

Landauer-Büttiker equation for bosonic carriers

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(Dated: July 19, 2018)

We study the current of Bose particles between two reservoirs connected by a one-dimensional channel. We analyze the problem from first principles by considering a microscopic model of conductivity in the noninteracting limit. Equations for the transient and the stationary current are derived analytically. The asymptotic current has a form similar to the Landauer-Büttiker equation for electronic current in mesoscopic devices.

Keywords: Bose-Einstein condensates, ultracold atoms, quantum transport, open quantum systems

Recent progress in cold-atom physics witnesses the emergency of the new field atomtronics [1–3], which deals with atom-based setups which are similar to crystal-based electronic devices. In particular, the recent series of experiments at ETH [4, 5] analyzes a current of fermionic atoms between two atomic reservoirs connected by a point contact [4], or even by quasi one-dimensional channels with periodic structure [5]. To explain their experimental results in the case of weakly interacting atoms the authors of [4, 5] appeal to the Landauer-Büttiker theory [6], which has been proved to be very successful in describing ballistic transport of electrons in mesoscopic solid-state devices.

According to the Landauer-Büttiker approach [6] the electron current j is given by the equation

$$j = \sum_n \int f(E) |t_n(E)|^2 dE. \quad (1)$$

Here n labels the transmission channels, $t_n(E)$ is the transmission amplitude at the energy E of each channel, and the function $f(E)$ is determined by the chemical potentials of the left and right reservoir through the Fermi-Dirac distribution $f_{FD}(E)$ as $f(E) \sim f_{FD}(E - \mu_L) - f_{FD}(E - \mu_R)$. It was demonstrated in the ETH experiments that Eq. (1) describes reasonably well the current of weakly interacting fermionic atoms in engineered optical potentials. A unique property of atomtronic devices is that they may use Fermi as well as Bose atoms. This rises the question about an analogue of the Landauer-Büttiker equation for bosonic transport [7]. To obtain such an analogue is the main goal of this paper.

In what follows we illustrate the derivation of the bosonic Landauer-Büttiker equation by considering a simple microscopic model that is a modification of the model introduced in Ref. [8]. It consists of two reservoirs of Bose particles connected by the transport channel, see Fig. 1 (upper panel). The reservoirs are described by the

Bose-Hubbard Hamiltonians \hat{H}_b ,

$$\hat{H}_b = -\frac{J}{2} \sum_{m=1}^{M-1} (\hat{b}_{m+1}^\dagger \hat{b}_m + h.c.) + \frac{W}{2} \sum_{m=1}^M \hat{n}_m (\hat{n}_m - 1), \quad (2)$$

where $W \neq 0$ is the interaction constant and we implicitly assume the thermodynamic limit with a fixed filling factor $\bar{n} = N/M$. The reservoirs are connected to the transport channel described by the Hamiltonian \hat{H}_s ,

$$\hat{H}_s = -\frac{J}{2} \sum_{l=1}^{L-1} (\hat{a}_{l+1}^\dagger \hat{a}_l + h.c.) + \sum_{l=1}^L \left(E_l \hat{n}_l + \frac{U}{2} \hat{n}_l (\hat{n}_l - 1) \right), \quad (3)$$

where the on-site energies E_l correspond to a scattering potential. Finally, the channel is coupled to the left reservoir by the Hamiltonian \hat{H}_{int}

$$\hat{H}_{int} = \varepsilon (\hat{b}_M \hat{a}_1^\dagger + h.c.), \quad (4)$$

where the hopping matrix element ε plays the role of the coupling constant. The coupling Hamiltonian to the right reservoir (which is described by its own Bose-Hubbard Hamiltonian) has the form $\hat{H}_{int} = \varepsilon (\hat{a}_L \hat{b}_1^\dagger + h.c.)$.

To avoid a possible confusion we stress that, in spite of using different notations for the creation and annihilation operators for Bose particles in the transport channel and reservoirs, the total Hamiltonian describes a system of indistinguishable particles. The main assumption of the model is that the interaction constants W and U in the Hamiltonians (2) and (3) can be varied independently, where we will mainly focus on the case $U = 0$ but $W \neq 0$. The advantage of using the interacting Bose-Hubbard model (2) as a bath is that it is generally a quantum chaotic system with universal properties of the energy spectrum and eigenstates [9, 10]. These properties help us to justify the master equation that will be derived below. The advantage of considering a non-interacting channel is that the obtained master equation

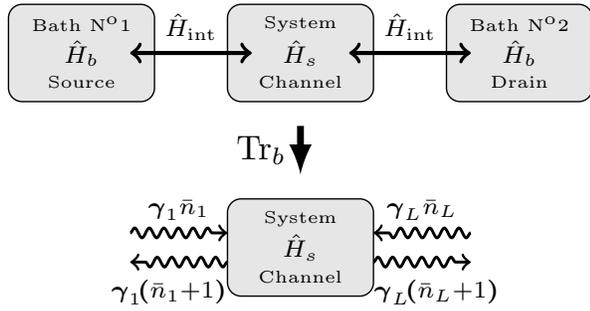


FIG. 1: Schematic representation of the microscopic model (upper panel) from which the effective dissipative Bose-Hubbard chain description is derived with gain and loss at sites 1 and L (bottom panel).

can be solved analytically without any further approximations.

The first step is to derive the master equation for the reduced density matrix describing the carriers in the transport channel, $\rho_s(t) = \text{Tr}_b[\rho_{tot}(t)]$, where $\text{Tr}_b[\dots]$ denotes the partial trace over the bath variables. A master equation in Lindblad form can be obtained for $\rho_s(t)$ within the so-called Born-Markov approximation [11]. This approximation assumes that (i) the total density matrix factorizes into the tensor product of the reduced density matrices for all times, $\rho_{tot}(t) = \rho_b(t) \otimes \rho_s(t)$, (here for simplicity we temporally discuss the case of a single bath) and that (ii) bath degrees of freedom are δ -correlated, i.e., $\text{Tr}_b[\hat{b}(t)\hat{b}^\dagger(t')\rho_b(t=0)] \sim \delta(t-t')$. We mention, in passing, that the former approximation is actually never satisfied because the coupling Hamiltonian entangles the particles in the channel and the bath. However, one can justify a weaker approximation [12], $\text{Tr}_b[F(\hat{b}, \hat{b}^\dagger)\rho_{tot}(t)] = \text{Tr}_b[F(\hat{b}, \hat{b}^\dagger)\rho_b(t)]\rho_s(t)$, which is sufficient to eliminate the bath ($F(\dots)$ is an arbitrary operator-valued function of the bath variables). The required property behind the previous equation is a quantum counterpart of the mixing property of classically chaotic systems and the interacting Bose-Hubbard model possesses this property [9].

Using the explicit form of the coupling Hamiltonian (4), the result is a Lindblad master equation for the reduced density matrix of the channel, see, e.g., [13]. This provides an effective model for the reduced dynamics in the channel, as sketched in Fig. 1 (bottom panel). The channel is now a dissipative Bose-Hubbard chain subject to single-particle loss processes at rates $\gamma_{1,L}$ as well as incoherent pumping at the same rates around the populations $\bar{n}_{1,L}$ at both ends, labelled 1 and L, respectively. Explicitly we have

$$\begin{aligned} \partial_t \hat{\rho} = & -i[\hat{H}_s, \hat{\rho}_s] \\ & + \sum_{j=1,L} \gamma_j (\bar{n}_j \mathcal{D}[\hat{a}_j^\dagger] \hat{\rho}_s + (\bar{n}_j + 1) \mathcal{D}[\hat{a}_j] \hat{\rho}_s) \end{aligned} \quad (5)$$

where the dissipator is defined as $\mathcal{D}[\hat{a}] \hat{\rho}_s = \hat{a} \hat{\rho}_s \hat{a}^\dagger - 1/2\{\hat{a}^\dagger \hat{a}, \hat{\rho}_s\}$. In terms of the microscopic model of Eqs. (2-4), the parameters \bar{n}_1 and \bar{n}_L are given by the filling factor of the Bose-Hubbard reservoirs and the parameters $\gamma_{1,L}$ are proportional to the square of the lead-channel coupling constant, $\gamma_{1,L} \sim \varepsilon^2$. Notice that, besides the particle exchange between the system and the bath, the relaxation terms Eq. (5) are responsible for decoherence processes as well. The latter is a consequence of the mentioned system-bath entanglement.

With respect to the microscopic model Eqs. (2-4), the validity of the master Eq. (5) was tested in ref. [8]. It was found that it is well justified in the high-temperature limit, where the overwhelming majority of bath states are chaotic. However, it may give wrong results in the low-temperature limit, where most of the populated bath states (including the ground state) are regular states. The high-temperature limit (which we shall assume from now on) implies that all Bloch states for a particle in the bath are equally populated. Thus a particle coming into the channel may have an arbitrary quasimomentum. Let us also mention that the master Eq. (5) is used as the starting point in many papers on conductivity with bosonic and fermionic carriers [14–16], where in the latter case the bosonic annihilation and creation operator should be substituted by fermionic ones.

The reduced density matrix $\rho_s(t)$ entering the master Eq. (5) carries the whole information about the atoms in the transport channel but has a huge dimension which grows exponentially with L . Fortunately, for many purposes, it suffices to know only the single-particle density matrix (SPDM), which has the fixed dimension $L \times L$ and is defined as

$$\sigma_{lm}(t) = \text{Tr}[\hat{\rho}_s(t) \hat{a}_l^\dagger \hat{a}_m] \equiv \langle \hat{a}_l^\dagger(t) \hat{a}_m(t) \rangle. \quad (6)$$

The SPDM is easily shown to satisfy the following set of equations of motion

$$\begin{aligned} \partial_t \sigma_{lm} = & i \frac{J}{2} (\sigma_{l,m+1} + \sigma_{l,m-1} - \sigma_{l+1,m} - \sigma_{l-1,m}) \\ & + i(E_l - E_m) \sigma_{lm} - iU (\langle \hat{a}_l^\dagger \hat{a}_m \hat{a}_m^\dagger \hat{a}_m \rangle - \langle \hat{a}_l^\dagger \hat{a}_l \hat{a}_l^\dagger \hat{a}_m \rangle) \\ & - \sum_{j=1,L} \frac{\gamma_j}{2} (\delta_{l,j} + \delta_{m,j}) (\sigma_{lm} - \delta_{l,m} \bar{n}_j). \end{aligned} \quad (7)$$

These equations can be put into a closed form using an appropriate truncation scheme such as mean field or the beyond-mean-field Bogoliubov back-reaction method [14, 17]. Fortunately, in the case of non-interacting bosons ($U = 0$), considered throughout this paper, the equations are already in closed form. This holds for any master equation with Hamiltonian terms and Lindblad operators at most quadratic on the creation and annihilation operators [11].

We are interested in the current across the chain. By building a vector $\vec{\sigma}$ out of the SPDM's matrix elements,

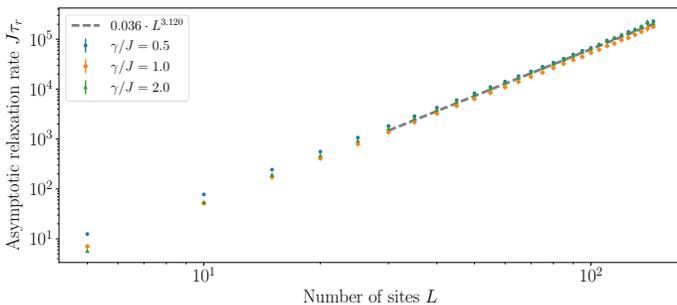


FIG. 2: Asymptotic relaxation time τ_r vs. L for $\bar{n}_1 = 0.02$, $\bar{n}_L = 0$, and various ratios γ/J as shown in the legend. The dashed line shows a fit approximately cubic in L .

Eq. (7) can be rewritten in the form

$$\partial_t \vec{\sigma}(t) = \mathbf{A} \vec{\sigma}(t) + \vec{b}, \quad (8)$$

with \mathbf{A} a diagonally dominant complex symmetric matrix. The general solution of such a system is

$$\vec{\sigma}(t) = e^{\mathbf{A}t} \vec{\sigma}(0) + \mathbf{A}^{-1} (\mathbf{1} - e^{\mathbf{A}t}) \vec{b}, \quad (9)$$

which can be explicitly obtained for a few-site chain, for example the two-site system, see the Supplementary Material. However, explicit expressions get more involved for larger systems, for which numerical diagonalization can be efficiently used. This is the reason why we will now study the limit of the stationary current. Indeed, it follows from Eq. (9) that, independent of the initial condition, the SPDM $\sigma_{l,m}(t)$ relaxes to some stationary matrix $\bar{\sigma}_{l,m}$. Relaxation towards this steady state occurs on a time scale of the order of the asymptotic relaxation time, defined as $\tau_r = \inf_{\ell} (|\lambda_{\ell}|)^{-1}$, where $\{\lambda_{\ell}\}$ denotes the set of eigenvalues of the matrix \mathbf{A} of Eq. (8). We find that the relaxation time τ_r increases with the chain length L . This rises the question of its asymptotic scaling. Fig. 2 shows that τ_r scales with the number of sites L as an approximate cubic power law.

To analyse the regime of stationary currents, we first consider the case of identical on-site energies E_l , where the transmission probability is unity. In this case the SPDM relaxes to a tridiagonal matrix $\bar{\sigma}_{l,m}$ shown in Fig. 3(a). This matrix is uniquely characterized by four quantities: the value of its diagonal elements A (except for the first and last sites), the value of its off-diagonal elements $\pm iB$, and $\bar{\sigma}_{1,1} = C$ and $\bar{\sigma}_{L,L} = D$. To simplify the equations we shall restrict ourselves to the parameter region $\gamma_1 = \gamma_L \equiv \gamma$. Setting the left-hand-side of Eq. (7) to zero for $U = 0$, we obtain the following system of algebraic equations for the unknown matrix parameters

$$\gamma C + JB = \gamma \bar{n}_1, \quad (10)$$

$$\gamma B - JC + JA = 0, \quad (11)$$

$$\gamma B - JA + JD = 0, \quad (12)$$

$$\gamma D - JB = \gamma \bar{n}_L, \quad (13)$$

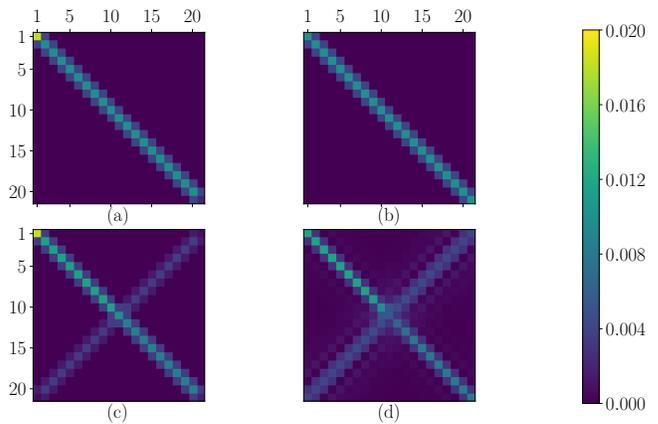


FIG. 3: Absolute values of the steady state SPDM for $L = 21$, $\bar{n}_1 = 0.02$, $\bar{n}_L = 0$, $\gamma/J = 2$ and either $F/J = 0$ (upper panels) or $F/J = 0.5$ (bottom panels) for the V_1 scattering potential. Exact numerical results (left) are to be compared to the Landauer-Büttiker ones (right), computed from Eq. 16.

which gives

$$A = \frac{C + D}{2} = \frac{\bar{n}_1 + \bar{n}_L}{2}, \quad (14)$$

and

$$B = \frac{J\gamma}{\gamma^2 + J^2} \frac{\bar{n}_1 - \bar{n}_L}{2}. \quad (15)$$

Keeping in mind the matrix of the current operator, $j = j_0(\delta_{l,m+1} - \delta_{l+1,m})/2i$, we conclude that Eq. (15) determines the stationary current in the channel as $j = j_0 B$, where $j_0 = Jd/\hbar$, with d being the lattice period which we set to unity from now on. As expected, j is proportional to the population difference $\bar{n}_1 - \bar{n}_L$ between the two reservoirs and to the relaxation rate γ , provided that $\gamma \ll J$. It follows from Eq. (14) that the mean number of carries in the lead is $\langle N \rangle = (\bar{n}_1 + \bar{n}_L)L/2$. This information may be relevant for a numerical simulation of the system dynamics using approximate, e.g., Hilbert-space truncation methods.

Next we analyze the case of a non-vanishing scattering potential. As an example, we consider the potential V_1 corresponding to a point-like scatter $E_l = F\delta_{l,L/2}$. Fig. 3(c) presents the stationary density matrix for $F = 0.5J$. As expected, the diagonal elements $\bar{\sigma}_{l,l}$ now show a jump at the scatterer's position. Yet, the nearest elements to the main diagonal, which determine the current in the system, have constant value, which is a consequence of the continuity equation. We also notice non-negligible anti-diagonal matrix elements, which reflect strong spatial correlations between the transmitted and reflected particles.

For a more complicated scattering potential, for example the potential V_2 defined by $E_l = F(\delta_{l,L/2-1} +$

$\delta_{l,L/2+1}$), where one meets the phenomenon of resonant scattering, the stationary density matrix has an even more involved structure which is hard to reproduce by means of an algebraic approach. However, we can fairly well reproduce this structure by employing the Landauer-Büttiker approach [6]. For this, it is instructive to discuss the result depicted in Fig. 3(a) in terms of the Bloch waves $|\kappa\rangle \sim \sum_l \exp(i\kappa l)|l\rangle$, where we formally consider the limit $L \rightarrow \infty$ and, hence, the quasimomentum κ is a continuous quantity. This limit eliminates the boundary effects and the stationary matrix $\bar{\sigma}_{l,m}$ is approximated by the average matrix $\bar{\sigma}$,

$$\bar{\sigma} = \int_{-\pi}^{\pi} |\kappa\rangle\langle\kappa| f(\kappa) \frac{d\kappa}{2\pi}, \quad (16)$$

where

$$f(\kappa) = A + 2B \sin(\kappa). \quad (17)$$

Remarkably, the case of a non-vanishing scattering potential is reproduced by substituting in Eq.(16) the Bloch wave $|\kappa\rangle$ by the scattered Bloch waves $|\kappa'\rangle$:

$$\langle l|\kappa'\rangle \sim \begin{cases} \exp(i\kappa l) + r(\kappa) \exp(-i\kappa l) & , l < L/2 \\ t(\kappa) \exp(i\kappa l) & , l > L/2 \end{cases}. \quad (18)$$

Fig. 3 compares the exact steady-state SPDM (left panels) with those obtained from Eq. (16) (right panels) for both above-defined scattering potentials, V_1 (upper panels) and V_2 (bottom panels). The observed agreement suggests the following equation for the stationary current,

$$j = j_0 \int_{-\pi}^{\pi} \sin(\kappa) f(\kappa) |t(\kappa)|^2 \frac{d\kappa}{2\pi}, \quad (19)$$

where the function $f(\kappa)$ was defined in Eq. (17). In principle, the integration over quasimomentum in Eq. (19) can be substituted by an integration over the energy with $dE = J \sin(\kappa) d\kappa$. Then Eq. (19) takes the same form as the celebrated Landauer-Büttiker Eq. (1). The usage of quasimomentum, however, has the advantage that we obtain not only the current but also reproduce the SPDM. The lower panel of Fig. 4 shows the stationary current across the chain as a function of F/J obtained from the analytical expression (19) (solid lines), as compared to numerical results based on simulations of the reduced density matrix (symbols) for both potentials V_1 and V_2 . The agreement of the analytical result based on the Landauer-Büttiker approach with the exact data is striking.

To conclude, we studied the stationary current of Bose particles between two reservoirs connected by a one-dimensional transport channel. We analyzed the problem from first principles, i.e., without using uncontrolled assumptions or approximations. The obtained equation for the stationary current has the same structure as the

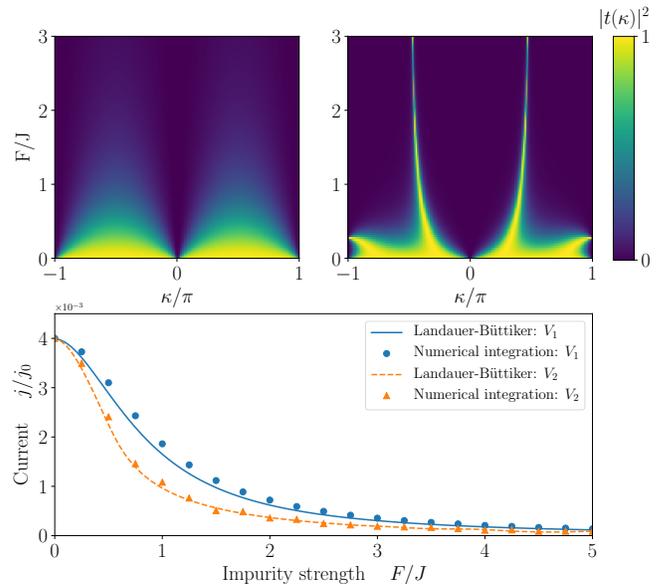


FIG. 4: Squared modulus of the transmission coefficient corresponding to the scattering potentials V_1 (upper left) and V_2 (upper right) as a function of F/J and the quasimomentum κ . (Bottom panel) Steady state currents across a $L = 20$ chain for both potentials and $\bar{n}_1 = 0.02$, $\bar{n}_L = 0$, $\gamma/J = 2$. Results predicted by Eq. (19) (solid lines) are compared to exact numerical simulations (symbols).

fermionic Landauer-Büttiker equation and involves an integration over the energy/quasimomentum of the transmission probability for the carriers weighted by some function $f(\kappa)$. Similar to the fermionic case, this weight function is determined by the chemical potentials of the reservoirs. Additionally, $f(\kappa)$ was found to depend on the relaxation constant γ , whose value is determined by the coupling constant ε as $\gamma \sim \varepsilon^2$. This result goes beyond the common Landauer-Büttiker approach because it explicitly takes into account a particular form of coupling between the lead and reservoirs. It should also be mentioned that the obtained Eq. (19) requires infinite temperature of the reservoirs – the assumption we need to justify the master Eq. (7). It is an open problem to obtain the bosonic Landauer-Büttiker equation for a finite temperature where the Markovian approximation may be not justified and, hence, the equation on the reduced density matrix may include non-Markovian terms.

The authors thank very much Giulio Amato for a critical reading of the manuscript.

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