

# Electronic transport calculations in the ONETEP code: Implementation and applications



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## ABSTRACT

We present an approach for computing Landauer–Büttiker ballistic electronic transport for multi-lead devices containing thousands of atoms. The method is implemented in the ONETEP linear-scaling density-functional theory code and uses matrix elements calculated from first-principles. Using a compact yet accurate basis of atom-centred non-orthogonal generalised Wannier functions that are optimised *in situ* to their unique local chemical environment, the transmission and related properties of very large systems can be calculated efficiently and accurately. Other key features include the ability to simulate devices with an arbitrary number of leads, to compute eigenchannel decompositions, and to run on highly parallel computer architectures. We demonstrate the scale of the calculations made possible by our approach by applying it to the study of electronic transport between aligned carbon nanotubes, with system sizes up to 2360 atoms for the underlying density-functional theory calculation. As a consequence of our efficient implementation, computing electronic transport from first principles in systems containing thousands of atoms should be considered routine, even on relatively modest computational resources.

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## 1. Introduction

As a result of the drive towards miniaturisation of electronic devices and the fabrication of nanostructured materials, there is great interest in theoretical methods to calculate their charge transport characteristics. Approaches that provide a full atomistic description are particularly appealing, and are invaluable in improving our understanding of such devices, and optimising their performance.

A popular method to determine the conductance properties of nanoelectronic devices combines the framework of Landauer transport [1–3] with a description of electronic structure determined from first-principles [4,5]. The advantage of this approach is in its predictive power that comes from a fully-quantum mechanical treatment of conductance with an unbiased and accurate description of electronic structure. Whilst there are limitations regarding its validity in certain situation [6], approaches combining

Landauer transport with density functional theory (DFT) [4,5] have been remarkably successful in describing a wide variety of materials [7–9].

Several computational implementations of this approach exist [10–20] adopting either a non self-consistent approximation, valid at zero bias, or employing the non-equilibrium Green's function approach to account for the self-consistent rearrangement of electronic charge when under bias [21,22]. Many of these implementations focus on transport between two-terminal devices, however there has been recent interest and success in developing approaches to simulate multi-terminal devices [23,24].

Common amongst all these implementations is that, for a given amount of available computing resource, there is a trade-off to be made between accuracy and the size of the system that can be simulated. Existing implementations can be broadly categorised into two classes.

The first approach relies on very large sets of simple basis functions, such as plane-waves, in order to compute the electronic structure accurately and with systematically improvable accuracy, within the limitations of the underlying theory (e.g., the choice of exchange–correlation functional, pseudopotentials, etc.). A subsequent transformation to a much smaller, if not minimal, set of

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localised Wannier functions then enables efficient transport calculations [13,19,20,25,26]. In this approach it is the computational cost of the underlying electronic structure calculation, which scales asymptotically cubically with respect to system size for traditional methods, that severely limits the ability of this method to study realistic devices.

In a second class of methods, the electronic structure is calculated using a fixed basis set of localised functions, such as Gaussians [12,27] or numerical atomic orbitals [10,11,15], and the same basis set is then used to calculate the transport properties of the device. There are competing requirements here because an accurate description of the electronic structure often requires a large basis set, typically several times larger than the minimal Wannier function basis, yet using this same basis for also calculating transport properties results in much higher computational cost than if a minimal basis is used. In the case of an atomic-like orbital basis, therefore, it is the cost of computing transport properties that often restricts the accessible system size.

The trade-off between accuracy and system-size poses a problem for simulations of realistic devices as typically several thousands of atoms or more may need to be included in order to capture the characteristics of the device faithfully.

In this paper we present an approach that combines the advantages of both classes of method described above to calculate Landauer transport from first-principles using a small basis, whilst retaining plane-wave accuracy. Our implementation is within the ONETEP linear-scaling DFT project [28], which uses a small basis of localised orbitals, called non-orthogonal generalised Wannier functions (NGWFs) [29], that are represented in terms of an underlying systematic basis of Fourier–Lagrange, or *psinc*, functions equivalent to a set of plane-waves [30]. The NGWFs are optimised *in situ* to their unique chemical environment [29] such that plane-wave accuracy can be achieved. Zero-bias transport properties are calculated efficiently within the same basis using a non self-consistent approach.

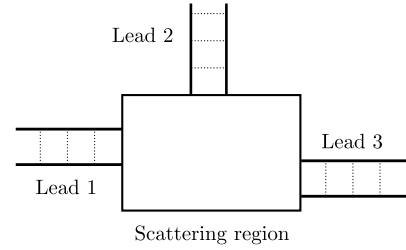
The method can be used to calculate transport through devices connected to an arbitrary number of leads and containing thousands of atoms on a routine basis using even relatively modest parallel computational resources. We demonstrate its scope and applicability through a study of inter-tube electron transport in carbon nanotube networks.

The rest of this paper is organised as follows: Section 2 describes the necessary background theory of computing Landauer–Büttiker electronic transport; Section 3 gives details of our specific implementation within the ONETEP code; we discuss the optimisations in our implementation that enable the study of transport in very large systems in Section 4, and the calculation of the bulk-lead band structures and eigenchannels in multi-lead devices in Section 5; in Section 6, we apply our implementation to the study of electronic transport in networks of carbon nanotubes; finally, we summarise our findings in Section 7.

## 2. Theoretical background

The standard geometry considered in the Landauer–Büttiker formalism is shown in Fig. 1, where the entire system consists of a number of semi-infinite leads connected to a central scattering region. The leads act as current sources and sinks, and are assumed to couple only through the device region. Current must flow through the device region to travel between two leads. Scattering occurs in the central region only, and is assumed to occur elastically.

Central to the Landauer formalism is the transmission between two leads,  $T_{ij}(E)$ , defined as the probability that a state of energy  $E$  injected from lead  $i$  is received in lead  $j$ . For a single conduction



**Fig. 1.** The schematic geometry of a three lead device, connected by a central scattering region. The dashed lines represent the periodically-repeating structure within the semi-infinite leads.

channel at energy  $E$  propagating through a device, the zero-bias conductance between these two leads is given by [2,21]

$$g_{ij}(E) = \frac{2e^2}{h} T_{ij}(E). \quad (1)$$

Eq. (1) is generalised to leads with multiple conduction channels by summing over contributions from each channel. Throughout this work we will assume the system to be spin degenerate, however spin-polarised systems can also be calculated using our implementation.

### 2.1. Transmission from Green's functions

The key task is to compute the transmission coefficients, which we do using a Green's function formalism [21]. This formalism employs a set of localised basis functions so that matrix elements can be unambiguously assigned to a localised region in real space. The Green's function for a device is given by

$$G_d(E) = [(E + i\eta)S_d - H_d - \Sigma_1(E) - \Sigma_2(E) - \dots]^{-1}, \quad (2)$$

where  $H_d$  is the device Hamiltonian,  $S_d$  is the overlap matrix for the device basis functions, which are assumed not necessarily orthogonal, and  $\Sigma_i(E)$  is the self energy for lead  $i$ .

The transmission coefficient between leads  $i$  and  $j$  is then given by [21]

$$T_{ij}(E) = \text{tr}[\Gamma_i G_d \Gamma_j G_d^\dagger] \quad (3)$$

where  $\Gamma_i(E)$  are the coupling matrices defined in terms of the corresponding lead self energy as

$$\Gamma_j = i(\Sigma_j - \Sigma_j^\dagger). \quad (4)$$

In addition to the transmission coefficients, the device Green's function allows the device density of states to be computed using

$$\mathcal{N}_d(E) = -\frac{1}{\pi} \text{Im} \text{tr}[G_d S_d]. \quad (5)$$

The most general transport setup involves transmission between leads of different material or structure, through a central device region with arbitrary geometry. We refer to this transmission as *device* transmission. A special case is when the full device, i.e. central region and leads, is formed from the same bulk material. Such a system has no scattering and transmission takes an integer value determined by the number of transmission modes available at that energy. We refer to this special case as *bulk* transmission.

### 2.2. ONETEP and the NGWF basis

The platform for our implementation is ONETEP [28], a linear-scaling DFT code specifically designed to calculate electronic structures of systems containing thousands of atoms.

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