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# Definition of current density in the presence of a non-local potential

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## Abstract

In the presence of a non-local potential arising from electron–electron interaction, the conventional definition of current density  $\mathbf{J}_c = (e/2m)[(\mathbf{p} - e\mathbf{A})\psi]^*\psi - \psi^*[(\mathbf{p} - e\mathbf{A})\psi]$  cannot satisfy the condition of current conservation, i.e.,  $\nabla \cdot \mathbf{J}_c \neq 0$  in the steady state. In order to solve this problem, we give a new definition of current density including the contribution due to the non-local potential. We show that the current calculated based on the new definition of current density conserves the current and is the same as that obtained from the Landauer–Büttiker formula. Examples are given to demonstrate our results.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

With the recent development of nano-technology, predictions on transport properties of nano-devices such as current are becoming increasingly important. It is equally important for us to understand how current flows inside the nano-devices since the current distribution or current density  $\mathbf{J}$  gives information about the heat dissipation [1]. The divergence of current density  $\nabla \cdot \mathbf{J}(\mathbf{r}, t)$  represents the rate at which electrons are lost from the surrounding volume. It satisfies the current continuity equation  $\partial_t \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0$ , where  $\rho(\mathbf{r}, t)$  is the electron density<sup>4</sup>. At steady state,  $\partial_t \rho(\mathbf{r}, t) = 0$ , the divergence of current density has to be zero in order to satisfy current conservation. The general expression for current density is usually defined as  $\mathbf{J}_c = (e/2m)[(\mathbf{p} - e\mathbf{A})\psi]^*\psi - \psi^*[(\mathbf{p} - e\mathbf{A})\psi]$  [2], where  $\mathbf{p} = -i\hbar\nabla$  is the momentum operator,  $\mathbf{A}$  is the vector potential due to the magnetic field, and  $\psi$  the electron wavefunction. In most cases, this expression for current density is appropriate and the current calculated from  $\mathbf{J}_c$  is conserved as long as  $\nabla \cdot \mathbf{J}_c(\mathbf{r}, t)$  is equal to zero at steady state. However, as will be discussed in detail below, in the presence of a non-local potential  $V(\mathbf{r}, \mathbf{r}')$

the current calculated from the conventional current density  $\mathbf{J}_c$  defined above is not conserved. Why do people care about the non-local potential? Actually, in the first principles calculations of transport properties of nano-devices such as the density functional theory + non-equilibrium Green's function theory [3], there are a number of cases where the non-local potential is present. For instance, the exchange–correlation energy functional is non-local if one wants to go beyond the local density approximation [4]. The non-conserved current density cannot give a correct current. In addition, the non-local pseudo-potential is another source of non-local potential [5]. Due to the presence of non-local potential in the *ab initio* calculation [5], first principles calculation of conventional current density can give errors for current as large as 20% for molecular devices [6]. Due to the importance of the quantum transport problem in nano-devices, there is clearly a need to modify the conventional definition of the current density  $\mathbf{J}_c$  so that the current calculated from the current density gives the correct value. In general, there are two ways of calculating the current or conductance:

- (1) Define the Green's function of the scattering region and then calculate the transmission coefficient and hence the

<sup>4</sup> In the present paper, we assume that the strong electron–electron interaction can be neglected and the interaction is treated at mean field level.

current from Landauer–Büttiker formula [7],

$$I_\alpha = (2e/h) \sum_\beta \int dE (f_\alpha - f_\beta) \text{Tr}[G^r \Gamma_\alpha G^a \Gamma_\beta] \quad (1)$$

where  $G^r$  is the retarded Green's function.

- (2) Calculate the current density in the scattering region, and then the current is obtained by integrating the current density  $\mathbf{J}(\mathbf{r})$  over the interface between the scattering region and the lead  $\alpha$ ,

$$I_\alpha = \int d\sigma_\alpha \cdot \mathbf{J}(\mathbf{r}). \quad (2)$$

Obviously, the currents calculated from these two approaches must be equal. It is easy to see that the current obtained from equation (1) is conserved since  $\sum_\alpha I_\alpha = 0$  regardless of the presence of non-local potentials. Note that the conventional definition of current density in the absence of magnetic field and non-local potential is given by

$$\mathbf{J}_c(\mathbf{r}, t) = \frac{ie\hbar}{2m} [\psi(\mathbf{r}, t) \nabla \psi^*(\mathbf{r}, t) - \text{c.c.}] \quad (3)$$

The condition that the current calculated from equation (2) is conserved is given by  $\nabla \cdot \mathbf{J}(r) = 0$ . It will be shown later (see equation (8) below) that this condition is violated when a non-local potential is present. The purpose of this paper is to define a new current density in the presence of a non-local potential so that the current calculated from the current density is correct. In section 2, we provide such a formalism. In section 3, examples are given that demonstrate the conservation of current. Finally, our results are also summarized in section 3.

## 2. Theoretical formalism

In the presence of a non-local potential  $V(\mathbf{r}, \mathbf{r}')$ , the wavefunction obeys the following Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + \int d\mathbf{r}' V(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}', t) \quad (4)$$

where the gradient operator  $\nabla$  operates only on  $\mathbf{r}$ . The complex conjugate of the above equation can be written as

$$-i\hbar \frac{\partial}{\partial t} \psi^*(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi^*(\mathbf{r}, t) + \int d\mathbf{r}' V^*(\mathbf{r}, \mathbf{r}') \psi^*(\mathbf{r}', t). \quad (5)$$

From  $\psi(\mathbf{r}, t) \times$  equation (5)  $-\psi^*(\mathbf{r}, t) \times$  equation (4), we obtain

$$-\partial_t \rho(\mathbf{r}, t) = \nabla \cdot \mathbf{J}_c(\mathbf{r}, t) + \rho_n(\mathbf{r}, t) \quad (6)$$

where  $\rho(\mathbf{r}, t) = e|\psi(\mathbf{r}, t)|^2$  is the electron density and  $\mathbf{J}_c(\mathbf{r}, t)$  is the conventional current density in the absence of magnetic field defined in equation (3). Here we have introduced a new quantity, the non-local electron density  $\rho_n(\mathbf{r}, t)$ , due to the non-local potential,

$$\rho_n(\mathbf{r}, t) = \frac{e}{i\hbar} \int d\mathbf{r}' [\psi(\mathbf{r}, t) V^*(\mathbf{r}, \mathbf{r}') \psi^*(\mathbf{r}', t) - \text{c.c.}] \quad (7)$$

Note that this non-local electron density  $\rho_n(\mathbf{r}, t)$  has the dimension of volume current density not charge density. In the steady state,  $\partial_t \rho(\mathbf{r}, t) = 0$ . Equation (6) becomes

$$\nabla \cdot \mathbf{J}_c(\mathbf{r}) + \rho_n(\mathbf{r}) = 0. \quad (8)$$

If the potential is local, i.e.,  $V(\mathbf{r}, \mathbf{r}')$  is a diagonal matrix, the quantity  $\rho_n(\mathbf{r})$  vanishes. The current calculated from  $\mathbf{J}_c$  is conserved since  $\nabla \cdot \mathbf{J}_c(\mathbf{r}) = 0$ . However, in the presence of a non-local potential, the quantity  $\rho_n(\mathbf{r})$  is nonzero, and therefore  $\nabla \cdot \mathbf{J}_c(\mathbf{r}) \neq 0$ . As a result, the current calculated from the current density  $\mathbf{J}_c$  is not conserved. Therefore, we need to modify the conventional definition of current density to include the contribution of  $\rho_n(\mathbf{r})$  induced by the non-local potential.

We define the new current density in the presence of a non-local potential as

$$\mathbf{J}(\mathbf{r}) = \mathbf{J}_c(\mathbf{r}) + \mathbf{J}_n(\mathbf{r}) \quad (9)$$

where  $\mathbf{J}_n(\mathbf{r})$  is the non-local current density defined as

$$\mathbf{J}_n(\mathbf{r}) = -\nabla \varphi_n(\mathbf{r}) \quad (10)$$

and  $\varphi_n(\mathbf{r})$  is determined by the following Poisson equation,

$$\nabla^2 \varphi_n(\mathbf{r}) = -\rho_n(\mathbf{r}). \quad (11)$$

Note that  $\mathbf{J}_n(\mathbf{r})$  is a local quantity. We call it the non-local current density because it is solely due to the non-local potential. Once  $\rho_n(\mathbf{r})$  is known the quantity  $\varphi_n(\mathbf{r})$  and hence  $\mathbf{J}_n(\mathbf{r})$  can be calculated by solving the Poisson equation with proper boundary conditions. It is obvious that the newly defined current density satisfies  $\nabla \cdot \mathbf{J}(\mathbf{r}) = 0$ , and therefore the current calculated from this current density satisfies the current conservation.

In the following we show that the current calculated from equation (2) using the new definition of current density is the same as that obtained from the Landauer–Büttiker formula, equation (1). To do that, we express the conventional current density and non-local electron density in terms of Green's functions. This has been done in [2] when the non-local potential is absent, and we will be following exactly the same approach as that of [2]. We divide the system into three parts: the central scattering region and two leads. The influence of the lead on the scattering region is considered by the self-energy  $\Sigma^{r,a}$ . The retarded Green's function of the scattering region is defined as  $G^r = 1/(E - H - \Sigma^r)$ . The density matrix of the central scattering region is the lesser Green's function  $-iG^<$  that can be obtained by replacing the scattering wavefunction in the central region  $\psi(\mathbf{r})\psi^*(\mathbf{r}')$  with  $(-i/2\pi)G^<(\mathbf{r}, \mathbf{r}')$  (see [2]). With this observation, the conventional current density  $\mathbf{J}_c(\mathbf{r})$  can be expressed as

$$\mathbf{J}_c(\mathbf{r}) = \int \frac{dE}{2\pi} \mathbf{J}_c(\mathbf{r}, E) \quad (12)$$

where

$$\mathbf{J}_c(\mathbf{r}, E) = -\frac{e\hbar}{4\pi m} [(\nabla - \nabla') G^<(\mathbf{r}, \mathbf{r}', E)]_{\mathbf{r}=\mathbf{r}'}, \quad (13)$$

the same expression as obtained in [2]. Using the same approach, the non-local electron density can also be obtained,

$$\rho_n(\mathbf{r}, E) = \frac{e}{2\pi\hbar} \int d\mathbf{r}' [V(\mathbf{r}, \mathbf{r}')G^<(\mathbf{r}, \mathbf{r}', E) - V^*(\mathbf{r}, \mathbf{r}')G^<(\mathbf{r}', \mathbf{r}, E)]. \quad (14)$$

Now we have expressed all the quantities needed in terms of non-equilibrium Green's functions  $G^r$  and  $G^<$ , where  $G^< = G^r\Sigma^<G^a$  from the Keldysh equation and  $\Sigma^< = i\sum_\alpha \Gamma_\alpha f_\alpha$  [8]. Here  $\Gamma_\alpha$  is the linewidth function of lead  $\alpha$  and  $f_\alpha = f(E - qv_\alpha)$  is the Fermi distribution function of lead  $\alpha$  with bias  $v_\alpha$ . Thus once the Green's functions for the system are calculated, we can obtain the local current density  $\mathbf{J}_c(\mathbf{r}, E)$  and the non-local electron density  $\rho_n(\mathbf{r}, E)$ .

From equation (13), the divergence of current density can also be written as

$$\nabla \cdot \mathbf{J}_c(\mathbf{r}, E) = -\frac{e\hbar}{4\pi m} [(\nabla^2 - \nabla'^2)G^<(\mathbf{r}, \mathbf{r}', E)]_{\mathbf{r}=\mathbf{r}'}. \quad (15)$$

Since  $\rho_n = \nabla \cdot \mathbf{J}_n$ , combining equations (14) and (15), we have

$$\int \frac{dE}{2\pi} \nabla \cdot \mathbf{J}(\mathbf{r}, E) = \frac{e}{h} [HG^< - G^<H]_{\text{rr}} \quad (16)$$

where  $\mathbf{J}(\mathbf{r}, E) = \mathbf{J}_c(\mathbf{r}, E) + \mathbf{J}_n(\mathbf{r}, E)$ ,  $H = -(\hbar^2/2m)\nabla^2 + V(\mathbf{r}, \mathbf{r}')^5$ , and  $G^<(\mathbf{r}, \mathbf{r}') = \int (dE/2\pi)G^<(\mathbf{r}, \mathbf{r}', E)$ . Using the relation [2]

$$HG^< - G^<H = G^r\Sigma^< - \Sigma^<G^a - \Sigma^rG^< + G^<\Sigma^a \quad (17)$$

equation (15) becomes

$$\int \frac{dE}{2\pi} \nabla \cdot \mathbf{J}(\mathbf{r}, E) = \frac{e}{h} \sum_\alpha [G^r\Sigma_\alpha^< - \Sigma_\alpha^<G^a - \Sigma_\alpha^rG^< + G^<\Sigma_\alpha^a]_{\text{rr}} \quad (18)$$

where  $\sum_\alpha \Sigma_\alpha^\gamma = \Sigma^\gamma$  with  $\gamma = r, a, <$  and  $\Sigma^<$  is the lesser self-energy. The terminal current can be obtained by integrating the current density over the cross-section of the corresponding contact  $\alpha$ :

$$I_\alpha = 2 \int \left[ \int \mathbf{J}(\mathbf{r}, E) \cdot d\sigma_\alpha \right] dE \quad (19)$$

where the factor of two comes from spin degeneracy. Alternatively, the terminal current can also be calculated by

$$I_\alpha = \frac{2e}{h} \int dE \text{Tr}[G^r\Sigma_\alpha^< - \Sigma_\alpha^<G^a - \Sigma_\alpha^rG^< + G^<\Sigma_\alpha^a] \quad (20)$$

which is the Landauer-Büttiker formula. Taking the trace over both sides of equation (18) gives the relation between the currents calculated from the current density and the Landauer-Büttiker formula. In addition, equation (18) ensures the conservation of current calculated using either equation (19) or (20).

Using the relation

$$G^< = iG^r\Gamma G^a f_L + iG^r\Gamma_R G^a (f_R - f_L) \quad (21)$$

<sup>5</sup> Here the non-local Hamiltonian means  $H\psi(\mathbf{r}) = -(\hbar^2/2m)\nabla^2\psi(\mathbf{r}) + \int d\mathbf{r}' V(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}')$ .

we can partition the current density into two parts: equilibrium and non-equilibrium contributions. In the absence of magnetic field, the equilibrium current density (contributed from the first term of equation (21)) is zero. In the presence of magnetic field, it is nonzero but does not contribute to the transport current. From now on, we keep only the non-equilibrium part of the current density. With this in mind we rewrite equations (13) and (14) as follows.

$$\mathbf{J}_c(\mathbf{r}, E) = \frac{ie\hbar}{4\pi m} [(\nabla - \nabla')D_R(\mathbf{r}, \mathbf{r}', E)]_{\mathbf{r}=\mathbf{r}'} (f_L - f_R) \quad (22)$$

and

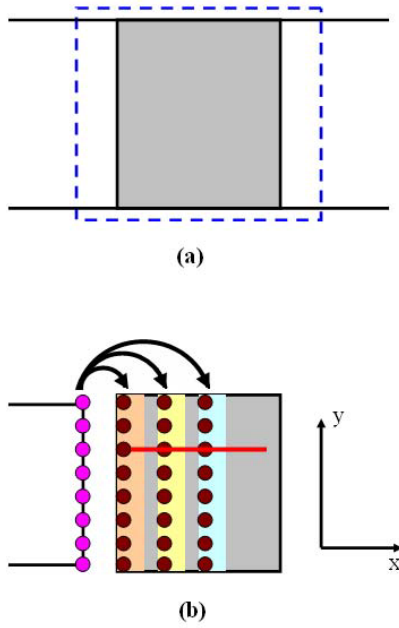
$$\rho_n(\mathbf{r}, E) = \frac{ie}{2\pi\hbar} \int d\mathbf{r}' [V(\mathbf{r}, \mathbf{r}')D_R(\mathbf{r}, \mathbf{r}', E) - V^*(\mathbf{r}, \mathbf{r}')D_R(\mathbf{r}', \mathbf{r}, E)] (f_R - f_L) \quad (23)$$

where  $D_R \equiv G^r\Gamma_R G^a$ . Note that if we are only interested in the current density in the linear response regime at zero temperature, the calculation is simplified drastically since the integral over energy is no longer needed due to the  $\delta$  function  $\partial_E f(E)$  from the expansion of  $f_\alpha$ .

To summarize briefly, in the presence of a non-local potential the current density consists of two parts: conventional current density and non-local current density. They can be calculated as follows: (1) We first calculate the conventional current density  $\mathbf{J}_c(\mathbf{r}, E)$  and the non-local electron density  $\rho_n(\mathbf{r}, E)$  according to equations (22) and (23). (2) We then solve the Poisson equation, equation (11), with proper boundary conditions to find the non-local current density  $\mathbf{J}_n(\mathbf{r}, E)$ . (3) The total current density is given by  $\mathbf{J}(\mathbf{r}) = \int (dE/2\pi)[\mathbf{J}_c(\mathbf{r}, E) + \mathbf{J}_n(\mathbf{r}, E)]$ .

### 3. Numerical implementation

To illustrate this procedure we discuss two examples in the following by calculating the current density in the linear regime so that both current and current density are proportional to the bias voltage, i.e.,  $I = G(v_L - v_R)$ . In the first example, the non-local potential is present only in the scattering region and is zero in the lead. In the second example, in addition to the non-local potential in the central region a periodic non-local potential is present in the lead. The boundary conditions are different in these two examples. We first consider a system with non-local potential in the central scattering region connected by two ideal leads without non-local potential, as shown in figure 1(a). To match the boundary conditions, we have added part of the leads into our central simulation box (see figure 1(a)). The non-local potential in the central box is nonzero when  $x$  is from 5 to 25 along the  $x$ -direction. The non-local potential is chosen as  $V(x, y; x', y') = 0.2 \sin[\pi(x - 5)/20](\delta_{x+1, x'} + \delta_{x-1, x'})\delta_{y, y'}$  in the shadowed region in figure 1. In the calculation, the energy is measured in e.u. (energy units), which is  $\hbar^2/2ma^2$ , the length is measured in  $a$  which is the lattice constant, and the current is measured in  $(2e^2/h)$  V. In the numerical calculation, we first calculate the self-energy of both leads using a transfer matrix method [9] and then obtain the Green's functions for the system. Once the Green's functions are obtained, we can calculate the conventional



**Figure 1.** (a) Schematic picture of the model. The shadowed region represents the scattering region with a non-local potential and the dashed line marks our central simulation box in the numerical calculation. (b) The coupling between the lead and the simulation box is labeled by arrows. In the figure, the lead couples to the simulation box through three layers of lattice sites.

current density  $\mathbf{J}_c(\mathbf{r})$  at each point according to equation (22). The non-local current density  $\mathbf{J}_n$  can be calculated by solving the Poisson equation with the Neumann boundary condition where the normal derivative of the function is specified on all boundaries. In our system, we have chosen the dashed line in figure 1(a) as our boundaries.

In the first example, the normal derivatives of function  $\varphi_n$  in equation (11) are zero on the four boundaries, i.e.,  $\hat{\mathbf{x}}_\alpha \cdot \mathbf{J}_n = \hat{\mathbf{x}}_\alpha \cdot \partial\varphi_n = 0$ , where  $\hat{\mathbf{x}}_\alpha$  is the normal direction of a particular interface located at  $\mathbf{x}_\alpha$ . The reason is the following. On the up and down boundaries, the normal derivative of the function  $\varphi_n$  is along the  $y$ -direction and there is no current flow along the  $y$ -direction across the up and down boundaries. On the left and right boundaries, there are no non-local potentials near the boundaries. Therefore the non-local current density  $\mathbf{J}_n$  is zero on the left and right boundaries. Hence, in this case, we have  $\mathbf{J}_{nL} = \mathbf{J}_{nR} = 0$  and  $\hat{\mathbf{x}}_U \cdot \mathbf{J}_{nU} = \hat{\mathbf{x}}_D \cdot \mathbf{J}_{nD} = 0$ .

In the second example, we allow a non-local potential in the lead. In this case, we also choose Neumann boundary conditions in solving the Poisson equation. On the up and down boundaries, the normal derivative of the function  $\varphi_n$  is along the  $y$ -direction and equal to zero, so we have  $\hat{\mathbf{x}}_U \cdot \mathbf{J}_{nU} = \hat{\mathbf{x}}_D \cdot \mathbf{J}_{nD} = 0$ . Now we consider the case where periodic non-local potentials are present in the left and right leads. Here again we include a portion of the lead into the simulation box. Obviously,  $\mathbf{J}_n$  is nonzero on the left and right boundaries because a non-local potential is present in the leads. We will determine their values through the relation  $\mathbf{J} = \mathbf{J}_c + \mathbf{J}_n$ . The conventional current density  $\mathbf{J}_c(x, y)$  can be calculated on the left and right boundaries. The total current density  $\mathbf{J}(x, y)$

can also be determined by the transmission function at the boundaries. Therefore the normal derivatives of the function  $\varphi_n$  on the left and right boundaries are determined by  $\mathbf{J}_n(x, y) = \mathbf{J}(x, y) - \mathbf{J}_c(x, y)$ . Now we explain how to obtain  $\hat{\mathbf{x}}_\alpha \cdot \mathbf{J}(x, y)$  at the boundary  $x_\alpha$  from the transmission function for a two-probe structure. We define a position-dependent transmission coefficient  $\mathcal{T}_\alpha(r)$  in the coupling region between the scattering region and the lead  $\alpha$ :

$$\mathcal{T}_\alpha(r) = [G^\dagger \Gamma_\beta G^a \Gamma_\alpha]_{rr} \quad (24)$$

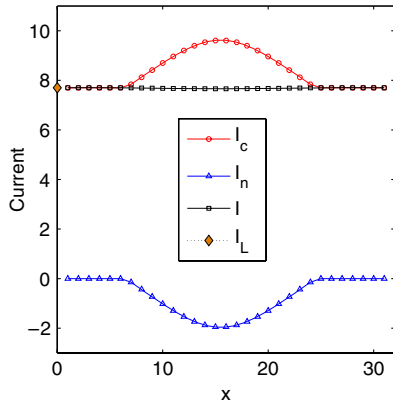
where  $r$  labels all the sites of the scattering region that are coupled to the lead  $\alpha$  and  $\beta \neq \alpha$ . Note that the coupling region depends on the unit cell of the lead. For the tight binding model, the coupling region contains just one layer of lattice sites. For graphene, the coupling region contains two layers of lattice sites. The physical meaning of  $\mathcal{T}_{\alpha(r)}$  is the transmission probability from the lead  $\alpha$  to the site  $r$  inside the scattering region. Obviously  $\sum_r \mathcal{T}_{\alpha(r)}$  is the transmission coefficient. The current density at the interface  $\alpha$  with the site labeled by  $y$  is obtained from  $\mathcal{T}_{\alpha(r)}$  with  $r = (x, y)$ :

$$\hat{\mathbf{x}}_\alpha \cdot \mathbf{J}(y) = \frac{2e}{h} \int dE (f_\alpha - f_\beta) \int dx [G^\dagger \Gamma_\beta G^a \Gamma_\alpha]_{rr} \quad (25)$$

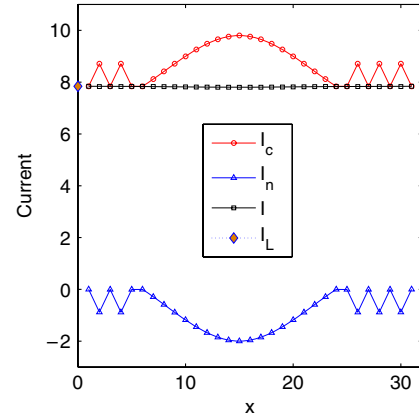
where the summation is over all the sites with the same  $y$ -coordinate in the coupling region (see the solid line in the scattering region of figure 1(b) for illustration). For the tight binding model on a square lattice, the linewidth function couples only to the boundary sites. Hence  $\hat{\mathbf{x}}_\alpha \cdot \mathbf{J}(y) = (2e/h) \int dE (f_\alpha - f_\beta) [G^\dagger \Gamma_\beta G^a \Gamma_\alpha]_{yy}$ .

In order to demonstrate the current conservation, we calculate the current across different cross-sections perpendicular to the  $x$ -direction inside the simulation box. The current is obtained by summing over the current density at all the  $y$  points on a cross-section at a fixed  $x$  inside the scattering region. We define the conventional current across the cross-section located at  $x$  as  $I_c(x) = \int dy \hat{\mathbf{x}} \cdot \mathbf{J}_c(x, y)$  and the non-local current  $I_n(x) = \int dy \hat{\mathbf{x}} \cdot \mathbf{J}_n(x, y)$ . If the total current of the system is conserved, the total current  $I(x) = \int dy \hat{\mathbf{x}} \cdot \mathbf{J}(x, y)$  should be a constant independent of  $x$  and must be equal to the current obtained from the Landauer–Büttiker formula.

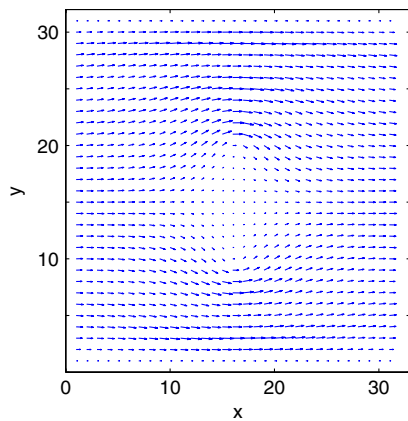
In figure 2, we plot the conventional current  $I_c$  and non-local current  $I_n$  across different cross-sections along the  $x$ -direction. Here we have fixed the energy of the incoming electron to be 1 e.u., so that there are ten subbands participating in the transport. Due to the scattering of non-local potential, the conductance is less than eight. Importantly, we see that the conventional current varies at different  $x$ . Since the simulation box includes part of the lead where the non-local potential is absent, the conventional current is a constant in the lead region  $x = [1, 4]$  and  $x = [26, 31]$ . When the non-local current is included, the total current  $I(x)$  obtained from the current density is a constant in the whole simulation box. We have also confirmed numerically that the current obtained from the current density inside the scattering region is the same as the current calculated from the Landauer–Büttiker formula. This indicates that the current calculated from the new definition of current density is conserved in the presence of a non-local



**Figure 2.** Local current  $I_c$ , non-local current  $I_n$  and total current  $I$  along the  $x$ -direction when there are no non-local potentials in the leads. Here the diamond symbol indicates the current calculated from the Landauer–Büttiker formula. The unit for the current is  $2(e^2/h)(v_L - v_R)$  and the distance  $x$  is measured in units of lattice constant  $a$ .



**Figure 4.** Local current  $I_c$ , non-local current  $I_n$  and total current  $I$  along the  $x$ -direction with periodical non-local potentials in the leads. In the figure the diamond symbol indicates the current calculated from the Landauer–Büttiker formula. The units of current and distance are the same as in figure 2.



**Figure 3.** Distribution of current density  $\mathbf{J}(x, y)$  in the  $x$ - $y$  plane. For illustration purposes, we have added impurity potentials in the regime  $x = 15$  and  $y = [10, 20]$  with impurity strength 2 e.u. The distances  $x$  and  $y$  are measured in units of lattice constant  $a$ .

potential. In figure 3, we plot the distribution of current density in the presence of a non-local potential only in the central box but not the leads. For illustration purposes, we have added impurity potentials in a small region<sup>6</sup>. We can see the current pattern in the scattering region. When there are non-local potentials in the leads, we can also calculate current density  $\mathbf{J}_c$  and non-local current density  $\mathbf{J}_n$ . For the convenience of solving the Poisson equation, the non-local potential in the leads is chosen as periodic<sup>7</sup>. Figure 4 plots the conventional current  $I_c$ , non-local current  $I_n$ , and total current  $I$  versus positions along  $x$  when the energy of the incoming electron is 1 e.u. We see that the total current calculated from the current density is again a constant that is equal to the current calculated from the Landauer–Büttiker formula.

<sup>6</sup> The impurity potential is a diagonal potential added on all the lattice points in the regime ( $x = 15, 10 \leq y \leq 20$ ). The amplitude of the impurity potential is chosen as 2 e.u.

<sup>7</sup> The non-local potential in the leads is chosen as  $V(x, y; x', y') = 0.1\delta_{x+1, x'}\delta_{y, y'}$  when  $x$  is an odd number and  $V(x, y; x', y') = 0$  when  $x$  is an even number.

## 4. Summary

In summary, we have addressed the issue of current density in the presence of a non-local potential. We found that the current density using the conventional definition is not suitable for describing the current density in the presence of a non-local potential. A new definition of current density is suggested. With this definition, the current inside the scattering region across any interface perpendicular to the direction of current flow is a constant and is equal to the current calculated from the Landauer–Büttiker formula. We have numerically confirmed the above conclusion by studying two examples.

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