Boltzmann Description of Non-Interacting Electrons in Weakly Localized Regime

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Abstract. Transport process of non-interacting electrons is reformulated, in view of the exact treatment of interacting fermions reported by the present authors in this conference. It makes correspondence to the Boltzmann theory, covering the weakly localized regime, and also eliminates the hidden ultraviolet divergence by incorporating the particle-particle and hole-hole pairs. A mass renormalization of purely two-particle nature appears in the transport equation, giving rise to the conductivity of the Drude form. Taking the maximally crossed diagrams, the 2D conductivity is shown to vanish in the elastic scattering limit, while the distribution function preserves its sharp peak and the transport mass reduces to the free-electron value. The description differs from the self-consistent theory by Vollhardt and Wölfle, in which the Bethe-Salpeter structure of the scattering vertex is abandoned in favour of the time-reversal symmetry so the correspondence to the Boltzmann theory is lost.

1. Introduction
Quantum interference is known to cause vanishing of the conductivity for one and two dimensions. It seems to be a common consensus that the relevant transport processes are purely quantum, being out of the scope of the Boltzmann picture. For instance, the self-consistent theory by Vollhardt and Wölfle [1], which successfully described the weak localization (WL), is not compatible with the classical transport equation.

Recently, the present authors have shown that the exact transport equation for interacting fermions is nothing but a different form of the Ward identity [2]. This implies that all transport processes can be treated quantum mechanically, without loosing contact with the classical theory, irrespective of the strength of the scattering. They also point out that the conventional treatments involve ultraviolet divergence in the conductivity, and show a correct way to remove it. In the present contribution, we attempt a similar argument to non-interacting electrons in the WL regime, in order to have a macroscopic understanding of the phenomenon in the framework of the Fermi liquid theory (FLT). A new renormalization due to the particle-particle (p-p) and hole-hole (h-h) pairs plays important roles in this treatment.

2. Divergence and the exact transport equation
We deal with non-interacting electrons with random scatterers in the general framework. We first discuss the hidden divergence of the transport coefficients in the conventional treatment.
The electrical conductivity for finite $\omega$ and $k$ is given by the Kubo-Greenwood formula as

$$\sigma_{\alpha\beta}(k, \omega) = \frac{K_{\alpha\beta}(k, \omega) - K_{\alpha\beta}(k, 0)}{i\omega}$$

$$K_{\alpha\beta}(k, \omega) = \frac{ie^2}{\pi m \Omega} \int d\epsilon \int \frac{d^3p}{(2\pi)^3} \left\{ \left( f_0(\epsilon - \omega/2) - f_0(\epsilon + \omega/2) \right) p^\alpha g_2(p) V_2^\beta(p) 
- f_0(\epsilon - \omega/2) p^\alpha g_1(p) V_1^\beta(p) + f_0(\epsilon + \omega/2) p^\alpha g_3(p) V_3^\beta(p) \right\}. \quad (2)$$

Here, as in Ref.[2], $g_1(p) \equiv G^R(p + k/2)G^R(p - k/2)$, $g_2(p) \equiv G^R(p + k/2)G^A(p - k/2)$ and $g_3(p) \equiv G^A(p + k/2)G^A(p - k/2)$ with $p \equiv (p, \epsilon)$ and $k \equiv (k, \omega)$. Also $V_i(p)$ ($i = 1, 2, 3$) denotes the three different analytical continuations of the current vertex function. The above formula gives the conductivity in the form

$$\sigma_{\alpha\beta}(k, \omega) = \frac{\hbar e^2}{\pi m \Omega} \int d\epsilon \left( -\frac{\partial f_0}{\partial \epsilon} \right) \times \left\{ \int \frac{d^3p}{(2\pi)^3} p^\alpha g_2(p) V_2^\beta(p) - \text{Re} \int \frac{d^3p}{(2\pi)^3} p^\alpha g_1(p) V_1^\beta(p) \right\}, \quad (3)$$

which is exact to the linear order in $\omega$.

In making correspondence to the Boltzmann theory, it is customary to take only the term involving the factor of $g_2(p)$ in the above expression. Also this factor is treated as being proportional to a delta function, which hides the ultraviolet divergence in the corresponding integral, as is seen by examining the asymptotic behaviour of the integrand at large $p$. Furthermore, the mass renormalization is missed out by this procedure [3].

The correct correspondence is discussed by Yamane and Itoh [2]. Although it is applicable to the present case in principle, we give an alternative argument adapted to non-interacting electrons. It involves some approximation but the treatment is much more simplified. We return to the conductivity expression in terms of the resolvent operators $\hat{G}(z) = (z - \hat{H})^{-1}$. We then note that the contributions with $f_0(\epsilon - \omega/2)$ and those with $f_0(\epsilon + \omega/2)$ in Eq(2) involve different combinations of resolvents. We use the optical theorem $\hat{G}(z_1)\hat{G}(z_2) = -(\hat{G}(z_1) - \hat{G}(z_2))/(z_1 - z_2)$ for each, converting it into a product of the three resolvents. They are then represented by diagrams with three vertices (Fig.1). We renormalize the propagators and vertices independently. The particle-number vertex is reduced by using the Ward identity. By further noting that $\{V_1(p) + V_3(p)/2 \equiv v_p$ is the group velocity, we obtain for an isotropic system

$$j = 2e \int \frac{d^3p}{(2\pi)^3} v_p \tilde{\varphi}_p(\mu)$$

and

$$\tilde{\varphi}_p(\epsilon) = \frac{1}{2\pi z_p} \left\{ g_2(p) - \frac{g_1(p) + g_3(p)}{2} \right\} V_2(p) \cdot (\epsilon E), \quad (5)$$

**Figure 1.**

Three-vertex representation of the conductivity. The vertex for $N$ corresponds to the unit operator. $p_\pm$ and $\epsilon_\pm$ are the short-hand notations of $p \pm k/2$ and $\epsilon \pm \omega/2$, respectively.
where \( \tilde{\varphi}_p(\mu) \), with \( \mu \) being the chemical potential, is the proper distribution function involving p-p and h-h corrections. The same expression has been derived in a different way in the self-consistent Born approximation [3].

The expressions (4) and (5) are free of divergence and in conformity with the results obtained for interacting electrons [2], except for the renormalizations in \( v_p \) and \( z_p \). We may also derive the transport equation for \( \tilde{\varphi}_p \) (Eq(6) below). It again coincides with the result in Ref.[2] (Eqs (19) and (20) therein; note that we do not have "interaction" \( T(p,p') \) in the present case). The details will be published elsewhere, and we summarize the result below:

\[
-i[\omega \tilde{S}(p) - k \cdot \tilde{Q}(p)]\tilde{\varphi}_p + \tilde{\Delta}(\epsilon_p - \mu)\tilde{Q}(p) \cdot eE = -\int \frac{d^3p'}{(2\pi)^3} \tilde{W}(p,p')z_{p'} \{ \tilde{\Delta}(\epsilon_p - \mu)\tilde{\varphi}_{p'} - \tilde{\Delta}(\epsilon_{p'} - \mu)\tilde{\varphi}_p \},
\]

where \( W(p,p') \) is the proper (non-separable) scattering vertex for the p-h pair, and \( \tilde{\Delta}(\epsilon_p - \mu) \) is defined by

\[
\tilde{\Delta}(\epsilon_p - \mu) \equiv \frac{\hbar}{2\pi z_p} \{ G^R(p+k/2) - G^A(p-k/2) \} \left[ 1 - \frac{g_1(p) + g_3(p)}{g_2(p)} \right].
\]

In all the equations above, the energy arguments are fixed to be equal to the chemical potential. The tildes on \( \tilde{Q}, \tilde{S} \) and \( \tilde{W} \) represent renormalizations due to p-p and h-h pairs. This is a new type of renormalization. The \( \tilde{\Delta}(\epsilon_p - \mu) \) may be replaced by \(-\partial f_0/\partial \epsilon_p \) in Eq(6), \textit{irrespective of the strength of} \( \tilde{W}(p,p') \), as far as the imaginary part of the electron self energy is small. This implies that quasiparticle concept can be made use of even for non-interacting electrons. \( \tilde{Q}(p) \) and \( \tilde{S}(p) \) give the transport effective mass by \( p/\tilde{m}_p^* \equiv \tilde{Q}(p)/\tilde{S}(p) \), while \( \tilde{W}(p,p')z_{p'}/\tilde{S}(p) \) represents the renormalized collision among quasiparticles.

3. Maximally crossed diagrams and dc conductivity

We apply the preceding formalism to the maximally crossed diagrams of 2-dimensional electrons, with randomly distributed impurities of short range potentials. After Vollhardt and Wölflle [1] we assume \( G^{R,A}(p) = |\epsilon - p^2/2m \pm 2i/\tau|^{-1} \) with \( 1/\tau = n_i v^2 \rho \). The proper scattering vertex is, in this case,

\[
W(p,p') = n_i v^2 \frac{1}{\Omega \tau} \frac{1}{D(p + p')^2 + \gamma^2}
\]

where we have introduced a small parameter \( \gamma \) to represent inelastic scatterings. Eqs (6)-(9) may then be solved simultaneously; we solved the Bethe-Salpeter equation for \( V_2(p,\mu) \) to obtain an equivalent solution for \( \tilde{\varphi}_p \) through Eq(5).

In Fig.2 we show the calculated dc conductivity and the distribution function. The \( \gamma \) has been extrapolated to zero, numerically. Other parameters are fixed so that \( p_F = 2 \) and \( 1/\tau = 0.02 \). The distribution function is displayed for \( \gamma = 10^{-9.977} \), the smallest value we have examined. Although \( \tilde{\varphi}_p \) must collapse ultimately, its peak is seen to remain sufficiently sharp, even though
the conductivity is virtually zero for this value of $\gamma$, as compared to the saturated values at larger inelastic scatterings. We therefore consider that the FLT description is valid even in the vicinity of the WL. We have also plotted in Fig. 3 $\tilde{Q}(p)$ and $\tilde{S}(p)$, obtained by solving Eqs (7) and (8), as functions of $|p|$. Both quantities diverge at $|p| = p_F$ as $\gamma \to 0$, due to the interplay between the singularity in the backscattering and the structure of $g_1 + g_3$ in its neighbourhood. In fact the peak suddenly turns negative at certain point, and we were unable to obtain numerically stable solutions for $\gamma$ smaller than $\approx 10^{-71}$. In the calculable range, the evaluated effective mass was found to be equal to the free electron mass up to the six digits, because the two divergences in $\tilde{Q}(p)$ and $\tilde{S}(p)$ have equal weights. With this effective mass, Eq (4) gives the Drude formula $\sigma = ne^2 \tau_{tr}/m^*$, with $\tau_{tr}$ being evaluated by the collision integral in Eq (6).

![Figure 2](image1.png)

**Figure 2.** Left: dc conductivity as a function of $-1/\log_{10} \gamma$, Right: distribution function (5) as a function of $|p|$. The Green line shows the conventional definition without p-p and h-h corrections (lacking $g_1$ and $g_3$).

![Figure 3](image2.png)

**Figure 3.** Plots of $\tilde{Q}(p)$ and $\tilde{S}(p)$ ($\tilde{Q}(p) \equiv \tilde{Q}(p/|p|)$) as functions of $|p|$, for three different $\gamma$ values. On the right the peak structure is shown in the inset in a magnified scale. The correspondence between the colour and the value of $\gamma$ is indicated on the left. The two quantities simultaneously turn to negative around $\gamma = 10^{-70}$.

### 4. Conclusion

The WL of two-dimensional non-interacting electrons has been treated in the framework of the FLT by Yamane and Itoh [2]. The role of the p-p and h-h contributions has been emphasized, and we observed that the quantum interference reduced the transport effective mass to the free electron value, while the classical Boltzmann picture was valid until fairly close to the localization. The validity of the present approximation shown by Fig.1, which appears to lack some of the renormalizations derived in Ref.[2], is to be further examined, and we hope to discuss it in future publications.

### References

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