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1998 J. Phys. A: Math. Gen. 31 465

(http://iopscience.iop.org/0305-4470/31/2/008)

J. Phys. A: Math. Gen. **31** (1998) 465–474. Printed in the UK PII: S0305-4470(98)87971-7

Exact Drude weight for the one-dimensional Hubbard model at finite temperatures

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Received 29 September 1997

Abstract. The Drude weight for the one-dimensional Hubbard model is investigated at finite temperatures by using the Bethe ansatz solution. Evaluating finite-size corrections to the thermodynamic Bethe ansatz equations, we obtain the formula for the Drude weight as the response of the system to an external gauge potential. We perform low-temperature expansions of the Drude weight in the case of half-filling as well as away from half-filling, which clearly distinguish the Mott-insulating state from the metallic state.

1. Introduction

The Mott–Hubbard metal–insulator transition (MIT) is one of the long-standing important issues in strongly-correlated electron systems. The one-dimensional (1D) Hubbard model is a fundamental model which describes the MIT. This model is exactly solvable in terms of the Bethe ansatz method [1]. Various thermodynamic quantities such as the specific heat and the spin and charge susceptibilities which characterize the MIT have been obtained exactly [2–4]. However, the study on transport properties, such as the Drude weight, based upon the Bethe ansatz method have been restricted to the zero temperature case [5–7]. The Drude weight at finite temperatures has so far been investigated only by using numerical methods [8, 9]. Since the Drude weight is a direct probe for the MIT [5, 10], it is desirable to obtain the exact results at finite temperatures. This is the main purpose of this paper. In order to obtain the Drude weight, it is necessary to calculate the finite-size corrections to the energy spectrum, so that we need to evaluate the finite-size corrections to the thermodynamic Bethe ansatz equations. For this purpose, we generalize standard methods for finite-size corrections based on the Euler–Maclaurin formula to the case of finite temperatures, and obtain the leading temperature dependence of the Drude weight at low temperatures.

It is easily seen from the Kubo formula that the Drude weight in translationally invariant systems is independent of temperature. Then the temperature dependence of the Drude weight for the Hubbard model comes from the interactions such as the Umklapp scattering which break translational symmetry. This implies that its temperature dependence carries information concerning how the electron correlations which control the MIT develop in low temperatures. In the case of half-filling, we indeed show how the system approaches the Mott insulator as the temperature is decreased.

The organization of this paper is as follows. In section 2, the formulation for the finite-size corrections to thermodynamic Bethe ansatz equations is given. The procedure is not

0305-4470/98/020465+10$19.50

restricted to the Hubbard model, but is also applicable to any other solvable models. In section 3, we obtain the general expression for the Drude weight at finite temperatures. The low-temperature expansion for the Drude weight is derived in section 4 both in the case of half-filling as well as away from half-filling. The leading temperature dependence is evaluated at low temperatures. A brief summary is given in section 5.

2. Finite-size corrections to the thermodynamic Bethe ansatz equations

In this section we consider finite-size effects on the Bethe ansatz solutions of the 1D Hubbard model at finite temperatures. Finite-size effects at zero temperature have been studied by many authors in connection with the application of conformal field theory [11–14]. We generalize their method to the case of finite temperatures. The Hamiltonian of the 1D Hubbard model reads

$$H = -\sum_{\sigma i} c^{\dagger}_{\sigma i} c_{\sigma i+1} + \mathrm{HC} + U \sum_{i} c^{\dagger}_{\uparrow i} c_{\uparrow i} c^{\dagger}_{\downarrow i} c_{\downarrow i}. \tag{1}$$

It is necessary to introduce the Aharonov–Bohm (AB) flux Φ to formulate the Drude weight as the response to an external gauge potential. Alternatively, the effect of the AB flux is incorporated into the twisted boundary condition for the wavefunction, $\Psi(x+L) = \mathrm{e}^{\mathrm{i}\Phi}\Psi(x)$ [15]. The Bethe ansatz equations in the presence of the AB flux are given by [1, 16],

$$\mathrm{e}^{\mathrm{i}k_j L} = \mathrm{e}^{\mathrm{i}\Phi} \prod_{\alpha=1}^{M} \frac{\sin k_j - \Lambda_\alpha + \mathrm{i}u}{\sin k_j - \Lambda_\alpha - \mathrm{i}u} \tag{2}$$

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

Here k_j and Λ_α are, respectively, the rapidities for the charge and spin degrees of freedom, and we have introduced $u = U/4$. N and M are the total number of electrons and down spins.

Thermodynamic Bethe ansatz solution for the 1D Hubbard model was obtained by Takahashi many years ago with the use of so-called string hypothesis [2]. The validity of the string hypothesis is justified only for the thermodynamic limit $L \to \infty$. In order to calculate the Drude weight, we should evaluate the energy for a finite-size system, because the effect of Φ vanishes in the thermodynamic limit. Thus one may worry about whether the string hypothesis can be applied to the calculation of the Drude weight. However, by recalling the following fact we can still adopt the string hypothesis for our purpose: the corrections to the string hypothesis for a finite-size system are estimated as $\sim\mathrm{O}(\mathrm{e}^{-cL})$, where c is a constant which depends on the temperature. On the other hand, the dependence of the energy on the AB flux appears of the order of $1/L^2$. Thus the correction to the string hypothesis for the finite-size system is much smaller than the finite-size corrections to the energy spectrum which we need for the calculation of the Drude weight. This situation is analogous to that for the Kondo model [17] or the impurity Anderson model [18, 19], where the local electron correlations, which are given by the $1/L$ corrections to the bulk quantities, are correctly evaluated based upon the string hypothesis.

Using the string hypothesis, we can thus write down the thermodynamic Bethe ansatz equations. After taking the logarithm of the above equations, we end up with

$$k_j L = 2\pi I_j + \Phi - \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} \theta\left(\frac{\sin k_j - \Lambda_\alpha^n}{nu}\right) - \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M'_n} \theta\left(\frac{\sin k_j - \Lambda_\alpha'^n}{nu}\right) \tag{4}$$

$$L(\sin^{-1}(\Lambda'^n_\alpha + \mathrm{i}nu) + \sin^{-1}(\Lambda'^n_\alpha - \mathrm{i}nu)) = 2\pi J'^n_\alpha + 2n\Phi + \sum_{j=1}^{N-2M'} \theta\left(\frac{\sin k_j - \Lambda'^n_\alpha}{nu}\right) + \sum_{m=1}^{\infty}\sum_\beta \Theta_{nm}\left(\frac{\Lambda'^n_\alpha - \Lambda'^m_\beta}{u}\right) \tag{5}$$

$$\sum_{j=1}^{N-2M'} \theta\left(\frac{\sin k_j - \Lambda^n_\alpha}{nu}\right) = 2\pi J^n_\alpha + \sum_{m=1}^{\infty}\sum_\beta \Theta_{nm}\left(\frac{\Lambda^n_\alpha - \Lambda^m_\beta}{u}\right) \tag{6}$$

with $\theta(x) = 2\tan^{-1} x$ and

$$\Theta_{nm}(x) = \begin{cases} \theta\left(\frac{x}{|n-m|}\right) + 2\theta\left(\frac{x}{|n-m|+2}\right) + \cdots \\ \qquad +2\theta\left(\frac{x}{n+m-2}\right) + \theta\left(\frac{x}{n+m}\right) & n \neq m \\ 2\theta\left(\frac{x}{2}\right) + \cdots + 2\theta\left(\frac{x}{2n-2}\right) + \theta\left(\frac{x}{2n}\right) & n = m. \end{cases} \tag{7}$$

Here k_j is the rapidity for charge excitations which are not in bound states, Λ^n_α is that for spin excitations, and Λ'^n_α is that for bound states. I_j, J^n_α, and J'^n_α are the corresponding quantum numbers which specify the above excitations, respectively. M_n is the number of n-strings for spin excitations. $2M'$ is the total number of electrons which make bound states.

In order to calculate the finite-size corrections to the energy spectrum, we expand the rapidities in terms of $1/L$ following Berkovich and Murthy [20],

$$\begin{aligned} k_j &= k_j^\infty + \frac{f_1}{L} + \frac{f_2}{L^2} + \mathrm{O}(1/L^3) \\ \Lambda^n_\alpha &= \Lambda^{n\infty}_\alpha + \frac{g_{1n}}{L} + \frac{g_{2n}}{L^2} + \mathrm{O}(1/L^3) \\ \Lambda'^n_\alpha &= \Lambda'^{n\infty}_\alpha + \frac{h_{1n}}{L} + \frac{h_{2n}}{L^2} + \mathrm{O}(1/L^3). \end{aligned} \tag{8}$$

The lowest-order contributions in $1/L$ give the conventional thermodynamic Bethe ansatz equations which read [2]

$$(1+\zeta(k))\rho(k) = \frac{1}{2\pi} + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \frac{\mathrm{d}\Lambda}{\pi} \frac{nu\cos k(\sigma_n(\Lambda) + \sigma'_n(\Lambda))}{(nu)^2 + (\sin k - \Lambda)^2} \tag{9}$$

$$\eta_n(\Lambda)\sigma_n(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m(\Lambda) = \int_{\infty}^{\infty} \frac{\mathrm{d}k}{\pi} \frac{nu\rho(k)}{(nu)^2 + (\sin k - \Lambda)^2} \tag{10}$$

$$\eta'_n(\Lambda)\sigma'_n(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma'_m(\Lambda) = \frac{1}{\pi}\,\mathrm{Re}\,\frac{1}{\sqrt{1-(\Lambda - \mathrm{i}nu)^2}} - \int_{\infty}^{\infty} \frac{\mathrm{d}k}{\pi} \frac{nu\rho(k)}{(nu)^2 + (\sin k - \Lambda)^2} \tag{11}$$

$$\ln\zeta(k) = \frac{-2\cos k - \mu_0 H - A}{T} + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \frac{\mathrm{d}\Lambda}{\pi} \frac{nu(\ln(1+\eta'^{-1}_n(\Lambda)) - \ln(1+\eta^{-1}_n(\Lambda)))}{(nu)^2 + (\sin k - \Lambda)^2} \tag{12}$$

$$\ln(1+\eta_n(\Lambda)) + \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{\pi} \frac{nu\cos k\ln(1+\zeta^{-1}(k))}{(nu)^2 + (\sin k - \Lambda)^2} = \frac{2n\mu_0 H}{T} + \sum_{m=1}^{\infty} A_{nm} * \ln(1+\eta^{-1}_m(\Lambda)) \tag{13}$$

$$\ln(1+\eta_n'(\Lambda)) + \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{\pi} \frac{nu \cos k \ln(1+\zeta^{-1}(k))}{(nu)^2 + (\sin k - \Lambda)^2} = \frac{4\,\mathrm{Re}\sqrt{1-(\Lambda - \mathrm{i}nu)^2} - 2nA}{T} + \sum_{m=1}^{\infty} A_{nm} * \ln(1+\eta_m'^{-1}(\Lambda)) \tag{14}$$

where

$$A_{nm} * \phi(x) = \delta_{nm}\phi(x) + \frac{\mathrm{d}}{\mathrm{d}x}\int_{-\infty}^{\infty} \frac{\mathrm{d}x'}{2\pi}\Theta_{nm}\left(\frac{x-x'}{u}\right)\phi(x').$$

$\rho(k)$, $\sigma_n(\Lambda)$, and $\sigma_n'(\Lambda)$ are the distribution functions for the rapidities k_j, Λ_α^n, and $\Lambda_\alpha'^n$, respectively, and $\zeta(k) \equiv \rho^h/\rho$, $\eta_n(\Lambda) \equiv \sigma_n^h/\sigma_n$, $\eta_n'(\Lambda) \equiv \sigma_n'^h/\sigma_n'$ with the distribution functions for the holes ρ^h, σ_n^h, and $\sigma_n'^h$. We have introduced an external magnetic field H and a chemical potential A.

Using the Euler–Maclaurin formula and equations (4)–(6) and (8), we obtain the $1/L$ and $1/L^2$ corrections to the Bethe ansatz equations which determine $f_{1,2}$, $g_{1,2n}$, and $h_{1,2n}$. Taking a continuum limit, we consequently have,

$$(1+\zeta(k))\rho(k) f_1(k) = \frac{\Phi}{2\pi} + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda}{\pi}\frac{nu}{(nu)^2+(\sin k-\Lambda)^2} \times (g_{1n}(\Lambda)\sigma_n(\Lambda) + h_{1n}(\Lambda)\sigma_n'(\Lambda)) \tag{15}$$

$$\sigma_n(\Lambda)\eta_n(\Lambda)g_{1n}(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m(\Lambda)g_{1n}(\Lambda) = \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu\cos k}{(nu)^2+(\sin k-\Lambda)^2} f_1(k)\rho(k) \tag{16}$$

$$\sigma_n'(\Lambda)\eta_n'(\Lambda)h_{1n}(\Lambda) + \sum_{m=1}^{\infty} A_{nm} * \sigma_m'(\Lambda)h_{1n}(\Lambda) = \frac{n\Phi}{\pi} - \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu\cos k}{(nu)^2+(\sin k-\Lambda)^2} f_1(k)\rho(k) \tag{17}$$

$$\begin{aligned}(1+\zeta(k))\rho(k) f_2(k) = {}& \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda}{\pi}\frac{nu}{(nu)^2+(\sin k-\Lambda)^2}(g_{2n}(\Lambda)\sigma_n(\Lambda) + h_{2n}(\Lambda)\sigma_n'(\Lambda)) \\ &+ \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}k}[(1+\zeta(k))\rho(k)f_1^2(k)] \\ &+ \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda}{\pi}\frac{nu(\sin k-\Lambda)}{((nu)^2+(\sin k-\Lambda)^2)^2}(g_{1n}^2(\Lambda)\sigma_n(\Lambda) + h_{1n}^2(\Lambda)\sigma_n'(\Lambda))\end{aligned} \tag{18}$$

$$\begin{aligned}(1+\eta_n(\Lambda))\sigma_n(\Lambda)g_{2n}(\Lambda) = {}& \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\Lambda}[(1+\eta_n(\Lambda))\sigma_n(\Lambda)g_{1n}^2(\Lambda)] \\ &+ \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu\cos k}{(nu)^2+(\sin k-\Lambda)^2} f_2(k)\rho(k) \\ &+ \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu(\sin k-\Lambda)\cos^2 k}{((nu)^2+(\sin k-\Lambda)^2)^2} f_1^2(k)\rho(k) \\ &- \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu\sin k}{(nu)^2+(\sin k-\Lambda)^2}\frac{f_1^2(k)\rho(k)}{2} \\ &+ \sum_{m=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda'}{2\pi}\Theta'\left(\frac{\Lambda-\Lambda'}{u}\right)\frac{g_{2m}(\Lambda')\sigma_m(\Lambda')}{u}\end{aligned}$$

$$+\sum_{m=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda'}{2\pi}\Theta''\left(\frac{\Lambda-\Lambda'}{u}\right)\frac{g_{1m}^2(\Lambda')\sigma_m(\Lambda')}{2u^2}$$
$$+\lim_{\Lambda_0\to\infty}\frac{1}{48\pi u}\sum_{m=1}^{\infty}\left[\frac{\Theta'((\Lambda-\Lambda_0)/u)}{(1+\eta_m(\Lambda_0))\sigma_m(\Lambda)}-\frac{\Theta'((\Lambda+\Lambda_0)/u)}{(1+\eta_m(-\Lambda_0))\sigma_m(-\Lambda)}\right] \quad (19)$$

$$(1+\eta_n'(\Lambda))\sigma_n'(\Lambda)h_{2n}(\Lambda)=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\Lambda}[(1+\eta_n'(\Lambda))\sigma_n'(\Lambda)h_{1n}^2(\Lambda)]$$
$$-\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu\cos k}{(nu)^2+(\sin k-\Lambda)^2}f_2(k)\rho(k)$$
$$-\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu(\sin k-\Lambda)\cos^2 k}{((nu)^2+(\sin k-\Lambda)^2)^2}f_1^2(k)\rho(k)$$
$$+\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{nu\sin k}{(nu)^2+(\sin k-\Lambda)^2}\frac{f_1^2(k)\rho(k)}{2}$$
$$+\sum_{m=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda'}{2\pi}\Theta'\left(\frac{\Lambda-\Lambda'}{u}\right)\frac{h_{2m}(\Lambda')\sigma_m'(\Lambda')}{u}$$
$$+\sum_{m=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda'}{2\pi}\Theta''\left(\frac{\Lambda-\Lambda'}{u}\right)\frac{h_{1m}^2(\Lambda')\sigma_m'(\Lambda')}{2u^2}$$
$$+\lim_{\Lambda_0\to\infty}\frac{1}{48\pi u}\left[\frac{\Theta'((\Lambda-\Lambda_0)/u)}{(1+\eta_m'(\Lambda_0))\sigma_m'(\Lambda)}-\frac{\Theta'((\Lambda+\Lambda_0)/u)}{(1+\eta_m'(-\Lambda_0))\sigma_m'(-\Lambda))}\right] \quad (20)$$

where $\Theta'(x)$ and $\Theta''(x)$ are, respectively, the first and second derivative of $\Theta(x)$. This gives our starting equations for the following discussions. Using these equations, we shall investigate finite-size effects to obtain the Drude weight at finite temperatures.

3. Drude weight at finite temperatures

Here we derive the expression for the Drude weight at finite temperatures using the formulation in the previous section. The Drude weight at finite temperatures is given by the second derivative of the energy spectrum with respect to the AB flux Φ [10],

$$D=\frac{L}{2}\left\langle\frac{\mathrm{d}^2E_n}{\mathrm{d}\Phi^2}\right\rangle\Bigg|_{\phi=0}. \quad (21)$$

Here $\langle\cdots\rangle$ is the thermal average for a canonical ensemble. Note that the above Drude weight D is different from the second derivative of the free energy, which denotes a Meissner fraction [21].

We now wish to evaluate D from the finite-size corrections to the energy. To this end, we first write down the total energy,

$$\frac{E}{L}=-\sum_{j=1}^{N-2M'}(\cos k_j+\mu_0H+A)+\sum_{n=1}^{\infty}\sum_{\alpha}4\,\mathrm{Re}\sqrt{1-(\Lambda_\alpha'^n-\mathrm{i}nu)^2}$$
$$+2\mu_0H\sum_{n=1}^{\infty}nM_n-2A\sum_{n=1}^{\infty}nM_n'. \quad (22)$$

We then expand the energy in powers of $1/L$ using equation (8),

$$\frac{E}{L}=E_0+\frac{E_1}{L}+\frac{E_2}{L^2}. \quad (23)$$

The first-order correction term E_1 is given by

$$E_1 = 2\int_{-\pi}^{\pi} \mathrm{d}k\ \sin k f_1(k)\rho(k) + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, 4\,\mathrm{Re}\,\frac{-(\Lambda - \mathrm{i}nu)}{\sqrt{1-(\Lambda-\mathrm{i}nu)^2}} h_{1n}(\Lambda)\sigma_n'(\Lambda). \tag{24}$$

Differentiating equations (12)–(14) with respect to rapidities, and substituting them into equation (24), we easily find that $E_1 = 0$. We now consider the second-order term which is

$$\begin{aligned} E_2 = {} & 2\int_{-\pi}^{\pi} \mathrm{d}k\ \sin k f_2(k)\rho(k) + 2\int_{-\pi}^{\pi} \mathrm{d}k\ \cos k\,\frac{f_1^2(k)\rho(k)}{2} \\ & + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, 4\,\mathrm{Re}\,\frac{-(\Lambda-\mathrm{i}nu)}{\sqrt{1-(\Lambda-\mathrm{i}nu)^2}} h_{2n}(\Lambda)\sigma_n'(\Lambda) \\ & + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\, 4\,\mathrm{Re}\left[\frac{-1}{(1-(\Lambda-\mathrm{i}nu)^2)^{3/2}}\right]\frac{h_{1n}^2(\Lambda)\sigma_n'(\Lambda)}{2}. \end{aligned} \tag{25}$$

Using equations (12)–(20), we can rewrite this expression as

$$\begin{aligned} E_2 = {} & \frac{T}{2}\int_{-\pi}^{\pi} \mathrm{d}k\ \frac{\rho(k) f_1^2(k)}{\zeta(k)(1+\zeta(k))}\left(\frac{\mathrm{d}\zeta(k)}{\mathrm{d}k}\right)^2 + \frac{T}{2}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\ \frac{\sigma_n(\Lambda) g_{1n}^2(\Lambda)}{\eta_n(\Lambda)(1+\eta_n(\Lambda))}\left(\frac{\mathrm{d}\eta_n(\Lambda)}{\mathrm{d}\Lambda}\right)^2 \\ & + \frac{T}{2}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\ \frac{\sigma_n'(\Lambda) h_{1n}^2(\Lambda)}{\eta_n'(\Lambda)(1+\eta_n'(\Lambda))}\left(\frac{\mathrm{d}\eta_n'(\Lambda)}{\mathrm{d}\Lambda}\right)^2. \end{aligned} \tag{26}$$

Note that the dependence on the AB flux appears only through $f_1(k)$, $g_{1n}(\Lambda)$, and $h_{1n}(\Lambda)$. We can obtain the Drude weight by differentiating E_2 twice with respect to Φ. We see from equations (15)–(17) that the equations for $\mathrm{d}f_1/\mathrm{d}\Phi$, $\mathrm{d}g_{1n}/\mathrm{d}\Phi$, and $\mathrm{d}h_{1n}/\mathrm{d}\Phi$ do not depend on Φ. Thus, we have

$$\frac{\mathrm{d}^2 f_1}{\mathrm{d}\Phi^2} = \frac{\mathrm{d}^2 g_{1n}}{\mathrm{d}\Phi^2} = \frac{\mathrm{d}^2 h_{1n}}{\mathrm{d}\Phi^2} = 0. \tag{27}$$

Then the Drude weight is given by

$$\begin{aligned} D = {} & \frac{1}{2}\frac{\mathrm{d}^2 E_2}{\mathrm{d}\Phi^2}\bigg|_{\Phi=0} = \frac{1}{2}\int_{-\pi}^{\pi} \mathrm{d}k\ \left\{(1+\zeta(k))\rho(k)\frac{\mathrm{d}f_1}{\mathrm{d}\Phi}\right\}^2 \frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{-1}{1+\mathrm{e}^{\kappa(k)/T}}\right) \\ & \times\frac{1}{(1+\zeta(k))\rho(k)}\frac{\mathrm{d}\kappa(k)}{\mathrm{d}k} + \frac{1}{2}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\ \left\{(1+\eta(\Lambda))\sigma(\Lambda)\frac{\mathrm{d}g_{1n}}{\mathrm{d}\Phi}\right\}^2 \\ & \times\frac{\mathrm{d}}{\mathrm{d}\Lambda}\left(\frac{-1}{1+\mathrm{e}^{\varepsilon_n(\Lambda)/T}}\right)\frac{1}{(1+\eta(\Lambda))\sigma(\Lambda)}\frac{\mathrm{d}\varepsilon_n(\Lambda)}{\mathrm{d}\Lambda} \\ & + \frac{1}{2}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda\ \left\{(1+\eta'(\Lambda))\sigma'(\Lambda)\frac{\mathrm{d}h_{1n}}{\mathrm{d}\Phi}\right\}^2 \\ & \times\frac{\mathrm{d}}{\mathrm{d}\Lambda}\left(\frac{-1}{1+\mathrm{e}^{\varepsilon_n'(\Lambda)/T}}\right)\frac{1}{(1+\eta'(\Lambda))\sigma'(\Lambda)}\frac{\mathrm{d}\varepsilon_n'(\Lambda)}{\mathrm{d}\Lambda}. \end{aligned} \tag{28}$$

Here we have used the conventional notation, $\kappa(k) \equiv T\ln\zeta(k)$, $\varepsilon_n(\Lambda) \equiv T\ln\eta_n(\Lambda)$, and $\varepsilon_n'(\Lambda) \equiv T\ln\eta_n'(\Lambda)$. In order to simplify the expression, it is convenient to define the following quantities,

$$\xi_{\mathrm{c}}(k) \equiv 2\pi(1+\zeta(k))\rho(k)\frac{\mathrm{d}f_1}{\mathrm{d}\Phi} \tag{29}$$

$$\xi_{\mathrm{s}n}(\Lambda) \equiv 2\pi(1+\eta(\Lambda))\sigma(\Lambda)\frac{\mathrm{d}g_{1n}}{\mathrm{d}\Phi} \tag{30}$$

$$\xi_{\mathrm{b}n}(\Lambda) \equiv 2\pi(1+\eta'(\Lambda))\sigma'(\Lambda)\frac{\mathrm{d}h_{1n}}{\mathrm{d}\Phi} \tag{31}$$

$$2\pi v_{\mathrm{c}}(k) \equiv \frac{1}{(1+\zeta(k))\rho(k)}\frac{\mathrm{d}\kappa(k)}{\mathrm{d}k} \tag{32}$$

$$2\pi v_{\mathrm{s}n}(\Lambda) \equiv \frac{1}{(1+\eta(\Lambda))\sigma(\Lambda)}\frac{\mathrm{d}\varepsilon_n(\Lambda)}{\mathrm{d}\Lambda} \tag{33}$$

$$2\pi v_{\mathrm{b}n}(\Lambda) \equiv \frac{1}{(1+\eta'(\Lambda))\sigma'(\Lambda)}\frac{\mathrm{d}\varepsilon'_n(\Lambda)}{\mathrm{d}\Lambda}. \tag{34}$$

These quantities have simple physical meanings: ξ_{c}, $\xi_{\mathrm{s}n}$ and $\xi_{\mathrm{b}n}$ correspond to the dressed charges generalized to finite temperature. v_{c}, $v_{\mathrm{s}n}$, and $v_{\mathrm{b}n}$ are the velocities for charge excitations, spin excitations, and bound states, respectively. Consequently, we end up with the simple formula for the Drude weight expressed in terms of these quantities,

$$\begin{aligned} D = {} & \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{4\pi}\frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{-1}{1+\mathrm{e}^{\kappa(k)/T}}\right)\xi_{\mathrm{c}}^2(k)v_{\mathrm{c}}(k)+\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda}{4\pi}\frac{\mathrm{d}}{\mathrm{d}\Lambda}\left(\frac{-1}{1+\mathrm{e}^{\varepsilon_n(\Lambda)/T}}\right)\xi_{\mathrm{s}n}^2(\Lambda)v_{\mathrm{s}n}(\Lambda) \\ & +\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}\Lambda}{4\pi}\frac{\mathrm{d}}{\mathrm{d}\Lambda}\left(\frac{-1}{1+\mathrm{e}^{\varepsilon'_n(\Lambda)/T}}\right)\xi_{\mathrm{b}n}^2(\Lambda)v_{\mathrm{b}n}(\Lambda). \end{aligned} \tag{35}$$

Note that at finite temperatures not only the charge degrees of freedom but also the spin degrees of freedom contribute to the Drude weight. The above formula is one of our main results in this paper.

To conclude this section, we check that the above formula reproduces the known results [6, 7] by taking the zero temperature limit $T \to 0$. Since $\varepsilon_n(\Lambda) > 0$ for $n = 2, 3, \ldots$ and $\varepsilon'_n(\Lambda) \geqslant 0$ for $n = 1, 2, 3, \ldots,$ the contributions from spin excitations with $n > 1$ and bound states to the Drude weight vanish for $T \to 0$. Moreover, from equations (15) and (16) we have $\xi_{\mathrm{s}1}(\pm B) = 0$ for $T \to 0$ where $\pm B$ are the zeros of $\varepsilon_1(\Lambda)$. Thus, only the contribution from the charge degrees of freedom to the Drude weight survives,

$$D = \int \mathrm{d}\kappa \sum_{\text{zeros of }\kappa}\delta(\kappa)\frac{\xi_{\mathrm{c}}^2(k)v_{\mathrm{c}}(k)}{4\pi} = \frac{K_{\mathrm{c}}v_{\mathrm{c}}}{\pi}. \tag{36}$$

Here $K_{\mathrm{c}} = \xi_{\mathrm{c}}^2(k_0)/2$, and $v_{\mathrm{c}} = v_{\mathrm{c}}(k_0)$ with $\kappa(\pm k_0) = 0$. Then we reproduce the well known result for zero temperature.

4. Low temperature expansion

4.1. Case of half-filling

In this section, we explicitly derive the temperature dependence of the Drude weight in the case of half-filling at low temperatures. In this case, the system is in the Mott-insulating state with the charge excitation gap. Thus we immediately find $D = 0$ at zero temperature. However, at finite temperatures it can have finite values as we will see presently. We consider the case that $2u - A \geqslant 0$, $\mu_0 H < 2(\sqrt{1+u^2} - u)$, and $2 - \mu_0 H - A \leqslant 0$, i.e. the charge excitation is gapful, whereas the spin excitation is gapless. In order to obtain the temperature dependence of the Drude weight, we need to take a thermal average over a canonical ensemble and consider the temperature dependence of the chemical potential A. However, in the presence of the Mott–Hubbard gap, the temperature dependence of A appears only through that of the Mott–Hubbard gap, which gives a subleading contribution to the temperature dependence of the Drude weight, as is shown later. Thus we can safely ignore the temperature dependence of A.

Following Takahashi's method, we perform low-temperature expansions [3]. As a result, we find that at low temperatures the Drude weight is mainly controlled by the contributions from the charge excitation, the spin excitation with $n = 1$, and the bound-state excitation with $n = 1$. At low temperatures equation (12) and (13) for $n = 1$, and (14) for $n = 1$ are rewritten as

$$\kappa(k) = -2\cos k - \mu_0 HA + \int_{-B}^{B} \frac{\mathrm{d}\Lambda}{\pi} \frac{u}{u^2 + (\sin k - \Lambda)^2} \varepsilon_1(\Lambda) + C_1 T^{\gamma} \tag{37}$$

$$\varepsilon_1(\Lambda) = 2\mu_0 H - 4(\mathrm{Re}\sqrt{1-(\Lambda - \mathrm{i}u)^2} - u) - \int_{-B}^{B} \frac{\mathrm{d}\Lambda'}{\pi} \frac{2u}{4u^2 + (\Lambda - \Lambda')^2} \varepsilon_1(\Lambda') + C_2 T^{\gamma} \tag{38}$$

$$\varepsilon_1'(\Lambda) = 4u - 2A - C_3 T^{3/2}\, \mathrm{e}^{\kappa(\pi)/T} \frac{u}{u^2 + \Lambda^2} + C_4 T^{3/2}\, \mathrm{e}^{-(4u-2A)/T} \tag{39}$$

where $\gamma = 2$ for $H \neq 0$ and $\gamma = 3/2$ for $H = 0$. B is defined by the condition $\varepsilon_1(\pm B) = 0$. In the absence of magnetic fields, $H = 0$, $B \to +\infty$. $\varepsilon_1(\Lambda)$ is obtained from equation (38) by using the Wiener–Hopf method. Substituting the solution into equations (37) and (39), we obtain $\kappa(k)$ and $\varepsilon_1'(\Lambda)$. The generalized dressed charges ξ_{c}, $\xi_{\mathrm{s}1}$, and $\xi_{\mathrm{b}1}$ are now determined by the derivative of equations (15), (16), and (17) with respect to Φ, which are given in the low-temperature limit,

$$(1 + \mathrm{e}^{\kappa(k)/T})\xi_{\mathrm{c}}(k) = 1 + \int_{-B}^{B} \frac{\mathrm{d}\Lambda}{\pi} (\xi_{\mathrm{s}1}(\Lambda) + \xi_{\mathrm{b}1}(\Lambda)) \tag{40}$$

$$(1 + \mathrm{e}^{\varepsilon_1(\Lambda)/T})\xi_{\mathrm{s}1}(\Lambda) = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{\pi} \frac{u\cos k}{u^2 + (\sin k - \Lambda)^2} \xi_{\mathrm{c}}(k) - \int_{-B}^{B} \frac{\mathrm{d}\Lambda'}{\pi} \frac{2u}{4u^2 + (\Lambda - \Lambda')^2} \xi_{\mathrm{s}1}(\Lambda) \tag{41}$$

$$\begin{aligned}(1 + \mathrm{e}^{\varepsilon'(\Lambda)/T})\xi_{\mathrm{b}1}(\Lambda) = 2 &+ \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{\pi} \frac{u\cos k}{u^2 + (\sin k - \Lambda)^2} \xi_{\mathrm{c}}(k) \\ &- \int_{-B}^{B} \frac{\mathrm{d}\Lambda'}{\pi} \frac{2u}{4u^2 + (\Lambda - \Lambda')^2} \xi_{\mathrm{b}1}(\Lambda).\end{aligned} \tag{42}$$

Solving these equations we have $\xi_{\mathrm{c}}(k) = 1$ and

$$\xi_{\mathrm{s}1}(\Lambda) \sim D_1\sqrt{T}\, \mathrm{e}^{(2-\mu_0 H - A + \Delta(B))/T} \tag{43}$$

$$\xi_{\mathrm{b}1}(\Lambda) \sim D_2\, \mathrm{e}^{-\varepsilon_1'(\Lambda)/T} \tag{44}$$

where

$$\Delta(B) \equiv \int_{-B}^{B} \frac{\mathrm{d}\Lambda}{\pi} \frac{u}{u^2 + \Lambda^2} \varepsilon_1(\Lambda). \tag{45}$$

The distribution functions for rapidities, $\rho(k)$ and $\sigma_1(\Lambda)$, are given by those for zero temperature. Also, $\sigma_1'(\Lambda)$ is estimated as

$$\sigma_1'(\Lambda) \sim C'\sqrt{T}\, \mathrm{e}^{(2-\mu_0 H - A + \Delta(B))/T}\, \mathrm{e}^{-\varepsilon_1'(\Lambda)/T}. \tag{46}$$

Using equations (35) and (37)–(46), we finally end up with

$$D = \frac{\sqrt{T}}{\sqrt{\pi}\,\tilde{\rho}}\, \mathrm{e}^{-\Delta_{\mathrm{MH}}/T} + \mathrm{O}(T\, \mathrm{e}^{2(2-\mu_0 H - A + \Delta(B))/T}) + \mathrm{O}(T^{3/2}\, \mathrm{e}^{-(4u-2A)/T}\, \mathrm{e}^{(2-\mu_0 H - A + \Delta(B))/T}) \tag{47}$$

where $\Delta_{\mathrm{MH}} \equiv -2 + \mu_0 H + A - \Delta(B)$ is nothing but the Mott–Hubbard gap, and

$$\tilde{\rho} = \frac{1}{2\pi} - \int_{-B}^{B} \frac{\mathrm{d}\Lambda}{\pi} \frac{u\sigma_0(\Lambda)}{u^2 + \Lambda^2} \tag{48}$$

$$\sigma_0(\Lambda) = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{8\pi u \cosh(\pi(\Lambda - \sin k)/2u)}. \tag{49}$$

Here the first term of equation (47), which is most dominant, comes from the charge degrees of freedom, whereas the second and third terms are the contributions from spin degrees of freedom and bound states, respectively. As seen from the above equations, the Drude weight vanishes exponentially at half-filling at low temperatures, reflecting the presence of the Mott–Hubbard gap. It is noted that the temperature dependence of equation (47) is similar to the system-size dependence of the Drude weight obtained by Stafford and Millis [22]. It implies that the hyperscaling behaviour found at $T = 0$ by them may hold at finite low temperatures.

4.2. Case away from half-filling

We next consider the case away from half-filling in the absence of magnetic fields, i.e. $\kappa(\pi) > 0$. We first estimate the contribution from the charge degrees of freedom. Since we are concerned with a canonical ensemble, we must take into account the temperature dependence of the chemical potential A or k_0 in the case that the number of electrons

$$\frac{N}{L} = \int_{-\pi}^{\pi} \mathrm{d}k\, \rho(k) + \sum_{n=1}^{\infty} 2n \int_{-\infty}^{\infty} \mathrm{d}\Lambda\, \sigma_n'(\Lambda) \tag{50}$$

is fixed. At low temperatures equation (50) is approximated by

$$\begin{aligned}\frac{N}{L} &\approx \int_{-\pi}^{\pi} \mathrm{d}k \frac{\rho_0(k)}{1 + \mathrm{e}^{\kappa(k)/T}} \approx \frac{k_0}{\pi} + 2\int_{-\infty}^{\infty} \frac{\Lambda}{\pi} \tan^{-1} \frac{\sin k_0 - \Lambda}{U} \sigma_1(\Lambda) \\ &\quad + \frac{\pi^2 T^2}{3} \frac{\partial}{\partial \kappa} \left(\frac{\rho_0(k)}{\kappa'(k)} \right)\bigg|_{k=k_0}\end{aligned} \tag{51}$$

where $\rho_0(k)$ is the distribution function for k at $T = 0$. Thus we have the temperature dependence of k_0,

$$\delta k_0 \equiv k_0 - \tilde{k}_0 = -\frac{\pi^2 T^2}{6\rho_0(\tilde{k}_0)} \frac{\partial}{\partial \kappa} \left(\frac{\rho_0(k)}{\kappa'(k)} \right)\bigg|_{k=\tilde{k}_0}. \tag{52}$$

Here $\tilde{k}_0$ is k_0 at $T = 0$. Then using equation (35), we obtain the contribution from the charge degrees of freedom to the Drude weight at low temperatures,

$$\begin{aligned}D_{\mathrm{charge}} &\approx \frac{\xi_{\mathrm{c}}^2(k_0) v_{\mathrm{c}}(k_0)}{2\pi} \frac{\pi T^2}{12} \frac{\partial^2}{\partial \kappa^2} (\xi_{\mathrm{c}}^2(k) v_{\mathrm{c}}(k))|_{k=k_0} \approx \frac{K_{\mathrm{c}} v_{\mathrm{c}}}{\pi} + \frac{\delta k_0}{2\pi} \frac{\partial}{\partial k_0} (\xi_{\mathrm{c}}^2(k_0) v_{\mathrm{c}}(k_0))|_{k_0=\tilde{k}_0} \\ &\quad + \frac{\pi T^2}{12} \frac{\partial^2}{\partial \kappa^2} (\xi_{\mathrm{c}}^2(k) v_{\mathrm{c}}(k))|_{k=\tilde{k}_0} = \frac{K_{\mathrm{c}} v_{\mathrm{c}}}{\pi} + CT^2\end{aligned} \tag{53}$$

where the coefficient of the quadratic term is

$$C = \frac{\pi}{12} \left[\frac{\partial^2}{\partial \kappa^2} (\xi_{\mathrm{c}}^2(k) v_{\mathrm{c}}(k))|_{k=\tilde{k}_0} - \frac{1}{\rho_0(\tilde{k}_0)} \frac{\partial}{\partial \kappa} \left(\frac{\rho_0(k)}{\kappa'(k)} \right)\bigg|_{k=\tilde{k}_0} \frac{\partial}{\partial k_0} (\xi_{\mathrm{c}}^2(k_0) v_{\mathrm{c}}(k_0))|_{k_0=\tilde{k}_0} \right]. \tag{54}$$

Here $\xi_{\mathrm{c}}(k)$ and $v_{\mathrm{c}}(k)$ are calculated at $T = 0$.

In a similar manner, we can evaluate the contributions from the spin degrees of freedom as well as from the bound states. As a consequence we find that they are subdominant compared to the contribution from the charge degrees of freedom at low temperatures. Therefore, the leading term of the Drude weight is given by equation (53). We expect that expression (53) and its temperature dependence $\sim D(0) + CT^2$ may be general for all integral models with massless excitations.

5. Summary

By using the Bethe ansatz solution, we have obtained the formula for the Drude weight of the Hubbard model at finite temperatures. The present general formulation is not restricted to the Hubbard model, but also applicable to any other integrable models. We have then performed low-temperature expansions both in the case of half-filling as well as away from half-filling. In the case of half-filling, the Drude weight decreases exponentially, as the temperature is lowered, reflecting the presence of the Mott–Hubbard gap. In the case away from half-filling, it behaves like $\sim D(0) + CT^2$, with the coefficient C expressed in terms of the velocity for charge excitations, the dressed charge, and their derivatives. Although the essential properties of the Drude weight can be seen through the present low-temperature expansion, it is interesting to obtain its full temperature dependence by solving the integral equations numerically, which should be done in a future study.

Acknowledgments

The authors are grateful to C Stafford for useful comments and drawing their attention to [22]. This work was partly supported by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture, Japan.

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