Nonequilibrium-current-induced corrections to the
one-particle-correlation function in a wire

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Abstract

Electron gas in a wire connected to two terminals with potential drop is studied with the
Schwinger-Keldysh formalism. Recent studies, where the current is enforced to flow with a
Lagrange-multiplier term, demonstrated that the current enhances the one-particle-correlation
function. We report that in our model, such enhancement is not guaranteed to occur, but
conditional both on the potential drop and the positions where we observe the correlation
function. That is, under a certain condition, spatially modulated pattern is formed in the wire
owing to the nonequilibrium current.

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devices (quantum dots, quantum wires, etc.))
Recently, Antal et al. have reported that nonequilibrium current enhances the one-particle-correlation function contrary to our naive expectation that nonequilibrium transport would destroy any orders [1, 2, 3]. They utilized a trick with which the nonequilibrium flow is introduced in a frame of equilibrium statistical mechanics. That is, they introduced a Lagrange multiplier $\lambda$, and investigated the (equilibrium) ground state of the Hamiltonian given by $\mathcal{H} - \lambda J$, where $\mathcal{H}$ denotes a model Hamiltonian of a wire and $J$ denotes the space integral of the current operator. Namely, the current flow is regarded as an environment variable, which is to be given ad hoc. As for an explicit example of $\mathcal{H}$, they took up the transverse Ising model and the $XY$ model in one dimension, and found that the above-mentioned behavior, namely, the transport-induced correlation enhancement, occurs in these models. Cardy extended their work for a nonintegrable case (a lattice scaler field theory), and confirmed their observation [4].

This enhancement due to nonequilibrium transport had been studied extensively in the field of classical statistical mechanics [5, 6, 7, 8, 9, 10]. It should be noted, however, that the quantum version has an advantage that the (nonequilibrium) dynamics is governed by the Hamiltonian itself, whereas the classical dynamics depends upon the kinetic rules which we implement.

In this letter, we investigate the spinless electron gas in a wire, which is connected to two leads with different chemical potentials. Hence, in our case, the current is driven to flow by the potential drop as in actual experimental situations. We stress that we have employed the Schwinger-Keldysh formalism [11, 12], that allows us to treat the transport phenomena driven far out of equilibrium. Thereby, we report that the enhancement due to nonequilibrium flow is not guaranteed to occur, but depends significantly both on the potential drop and the positions where we observe the correlation. As in the previous studies — note that the transverse Ising model and the $XY$ model are equivalent to free-spinless-fermion models — we supposed that the wire electrons are free (quadratic). We believe that the many-body-correlation effect would not change our essential conclusions.
Our model Hamiltonian is given by,

\[ \mathcal{H} = \sum_k \left( \varepsilon_k - \frac{eV}{2} \right) L_k^\dagger L_k + \sum_k \left( \varepsilon_k + \frac{eV}{2} \right) R_k^\dagger R_k + \sum_i t(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + T'(c_\alpha^\dagger c_1 + c_1^\dagger c_\alpha) + T'(c_\alpha^\dagger c_L + c_L^\dagger c_\alpha'). \]

The operator \( L_k^\dagger \) (\( R_k^\dagger \)) creates a conduction electron with wave number \( k \) in the left (right) lead. \( \varepsilon_k \) denotes the dispersion relation of these leads, and \( \mu = eV/2 \) (\( -eV/2 \)) give the chemical potential of the left (right) lead. Therefore, the parameter \( eV \) gives the chemical-potential drop between the leads. The scheme how we describe nonequilibrium flow is explicated afterwards.

The operator \( c_\alpha \) (\( c_{\alpha'} \)) is the annihilation operator at the left (right) terminal; namely, \( c_\alpha = (1/\sqrt{N}) \sum_k L_k \) and \( c_{\alpha'} = (1/\sqrt{N}) \sum_k R_k \) with the number of conduction electron levels \( N \).

The operator \( c_i^\dagger \) creates an electron at site \( i \) in the wire. We assume that the wire is sufficiently long, and the lead electrons are injected at the intermediate positions of \( i = 1 \) and \( L \) with the coupling (transfer) amplitude \( T' \). We could implement the open-boundary condition for our wire, for instance, with use of the Fabrizio-Gogolin Tomonaga-Luttinger-liquid formalism under the open-boundary condition [13]; it would just cause inessential complications.

Properties of quantum wire, especially, those on the electron conductance, have been studied extensively so far. It seems, however, that these studies have been rather inclined to the vicinity of equilibrium that can be managed within the Kubo formula, and little attention has been paid to the situation driven far out of equilibrium. The Schwinger-Keldysh formalism [11, 12] circumvents that restriction. Their formalism is demonstrated for nonequilibrium steady flow through a wire by Caroli et al. explicitly [14]. We follow this description in order to investigate the nonequilibrium flow. In their description, the nonequilibrium steady flow is realized through infinite-time evolution from such initial state where both leads are disconnected from the wire \( (T' = 0) \), and are staying at each ground state with different chemical potentials. With respect to such time-evolved nonequilibrium state \(| \rangle \rangle \), the following Green functions are defined;

\[ G^i_{ij}(t) = -i\theta(t)\langle\{c_i(t), c_j^\dagger\}\rangle \]

\[ G^a_{ij}(t) = i\theta(-t)\langle\{c_i(t), c_j^\dagger\}\rangle \]

\[ F_{ij}(t) = -i\langle[c_i(t), c_j^\dagger]\rangle. \]
They satisfy the following respective Dyson equations,

\[ G^r_{ij}(\omega) = g^r_{ij}(\omega) + g^r_{ik}(\omega)\Sigma_{kl}G^r_{lj}(\omega) \]  
(5)

\[ G^a_{ij}(\omega) = g^a_{ij}(\omega) + g^a_{ik}(\omega)\Sigma_{kl}G^a_{lj}(\omega) \]  
(6)

\[ F_{ij}(\omega) = f_{ij}(\omega) + g^r_{ik}(\omega)\Sigma_{kl}F_{lj}(\omega) + f_{ik}(\omega)\Sigma_{kl}G^r_{lj}(\omega), \]  
(7)

The small-letter ones are those for the (unperturbed) initial state, and the self energy is given by \( \Sigma_{kl} = T'(\delta_{kl}\delta_{11} + \delta_{k1}\delta_{al} + \delta_{ka}\delta_{ll} + \delta_{kl}\delta_{aa1}) \). It is notable that the Dyson equation of \( F_{ij} \) is rather involved, and as a matter of fact, nonequilibrium characteristics are included in \( F_{ij} \).

Quantity to be investigated below is the one-particle-correlation function, which is given by \( C_{ij} = \langle c_i^\dagger c_j + c_j^\dagger c_i \rangle \). This correlation function is the central concern of the previous papers \([1, 2]\), where it is represented in terms of the spin language; \( \langle S_i^x S_j^x \rangle \). In one dimension (Tomonaga-Luttinger liquid), (long-range asymptotic forms of) all the correlation functions are interlocked each other. Hence, one particular correlation function, for instance, the one-particle correlation, is sufficient to gain the essential physics. (For example, when the one-particle correlation is suppressed, the density-density correlation develops instead.) The one-particle-correlation function is expressed in terms of the Green function \( F_{ij} \),

\[ C_{ij} = -\frac{i}{2} (F_{ij}(t = 0) + F_{ji}(t = 0)) \]  
(8)

\[ = -\int \frac{d\omega}{2\pi} \frac{i}{2} (F_{ij}(\omega) + F_{ji}(\omega)). \]  
(9)

Therefore, we need to know \( F_{ij} \). By means of successive use of the above Dyson equations, \( F_{ij} \) can be expressed in terms of the unperturbed Green functions. Through a straightforward linear algebra, we arrive at the following expression;

\[ F_{ij} = f_{ij} + g^r_{iL}T'F_{a\alpha} + g^r_{iL}T'f_{a\alpha} + f_{i1}T'G^a_{a\alpha} + f_{i1}T'G^a_{a\alpha}, \]  
(10)

with

\[ F_{a\alpha} = \{(1 - g^r_{a\alpha}g^r_{a\alpha}T^2)(g^r_{a\alpha}T'f_{1j} + f_{1j}T'G^a_{a\alpha} + f_{1L}T'G^a_{a\alpha}) + f_{a\alpha}T'G^a_{ij}) \]

\[ +g^r_{a\alpha}g^r_{a\alpha}T^2g^r_{iL}(g^r_{a\alpha}T'(f_{Lj} + f_{L1}T'G^a_{a\alpha} + f_{LL}G^a_{a\alpha}) + f_{a\alpha}T'G^a_{Lj}) \} \]  
(11)
with the band width of the conduction-electron spectrum \( W \) dispersion is linear, and the Fermi points are shifted towards the origin; derive these expressions for a one-dimensional free-electron gas, assuming that the one-particle

with the density of states \( \rho \) namely,

is seen above, informations of the terminals are involved within the local Green functions at \( \alpha \) and \( \alpha' \). Here, we assume that the spectral property at the terminals is of the Lorentz type; namely,

\[
g^{r}_{\alpha\alpha',\alpha'}(\omega) = \frac{1}{(\omega + iW)} \tag{19}\]

\[
g^{a}_{\alpha\alpha',\alpha'}(\omega) = \frac{1}{(\omega - iW)} \tag{20}\]

\[
F_{\alpha\alpha}(\omega) = -2iW\text{sgn}(\omega - eV/2)/(\omega^2 + W^2) \tag{21}\]

\[
F_{\alpha'\alpha}(\omega) = -2iW\text{sgn}(\omega + eV/2)/(\omega^2 + W^2), \tag{22}\]

with the band width of the conduction-electron spectrum \( W \).

As for the wire Green functions, we used the following expressions:

\[
G^{a}_{ij}(\omega) = \frac{2\pi i\rho}{v_F} e^{-i\frac{\omega}{v_F}|i-j|} e^{-|\omega|/\omega_c} \tag{23}\]

\[
G^{r}_{ij}(\omega) = -\frac{2\pi i\rho}{v_F} e^{i\frac{\omega}{v_F}|i-j|} e^{-|\omega|/\omega_c} \tag{24}\]

\[
F_{ij}(\omega) = -\frac{4\pi i\rho}{v_F} \cos(\omega(i-j)/v_F)\text{sgn}(\omega)e^{-|\omega|/\omega_c}. \tag{25}\]

with the density of states \( \rho = 1/(2\pi) \). Let us mention some notions about these expressions: We derive these expressions for a one-dimensional free-electron gas, assuming that the one-particle dispersion is linear, and the Fermi points are shifted towards the origin; \( \omega = \pm v_Fk \). (We will
assume that the units of time and length are identical (isotropic); $v_F = 1$.) These prescriptions are common to those of the bosonization scheme, and thus the validity is guaranteed especially as far as the low-energy physics is concerned. Moreover, it is notable that we readily treat a many-body-correlated wire, just substituting the above expressions with those of Luther and Peschel [15]. The high-energy-cut-off factor $\omega_c$ stands for the band width of the wire electron, and is related to the lattice constant $a$; $\omega_c = v_F k_c = v_F \pi / a$. In the Tomonaga-Luttinger liquid theory, final expressions are obtained through setting $k_c \to \infty$, because one is motivated to know the long-wave-length physics, where the lattice constant is renormalized to zero. Here, we retain the cut-off factor, because our wire length is supposed to be finite, and the length is to be measured by the lattice constant. We set the lattice constant as the unit of length; $a = 1$.

The above formulae complete our scheme to calculate the one-particle-correlation function (8). In order to do the numerical integration of eq. (9), we adopted the Romberg algorithm [16]; we proceeded the Romberg iteration until the output result converges up to the tenth digit. All the data presented below are calculated for the condition of the lead-electron-band width $W = 2$, the coupling amplitude $T' = 0.5$ and the wire length $L = 20$.

Let us turn to present the numerical results. In Fig. 1, we plotted the correlation $C_{ij}$ against the voltage drop $eV$. According to the preceding reports, the correlation should be enhanced by the nonequilibrium potential drop $eV$ [1, 2, 4]. We found that in fact, the correlation $C_{ij}$ is influenced by $eV$. However, the dependence is not monotonic, but oscillates with respect to $eV$. In other words, our result indicates that it is not guaranteed whether the correlation is stabilized or not, but conditional on $eV$.

In order to clarify the parameter range where this non-equilibrium effect becomes significant, we had swept various parameter ranges. Thereby, we observed that the oscillation period is not influenced very much by $W$ and $T'$, but is proportional to $1/L$. Hence, it is suggested that the oscillation period is governed solely by the energy scale $\sim \omega_c/ L$. Note that the length of the wire does contribute to the energy scale, and thus the existence of the terminals is crucial in the present phenomenon.
Secondly, we report that the enhancement of \( C_{ij} \) depends on the distance \( i - j \) as well. In Figs. 2 and 3, we plotted the correlation \( C_{4,i} \) over various distances \( i \) at \( eV = 0.2 \) and \( eV = 1.6 \), respectively. At \( eV = 0.2 \) (Fig. 2), we see that in almost whole distance range, the correlation function decays monotonically, and for long-range distance \( (i - j \sim L) \), to our surprise, the sign of the correlation alternates. That is, the correlation function suffers long-wave-length modulation. At \( eV = 1.6 \) (Fig. 3), the alternation period becomes shortened. We observed that for larger \( eV \), in general, the correlation alternates more rapidly. We stress that the modulation period is not related to the (equilibrium) Fermi wave length like the Friedel oscillation, because in our formalism the Fermi points are shifted towards \( k = 0 \). Hence, we conclude that the nonequilibrium current does shift the Fermi points out of \( k = 0 \) effectively. The Fermi-point shift is found to take place actually in the aforementioned models in refs. 1, 2. In Figs. 2 and 3, we notice that the correlation of \( eV = 1.6 \) dominates that of \( eV = 0.2 \). One might think that the correlation is enhanced by the nonequilibrium driving force \( eV \). Yet, we found that this enhancement is rather accidental, and the correlation amplitude becomes suppressed gradually by \( eV \); remember the behavior shown in Fig. 1.

Next, we show the short-distance correlation \( C_{i,i+4} \) for various positions at \( eV = 1 \) in Fig. 4. We found that the correlation is spatially anti-symmetric with respect to the center of the terminals. Therefore, the correlation-function data presented so far change the signs, if we redefine \( C_{ij} \) so as to become closer to the opposite terminal instead: \( C_{ij} \leftrightarrow C_{L-i+1,L-j+1} \). This anti-symmetry may be plausible, if we notice the following symmetry of our model: \( i \leftrightarrow L - i + 1 \) and \( eV \leftrightarrow -eV \). Namely, owing to the anti-symmetry, the net enhancement of the correlation, which is integrated over the wire, is always vanishing. This feature is precisely due to the existence of terminals, which are not taken into account explicitly in the previous studies.

Finally, in Fig. 5, we plotted the electronic current \( I \) against \( eV \). The current is calculated by means of the following formula derived by Caroli et al. 14:

\[
I = \frac{eT''}{2\hbar} \int \frac{d\omega}{2\pi} G^\dagger_{i,i} G^\dagger_{j,j} \left\{ \left( g_{a\alpha}^* - g_{a\alpha}' \right) f_{\alpha'\alpha'} + f_{\alpha\alpha} \left( g_{a'\alpha'}^* - g_{a'\alpha'}^\dagger \right) \right\}.
\]

(26)

We found that the dependence of the current on \( eV \) is fairly monotonic; that does not exhibit
any oscillatory behaviors. Hence, it is shown that our observations presented above are not
directly related to the current flow strength.

To summarize, we have calculated the one-particle-correlation function in a wire (8), which
is subjected to two biased terminals. Being contrastive to the preceding report where the
nonequilibrium flow is introduced ad hoc, our results show that the enhancement of the corre-
lation function due to the nonequilibrium flow is conditional both on the bias and the positions
where we observe it. In particular, at a certain condition, the nonequilibrium flow gives rise
to spatially modulated structures. These features are related closely to the existence of termi-
nals, which are implicit in the previous Lagrange-multiplier formalism. The situation that we
had studied in this letter is quite realistic, and it may be realized in nano-technology devises.
However, because we are concerned in the longstanding statistical-mechanical problem whether
non-equilibrium transport enhances correlation or not, we concentrated deeply on the one-
particle correlation function, that may not be measurable directly in experiments. It remains
for future study to calculate quantities directly accessible in experiments.

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Figure 1: The one-particle-correlation function $C_{4,8}$ for various chemical-potential drop $eV$. 
Figure 2: The one-particle-correlation function $C_{4i} \ (8)$ for various distances $i$ over the wire for $\epsilon V = 0.2$. 
Figure 3: The one-particle-correlation function $C_{4,i}$ for various distances $i$ over the wire for $eV = 1.6$. 
Figure 4: The one-particle-correlation function $C_{i,i+4}$ at various positions $i$ in the wire for $eV = 1$. We see that the spatial distribution of the correlation enhancement is anti-symmetric.
Figure 5: Electric current against the potential drop $eV$. 