Landauer-type transport theory for interacting quantum wires: Application to carbon nanotube Y junctions

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We propose a Landauer-like theory for nonlinear transport in networks of one-dimensional interacting quantum wires (Luttinger liquids). A concrete example of current experimental focus is given by carbon nanotube Y junctions. Our theory has three basic ingredients that allow to explicitly solve this transport problem: (i) radiative boundary conditions to describe the coupling to external leads, (ii) the Kirchhoff node rule describing charge conservation, and (iii) density matching conditions at every node.

We study \( N \) single-channel spinless QWs at \(-L < x < 0\) described by LL theory merging at a common node at \( x = 0 \). For simplicity, we assume the same interaction constant \( g \) and Fermi velocity \( v_F \) in each QW, with straightforward generalization also to include spin and flavor degrees of freedom \([1]\). Theory then has to address (i) the inclusion of applied voltage sources and (ii) how a consistent treatment of the node can be achieved. Let us start with the first issue. Like in the two-terminal case, adiabatically coupled external reservoirs held at electrochemical potentials \( \mu_i \) lead to radiative boundary conditions \([2]\) (we put \( \hbar = 1 \))

\[
\frac{g^2}{2} + 1 \frac{\rho_{\nu,R}(-L)}{2} + \frac{g^2}{2} - 1 \frac{\rho_{\nu,L}(-L)}{2} = \frac{\mu_i}{2\pi v_F},
\]

where \( \rho_{\nu,R/L}(x) \) is the right/left-moving part of the density in QW \( i \). These boundary conditions only depend on the current injected into each QW from the respective reservoir, which in turn does not depend on the backscattering happening later on at the node or within the QW. Here we discuss the computation of the nonlinear conductance matrix normalized to \( e^2/h \),

\[
G_{ij} = \hbar \frac{\partial I_i}{\partial \mu_j},
\]

where the current \( I_i \) flowing through QW \( i \) is oriented towards the node, leaving noise properties to a future publication. Below applied voltages \( U_i \) are defined as

\[
e U_i = \mu_i - \bar{\mu}, \quad \bar{\mu} = \frac{1}{N} \sum_i \mu_i.
\]

Under this definition, gauge invariance (conductance matrix is invariant under a uniform change of all \( \mu_i \)) is automatically fulfilled if the \( G_{ij} \) depend only on the \( U_i \).
Next we address the physics arising at the node $x = 0$. Conservation of charge enforces the Kirchhoff node rule
\[ \sum_i I_i = 0. \] (4)

A second requirement at the node is the wavefunction matching via the $S$ matrix \[ S \Psi_L(0) = \Psi_R(0), \] (5)
where $\Psi(x) = (\psi_1, \ldots, \psi_N)$ contains the wavefunctions for the $N$ QWs, and the outgoing (left-moving) components $\Psi_L$ are connected to the incoming (right-moving) states $\Psi_R$ via an appropriate $N \times N$ matrix $S$, see, e.g. Ref. [19], for specific choices at $N = 3$. Note that the scattering matrix in Eq. (5) provides a “bare” (microscopic) description of the node properties, while interactions could dynamically generate some different boundary condition at low energy scales.

Unfortunately, a boundary condition like Eq. (3) is very difficult to handle for correlated electronic systems and typically does not allow for progress. Here we proceed differently by constructing a wide class of practically important $S$ matrices (albeit not all possible ones [19]) in the following way. We first consider an ideal system composed of impurity-free QWs symmetrically connected at the node. Microscopically, the corresponding non-interacting problem could be modelled as $N$ tight-binding chains with equal hopping matrix element $t_0$, where the “last” site of each chain is connected to the common node site via the same $t_0$ and all on-site energies are equal. Such a node corresponds to the special highly symmetric $S$ matrix
\[ S = \begin{pmatrix} (2 - N)/N & 2/N & \cdots & 2/N \\ 2/N & (2 - N)/N & \cdots & 2/N \\ \vdots & \vdots & \ddots & \vdots \\ 2/N & 2/N & \cdots & (2 - N)/N \end{pmatrix}. \] (6)

For this $S$ matrix, Eq. (3) directly implies $\psi_1(0) = \cdots = \psi_N(0)$ for the components of $\Psi = \Psi_L + \Psi_R$. Since phases in $\psi_i(0)$ can be gauged away, a density matching condition upon approaching the node results,
\[ \rho_1(0) = \cdots = \rho_N(0), \] (7)
where $\rho_i(0)$ denotes the total electronic density in QW $i$ close to the node. Remarkably, the conditions (7), (4) and (1) then allow to explicitly solve this transport problem for arbitrary interactions because the condition (7) does not involve wavefunction phases but only amplitudes. To arrive at more general $S$ matrices, in a second step we then consider additional impurities in the different QWs displaced slightly away from the node. Inclusion of impurities does not cause conceptual difficulties, and such a modelling allows to construct all $S$ matrices of practical interest.

Let us first discuss the ideal node defined by the bare scattering matrix (4). For $g = 1$, the conditions (5) and (6) are in fact equivalent to the standard Landauer-Büttiker approach. This is easily seen by using the usual scattering states, e.g. the state injected into QW $i = 1$:
\[ \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} = \begin{pmatrix} e^{ikx} + re^{-ikx} \\ te^{-ikx} \\ \vdots \\ te^{-ikx} \end{pmatrix}, \] (8)
with reflection (transmission) amplitude $r$ ($t$). For $g = 1$, the boundary conditions (5) are equivalent to a Fermi distribution for occupying the states (8), while Eq. (6) gives $1 = r + (N - 1)t$. Furthermore, the density matching condition (7) yields $|1 + r|^2 = |t|^2$. Combining both equations immediately gives $r = (2 - N)/N$ and $t = 2/N$, and hence reproduce Eq. (5). The conductance matrix is then
\[ G_{ii} = 1 - (1 - 2/N)^2, \quad G_{ij} = -(2/N)^2. \] (9)

Will the conductance matrix for this ideal case be affected by interactions ($g < 1$)? Based on the two-terminal case [2], one might suspect that there is no renormalization because of the Fermi-liquid character of the leads, and hence Eq. (9) would stay valid for arbitrary $g$. However, it turns out that for small applied voltages and low temperatures, the system always flows to the disconnected-node fixed point,
\[ G_{ij} = 0. \] (10)
Thus the only stable generic fixed point of this system for any $g < 1$ represents an isolated node weakly connected to $N$ broken-up QWs, even for an arbitrary $S$ matrix of the node. The corrections to Eq. (10) due to finite $U_i$ or $T$ are then sensitive to interactions. This phenomenon is a consequence of the strong correlations in the LL, which here induce asymptotically vanishing currents even in a perfectly clean (impurity-free) system. Equation (10) also implies that open boundary bosonization [20] allows to access the asymptotic low-energy transport properties of a QW network.

For arbitrary $g$ and sufficiently far away from the node such that Friedel oscillations [21] have decayed and the boundary conditions (6) hold, the left- and right-moving densities must combine to give
\[ I_i = ev_F(\rho_{i,R} - \rho_{i,L}) = \frac{e^2}{2\pi} \left( U_i - \sum_j T_{ij} U_j \right), \] (11)
\[ \rho_i = \rho_{i,R} + \rho_{i,L} = \frac{eg^2}{2\pi v_F} \left( U_i + \sum_j T_{ij} U_j \right). \] (12)
Here the matrix $T_{ij}$ has been defined whose entries depend on $g$ and all $U_i$. The $T_{ij}$ reduce to standard
Landauer-Büttiker transmission probabilities for $g = 1$, but in general cannot be interpreted as single-particle quantities. It is important to stress that Eqs. (11) and (12) are consistent with both the LL equation of motion and the boundary conditions (6) for arbitrary $T_{ij}$. The Kirchhoff node rule can then be satisfied by requiring

$$
\sum_{i=1}^{N} T_{ij} = 1,
$$

and we now use the density matching conditions (10) to obtain the $T_{ij}$ and hence the conductance matrix. We mention in passing that the usual relation $\sum_j T_{ij} = 1$ should not be enforced since gauge invariance under uniform potential shifts in all reservoirs has been encoded in Eq. (8) already.

At this point it is crucial to realize that close to the node, the density $\rho_i(x)$ will deviate from the spatially homogeneous value $\rho_i$ in Eq. (12) due to Friedel oscillations. This happens already for $g = 1$, as can be easily checked from Eq. (8) and the subsequent solution. The total density very close to the node is $\rho_i(0) = \rho_i + \delta \rho_i(0)$, where $\delta \rho_i(0)$ is the Friedel oscillation amplitude at the node location. The $2k_F$ oscillatory Friedel contribution $\delta \rho_i(x)$ in QW $i$ arises due to interference of the incoming right-movers and the left-movers that are backscattered at the node. Importantly, left-movers that are transmitted from the other $N-1$ QWs into QW $i$ cannot interfere with the incoming right-movers and will therefore not contribute to $\delta \rho_i(x)$. This implies that $\delta \rho_i(x)$ is identical to the corresponding Friedel oscillation in a two-terminal setup with the same (bare) reflection coefficient as the one induced by the clean node, $R = (1 - 2/N)^2$. Fortunately, this allows us to obtain $\delta \rho_i(0)$ in an exact manner using the relation (3)

$$
\delta \rho_i(0) = -\frac{g^2 e V_i}{\pi v_F},
$$

where the “four-terminal voltage” parameter $V_i$ is found from a self-consistency equation. This equation is explicitly given and solved for arbitrary $g$ in Ref. [3], and using this solution, we also have the pinning amplitude (14) of the Friedel oscillation for any value of $g$. The relation to the two-terminal problem is not a necessary ingredient for our calculation, but quite convenient in allowing to compute $\delta \rho_i(0)$ from known results.

For concreteness, in what follows we consider $g = 1/2$ where this self-consistency equation is quite simple ($k_B = 1$),

$$
\frac{e V_i}{2T_B} = \text{Im} \psi \left( 1 + \frac{T_B + i e(U_i - V_i/2)}{2\pi T} \right),
$$

where $\psi$ is the digamma function and $T_B = \pi \lambda^2/\omega_c$ for bandwidth $\omega_c$ and impurity strength $\lambda$ of the corresponding two-terminal problem. (Specifically, for $N = 3$, to match the reflection coefficient of the ideal Y junction, $(\pi \lambda/\omega_c)^2 = 1/(1 + N/(N - 2))$. The solution to Eq. (15) then yields $V_i$ as a function of $U_i$, alone, which, however, itself depends on all the chemical potentials, see Eq. (3). The density matching conditions (10) are then solved by enforcing

$$
(1 + T_{ij})U_j - 2V_j = T_{kj} U_j
$$

for all pairs $k \neq j = 1, \cdots, N$, and with the Kirchhoff rule we find

$$
T_{ii} = \frac{2 - N}{N} + \frac{2(N - 1)V_i}{NU_i},
$$

$$
T_{k\neq i} = \frac{2 - 2V_i}{NU_i},
$$

Note that the $T_{ij}$ depend only on the applied voltages $U_i$ but not on the $\mu_i$. As a result, gauge invariance is ensured. The relations (16) and (17) represent the complete solution for the special $S$ matrix (4).

Before proceeding to more general $S$ matrices, let us discuss these results for the ideal Y junction ($N = 3$) at $g = 1/2$. From Eq. (3), we get

$$
G_{ii} = \frac{8}{9} \left( 1 - \frac{\partial V_i}{\partial U_i} \right) + \frac{2}{9} \sum_{j \neq i} \left( 1 - \frac{\partial V_j}{\partial U_j} \right),
$$

$$
G_{j\neq i} = \frac{4}{9} \left( \frac{\partial V_i}{\partial U_i} - 1 \right) + \frac{4}{9} \left( \frac{\partial V_j}{\partial U_j} - 1 \right) - \frac{2}{9} \left( \frac{\partial V_k}{\partial U_k} - 1 \right)
$$

where $i \neq j \neq k$ in the second equation. Note that the conductance matrix is symmetric. For $eU_i \ll T$, the linear conductances follow:

$$
G_{ij} = (2\delta_{ij} - 2/3) \frac{1 - e\psi'(c + 1/2)}{1 + e\psi'(c + 1/2)},
$$

where $c = T_B/2\pi T$ and $\psi'$ is the trigamma function. As $T \to 0$, the conductance matrix approaches the stable fixed point (10), $G_{ij} \sim (T/T_B)^2$. In general, for $g < 1$, we find $G_{ij} \sim (T/T_B)^2$ as $T \to 0$. Since this power law coincides with the prediction of open boundary bosonization around (4), this also provides a consistency check for our calculation. Corresponding power laws also govern the nonlinear conductances. This is shown in Fig. 2 for $g = 1/2$, depicting $G_{11}(U)$ at different temperatures. In the $T = 0$ limit, $G_{11} \sim U^2$. Clearly, interactions have a rather spectacular effect on the transport properties of this system.

Next we briefly outline how to construct more general node $S$ matrices based on this solution of the ideal junction for arbitrary $g$. The idea is to add impurities of strength $\lambda_i$ in each QW close to the node, $x_i \approx -1/k_F$, which will modify the bare $S$ matrix; for explicit calculations, see Ref. [4]. One can then compute the $G_{ij}$ for this more general case, but still allowing for arbitrary $g < 1$, e.g. by using perturbation theory around the above
solution of the ideal junction. Focusing on $N = 3$ and just one impurity, $\lambda_2 = \lambda_3 = 0$, to lowest order in $\lambda_1$, a straightforward calculation gives $I_i = I_0^i + \delta I_i$, where $I_0^i$ is the current through QW $i$ for $\lambda_i = 0$ discussed above, and

$$
\delta I_i = -2e g_i \frac{\lambda_i^2}{\omega_c} \sin(\pi g_i) \cos(\pi g_i) \times \Gamma(1 - 2g_i)(2\pi R_0^i/\omega_c)^{2g_i-1},
$$

(18)

where $g_i = 4g/3$ and $\delta I_{k\neq i} = -\delta I_i/2$. Obviously, this perturbative estimate breaks down at very small energy scales for $g_i < 1$ but is valid for all energies at $g_i > 1$. It is straightforward to perform similar calculations for more than one impurity, other $N$, and/or higher orders in the $\lambda_i$. From Eq. (18) and generalizations, we infer that $G_{ij} = 0$ is indeed the only stable fixed point. It is also clear that for at least one very strong impurity $\lambda_i$, the system will reduce to one of the special cases considered previously. For $g$ close to 1, we can also make explicit contact to Ref. [1]. For $S$ matrices close to Eq. (3) and weak interactions, our solution indeed reproduces the results of Ref. [4]. Note that the restriction to weak interactions allows to easily treat more general $S$ matrices.

To conclude, we have proposed a Landauer-type theory for strongly interacting electrons in branched quantum wires such as carbon nanotube Y junctions. A broad class of $S$ matrices can be covered by formulating a suitable boundary condition (“density matching”) to describe an ideal symmetric junction, and on top adding effective impurities in the individual wires. The only stable fixed point corresponds to disconnected quantum wires, with corrections revealing the Luttinger liquid physics via various power laws.

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