\sum_{j=1}^{N-2M'}I_j+\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n}J_\alpha^n-\sum_{n=1}^{\infty}\sum_{\alpha=1}^{M'_n}K_\alpha^n\right)+\sum_{n=1}^{\infty}(n+1)M'_n\pi. \tag{15}$$

In the thermodynamic limit, equations (9)–(11) are reduced to the set of the following integral equations:

$$\frac{1}{2\pi}=\rho(k)+\rho^h(k)-\cos k\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}\Lambda\, F_n(\sin k-\Lambda)[\sigma_n(\Lambda)+\sigma'_n(\Lambda)] \tag{16}$$

$$\frac{1}{\pi}\mathrm{Re}\frac{1}{\sqrt{1-(\Lambda-\mathrm{i}nU)^2}}-\int_{-\pi}^{\pi}\mathrm{d}k\, F_n(\Lambda-\sin k)\rho(k)=\sigma_n'^h(\Lambda)+\sum_{m=1}^{\infty}A_{nm}(\Lambda)*\sigma'_m(\Lambda) \tag{17}$$

$$\int_{-\pi}^{\pi}\mathrm{d}k\, F_n(\Lambda-\sin k)\rho(k)=\sigma_n^h(\Lambda)+\sum_{m=1}^{\infty}A_{nm}(\Lambda)*\sigma_m(\Lambda) \tag{18}$$

where $\rho(k)$, $\sigma'_n(\Lambda)$ and $\sigma_n(\Lambda)(\rho^h(k)$, $\sigma_n'^h(\Lambda)$ and $\sigma_n^h(\Lambda))$ are the distribution functions for the particle(hole) states of k_j, λ_α^n and Λ_α^n, and an asterisk denotes convolution. $F_n(x)$ and $A_{nm}(x)$ are defined as

$$F_n(x)=\frac{1}{\pi}\frac{nU}{x^2+(nU)^2} \tag{19}$$

$$A_{nm}(x)=\delta_{nm}\delta(x)+\frac{1}{2\pi}\frac{\mathrm{d}}{\mathrm{d}x}\Theta_{nm}\left(\frac{x}{U}\right). \tag{20}$$

At temperature T ($k_B=1$), the distribution functions at thermal equilibrium must minimize the thermodynamic potential $\Omega=E-TS-\mu N$ [10], where μ is the chemical potential. From the condition $\delta\Omega=0$ the following equations are derived:

$$\frac{\kappa(k)}{T}=\frac{-2\cos k-\mu_0H-\mu}{T}+\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}\Lambda\, F_n(\sin k-\Lambda)$$

$$\times\{\ln[1+\exp(-\varepsilon_n'(\Lambda)/T)] - \ln[1+\exp(-\varepsilon_n(\Lambda)/T)]\} \tag{21}$$

$$\ln[1+\exp(\varepsilon_n'(\Lambda)/T)] = \frac{4\mathrm{Re}\sqrt{1-(\Lambda-\mathrm{i}nU)^2} - 2n\mu}{T} - \int_{-\pi}^{\pi} \mathrm{d}k \cos k F_n(\Lambda - \sin k) \ln[1+\exp(-\kappa(k)/T)] + \sum_{m=1}^{\infty} A_{nm}(\Lambda) * \ln[1+\exp(-\varepsilon_m'(\Lambda)/T)] \tag{22}$$

$$\ln[1+\exp(\varepsilon_n(\Lambda)/T)] = \frac{2n\mu_0 H}{T} - \int_{-\pi}^{\pi} \mathrm{d}k \cos k F_n(\Lambda - \sin k) \ln[1+\exp(-\kappa(k)/T)] + \sum_{m=1}^{\infty} A_{nm}(\Lambda) * \ln[1+\exp(-\varepsilon_m(\Lambda)/T)]. \tag{23}$$

Here $\kappa(k)$, $\varepsilon_n'(\Lambda)$ and $\varepsilon_n(\Lambda)$ are the pseudo-energies defined as

$$\kappa(k) \equiv T\ln[\rho^h(k)/\rho(k)] \qquad \varepsilon_n'(\Lambda) \equiv T\ln[\sigma_n'^h(\Lambda)/\sigma_1'(\Lambda)]$$

and

$$\varepsilon_n(\Lambda) \equiv T\ln[\sigma_n^h(\Lambda)/\sigma_n(\Lambda)]$$

respectively.

The equations presented above are the Bethe ansatz solutions of the 1D Hubbard model at finite temperatures, which were given by Takahashi [10]. Using these results, we derive the expression for the elementary excitations at finite temperatures and give numerical results in the next section.

3. Elementary excitations at finite temperatures

In order to investigate the elementary excitations at finite temperatures, let us recall here that the ground state is described by real charge and spin rapidities [1], and that the free-energy functional at thermal equilibrium is expressed only by real rapidities [10]. Therefore, it is probable that low-temperature properties of the system are mainly controlled by real rapidities. Based on these observations, the elementary excitations at finite temperatures are considered to be obtained by removing one of real rapidities, with the total electron number being fixed. In this section, we derive the formulae for the shifts of the energy and the momentum due to the excitation, following the method of Yang and Yang [8]. The formulation is made for the charge excitation in the cases of $N/N_a < 1$ and $N/N_a = 1$, and also for the spin excitation. Based on the derived formulae, numerical results for the dispersion curves and the excitation spectrums are presented.

3.1. Charge excitations

3.1.1. $N/N_a < 1$*.* First, we consider the case of $N/N_a < 1$. As mentioned above, we insert a hole into the real charge rapidity at a value k_h or the corresponding quantum number I_h, and add a particle to the real charge rapidity at k_p or I_p, other quantum numbers remaining unchanged. This procedure corresponds to the particle–hole excitation. Because of this procedure, the distribution of rapidities is rearranged through the phase shift described by the equations (9)–(11) (the back-flow effect). After the excitation, the basic equations (9)–(11) are expressed in terms of $\{k_j'\}$, $\{\lambda_\alpha^{n'}\}$ and $\{\Lambda_\alpha^{n'}\}$, where $\{k_j'\}$, $\{\lambda_\alpha^{n'}\}$ and $\{\Lambda_\alpha^{n'}\}$ are the new sets of rapidities. We write the shifts of rapidities as

$$\frac{1}{N_a}\Delta k_j = k_j' - k_j \tag{24}$$

$$\frac{1}{N_a}\Delta\lambda_\alpha^n = \lambda_\alpha^{n'} - \lambda_\alpha^n \tag{25}$$

$$\frac{1}{N_a}\Delta\Lambda_\alpha^n = \Lambda_\alpha^{n'} - \Lambda_\alpha^n. \tag{26}$$

Since the shifts of rapidities $(1/N_a)\Delta k_j$, $(1/N_a)\Delta\lambda_\alpha^n$ and $(1/N_a)\Delta\Lambda_\alpha^n$ are sufficiently small, we take them into account to only lowest order in the basic equations. Expanding basic equations in terms of the shifts of rapidities, we obtain the following equations:

$$\frac{1}{2\pi}\Delta k_j = -\frac{1}{N_a}\sum_{n=1}^{\infty}\left[\sum_{\alpha=1}^{M_n} F_n(\sin k_j - \Lambda_\alpha^n)\cdot(\cos k_j \Delta k_j - \Delta\Lambda_\alpha^n) + \sum_{\alpha=1}^{M_n'} F_n(\sin k_j - \lambda_\alpha^n) \times(\cos k_j \Delta k_j - \Delta\lambda_\alpha^n)\right] \tag{27}$$

$$\frac{1}{\pi}\mathrm{Re}\frac{1}{\sqrt{1-(\lambda_\alpha^n - \mathrm{i}nU)^2}}\Delta\lambda_\alpha^n = \frac{1}{N_a}\sum_{j=1}^{N-2M'} F_n(\lambda_\alpha^n - \sin k_j)\cdot(\Delta\lambda_\alpha^n - \cos k_j \Delta k_j) + \frac{1}{N_a}\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m'} B_{nm}(\lambda_\alpha^n - \lambda_\beta^m)\cdot(\Delta\lambda_\alpha^n - \Delta\lambda_\beta^m) + \frac{1}{2\pi}\left[\theta\left(\frac{\lambda_\alpha^n - \sin k_p}{nU}\right) - \theta\left(\frac{\lambda_\alpha^n - \sin k_h}{nU}\right)\right] \tag{28}$$

$$\frac{1}{N_a}\sum_{j=1}^{N-2M'} F_n(\Lambda_\alpha^n - \sin k_j)\cdot(\Delta\Lambda_\alpha^n - \cos k_j \Delta k_j) = \frac{1}{N_a}\sum_{m=1}^{\infty}\sum_{\beta=1}^{M_m} B_{nm}(\Lambda_\alpha^n - \Lambda_\beta^m) \times(\Delta\Lambda_\alpha^n - \Delta\Lambda_\beta^m) - \frac{1}{2\pi}\left[\theta\left(\frac{\Lambda_\alpha^n - \sin k_p}{nU}\right) - \theta\left(\frac{\Lambda_\alpha^n - \sin k_h}{nU}\right)\right] \tag{29}$$

where $B_{nm}(x) \equiv A_{nm}(x) - \delta_{nm}\delta(x)$. In the thermodynamic limit, the set of coupled integral equations is derived:

$$[\rho(k) + \rho^h(k)]\Delta k(k) = \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, F_n(\sin k - \Lambda)[\sigma_n(\Lambda)\Delta\Lambda_n(\Lambda) + \sigma_n'(\Lambda)\Delta\lambda_n(\Lambda)] \tag{30}$$

$$\sigma_n'^h(\Lambda)\Delta\lambda_n(\Lambda) = -\int_{-\pi}^{\pi} \mathrm{d}k \cos k\, F_n(\Lambda - \sin k)\rho(k)\Delta k(k) - \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m'(\Lambda)\Delta\lambda_m(\Lambda)] + \frac{1}{2\pi}\left[\theta\left(\frac{\Lambda - \sin k_p}{nU}\right) - \theta\left(\frac{\Lambda - \sin k_h}{nU}\right)\right] \tag{31}$$

$$\sigma_n^h(\Lambda)\Delta\Lambda_n(\Lambda) = \int_{-\pi}^{\pi} \mathrm{d}k \cos k\, F_n(\Lambda - \sin k)\rho(k)\Delta k(k) - \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m(\Lambda)\Delta\Lambda_m(\Lambda)] - \frac{1}{2\pi}\left[\theta\left(\frac{\Lambda - \sin k_p}{nU}\right) - \theta\left(\frac{\Lambda - \sin k_h}{nU}\right)\right]. \tag{32}$$

In this way, the shifts of rapidities due to the back-flow effect are determined completely by the above set of integral equations.

Now we can calculate the energy increment associated with the elementary excitation. The excitation energy is given by the sum of the bare energy change and the energy change due to the back-flow effect:

$$\Delta E\left(k_p, k_h\right) = -2\cos k_p + 2\cos k_h + \int_{-\pi}^{\pi} \mathrm{d}k\, \rho(k)\Delta k(k) 2\sin k + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \sigma_n'(\Lambda)\Delta\lambda_n(\Lambda)\left[\frac{\mathrm{d}}{\mathrm{d}\Lambda} 4\mathrm{Re}\sqrt{1-(\Lambda - \mathrm{i}nU)^2}\right]. \tag{33}$$

Differentiating the equations (21)–(23) with respect to rapidities and substituting them into the expression (33), we obtain

$$\begin{aligned}\Delta E(k_p, k_h) = {}& -2\cos k_p + 2\cos k_h + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda \Big\{\sigma_n'^h(\Lambda)\Delta\lambda_n(\Lambda) \\ & + \int_{-\pi}^{\pi} \mathrm{d}k \cos k F_n(\Lambda - \sin k)\rho(k)\Delta k(k) + \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m'(\Lambda)\Delta\lambda_m(\Lambda)]\Big\} \\ & \times \frac{1}{1+\exp(\varepsilon_n'(\Lambda)/T)}\frac{\mathrm{d}\varepsilon_n'(\Lambda)}{\mathrm{d}\Lambda} + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda \Big\{\sigma_n^h(\Lambda)\Delta\Lambda_n(\Lambda) \\ & - \int_{-\pi}^{\pi} \mathrm{d}k \cos k F_n(\Lambda - \sin k)\rho(k)\Delta k(k) + \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m(\Lambda)\Delta\Lambda_m(\Lambda)]\Big\} \\ & \times \frac{1}{1+\exp(\varepsilon_n(\Lambda)/T)}\frac{\mathrm{d}\varepsilon_n(\Lambda)}{\mathrm{d}\Lambda} + \int_{-\pi}^{\pi} \mathrm{d}k \Big\{[\rho(k) + \rho(k)h]\Delta k(k) \\ & - \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda F_n(\sin k - \Lambda)[\sigma_n(\Lambda)\Delta\Lambda_n(\Lambda) + \sigma_n'(\Lambda)\Delta\lambda_n(\Lambda)]\Big\} \\ & \times \frac{1}{1+\exp(\kappa(k)/T)}\frac{\mathrm{d}\kappa(k)}{\mathrm{d}k}. \end{aligned} \tag{34}$$

Using equations (30)–(32), we find finally the simple formula for the excitation energy renormalized by the back-flow effect as

$$\Delta E(k_p, k_h) = \kappa(k_p) - \kappa(k_h). \tag{35}$$

It is noted that the excitation energy can be expressed by using only the pseudo-energy for the real charge rapidity at thermal equilibrium.

The total momentum after the particle–hole excitation is evaluated as

$$P' = \frac{2\pi}{N_a}\left[\left(\sum_{j=1}^{N-2M'} I_j' - I_h' + I_p'\right) + \sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n} J_\alpha^{n'} - \sum_{n=1}^{\infty}\sum_{\alpha=1}^{M_n'} K_\alpha^{n'}\right] + \sum_{n=1}^{\infty}(n+1)M_n'\pi \tag{36}$$

where $\{I_j'\}$, $\{K_\alpha^{n'}\}$ and $\{J_\alpha^{n'}\}$ are the new sets of the quantum numbers, which satisfy the relations $I_j' = I_j$ $(I_j \neq I_p, I_j \neq I_h)$, $K_\alpha^{n'} = K_\alpha^n$ and $J_\alpha^{n'} = J_\alpha^n$. Subtracting (15) from (36), we derive the shift of the total momentum due to the elementary excitation as follows,

$$\Delta P(I_p, I_h) = \frac{2\pi}{N_a}(I_p - I_h). \tag{37}$$

In the thermodynamic limit, (37) can be written as

$$\Delta P(k_p, k_h) = p_c(k_p) - p_c(k_h) \tag{38}$$

$$p_c(k) = \frac{k}{2\pi} + \frac{1}{2\pi}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda \left[\theta\left(\frac{\sin k - \Lambda}{nU}\right)\sigma_n(\Lambda) + \theta\left(\frac{\sin k - \Lambda}{nU}\right)\sigma_n'(\Lambda)\right]. \tag{39}$$

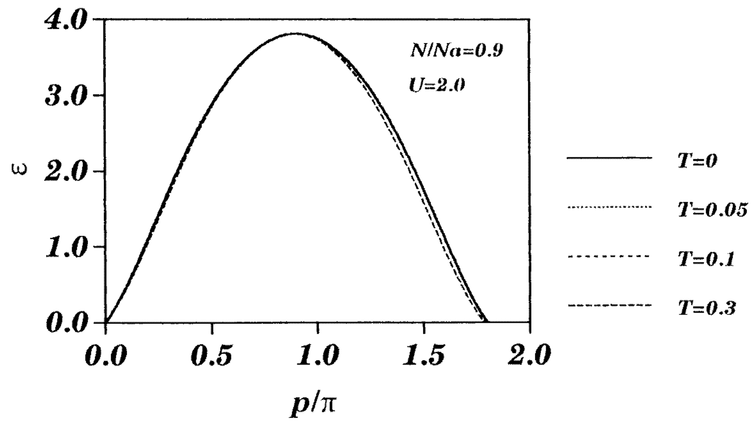


Figure 1. Dispersion relations of the charge excitation for $N/N_a = 0.9$ and $U = 2.0$ with k_p being fixed at Q, where Q is the cut-off at zero temperature.

As seen in (38), the shift of the total momentum is also written in a simple form by using $p_c(k)$. This expression is recast into the following formula:

$$\Delta P(k_p, k_h) = 2\pi \int_{k_h}^{k_p} \mathrm{d}k[\rho(k) + \rho^h(k)]. \tag{40}$$

Using (35) and (40), the dispersion curves for the model at finite temperatures are obtained. At zero temperature, the real charge rapidity occupies the region $[-Q, Q]$ fully, and the lower bound of the dispersion curve is obtained when k_p is fixed at Q or $-Q$. At finite temperatures, however, a clear cut-off of the rapidity does not exist because particles and holes are distributed randomly. Therefore, we have to determine the position of k_p in order to obtain the energy of the elementary excitation. In the previous papers for other models [9, 11, 12], the excitation energy was defined as $\Delta E(\Lambda) = \varepsilon(-\infty) - \varepsilon(\Lambda)$, where $\varepsilon(\Lambda)$ is the pseudo-energy for the rapidity Λ and $\Lambda = -\infty$ corresponds to the cut-off at zero temperature. As a reference, we have calculated the dispersion relations of the charge excitation for $N/N_a < 1$, taking k_p as $k_p = Q$. Numerical results are shown in figure 1 in the case of $U = 2.0$.

In the present calculation, however, we make more plausible choice: we take k_p as $Q(T)$ which satisfies $\kappa(Q(T)) = 0$. In the limit of $T \to 0$, the pseudo-energy $\kappa(k)$ satisfies $\kappa(Q) = 0$. We extend this relation between the pseudo-energy and the cut-off to the case of finite temperatures. It should be noted that for both choices of k_p, the excitation energy and the shift of the total momentum in the limit of $T \to 0$ coincide with those at zero temperature. In figure 2, we show the temperature dependence of the dispersion curves in the case of $N/N_a = 0.9$. In these figures, $\varepsilon \equiv \Delta E(k_p, k) = \kappa(k_p) - \kappa(k)$ and $p \equiv \Delta P(k_p, k) = 2\pi \int_k^{k_p} \mathrm{d}k' [\rho(k') + \rho^h(k')]$ with fixed k_p, and $k(\geqslant 0)$ denotes k_h. Numerical results are shown for $U = 0.5$ and 2.0 in the case of $H = 0$. Note that for $U = 2.0$ the system can be regarded as being in the strong coupling regime, because the temperature dependence of the spin susceptibility of the 1D Hubbard model is fairly well described by the 1D Heisenberg antiferromagnet, in the case of $U = 2.0$ and 3.0 [13]. For $U = 0.5$, the dispersion curve seems to be linear in the vicinity of $p = 0$ and has little temperature dependence. On the other hand, for $U = 2.0$, the velocity near $p = 0$ tends to decrease and the maximum of the excitation energy is enhanced slightly, as temperature is increased.

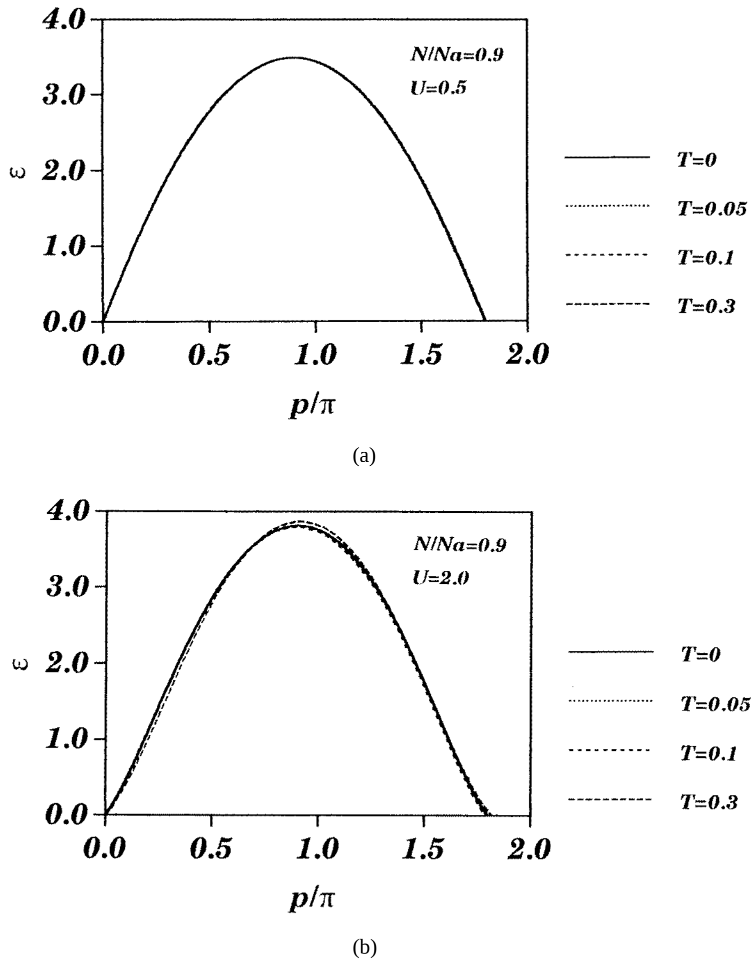


Figure 2. Dispersion relations of the charge excitation at $N/N_a = 0.9$ for several values of temperature T. The results for (a) $U = 0.5$ and (b) $U = 2.0$ are shown.

We now introduce the spectral density for the charge excitation as a function of the excitation energy. This is given by counting the number of particle states in a given range of the excitation energy $[\varepsilon, \varepsilon + \mathrm{d}\varepsilon]$,

$$D_c(\varepsilon(k)) = 2\frac{\rho(k)}{|\mathrm{d}\varepsilon(k)/\mathrm{d}k|}. \tag{41}$$

In order to see the temperature dependence of the spectral density for the charge excitation clearly, it is helpful to introduce the *whole* excitation spectrum

$$D_c^{whole}(\varepsilon(k)) = 2\frac{\rho(k) + \rho^h(k)}{|\mathrm{d}\varepsilon(k)/\mathrm{d}k|} \tag{42}$$

which is obtained by counting the number of both particle and hole states in a range of the excitation energy $[\varepsilon, \varepsilon + \mathrm{d}\varepsilon]$. These spectral densities satisfy the relation

$$D_c(\varepsilon(k)) = \frac{1}{\exp[(-\varepsilon(k) + \kappa(k_p))/T] + 1} D_c^{whole}(\varepsilon(k)). \tag{43}$$

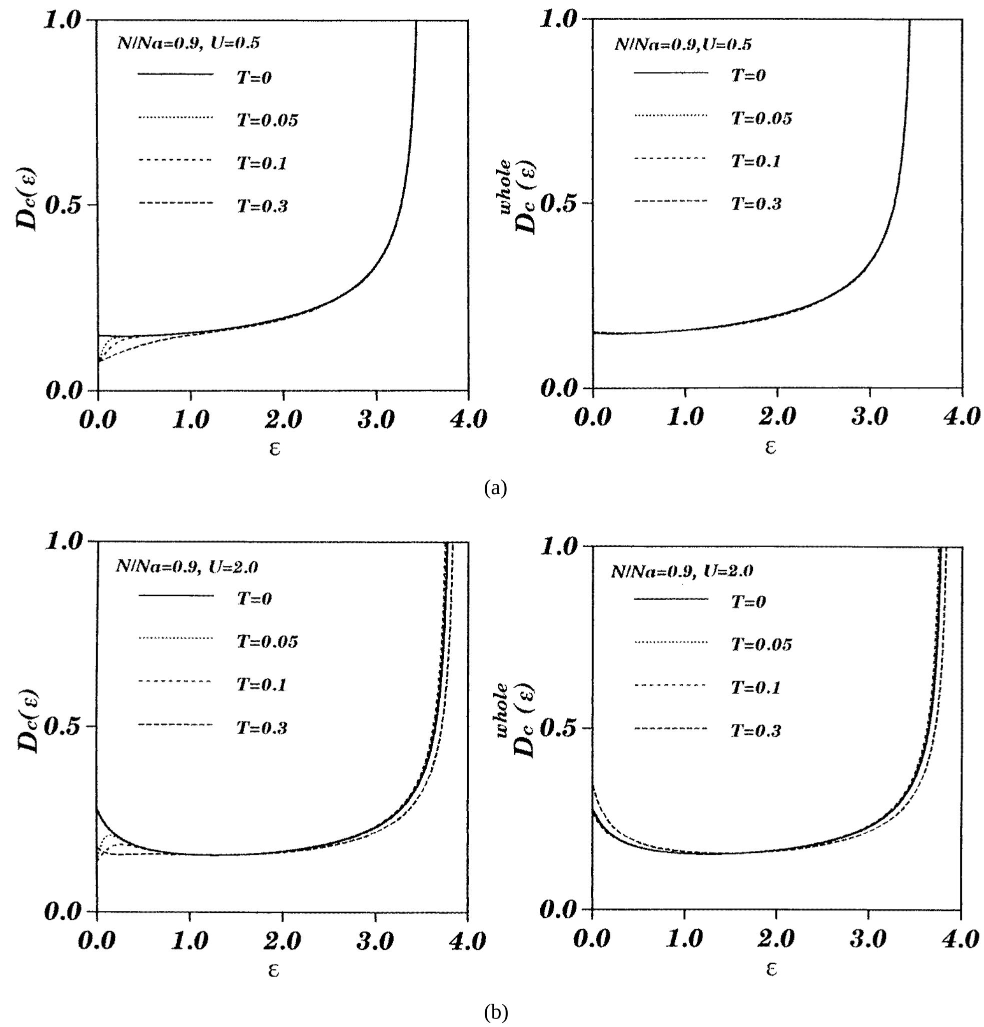


Figure 3. Charge excitation spectrums $D_c(\varepsilon)$ and $D_c^{whole}(\varepsilon)$ defined in the equations (41) and (42) for $N/N_a = 0.9$. The results in the case of (a) $U = 0.5$ and (b) $U = 2.0$ are shown for the same values of T as figure 2.

In figure 3, we show the results for $D_c(\varepsilon)$ and $D_c^{whole}(\varepsilon)$ in the case of $H = 0$. For both $U = 0.5$ and 2.0, the whole excitation spectrum is nearly identical. Therefore, the temperature dependence of the excitation spectrum $D_c(\varepsilon)$ in the low-energy region is caused mainly by that of the 'Fermi distribution function' in (43).

In the present paper, we could not make a definite choice for the position of the rapidity being added. This difficulty is inherent in the calculation of the excitation spectrum using the method of Yang and Yang. We leave this problem for future investigation.

3.1.2. $N/N_a = 1$ (half-filled case). At zero temperature, we cannot treat the particle–hole excitation within the real charge rapidity in the half-filled case, since the available region $[-\pi, \pi]$ is occupied fully. This is due to the fact that real charge rapidities can describe only the excitation within the lower band. In order to treat a particle excitation to the upper band, we should introduce a two-string solution for the charge rapidity [14, 15]. In this way, the particle–hole excitation is formulated for the charge excitation in the half-filled case. It is noted that in this treatment, the total electron number is conserved. We will extend the formulation for the particle–hole excitation to the case of finite temperatures.

Now we remove the real rapidities k_{h1} and k_{h2} and add a pair of complex charge rapidity $k_\pm(k_\pm = \pi - \sin^{-1}(\lambda_p \pm \mathrm{i}U))$. In the thermodynamic limit, the equations for the shifts of rapidities are obtained as follows:

$$[\rho(k) + \rho^h(k)]\Delta k(k) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, F_n(\sin k - \Lambda)[\sigma_n(\Lambda)\Delta\Lambda_n(\Lambda) + \sigma_n'(\Lambda)\Delta\lambda_n(\Lambda)] - \frac{1}{2\pi}\theta\left(\frac{\sin k - \lambda_p}{U}\right) \tag{44}$$

$$\sigma_n'^h(\Lambda)\Delta\lambda_n(\Lambda) = -\int_{-\pi}^{\pi} \mathrm{d}k \cos k\, F_n(\Lambda - \sin k)\rho(k)\Delta k(k) - \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m'(\Lambda)\Delta\lambda_m(\Lambda)] + \frac{1}{2\pi}\Theta_{n1}\left(\frac{\Lambda - \lambda_p}{U}\right) - \frac{1}{2\pi}\left[\theta\left(\frac{\Lambda - \sin k_{h1}}{nU}\right) + \theta\left(\frac{\Lambda - \sin k_{h2}}{nU}\right)\right] \tag{45}$$

$$\sigma_n^h(\Lambda)\Delta\Lambda_n(\Lambda) = \int_{-\pi}^{\pi} \mathrm{d}k \cos k\, F_n(\Lambda - \sin k)\rho(k)\Delta k(k) - \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m(\Lambda)\Delta\Lambda_m(\Lambda)] + \frac{1}{2\pi}\left[\theta\left(\frac{\Lambda - \sin k_{h1}}{nU}\right) + \theta\left(\frac{\Lambda - \sin k_{h2}}{nU}\right)\right]. \tag{46}$$

After the calculation similar to the case of $N/N_a < 1$, the excitation energy is derived as

$$\Delta E(\lambda_p, k_{h1}, k_{h2}) = \varepsilon_1'(\lambda_p) - \kappa(k_{h1}) - \kappa(k_{h2}) + C(T) \tag{47}$$

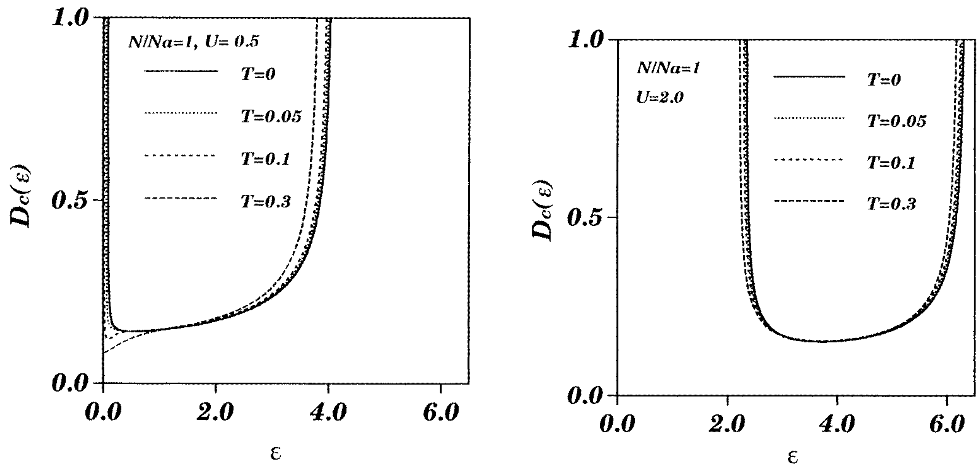
where $C(T) = -\varepsilon_1'(\pm\infty) + T\{2\ln 2 - 2\sum_{n=1}^{\infty} \ln[1 + \exp(-\varepsilon_n(\pm\infty)/T)]\}$.

In figure 4 we show the numerical results for $D_c(\varepsilon)$ in the half-filled case. Here $H = 0$ and λ_p is fixed at $\pm\infty$ to minimize the excitation energy. In this case, the excitation energy is written simply as $\Delta E(k_{h1}, k_{h2}) = -\kappa(k_{h1}) - \kappa(k_{h2})$, and we defined ε as $\varepsilon \equiv -\kappa(k)$. For $U = 0.5$, when temperature is increased, the spectrum shifts monotonously to the low-energy side and as a consequence the excitation gap disappears. In contrast, for $U = 2.0$ the width of the energy gap is kept nearly unchanged. The results imply that the charge excitation in the case of $N/N_a = 1$ is affected considerably by the strength of the Coulomb interaction.

3.2. Spin excitations

Next, we consider the spin excitation. As mentioned before, the spin excitation is given by inserting a hole into the real spin rapidity at Λ_h or J_h, and by adding a particle into the real spin rapidity at Λ_p or J_p. Expanding equations (9)–(11) in terms of the shifts of rapidities, we obtain the following set of equations for the shifts of rapidities:

$$[\rho(k) + \rho^h(k)]\Delta k(k) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, F_n(\sin k - \Lambda)[\sigma_n(\Lambda)\Delta\Lambda_n(\Lambda) + \sigma_n'(\Lambda)\Delta\lambda_n(\Lambda)] - \frac{1}{2\pi}\left[\theta\left(\frac{\sin k - \Lambda_p}{U}\right) - \theta\left(\frac{\sin k - \Lambda_h}{U}\right)\right] \tag{48}$$



(a) (b)

Figure 4. Charge excitation spectrums $D_c(\varepsilon)$ in the half-filled case for (a) $U = 0.5$ and (b) $U = 2.0$. Here $\varepsilon = 0$ corresponds to the centre of the energy gap.

$$\sigma_n^{\prime h}(\Lambda)\Delta\lambda_n(\Lambda) = -\int_{-\pi}^{\pi} \mathrm{d}k \cos k F_n(\Lambda - \sin k)\rho(k)\Delta k(k) - \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m'(\Lambda)\Delta\lambda_m(\Lambda)] \tag{49}$$

$$\sigma_n^{h}(\Lambda)\Delta\Lambda_n(\Lambda) = \int_{-\pi}^{\pi} \mathrm{d}k \cos k F_n(\Lambda - \sin k)\rho(k)\Delta k(k) - \sum_{m=1}^{\infty} A_{nm}(\Lambda) * [\sigma_m(\Lambda)\Delta\Lambda_m(\Lambda)] + \frac{1}{2\pi}\left[\Theta_{n1}\left(\frac{\Lambda - \Lambda_p}{U}\right) - \Theta_{n1}\left(\frac{\Lambda - \Lambda_h}{U}\right)\right]. \tag{50}$$

The excitation energy is given only by the contribution of the back-flow effect as

$$\Delta E(\Lambda_p, \Lambda_h) = \int_{-\pi}^{\pi} \mathrm{d}k\, \rho(k)\Delta k(k) 2\sin k + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \sigma_n'(\Lambda)\Delta\lambda_n(\Lambda) \times \left[\frac{\mathrm{d}}{\mathrm{d}\Lambda} 4\mathrm{Re}\sqrt{1 - (\Lambda - \mathrm{i}nU)^2}\right]. \tag{51}$$

Using the differentiation of equations (21)–(23) with respect to rapidities and equations (48)–(50), we can recast (51) into the simple formula with the use of the pseudo-energy of the real spin rapidity at thermal equilibrium,

$$\Delta E(\Lambda_p, \Lambda_h) = \varepsilon_1(\Lambda_p) - \varepsilon_1(\Lambda_h). \tag{52}$$

In the thermodynamic limit, the shift of the total momentum due to the spin excitation can be derived as

$$\Delta K(\Lambda_p, \Lambda_h) = p_s(\Lambda_p) - p_s(\Lambda_h) \tag{53}$$

$$p_s(\Lambda) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}k\, \theta\left(\frac{\Lambda - \sin k}{U}\right)\rho(k) - \frac{1}{2\pi}\sum_{m=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda'\, \Theta_{1m}\left(\frac{\Lambda - \Lambda'}{U}\right)\sigma_m(\Lambda') \tag{54}$$

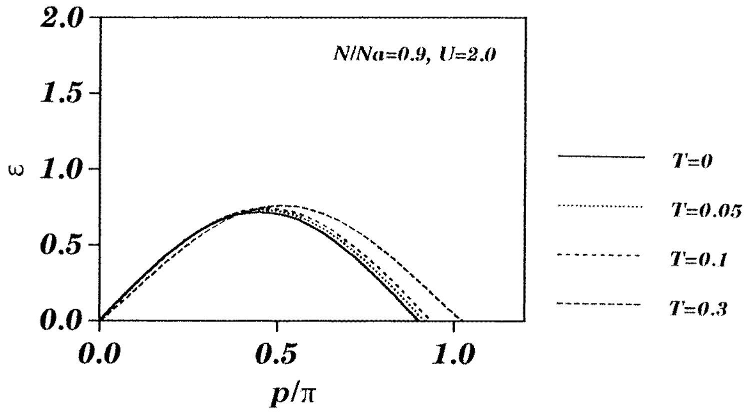


Figure 5. Dispersion relations of the spin excitation with Λ_p being fixed at ∞, where $\Lambda = \infty$ is the cut-off at zero temperature. Here $N/N_a = 0.9$ and $U = 2.0$.

then as

$$\Delta K(\Lambda_p, \Lambda_h) = 2\pi \int_{\Lambda_h}^{\Lambda_p} \mathrm{d}\Lambda\, [\sigma_1(\Lambda) + \sigma_1^h(\Lambda)]. \tag{55}$$

Note that $\Delta E(\Lambda_p, \Lambda_h)$ and $\Delta K(\Lambda_p, \Lambda_h)$ are determined only by real spin rapidities Λ_p and Λ_h.

Using (52) and (55), we obtain the dispersion curve for the spin excitation at finite temperatures. First, in figure 5, we show the dispersion curves for the spin excitation in the case where Λ_p is fixed at the cut-off of the spin rapidity at $T = 0$. The results agree qualitatively with those of the $S = 1/2$ 1D Heisenberg antiferromagnet at finite temperatures obtained previously [11].

In the present calculation, we take Λ_p as $B(T)$ which satisfies $\varepsilon_1(B(T)) = 0$, because $\varepsilon_1(\Lambda)$ satisfies $\varepsilon_1(B) = 0$ (B is the cut-off of the spin rapidity at zero temperature) in the limit of $T \to 0$. In figure 6, numerical results are shown for $U = 0.5$ and 2.0 in the case of $H = 0$. In the figures, $\varepsilon \equiv \Delta E(\Lambda_p, \Lambda) = \varepsilon_1(\Lambda_p) - \varepsilon_1(\Lambda)$ and $p \equiv \Delta K(\Lambda_p, \Lambda) = 2\pi \int_{\Lambda}^{\Lambda_p} \mathrm{d}\Lambda' [\sigma_1(\Lambda') + \sigma_1^h(\Lambda')]$ with Λ_p being fixed, and $\Lambda(\geqslant 0)$ is Λ_h. For both $U = 0.5$ and $U = 2.0$, the maxima of the excitation energy and the shift of the total momentum are reduced considerably with increasing temperature. The dispersion curve of the spin excitation shows qualitatively the same behaviour irrespective of the value of U and N/N_a.

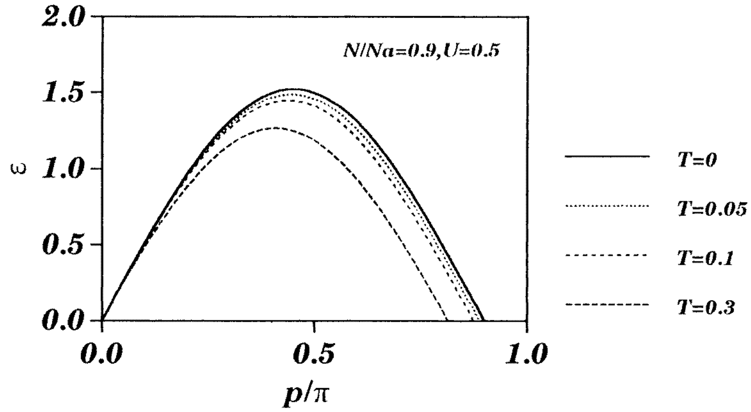
Similar to the case of the charge excitations, we define the spectral density for the spin excitation as follows,

$$D_s(\varepsilon(\Lambda)) = 2\frac{\sigma_1(\Lambda)}{|\mathrm{d}\varepsilon(\Lambda)/\mathrm{d}\Lambda|}. \tag{56}$$

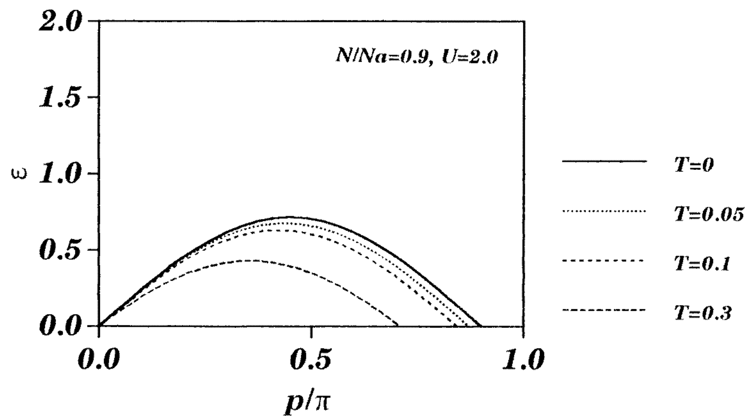
The whole excitation spectrum is given by

$$D_s^{whole}(\varepsilon(\Lambda)) = 2\frac{\sigma_1(\Lambda) + \sigma_1^h(\Lambda)}{|\mathrm{d}\varepsilon(\Lambda)/\mathrm{d}\Lambda|}. \tag{57}$$

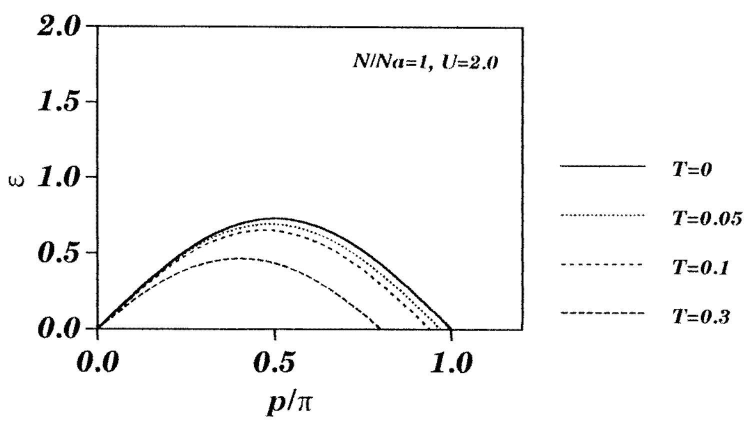
It is easily seen that $D_s(\varepsilon)$ and $D_s^{whole}(\varepsilon)$ fulfil the following relation: $D_s(\varepsilon(\Lambda)) = \{\exp[(-\varepsilon(\Lambda) + \varepsilon_1(\Lambda_p))/T] + 1\}^{-1} D_s^{whole}(\varepsilon(\Lambda))$. In figure 7 we show the numerical results for $D_s(\varepsilon)$ and $D_s^{whole}(\varepsilon)$ in the case of $H = 0$. As inferred from the dispersion curve, the width of the spectrum is reduced rapidly.



(a)



(b)



(c)

Figure 6. Dispersion relations of the spin excitation. The results at $N/N_a = 0.9$ are shown for (a) $U = 0.5$ and (b) $U = 2.0$. The results in the half-filled case are shown for $U = 2.0$ (c).

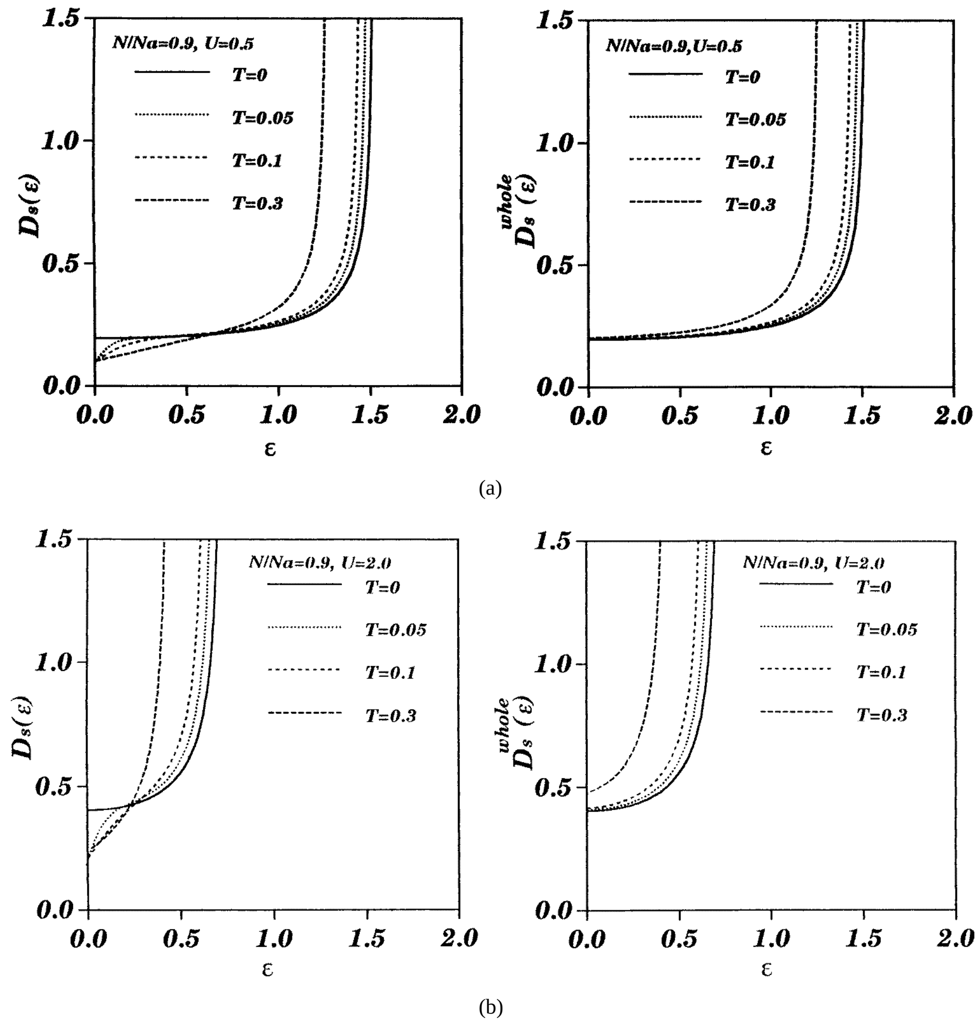


Figure 7. Spin excitation spectrums $D_s(\varepsilon)$ and $D_s^{whole}(\varepsilon)$ at $N/N_a = 0.9$ for (a) $U = 0.5$ and (b) $U = 2.0$.

4. Summary

We have investigated the elementary excitation for the 1D Hubbard model at finite temperatures, applying the method developed by Yang and Yang. It has been shown that, for both charge and spin excitations, the excitation energy can be described only by the pseudo-energy of the real rapidity, and that the shift of the total momentum is written only by using the distribution function of the real rapidity.

For both the charge and the spin degrees of freedom, the dispersion curves and the density of states for the elementary excitation have been calculated numerically, in the half-filled and near the half-filled cases.

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