Drude Weight at Finite Temperatures for Some Nonintegrable Quantum Systems in One Dimension

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Using conformal perturbation theory, we show that, for some classes of the one-dimensional quantum liquids that possess the Luttinger liquid fixed point in the low-energy limit, the Drude weight at finite temperatures is nonvanishing, even when the system is *nonintegrable* and the total current is not conserved. We also obtain the asymptotically exact low-temperature formula of the Drude weight for Heisenberg XXZ spin chains, which agrees quite well with recent numerical data.

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Quantum one-dimensional (1D) systems show anomalous transport properties quite different from higher dimensional systems [1–16]. In particular, Zotos and co-workers showed the remarkable fact that in integrable 1D systems the Drude weight is nonvanishing at finite temperatures T, and the transport is ballistic, because of the presence of nontrivial conservation laws [1,2]. The Drude weight is a coefficient of the singular part of the conductivity: $\sigma(\omega) = \pi D(T)\delta(\omega) +$ (regular part). Their proposal has been followed up by extensive studies based on various techniques, such as the Bethe ansatz [3–5,9], numerical methods [6–8,10], and bosonization [12]. Some authors also investigated how this anomalous transport is affected by the perturbations that break the integrability [6–8,10]. Recent numerical studies suggest that some classes of nonintegrable 1D systems may also show the nonzero Drude weight at finite temperatures, implying that the integrability is not a necessary condition for $D(T) \neq 0$ [6–8]. However, the relation between the finite Drude weight and nonintegrable perturbations has not yet been fully elucidated. The main purpose of this Letter is to address this issue. Using conformal perturbation theory, we explore the effects of integrability-breaking perturbations on the finite-temperature Drude weight in 1D Luttinger liquids including spin systems and one-component fermion systems. As a by-product, we also obtain the asymptotically exact low-temperature formula of the Drude weight for Heisenberg XXZ spin chains.

The Hamiltonian consists of the low-energy fixed point part H_{G} and the irrelevant perturbation H' that may render the system nonintegrable. Namely, $H = H_{\mathrm{G}} + H'$. H_{G} is given by the Hamiltonian of the $c = 1$ Gaussian model [17],

$$H_{\mathrm{G}} = \int_0^L \frac{dx}{2} v[(\partial_x \phi(x))^2 + (\partial_x \theta(x))^2], \qquad (1)$$

for the system of the linear size L with the velocity v. Here the boson fields ϕ and θ satisfy the canonical commutation relation, $[\phi(x), \partial_x \theta(x')] = i\delta(x - x')$. The charge density (or spin density) operator and the corresponding current operator, which satisfy the continuity equation, are, respectively, given by $\rho(x) = \sqrt{K}\partial_x \phi/\sqrt{\pi}$ and $J(x) = -\sqrt{K}\partial_t \phi/\sqrt{\pi}$. Here K is the Luttinger liquid parameter. The irrelevant perturbation H' is expressed in terms of primary fields of the $c = 1$ universality class. We are concerned with the case that the total current $J = \int dx J(x)$ is not conserved by the interaction H': $[H', J] \neq 0$. This happens when H' contains the cosine interaction $\cos[\alpha\phi(x)]$ which stems from Umklapp processes. In general, $H = H_{\mathrm{G}} + H'$ is not integrable. For instance, the multiple-frequency cosine interaction such as $\int dx \sum_n \{g_n \cos[\beta_n \phi(x)] + g'_n \cos[\gamma_n \theta(x)]\}$ breaks the integrability of the system [18].

To show the presence of nonvanishing Drude weight, following Zotos *et al.* [2], we exploit the Mazur inequality which gives the lower bound for the Drude weight. The lower bound is expressed in terms of nontrivial conserved quantities, which can be found in our case as follows. Introducing a cylindrical geometry with a system size L, we write the spatial translation operator as [19],

$$I \equiv \int_0^L \frac{dx}{2\pi}(T(x) - \bar{T}(x)) = \frac{2\pi}{L}(L_0 - \bar{L}_0), \qquad (2)$$

where $T(x)$ [$\bar{T}(x)$] is the holomorphic (antiholomorphic) part of the stress tensor. L_n and $\bar{L}_n$ are the Virasoro generators. For any local field $O(x)$, the commutation relation $[I, O(x)] = -i\partial_x O(x)$ holds. Note that $O(x)$ should not be multiplied by a c-number function $f(x)$, because I does not operate on $f(x)$ as translation [20]. In the case that the Hamiltonian is written in terms of local operators, $H = \int dx O(x)$, we have $[I, H] = 0$ under the periodic boundary condition. Thus, I is a nontrivial conserved quantity in the perturbed system. An important role played by the conservation law $[I, H] = 0$ for transport properties was also noticed by Rosch and Andrei previously [12,21]. For the $c = 1$ Gaussian model (1), I is expressed as $I = v \int dx \partial_x \theta(x) \partial_x \phi(x)$. This is nothing but the free field representation of the Virasoro generator (2). Using the equation of motion of $\phi(x)$ in the presence of

H', we rewrite I as $I = \int dx \partial_t \phi(x) \partial_x \phi(x) + I'$ with $I' = -i \int dx [H', \phi(x)] \partial_x \phi(x)$. The total momentum is given by $P = I + p_F J/K$, where p_F is the Fermi momentum. For the Hamiltonian $H = H_G + H'$, although the system is translationally invariant $[I, H] = 0$ as expected for continuum field theory, the charge current (or spin current) and the total momentum are not conserved, i.e., $[P, H] \neq 0$, and hence its transport property is nontrivial. With the conserved quantity I, the Mazur inequality reads [2]

$$D(T) \geq \frac{1}{LT} \frac{\langle JI \rangle^2}{\langle I^2 \rangle}. \tag{3}$$

In general, the system has the reflection symmetry (particle-hole symmetry in terms of fermion fields) $\phi \to -\phi$, which leads to $\langle JI \rangle = 0$. However, in the presence of a symmetry-breaking field $-h \partial_x \phi$ (magnetic field in spin systems or chemical potential in fermion systems), $\langle JI \rangle$ may be nonzero. We can easily see that this external field still conserves I. The symmetry-breaking field is incorporated into the shift of the boson field $\tilde{\phi}(x) = \phi(x) - hx$. Then we have

$$\begin{aligned} \frac{\langle JI \rangle}{LT} &= \frac{1}{LT} \left(-h \sqrt{\frac{\pi}{K}} \langle J^2 \rangle + \langle JI' \rangle \right) \\ &= \frac{-h}{T} \sqrt{\frac{\pi}{K}} \int_0^\infty d\omega \mathrm{Im} \Pi^R(\omega) \coth\left(\frac{\omega}{2T}\right) + \frac{\langle JI' \rangle}{LT}, \end{aligned} \tag{4}$$

with

$$\Pi^R(\omega) = \frac{-i}{L} \int_0^\infty dt \langle [J(q,t), J(-q,0)] \rangle e^{i\omega t}|_{q \to 0}. \tag{5}$$

Here we have used the fluctuation-dissipation theorem in the last line of (4). In the case of $\mathrm{Im}\Pi^R(\omega) \equiv 0$, the conductivity is given by $\mathrm{Re}[\sigma(\omega)] = Kv\delta(\omega)$, showing the presence of the finite-temperature Drude weight [see (6) below]. In the other cases, the first term of the right-hand side of (4) is nonvanishing, because $\mathrm{Im}\Pi^R(\omega)$ is non-negative. Note that the first term of (4) cannot be canceled with the second term for the following reason. Let a be the lattice constant and $s - 2$ the dimension of the leading term of H'. Then the second term of (4) is proportional to a^{s-2}, of which the order in terms of a is different from that of the first term. Hence, these two terms cannot be canceled with each other and give a nonzero lower bound for the Drude weight (3) provided that $\langle I^2 \rangle / LT$ is finite. It is easily seen that $\langle I^2 \rangle / LT$ is never divergent, since it is given by the derivative of the free energy, and the free energy has no thermodynamic singularities in 1D systems. As a result, we have shown that *as long as the translational invariance is recovered in the scaling limit (i.e., I is conserved), the Drude weight at finite temperatures is nonvanishing for the 1D systems that have the Luttinger liquid fixed point in the presence of particle-hole symmetry-breaking fields (magnetic fields in spin systems), even if the system is nonintegrable, and the charge current (or spin current) is not conserved.* One may question to what extent this argument is relevant to lattice systems, which are, at short-length scale, not translationally invariant. As the low-energy fixed point of the systems is the Luttinger liquid, the correlation length at $T = 0$ is infinite, characterizing the critical state described by the $c = 1$ universality class. Thus, at sufficiently low but finite temperatures, the correlation length is much longer than the lattice constant, rendering the systems approximately translationally invariant, provided that there exists no other length scale in the Hamiltonian. It should be stressed that, as mentioned before, to preserve the conservation law of I, the interaction H' must not contain the c-number function $f(x)$ that introduces another length scale [20].

Hitherto, our argument is based on the nonperturbative analysis. However, it is restricted to the case with symmetry-breaking fields. We investigate the case without the external fields, by computing the conductivity perturbatively from the Kubo formula,

$$\sigma(\omega) = \frac{i}{\omega} \left[\frac{Kv}{\pi} + \Pi^R(\omega) \right]. \tag{6}$$

For concreteness, we introduce a specific model given by

$$H' = \int dx \sum_{m=1} g_m \cos[\beta_m \phi(x)]. \tag{7}$$

In general, the multiple-frequency cosine terms (7) break the integrability of the system [18]. It is noted that the ratio of any two β_m's must be rational to ensure that the perturbative expansion in term of H' does not generate relevant interactions which invalidate the Luttinger liquid fixed point. For simplicity, we assume $\beta_m = m\beta_1$. Let us first consider the case that $g_n = 0$ for $n \geq 2$ and only a single cosine interaction exists. In this case, the system is the standard sine-Gordon model, which is integrable. We expand the imaginary time current-current correlation in terms of g_1,

$$\begin{aligned} \Pi(i\omega) = &\int dx \int_0^{1/T} d\tau \langle T \partial_\tau \phi(x,\tau) \partial_\tau \phi(0,0) \rangle_0 e^{-i\omega\tau} + \sum_{n=1}^\infty \left(\frac{g_1}{2}\right)^n \frac{1}{n!} \int dx \int_0^{1/T} d\tau \int d(1) \ldots d(n) e^{-i\omega\tau} \\ &\times \sum_{\alpha_i = \pm\beta_1} \langle T \partial_\tau \phi(x,\tau) \partial_\tau \phi(0,0) e^{i\alpha_1\phi(1)} e^{i\alpha_2\phi(2)} \ldots e^{i\alpha_n\phi(n)} \rangle_0. \end{aligned} \tag{8}$$

Here $\int d(n) = \int_0^L dx_n \int_0^{1/T} d\tau_n$, $\phi(n) = \phi(x_n, \tau_n)$, $\langle \cdots \rangle_0$ is the average with respect to H_G. Using the conformal Ward identity, we rewrite the nth order term of (8) as

$$-\frac{g_1^n}{2^n n!}\sum_{i,j}\alpha_i\alpha_j[G(i\omega)]^2F_{\alpha_1\alpha_2\ldots\alpha_n}[i\omega(1-\delta_{ij})], \tag{9}$$

where

$$F_{\alpha_1\alpha_2\ldots\alpha_n}[i\omega(1-\delta_{ij})]=\int d(1)\ldots d(j-1)d(j+1)\ldots d(n)\langle Te^{i\alpha_1\phi(1)}e^{i\alpha_2\phi(2)}\ldots e^{i\alpha_n\phi(n)}\rangle_0 e^{i\omega(\tau_i-\tau_j)}, \tag{10}$$

$$G(i\omega)=\int dx\int_0^{1/T}d\tau\langle T\partial_\tau\phi(x,\tau)\phi(0,0)\rangle_0 e^{-i\omega\tau}, \tag{11}$$

with $\langle T\partial_\tau\phi(x,\tau)\phi(0,0)\rangle_0 = i(T/4)\coth[(\pi T/v)(x+iv\tau)]$ + c.c. For $\omega\neq 0$, $G(i\omega)=v/(i\omega)$ and for $\omega=0$, $G(0)=v/T$. Correlators of vertex operators $\exp(i\alpha_i\phi)$ in (10) are nonvanishing only for $\sum_i^n\alpha_i=0$ because of U(1) symmetry. Then, without loss of generality, we can put $\alpha_{2m-1}=\beta_1$, $\alpha_{2m}=-\beta_1$, and $n=2m$. It is difficult to obtain the explicit expression of (10) as a function of ω. However, to show the presence of the Drude weight, it is sufficient to investigate the low-frequency behavior of $F_{\alpha_1\alpha_2\ldots\alpha_n}[i\omega(1-\delta_{ij})]$. For this purpose, using the conformal transformation $z=\exp(2\pi Tw/v)$ ($w=x+iv\tau$), we change the geometry of the system from a strip with a width $1/T$ to a two-dimensional plane. The correlator of vertex operators is transformed as

$$\int d(1)\ldots d(n-1)\langle e^{i\beta_1\phi(w_1,\bar{w}_1)}\ldots e^{-i\beta_1\phi(w_n,\bar{w}_n)}\rangle_0 e^{-i\omega(\tau_i-\tau_n)}$$
$$=\int d^2z_1|z_1|^{(\beta_1^2/4\pi)-2}\ldots d^2z_{n-1}|z_{n-1}|^{(\beta_1^2/4\pi)-2}|z_n|^{\beta_1^2/4\pi}e^{-i\omega(\tau_i-\tau_n)}\left(\frac{2\pi T}{v}\right)^{(\beta_1^2/2\pi)n-4n+2}\langle e^{i\beta_1\phi(z_1,\bar{z}_1)}\ldots e^{-i\beta_1\phi(z_n,\bar{z}_n)}\rangle_0. \tag{12}$$

Here we have relabeled the index as $n\rightarrow j$. Following Konik and LeClair [22], we map the IR region to the ultraviolet (UV) region by the conformal transformation $z'=1/z$. Note that under this transformation the expression of the right-hand side of (12) is unchanged. Thus, although the IR region of the w coordinate is mapped to both the IR and UV regions of the z coordinate, we need to consider only the UV behavior in the z coordinate. Exploiting the short distance expansion of operator product for the U(1) Gaussian theory [19], we find that the dimension of $\langle\exp[i\beta_1\phi(z_1,\bar{z}_1)]\ldots\exp[-i\beta_1\phi(z_n,\bar{z}_n)]\rangle_0$ in the UV region is $\beta_1^2 n/(2\pi)$, and hence the dimension of the right-hand side of (12) is zero. Therefore, the IR singularity of (10) is at most logarithmic, if it exists. We can apply the same argument to $d^kF_{\alpha_1\alpha_2\ldots\alpha_n}[i\omega(1-\delta_{ij})]/d(i\omega)^k$ and find that its dimension in the UV region of the z' coordinate is also zero, because the derivative with respect to ω does not give rise to an extra dimension in the right-hand side of (12). Hence, $F_{\alpha_1\alpha_2\ldots\alpha_n}[\omega(1-\delta_{ij})]$ has no singularity in the limit of $\omega\rightarrow 0$. After the analytic continuation in the upper half plane $i\omega\rightarrow\omega+i0$, we can expand (10) for small ω: $F_{\alpha_1\alpha_2\ldots\alpha_n}[\omega(1-\delta_{ij})]=a_0+a_1\omega(1-\delta_{ij})+a_2\omega^2(1-\delta_{ij})\cdots$. Substituting this into (9) and from $\sum_i\alpha_i=0$, we find that the expansion of $\Pi^R(\omega)$ in terms of g_1 does not give rise to singularity stronger than $1/\omega$. Thus, the Drude weight term of $\sigma(\omega)$ is not eliminated by resummation of higher-order singularities. A careful treatment of the limit $\omega\rightarrow 0$ for the second order term of (9) verifies that the strongest singularity of $\sigma(\omega)$ is not of order $\sim 1/\omega^2$, but $\sim 1/\omega$. Actually, the presence of the double pole $1/\omega^2$ is forbidden, because it breaks the nonnegativity of $\mathrm{Re}\sigma(\omega)$. Consequently, we have the Drude weight at finite temperatures as expected from the integrability of the model.

It is straightforward to generalize the above argument to the nonintegrable case with multiple cosine interactions (7). The perturbative expansion gives the same expressions as (8) and (9), except that α_i takes the values of β_1, $\beta_2=2\beta_1$, $\beta_3=3\beta_1,\ldots$, and so forth. Applying the above argument to this case, we also find that the dimension of $F_{\alpha_1\alpha_2\ldots\alpha_n}[i\omega(1-\delta_{ij})]$ and its derivative with respect to ω is zero, and that $F_{\alpha_1\alpha_2\ldots\alpha_n}[i\omega(1-\delta_{ij})]$ has no IR singularity for $\omega\rightarrow 0$. This observation leads to the conclusion that the $1/\omega$ singularity of $\sigma(\omega)$ cannot be eliminated by the resummation of higher-order singularities. *Therefore, the finite-temperature Drude weight exists for the nonintegrable model* (1) *and* (7). The above analysis generalizes Zotos *et al.*'s original proposal partially to nonintegrable systems. This remarkable result is physically understood as follows. The existence of nontrivial conservation law permits macroscopic numbers of level crossing [23]. It is expected that, even for nonintegrable systems, level crossing may be possible provided that a certain nontrivial conservation law holds. Then the presence of macroscopic numbers of degenerate levels results in the nonvanishing Drude weight at finite temperatures [6,11].

On the basis of the above perturbative analysis, we calculate the Drude weight at low temperatures for Heisenberg XXZ chains,

$$H_{XXZ}=J\sum_i[S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z], \tag{13}$$

where $\Delta=-\cos(\pi\beta^2)$. We consider only the massless regime $-1<\Delta\leq 1$. The low-energy effective Hamiltonian for this regime is completely obtained by Lukyanov [24]. Using his result, we obtain the leading temperature dependence of the Drude weight at low

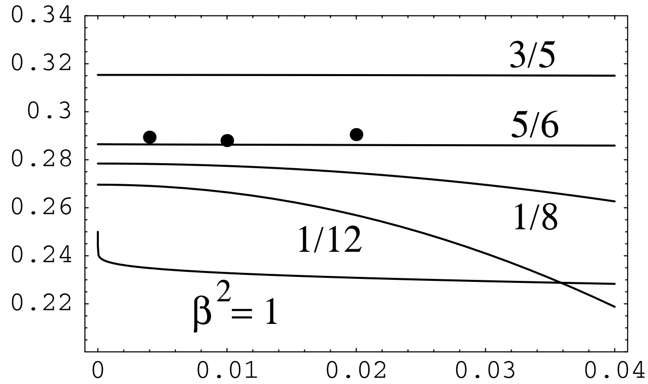

FIG. 1. Plot of $D(T)$ vs T for $\beta^2 = 1$, 1/12, 1/8, 5/6, 3/5 (from bottom to top). For comparison, the QMC data for $\beta^2 = 5/6$ is quoted from Ref. [10] (circles).

temperatures. For $2/3 < \beta^2 < 1$, up to logarithmic corrections, it is given by

$$D(T) = D(0)\left[1 - A\frac{\sin(2\pi/\beta^2)}{8\pi\beta^2}\lambda^2(2a\pi T)^{(4/\beta^2)-4}\right], \tag{14}$$

$$A = B^2\left(\frac{1}{\beta^2}, 1 - \frac{2}{\beta^2}\right)\left[2\pi^2\cot^2\left(\frac{\pi}{\beta^2}\right) + \psi'\left(\frac{1}{\beta^2}\right) - \psi'\left(1 - \frac{1}{\beta^2}\right)\right], \tag{15}$$

where $a = 2(1 - \beta^2)/[J\sin(\pi\beta^2)]$, $D(0) = 1/(2\pi a\beta^2)$, and $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$, $\psi(x) = \Gamma'(x)/\Gamma(x)$. For $0 < \beta^2 < 2/3$, we have

$$D(T) = D(0)\left[1 - \frac{6\lambda_- + \lambda_+}{12}(a\pi T)^2\right]. \tag{16}$$

The expressions for λ, λ_+, and λ_- are given by Eq. (2.24) in Ref. [24]. At the isotropic point $\beta^2 = 1$, logarithmic corrections caused by marginal interaction are incorporated into the renormalization of the running coupling constant, and we end up with

$$D(T) = \frac{J}{4}\left[1 - \frac{g}{2} + O(g^2)\right]. \tag{17}$$

Here g is determined by Eq. (3.18) in Ref. [24] with $h = 0$. $D(T)$ is nonvanishing at the isotropic point in accordance with Ref. [10]. The above formulas are applicable only in the low-temperature region $T \ll a^{-1}$. We show the plot of $D(T)$ as a function of T for several values of β^2 in Fig. 1. The result for $\beta^2 = 5/6$ agrees well with the recent quantum Monte Carlo (QMC) data obtained by Alvarez and Gros [10]. As β^2 decreases, the temperature dependence becomes stronger. However, it should be cautioned that, for small β^2, the applicable temperature range becomes narrower; e.g., for $\beta^2 = 1/12$, $a^{-1} = 0.1411$. In principle, we can improve the formulas by taking into account higher-order corrections.

In summary, we have shown that in a wide class of 1D integrable and nonintegrable systems with the Luttinger liquid fixed point, as long as the systems recover translational invariance in the scaling limit, the Drude weight is nonvanishing at finite temperatures, even when the charge current (or spin current) is not conserved.

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