Landauer-Type Transport Theory for Interacting Quantum Wires: Application to Carbon Nanotube Y Junctions

S. Chen,[1] B. Trauzettel,[2] and R. Egger[1]

[1]*Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany*

[2]*Fakultät für Physik, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany*

(Received 9 July 2002; published 8 November 2002)

We propose a Landauerlike 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 one 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.

DOI: 10.1103/PhysRevLett.89.226404 PACS numbers: 72.10.–d, 71.10.Pm, 73.63.–b

The Landauer-Büttiker approach to transport in mesoscopic systems has been very successful in describing noninteracting electrons by using a scattering matrix formulation [1]. It is an important challenge to generalize this approach to the case of strongly correlated electrons. Here we propose such a theory for N-terminal starlike networks of interacting 1D quantum wires (QWs) described by Luttinger liquid (LL) theory. The two-terminal setup ($N = 2$) has been formulated and solved previously [2,3]. However, the step from $N = 2$ to $N = 3$, where three individually contacted QWs meet at a single node ("Y junction"), see Fig. 1, is nontrivial yet essential for the development of a practically useful transport theory for interacting electrons. Recently, several works appeared where precisely this problem has been under study. While in Ref. [4] a weakly coupled "Kondo" node was considered, other authors used perturbation theory in the hopping [5] and/or the interaction [6]. At the same time, it has become clear that a more general approach is necessary to go beyond those special situations. Below we formulate boundary conditions that allow for the explicit solution of this transport problem. Progress along these lines is also likely to sharpen our understanding of conformal field theory with boundary conditions [7].

This problem is not only of intellectual interest but also of relevance to transport experiments for carbon nanotubes [8]. As has been predicted [9] and observed in a series of beautiful experiments [10], single-wall nanotubes provide a realization of LL physics. Electron-electron interactions cause remarkably pronounced non-Fermi liquid behaviors characterized by the standard LL parameter $g \approx 0.25$ (where $g = 1$ is the noninteracting value). Template-based chemical vapor deposition [11] and electron beam welding methods [12] allow one to fabricate and contact nanotube Y junctions, and the intrinsic nonlinear I-V characteristics of such a device have been observed recently [13]. In addition, the case $N = 4$ has been realized by several groups using two crossed nanotubes [14], providing another interesting application. Furthermore, semiconductor heterostructures [15] or ultracold trapped atomic gases [16] may allow for the systematic study of T or Y junctions as well. Eventually it could even be possible to access the fractional statistics of LL quasiparticles through the noise properties of such a device, thereby realizing a Hanbury-Brown-Twiss setup for fractionalized quasiparticles [5].

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 [9]. 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. As in the two-terminal case, adiabatically coupled external reservoirs held at electrochemical potentials μ_i lead to *radiative boundary conditions* [2] (we put $\hbar = 1$)

$$\frac{g^{-2}+1}{2}\rho_{i,R}(-L) + \frac{g^{-2}-1}{2}\rho_{i,L}(-L) = \frac{\mu_i}{2\pi v_F}, \quad (1)$$

where $\rho_{i,R/L}(x)$ is the right/left-moving part of the

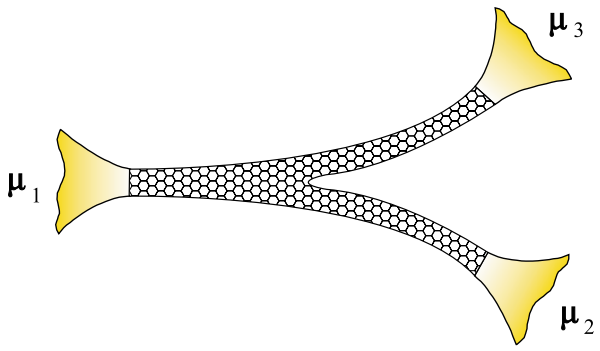

FIG. 1 (color online). Schematic view of a Y junction. QWs extend from adiabatically contacted reservoirs with electrochemical potential μ_i at $x = -L$ to the node at $x = 0$.

density in QW i. These boundary conditions depend only 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,

$$G_{ij} = \frac{h}{e}\frac{\partial I_i}{\partial \mu_j}, \tag{2}$$

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

$$eU_i = \mu_i - \bar{\mu}, \qquad \bar{\mu} = \frac{1}{N}\sum_i \mu_i. \tag{3}$$

Under this definition, gauge invariance (conductance matrix is invariant under a uniform change of all μ_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*

$$\sum_i I_i = 0. \tag{4}$$

A second requirement at the node is the wave function matching via the S matrix [17,18]

$$\Psi_L(0) = S\Psi_R(0), \tag{5}$$

where $\Psi(x) = (\psi_1, \ldots, \psi_N)$ contains the wave functions for the N QWs, and the outgoing (left-moving) components Ψ_L are connected to the incoming (right-moving) states Ψ_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. (5) 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 noninteracting problem could be modeled 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

$$S = \begin{pmatrix} (2-N)/N & 2/N & \cdots & 2/N \\ 2/N & (2-N)/N & \cdots & 2/N \\ \cdots & \cdots & \cdots & \cdots \\ 2/N & 2/N & \cdots & (2-N)/N \end{pmatrix}. \tag{6}$$

For this S matrix, Eq. (5) 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,

$$\rho_1(0) = \cdots = \rho_N(0), \tag{7}$$

where $\rho_i(0)$ denotes the *total* electronic density in QW i close to the node. Remarkably, the conditions (1), (4), and (7) then allow one to explicitly solve this transport problem for arbitrary interactions because the condition (7) does not involve wave function 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 modeling allows one to construct all S matrices of practical interest.

Let us first discuss the ideal node defined by the bare scattering matrix (6). For $g = 1$, the conditions (1), (4), and (7) 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 $i = 1$:

$$\begin{pmatrix} \psi_1 \\ \psi_2 \\ \cdots \\ \psi_N \end{pmatrix} = \begin{pmatrix} e^{ikx} + re^{-ikx} \\ te^{-ikx} \\ \cdots \\ te^{-ikx} \end{pmatrix}, \tag{8}$$

with reflection (transmission) amplitude r (t). For $g = 1$, the boundary conditions (1) are equivalent to a Fermi distribution for occupying the states (8), while Eq. (4) 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 reproduces Eq. (6). The conductance matrix is then

$$G_{ii} = 1 - (1 - 2/N)^2, \qquad G_{i\neq j} = -(2/N)^2. \tag{9}$$

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*,

$$G_{ij} = 0. \tag{10}$$

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

one 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 (1) hold, the left- and right-moving densities must combine to give

$$I_i = ev_F(\rho_{i,R} - \rho_{i,L}) = \frac{e^2}{2\pi}\Big(U_i - \sum_j T_{ij}U_j\Big), \quad (11)$$

$$\rho_i = \rho_{i,R} + \rho_{i,L} = \frac{eg^2}{2\pi v_F}\Big(U_i + \sum_j T_{ij}U_j\Big). \quad (12)$$

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 (1) for *arbitrary* T_{ij}. The Kirchhoff node rule can then be satisfied by requiring

$$\sum_{i=1}^{N} T_{ij} = 1, \quad (13)$$

and we now use the density matching conditions (7) 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. (3) 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 ρ_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 mover 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 [2]

$$\delta\rho_i(0) = -\frac{g^2 eV_i}{\pi v_F}, \quad (14)$$

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 one 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 ($k_B = 1$),

$$\frac{eV_i}{2T_B} = \mathrm{Im}\psi\Big(\frac{1}{2} + \frac{T_B + ie(U_i - V_i/2)}{2\pi T}\Big), \quad (15)$$

where ψ is the digamma function and $T_B = \pi\lambda^2/\omega_c$ for bandwidth ω_c and impurity strength λ of the corresponding two-terminal problem. Specifically, for $N = 3$, to match the reflection coefficient of the ideal Y junction, $\pi\lambda/\omega_c = 1/2$. 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 (7) are then solved by enforcing

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

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

$$T_{ii}(\{\mu_j\}) = \frac{2 - N}{N} + \frac{2(N - 1)V_i}{NU_i}, \quad (16)$$

$$T_{k\neq i}(\{\mu_j\}) = \frac{2}{N} - \frac{2V_i}{NU_i}. \quad (17)$$

Note that the T_{ij} depend only on the applied voltages U_i but not on the μ_i. As a result, gauge invariance is ensured. The relations (16) and (17) represent the complete solution for the special S matrix (6).

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. (2), we get

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

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

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:

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

where $c = T_B/2\pi T$ and ψ' 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 $G_{ij} \sim (T/T_B)^{2/g-2}$ as $T \to 0$. Since this power law coincides with the prediction of open boundary bosonization around (10), 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

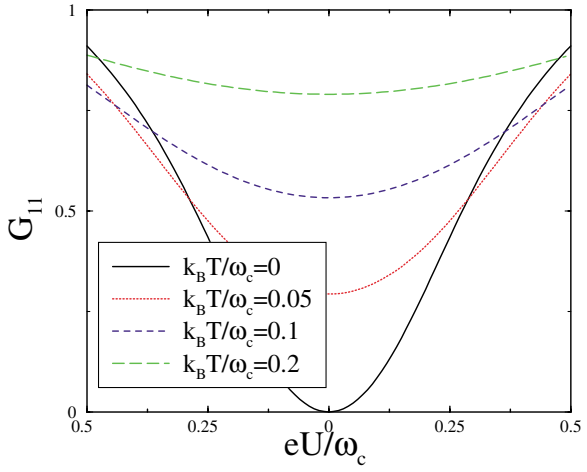

FIG. 2 (color online). Nonlinear conductance $G_{11}(U)$ for $N = 3$, $\mu_1 = E_F + U$, $\mu_2 = \mu_3 = E_F$, several temperatures and $g = 1/2$.

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 λ_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. [17]. 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 λ_1, a straightforward calculation gives $I_i = I_i^0 + \delta I_i$, where I_i^0 is the current through QW i for $\lambda_i = 0$ discussed above, and

$$\delta I_1 = -2eg_+ \frac{\lambda_1^2}{\omega_c} \sin(\pi g_+) \cos(\pi g_+) \times \Gamma(1 - 2g_+)(2\pi I_1^0/e\omega_c)^{2g_+ - 1}, \qquad (18)$$

where $g_+ = 4g/3$ and $\delta I_{k\neq 1} = -\delta I_1/2$. Obviously, this perturbative estimate breaks down at very small energy scales for $g_+ < 1$ but is valid for all energies at $g_+ > 1$. It is straightforward to perform similar calculations for more than one impurity, other N, and/or higher orders in the λ_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 λ_i, the system will reduce to one of the special cases considered previously [4–6]. For g close to 1, we can also make explicit contact to Ref. [6]. For S matrices close to Eq. (6) and weak interactions, our solution indeed reproduces the results of Ref. [6]. Note that the restriction to weak interactions allows one to easily treat more general S matrices [6].

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.

We thank H. Grabert and A. Komnik for useful discussions. Support by the DFG under the Gerhard-Hess program and under Grant No. GR 638/19 is acknowledged.

[1] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995).
[2] R. Egger and H. Grabert, Phys. Rev. Lett. **77**, 538 (1996); **80**, 2255(E) (1998); Phys. Rev. B **58**, 10 761 (1998).
[3] R. Egger *et al.*, Phys. Rev. Lett. **84**, 3682 (2000).
[4] C. Nayak *et al.*, Phys. Rev. B **59**, 15 694 (1999).
[5] I. Safi, P. Devillard, and T. Martin, Phys. Rev. Lett. **86**, 4628 (2001).
[6] S. Lal, S. Rao, and D. Sen, Phys. Rev. B 66, 165327 (2002).
[7] C. Itzykson and J. M. Drouffe, *Statistical Physics* (Cambridge University Press, Cambridge, 1989), Vol. 2.
[8] C. Dekker, Phys. Today **52**, No. 5, 22 (1999).
[9] R. Egger and A. O. Gogolin, Phys. Rev. Lett. **79**, 5082 (1997); C. Kane, L. Balents, and M. P. A. Fisher, *ibid.* **79**, 5086 (1997).
[10] M. Bockrath *et al.*, Nature (London) **397**, 598 (1999); Z. Yao *et al.*, *ibid.* **402**, 273 (1999); H. Postma *et al.*, Science **293**, 76 (2001).
[11] W. Z. Li, J. G. Wen, and Z. F. Ren, Appl. Phys. Lett. **79**, 1879 (2001).
[12] M. Terrones *et al.*, Phys. Rev. Lett. **89**, 075505 (2002).
[13] J. Li, C. Papadopoulos, and J. M. Xu, Nature (London) **402**, 253 (1999); C. Papadopoulos *et al.*, Phys. Rev. Lett. **85**, 3476 (2000).
[14] M. S. Fuhrer *et al.*, Science **288**, 494 (2000); J. Kim *et al.*, J. Phys. Soc. Jpn. **70**, 1464 (2001); J.W. Janssen *et al.*, Phys. Rev. B **65**, 115423 (2002).
[15] J. Hasen *et al.*, Nature (London) **390**, 54 (1997).
[16] D. S. Petrov, G.V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. Lett. **85**, 3745 (2000).
[17] S. Ami and C. Joachim, Phys. Rev. B **65**, 155419 (2002).
[18] A. N. Andriotis *et al.*, Phys. Rev. B **65**, 165416 (2002).
[19] T. Itoh, Phys. Rev. B **52**, 1508 (1995).
[20] M. Fabrizio and A. O. Gogolin, Phys. Rev. B **51**, 17 827 (1995).
[21] J. Friedel, Nuovo Cimento Suppl. **7**, 287 (1958).