Transport Properties in the Tomonaga-Luttinger Liquid

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We investigate the conductivity using Green's functions in the Tomonaga-Luttinger liquid. It is shown that the resistivity has a linear temperature dependence if we take account of the physical process that the accelerated electron decays into spinon and holon. The effect of impurity scattering becomes visible only below a crossover temperature which strongly depends on the impurity strength, every cutoff, and spin and charge velocities. The optical conductivity is also studied and it is shown that the relaxation rate has a linear frequency dependence.

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It is important to study the non-Fermi-liquid behaviors in high-T_c superconductors. The most prominent features are the temperature dependences of normal-state transport properties: the linear-T resistivity, the T^2 dependence of the Hall angle, and the c-axis resistivity, which are impossible to explain in the conventional Fermi-liquid theory. In the strong coupling regime to which the high-T_c materials belong, we expect spin-charge separation and the physics is determined by the strong-coupling fixed point. In this paper we study the transport properties in the one-dimensional Tomonaga-Luttinger (TL) liquid as one of the exact realizations of this strong-coupling fixed point [1]. The Green's function does not have quasiparticle poles but instead has a branch cut and different spin and charge velocities [2], so that non-Fermi-liquid transport properties are expected. So far the TL liquid is the only microscopic model with one band which is not a Fermi liquid. To investigate its transport properties is significant for strongly correlated systems as well as for quasi-one-dimensional conductors. We will point out the importance of the physical process that the electron after acceleration by the external field decays into spinon and holon.

Anderson and Zou [3] used resonating-valence-bond mean-field theory to calculate conductivity by a holon-spinon scattering mechanism. If the statistics of holons is taken into account seriously, the resistivity is proportional to $T^{3/2}$ in a dilute holon gas limit. It was pointed out, however, that for finite density of holons, linear-T resistivity is probable, but greater understanding of the spinon-holon system is required [4]. A recent Hall angle experiment strongly supports the spin-charge separation because of the existence of two kinds of relaxation rates observed in experiments [5]. Nagaosa and Lee [6] tried to explain the linear-T resistivity using a scattering mechanism of holons by the gauge field. However, their method is based on the slave-boson mean-field theory; the constraint conditions are only approximately taken into account. It is difficult to justify the mean-field treatment especially for the strong-coupling regime. On the other hand, in the one-dimensional (1D) Hubbard model we know that infinitesimal electron-electron interaction already leads the system to a strong-coupling fixed point and the system is always described as a TL liquid [2,7,8]. In other words, the Gutzwiller projection can be taken into account exactly. (Actually the 1D t-J model with a strict Gutzwiller projection is shown to behave as a TL liquid [9].) It is thus a big advantage to investigate transport properties in the TL liquid as an example of strongly correlated systems. Although the microscopic justification of the TL liquid in higher dimension is not widely understood [10,11], it is possible to demonstrate that the strong-coupling fixed point is likely to be the "tomographic" TL liquid [12], at least in two dimensions.

In this paper we find the linear-T resistivity ($1/\tau \sim k_B T$) and linear frequency dependence of the optical conductivity ($1/\tau \sim \omega$). We also show that the effect of impurities is different from the Fermi liquid and this may be the reason why the residual resistivity appears to be zero in most optimized samples.

First we consider the Kubo formula for conductivity at finite temperatures:

$$\sigma(\omega)=\frac{e^2}{\pi\omega m^2}\sum_k\int d\omega' k_x^2[f(\omega'-\omega)-f(\omega')]\chi(k,\omega',\omega'-\omega)G^R(k,\omega')G^A(k,\omega'-\omega)\,, \tag{1}$$

where $f(\omega)$ is a Fermi distribution function $1/(e^{\beta\omega}+1)$ and $\chi(k,\omega',\omega'-\omega)$ is a vertex correction. As a simple approximation we neglect vertex corrections. In the $\omega\to 0$ limit,

$$\sigma(\omega=0)=\frac{e^2}{\pi m^2}\sum_k\int d\omega' k_x^2[-f'(\omega')]|G^R(k,\omega')|^2\,. \tag{2}$$

This approximation involves a subtle problem of what is the conductivity in real systems. If we calculate the Kubo formula using the current-current correlation function, we get [13] $\sigma(\omega)=-ne^2K_\rho/mi\omega$, where K_ρ is a correlation exponent. This is because there is no dissipation mechanism in the TL liquid under the periodic boundary conditions. However, this is not a true description because the real physical process in the strongly correlated system is that an incident electron decays into

spinon and holon. Apparently we need to take account of a system with open boundary conditions instead of a closed system as implicitly assumed in the Kubo formula. In a sense, the transport problem in the strong-coupling regime is similar to the phonon-drag problem, where if the phonon-drag effect is completely taken into account, there is no dissipation. In the open boundary case we can think that the spinon and holon systems are in thermal equilibrium independent of the accelerated electron. As a result, even if there is a phonon-drag (in this case spinon-holon-drag) effect, the compensation is not complete and there is a dissipation for the electrons.

It is a long-standing question what the correct or reasonable conductivity formula is in such cases. Here we use a very rough approximation of neglecting vertex corrections, assuming that the open boundary effects or holon-drag type effects are partly taken into account. We have no formal way of doing this within the TL liquid, but using a phenomenological Boltzmann equation the thermal equilibrium of a spinon-holon system can be achieved by relaxation of spinons and holons due to impurity scattering. The resistivity becomes $\rho=1/\tau(1+\tau_{h,s}/\tau)$, where $1/\tau_{h,s}$ is the relaxation rate for holons or spinons. If there is no relaxation, then $\tau_{h,s}\to\infty$ and $\rho\to 0$ which means that the drag effect is completely taken into account. On the other hand when $\tau_{h,s}\ll\tau$, the contribution of the drag effect is $\tau_{h,s}/\tau^2\sim T^2\tau_{h,s}$ which is smaller than $1/\tau\sim T$. This corresponds to the case where the spinon and holon systems are almost in equilibrium. In order to see this mechanism in diagrammatic representation we check the effect of holon-impurity scattering in a phenomenological Hamiltonian. Some of the impurity scattering processes of holons do not contribute to the electron self-energy diagrams, but they are more effective in the diagrams representing the vertex corrections. These vertex corrections are analogous to the diagrams used by Holstein to represent phonon drag, and as in that case the vertex corrections may be neglected when the impurity scattering rate for the holon is fast compared with the holon's relaxation rate due to spinon-holon scattering, T^2. (The latter estimate is arrived at by use of detailed balance and the electron decay rate $\propto T$.) This indicates that the vertex corrections are to be suppressed to approximate the situation with a small $\tau_{h,s}$, or equivalently, almost equilibrium of holon and spin systems.

Moreover the conductivity formula (2) resembles the Landauer formula [14] which is appropriate for open boundary problems. The retarded Green's function represents the probability of finding the accelerated electron at a distance x and plays a role of transmittance coefficient. The relation between the Landauer formula and microscopic formula has not been clarified yet, but we expect that the formula (2) will serve as a kind of Landauer formula for metallic cases [15].

Let us proceed to calculate the conductivity using TL Green's functions [2]. In this paper to avoid unphysical complication of mathematical expressions, we use an approximate form of G^R which reproduces the correct behaviors of the original G^R in physically important regimes [16]:

$$G^R_{i\sigma}(x,t)=\pm\frac{ie^{\pm ik_Fx}}{\pi\Lambda^\alpha}\theta(t)\mathrm{Im}\left[\frac{B(x/v_c-t)^{1/2}B(x/v_s-t)^{1/2}B(2\tilde{x}/v_c)^\alpha}{(x\mp v_ct\pm i/\Lambda)^{1/2}(x\mp v_st\pm i/\Lambda)^{1/2}(2\tilde{x}\mp i/\Lambda)^\alpha}\right], \tag{3}$$

where $\pm$ corresponds to the two branches ($i=1,2$) in the vicinity of $\pm k_F$, respectively, Λ is a large-k cutoff of interactions, and $\tilde{x}=\max(x,v_ct)$. The temperature dependence shows up in $B(X)=(\pi X/\beta)/\sinh(\pi X/\beta)$ with $\beta=1/k_BT$. The exponent α is $\alpha=\frac{1}{4}(K_\rho+1/K_\rho-2)$ and $0\le\alpha\le\frac{1}{8}$ for the 1D Hubbard model. It is straightforward to compare the behavior of the Fourier transform in various limiting cases. The singularities in the vicinities of $\omega\sim v_ck$ and v_sk are $(\omega-v_ck)^{-1/2+\alpha}$ and $(\omega-v_sk)^{-1/2+\alpha}$, while the original G^R has $(\omega-v_ck)^{-(1-\alpha)/2}$ and $(\omega-v_sk)^{-1/2+\alpha}$. It can be checked that this difference does not change our final results. The differences are only harmless numerical prefactors. The singularity at $\omega+v_ck$ is omitted in (3), but even in the original G^R it is $(\omega-v_ck)^{\alpha/2}$ which does not diverge and makes no contribution to relevant physical quantities.

There are two typical parameter regions: $x<\beta v_-$ and $x>\beta v_-$ with $1/v_\pm=\frac{1}{2}(1/v_s\pm 1/v_c)$. In the region $x<\beta v_-$ including $T=0$, we can approximate $B(X)\sim 1$, and the Fourier transform of G^R becomes

$$G^R_{1\sigma}(x,\omega)=-\frac{ie^{ik_Fx+i(\omega/v_+)x}}{(v_cv_s)^{1/2}\Lambda^\alpha}\theta(x)J_0\left(\frac{\omega x}{v_-}\right)(2x-i/\Lambda)^{-\alpha}. \tag{4}$$

In the other region $x>\beta v_-$ for finite temperatures, the exponential decay of $B(X)$ becomes important. This is special for the TL liquid and its importance is discussed below. The integral in G^R is estimated from its behavior in the regions $|t-x/v_s|<\beta$ and $|t-x/v_c|<\beta$ to give $G^R_{1\sigma}(x,\omega)\propto e^{-(2\pi x/\beta)(1/2v_-+\alpha/v_c)}$.

Substituting these Green's functions into the conductivity formula, we obtain

$$\sigma(\omega=0)=-\frac{e^2k_F^2}{\pi m^2}\int d\omega' f'(\omega')\frac{v_-\beta^{1-2\alpha}}{v_cv_s(v_-\Lambda)^{2\alpha}}I(\beta\omega'),$$

where $I(\beta\omega')$ is a function of order 1. The integral over ω' may give a weak temperature dependence but the dominant temperature dependence is $\beta^{1-2\alpha}$. Since α is small we have roughly linear-T resistivity. Assuming v_c

$> v_s$, $\Lambda \sim 1/a$, $mv_c \sim k_F = n\pi/2$, and $v_s\Lambda \sim J$, we have

$$\sigma = \frac{ne^2\beta}{m}\frac{v_-}{2v_s}\left(\frac{1}{\beta J}\right)^{2\alpha}.$$

The relaxation time $1/\tau = k_B T$ shows up because the Green's function has an intrinsic decay proportional to $e^{-\pi x/\beta v_-}$. This comes from the fact that the accelerated electron cannot propagate coherently in the TL liquid, but decays into spinon and holon propagating with different velocities. This is characteristic for the TL liquid where $v_s \neq v_c$ and v_- is finite. Note that in a Fermi liquid with $\alpha = 0$ and $v_- = \infty$, the retarded Green's function is temperature independent and $G^R_{\uparrow\sigma}(x,\omega) = -[i\theta(x)/v] \times e^{ik_F x + i(\omega/v)x}$, showing that an electron propagates coherently. It is also worthwhile noticing that strictly at $T = 0$ the TL Green's function, Eq. (4), does not have an exponentially decaying factor. In other words thermal fluctuations destroy the coherence of electrons which propagate partly with the charge velocity and partly with the spin velocity. Anderson and Zou [3] described this effect as holon-spinon scattering. As mentioned before, if we use the current-current correlation function and periodic boundary conditions, this phenomenon is missed and electrons recover their total momentum via holon-drag processes. We believe that the real physical process is taken into account in our calculation.

Next we consider the effect of impurities. In the conventional diagrammatic procedure, the relevant self-energy is $|u|^2 \int^{k_c} G^R(q,\omega)dq$, where the impurity potential is approximated as a constant $|u|$ near the Fermi surface. In the Fermi liquid this self-energy is $-i\pi|u|^2/v_F$, independent of the energy cutoff k_c causing a relaxation $1/\tau_B$. In the present case, however, the TL Green's function gives

$$-\frac{i|u|^2 \sin(\pi\alpha/2)\Gamma(1-\alpha)}{(v_c v_s)^{1/2}\alpha}\left(\frac{k_c}{2\Lambda}\right)^{\alpha} \quad (5)$$

for $k_c\beta v_- \gg 1$, and

$$-\frac{i|u|^2 k_c \beta v_-}{(v_c v_s)^{1/2}(1-\alpha)}\left(\frac{1}{2\beta v_- \Lambda}\right)^{\alpha} \quad (6)$$

for $k_c\beta v_- < 1$. The important difference is that self-energy depends on the cutoff and has a different behavior compared to Fermi liquid. In the case where we expect $k_c \ll \Lambda$ the impurity effect can be very small. Moreover, the effect of impurities has a distinctive temperature dependence. In relatively higher temperature region, $T > k_c v_- \sim (k_c/\Lambda)J$, a simple partial summation of impurity diagrams leads to

$$\rho = \frac{m}{ne^2}\left\{T\left(\frac{J}{T}\right)^{2\alpha} + \frac{Jk_c}{\tau_B T\Lambda}\left(\frac{T}{2J}\right)^{\alpha}\right\}.$$

In this case the residual resistivity extrapolated from the high temperature behavior looks like zero. At low temperatures, $T < (k_c/\Lambda)J$, the resistivity becomes

$$\rho = \frac{m}{ne^2}\left\{T\left(\frac{J}{T}\right)^{2\alpha} + \frac{1}{\tau_B}\left(\frac{k_c}{2\Lambda}\right)^{\alpha}\right\}.$$

The effect of impurities becomes visible below a crossover temperature which is $\min[1/\tau_B, (Jk_c/\tau_B\Lambda)^{1/2}]$ for the small α limit. At very low temperatures and large $(k_c/\Lambda)^{\alpha}$, impurity scattering may lead to 1D Anderson localization insofar as we use the conventional Kubo formula. Renormalization group studies [13,17–19] use the self-energy (5) and show that the impurity effect is stronger than the noninteracting case. We would argue that the Anderson localization (if any) may take place below the crossover temperature which depends on impurity strength, cutoff, k_c, Λ, and velocity difference v_-. Above that temperature the dominant term is linear in T; below that crossover temperature the resistivity may begin to increase and eventually go into the Anderson localization regime which was discussed using the renormalization group.

Here we would like to insert another argument to support the weakness of the impurity effect in the TL liquid. The TL liquid used to derive $G^R(x,t)$ is based upon the perturbative renormalization group theory in the weak-coupling regime. It is possible to have a quantitative difference in the strong-coupling regime. Fortunately we know the ground state wave function of the 1D Hubbard model at $U \to \infty$ [8], so that we can calculate the matrix element of the impurity scattering Hamiltonian, $H_{\rm imp} = \sum_{i\sigma} u(2k_F) e^{2ik_F r_i} c^{\dagger}_{i\sigma} c_{i\sigma}$. We have chosen the $2k_F$ component of the impurity potential since it gives rise to the resistivity (and eventually localization) in the noninteracting case. The matrix element for the low energy limit, $\langle k_F|H_{\rm imp}|-k_F\rangle$, is most important for transport properties, where $|\pm k_F\rangle$ is an eigenstate with total momentum $\pm k_F$.

For the $U \to \infty$ Hubbard model the lowest energy state with $\pm k_F$ is given by $|\pm k_F\rangle = \mathcal{S}(\pm 2k_F)\Phi_H(\mp k_F)$, where $\mathcal{S}$ is a Slater determinant of spinless fermions representing the charge degrees of freedom and Φ_H is an eigenstate of the $S = \frac{1}{2}$ Heisenberg model with "squeezed" spin coordinates [8]. These states consist of a holon excitation just above its $\pm 2k_F$ Fermi surface as well as a spinon excitation above the $\mp k_F$ Fermi surface. Analysis of the quantum numbers in the Bethe ansatz shows that $\Phi_H(\pm k_F)$ is exactly the same as the eigenstate of the Heisenberg chain with total (crystal) momentum $\pm\pi/2$. Using these initial and final states, the matrix element $\langle k_F|H_{\rm imp}|-k_F\rangle$ becomes zero because $\langle\Phi_H(-k_F)|\Phi_H(k_F)\rangle = 0$. Here the charge part and spin parts are decomposed because of the summation over spin in $H_{\rm imp}$. The charge part can have a nonzero value but the spin part is identically zero. This fact shows that spin degrees of freedom are not scattered in the large-U limit [20].

Let us compare with the result of the TL liquid scheme. $H_{\rm imp}$ can be represented in terms of two Bose fields and it is straightforward to calculate the matrix element as $\langle k_F|H_{\rm imp}|-k_F\rangle = 1/L^{(1+K_\rho)/2}$. Its dependence on K_ρ essentially reproduces the result of renormalization group studies: For the repulsive case ($K_\rho < 1$) this matrix element has a stronger size dependence than in the noninteracting case ($K_\rho = 1$) and thus leads to Anderson localization. Comparison of the two matrix elements shows that the coefficient of $1/L^{(1+K_\rho)/2}$ can easily depend on U so that in the large-U regime, it can be zero or small if any. Therefore the crossover temperature, below which the effect of impurity becomes dominant, can be very low in the large-U region. This is consistent with our observation in the conductivity. The exponent α is largest ($\alpha = \frac{1}{8}$) at $U \to \infty$ and the impurity effect is weakest.

Next we study the optical conductivity. For this purpose the Green's function for $T < \omega$ is necessary. We use zero temperature Green's function for simplicity. Substitution of G^R into the conductivity formula gives

$$\sigma(\omega, T=0) = \frac{e^2 k_F^2}{\pi m^2} \frac{v_- \Gamma(1-2\alpha)}{4 v_c v_s \alpha \cos\pi\alpha} \left[\left(\frac{\omega}{2 v_s \Lambda} \right)^{2\alpha} - \left(\frac{\omega}{2 v_c \Lambda} \right)^{2\alpha} \right] \frac{1}{-i\omega + \omega \tan\pi\alpha} .$$

It is clear that the relaxation rate has a linear ω dependence and $1/\tau = \omega \tan\pi\alpha$. One interesting point is that the coefficient of ω is proportional to α for small α. It is independent of $v_c - v_s$, which was essential for $1/\tau \sim k_B T$. This small coefficient is required from the sum rule, $(2/\pi)\int_0^\infty d\omega \, {\rm Re}\sigma(\omega) = ne^2/m$, since the numerator of $\sigma(\omega)$ is proportional to $\omega^{2\alpha}$. Of course the sum rule is not completely satisfied because of the restriction of validity of TL liquid Green's function, which is only up to $\omega_c \sim v/\Lambda$.

Finally we briefly discuss the possible relation to experiments. As we can see, if the system approaches the Fermi liquid ($\alpha \to 0$, $v_c \to v_s$, and thus $v_- \to \infty$), the coefficient of the linear-T term becomes smaller and smaller. At the same time the impurity effect becomes stronger. It may happen in high-T_c materials in the overdoped regime as the hole doping increases. As we can see, the linear ω dependence of the relaxation rate also vanishes as the system approaches the Fermi liquid. On the other hand, when the system is a TL liquid and the crossover temperature is higher than T_c, a precursor of localization will be seen above T_c, as discussed above. For the application to higher dimensions, we assume the "tomographic" TL liquid which has a cut in the Green's function along the perpendicular direction of the Fermi surface. To estimate the Hall angle the spinon-spinon interaction causing relaxation time $\tau_\parallel$ has to be taken into account. Our calculation can be directly used for the quasi-one-dimen- sional conductors which will be realized in organic conductors and mesoscopic systems.

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