Kohn-Sham equations for nanowires with direct current

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Abstract

The paper describes the derivation of the Kohn-Sham equations for a nanowire with direct current. A value of the electron current enters the problem as an input via a subsidiary condition imposed by pointwise Lagrange multiplier. Using the constrained minimization of the Hohenberg-Kohn energy functional, we derive a set of self-consistent equations for current carrying orbitals of the molecular wire.

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I. INTRODUCTION

The goal of building real electronic devices from individual molecules 1 has spurred experimental and theoretical studies of molecular conductivities. Measurements of currentvoltage (I-V) characteristics have been reported for single molecules [2, 3] but mechanisms for electron transmissions through molecular interfaces remain largely unexplored and unexplained [4, 5]. It appears that the miniaturization of microelectronic devices shrinks the size of the system to a level when the simulations of transport characteristics of molecular electronic devices can be performed by *ab initio* electronic structure methods (with single benzene-1,4-dithiolate molecule as the molecular wire, the contact wire-contact "supermolecule" consists of just 32 atoms). However, the main principle hurdle for the application of the first principle electronic structure methods is not the size of the system but conceptually unsolved problems of modeling of the electronic current and interpretation of the applied voltage for correlated electronic systems. In traditional methods, which are based on the Landauer theory [6], the molecule and the edge part of the metal contacts can be in principle treated *ab initio*, e.g. in the density functional theory (DFT). But then to induce the electronic current it is assumed that the system is attached to two equilibrium electronic reservoirs with the different chemical potentials [7]. Being computationally not very efficient, since it requires to perform the calculations over the whole coordinate space, these traditional approaches are also pivotally relied on the electronic reservoir concept and often use *ad hoc* reservoir-molecule interaction as an essential input parameter.

We have previously shown that the reservoir model can be conceptually circumvented in electronic transport calculations if the electronic current is used as an input information instead the applied voltage bias [8, 9]. In our approach the electronic current enters a quantum variational problem via the corresponding Lagrange multiplier. In this paper, we continue development of our method and discuss detailed derivation of the Kohn-Sham equations for a nanowire with steady current. We begin by describing the variational principle for an inhomogeneous electron gas with steady current. We then derive the Kohn-Sham equations with steady current.

II. VARIATIONAL PRINCIPLE

We start our derivation by defining density and current density of an inhomogeneous, interacting N-electron gas in an external scalar potential $v(\mathbf{r})$ as (a.u. are used throughout the paper):

$$\rho(\mathbf{r}) = N \int \Psi(\mathbf{r}, \mathbf{r}_2, \dots; \mathbf{r}_N) \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \prod_{i=2}^N d\mathbf{r}_i , \qquad (1)$$

$$\mathbf{j}(\mathbf{r}) = N \int \operatorname{Im} \left\{ \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \nabla \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \right\} \prod_{i=2}^N d\mathbf{r}_i , \qquad (2)$$

where Ψ is the many-electron wave-function. For simplicity of notation we do not write explicitly the spin indeces but our derivation can be readily extended to spin-polarized systems.

Next, we introduce a subsidiary condition for the current density distribution by specifying the quantum wire constraint on the current [8, 9]:

$$\int dy \, dz \, j_x(\mathbf{r}) = I(x) \;, \tag{3}$$

where I(x) is a given input value of the steady current through the electronic device. With this constraint the current is aligned along the x-axis and the net current flow across a cross section $\int dy dz j_x(\mathbf{r})$ is constrained, and this quantity is available experimentally.

For an inhomogeneous, interacting electron gas in scalar external potential $v(\mathbf{r})$, the ground state energy is given by the Hohenberg-Kohn energy functional [10]:

$$E_{HK}[\rho] = T_o[\rho] + \int d\mathbf{r} v(\mathbf{r})\rho(\mathbf{r}) + \frac{1}{2} \int \int d\mathbf{r} d\mathbf{r}' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + E_{xc}[\rho] .$$
(4)

The first term, T_0 , is the kinetic energy functional of noninteracting electrons with given density and current density distribution. The second and third terms, are the interaction energy with external potential and the electrostatic interactions. The last term, $E_{xc}[\rho]$, is the exchange and correlation energy functional. The current dependent correction to the standard exchange-correlation energy functional is $O(j^2)$ [11]. A dependence of the exchange-correlation energy functional upon $\mathbf{j}(\mathbf{r})$ can be readily included in our approach, yielding the additional exchange-correlation vector potential [11]:

$$\mathbf{A}_{xc}[\rho, \mathbf{j}](\mathbf{r}) = \frac{\delta E_{xc}[\rho, \mathbf{j}]}{\delta \mathbf{j}(\mathbf{r})}$$
(5)

which modifies the kinetic energy operator in the final Kohn-Sham equation in the same way as an external vector potential does. The current dependent correction to the standard exchange-correlation energy functional is $O(j^2)$ [11]. Molecular and atomic wires can sustain a current of about $10^{-4}a.u$. for typical experiments on molecular conduction [2]. Therefore the direct current-dependent corrections to the total electronic energy are only of the order of $10^{-8}a.u$. and can be ignored in most molecular transport calculations.

Likewise our derivation of the Schrödinger equation for current carrying states [9], we use the constrained variational principle in our derivations. The problem is to minimize Hohenberg-Kohn energy functional (4) subject to the constraint on the current density (3). The constraint is explicitly achieved by introduction of an auxiliary functional

$$\Omega[\Psi] = E_{HK}[\rho] - \int dx a(x) \left(\int dy \, dz \, j_x(\mathbf{r}) - I(x) \right) \,. \tag{6}$$

The first term giving the total energy is standard in the variational formulation of the DFT. The second term with the Lagrange multipliers a(x) has been introduced to impose the subsidiary constraint for the current density (3).

III. KOHN-SHAM EQUATIONS WITH DIRECT CURRENT

Following the Kohn and Sham approach [12], we introduce a reference fermion system with orthonormal single-particle orbitals $\psi_i(\mathbf{r})$ and occupation numbers n_i to reproduce the charge and current densities:

$$\rho(\mathbf{r}) = \sum_{i} n_{i} \psi_{i}^{*}(\mathbf{r}) \psi_{i}(\mathbf{r}) , \qquad (7)$$

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2i} \sum_{i} n_i \left(\psi_i^*(\mathbf{r}) \nabla \psi_i(\mathbf{r}) - \psi_i(\mathbf{r}) \nabla \psi_i^*(\mathbf{r}) \right) .$$
(8)

According to the variational principle and assuming a fixed set of the occupation numbers n_i , we carry out the minimization of the Hohenberg-Kohn energy functional with respect to the single-electron orbitals $\psi_i(\mathbf{r})$ subject to the constraint for the current density (3), i.e. the variation of auxiliary functional $\Omega[\Psi]$. The minimization yields the following single-electron self-consistent equations:

$$\left(-\frac{1}{2}\nabla + v(\mathbf{r}) + \int d\mathbf{r} \frac{\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[\rho](\mathbf{r}) + \frac{1}{2i} \left[\partial_x, a(x)\right]_+\right) \psi_i(\mathbf{r}) = E_i \,\psi_i(\mathbf{r}) \,, \qquad (9)$$

where the anti-commutator term,

$$\left[\partial_x, a(x)\right]_+ = \partial_x(a(x)) + 2a(x)\partial_x \tag{10}$$

is the additional imaginary potential arising directly from the constraint on electronic current (Appendix A). This equation is a particular case of the more general equation derived recently by Kosov and Greer [8]. Relating a position gradient with the corresponding momentum operator ($\hat{p}_x = -i\partial_x$) we can rewrite the imaginary potential as the momentumdependent operator:

$$\frac{1}{2i} \left[\partial_x, a(x)\right]_+ = \frac{1}{2} \left[\hat{p}_x, a(x)\right]_+ \ . \tag{11}$$

Since the operator (11) is hermitian the Konh-Sham equation (9) is a hermitian eigenproblem.

We have not specified yet the occupation numbers n_i which enter the Kohn-Sham equations (9) via the density and the current density. To fix the set of occupation numbers, we need to know the number of electrons in the nanowire. Although we deal with the open quantum system where electrons can leave and enter the wire, we still can put a constraint on the total number of electrons because of time and space independence of the electronic current (i.e. steady state direct current). Then, the continuity equation tells us that the total number of electrons does not depend upon time. If we assume that the charge neutrality is maintained after the establishment of the current currying state, the average number of electrons in the nanowire N is the same as the number of electrons in the zero current wire. Therefore to obtain the occupation numbers we can minimize Ω (6) with respect to n_i subject to the particle conserving constraint imposed with the additional Lagrange multiplier μ (chemical potential):

$$\delta\left[\Omega - \mu(\sum_{i} n_i - N)\right] \ge 0.$$
(12)

The direct differentiation of the Hohenberg-Kohn energy is straitforward and results into the following expression (Janak theorem) [13]:

$$\frac{\partial E_{HK}}{\partial n_i} = \int d\mathbf{r} \psi_i^*(\mathbf{r}) \left(-\frac{1}{2} \nabla + v(\mathbf{r}) + \int d\mathbf{r} \frac{\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[\rho](\mathbf{r}) \right) \psi_i(\mathbf{r}) + \left[\sum_k n_k \int d\mathbf{r} \frac{\partial \psi_k^*(\mathbf{r})}{\partial n_i} \left(-\frac{1}{2} \nabla + v(\mathbf{r}) + \int d\mathbf{r} \frac{\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[\rho](\mathbf{r}) \right) \psi_k(\mathbf{r}) + c.c. \right]$$

The details of the differentiation of the constrained functional with respect to an occupation number n_i are given in Appendix B. The differentiation leads to the following expression for the derivative:

$$\frac{\partial \Lambda}{\partial n_{i}} = \frac{1}{2i} \int d\mathbf{r} \psi_{i}^{*}(\mathbf{r}) \left[\partial_{x}, a(x)\right]_{+} \psi_{i}(\mathbf{r}) + \left[\frac{1}{2i} \sum_{k} n_{k} \int d\mathbf{r} \frac{\partial \psi_{k}^{*}(\mathbf{r})}{\partial n_{i}} \left[\partial_{x}, a(x)\right]_{+} \psi_{k}(\mathbf{r}) + c.c.\right] .$$
(13)

Combining these two derivatives we arrive to the following expression for the derivative of the auxiliary functional:

$$\frac{\partial\Omega}{\partial n_{i}} = \int d\mathbf{r}\psi_{i}^{*}(\mathbf{r}) \left(-\frac{1}{2}\nabla + v(\mathbf{r}) + \int d\mathbf{r}\frac{\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[\rho](\mathbf{r}) + \frac{1}{2i}\left[\partial_{x}, a(x)\right]_{+}\right)\psi_{i}(\mathbf{r}) + \left[\sum_{k}n_{k}\int d\mathbf{r}\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}} \left(-\frac{1}{2}\nabla + v(\mathbf{r}) + \int d\mathbf{r}\frac{\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[\rho](\mathbf{r}) + \frac{1}{2i}\left[\partial_{x}, a(x)\right]_{+}\right)\psi_{k}(\mathbf{r}) + c.c.\right].$$
(14)

Given that ψ_i satisfy eq.(9) it is easy to see that:

$$\frac{\partial\Omega}{\partial n_i} = E_i \int d\mathbf{r} \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}) + \sum_k n_k E_k \frac{\partial}{\partial n_i} \int d\mathbf{r} \psi_k^*(\mathbf{r}) \psi_k(\mathbf{r}) = E_i .$$
(15)

From eq.(12) with the use of eq.(15) we arrive to the inequality

$$\sum_{i} (E_i - \mu) \delta n_i \ge 0 \tag{16}$$

which gives rise to the standard "build up principle" (orbitals with $E_i < \mu$ have $n_i = 1$ and those with $E_i > \mu$ have $n_i = 0$) which is still hold within our approach: a maximum two electrons are put into current carrying orbitals in the order of increasing orbital energy. The approach can be readily extended to the finite temperature case replacing of the integer $n_i = 0$ or 1 occupation number by the Fermi-Dirac expression. The formal aspects of the DFT with direct current and non-zero temperature are discussed elsewhere.

The Kohn-Sham equations with current (9) are not yet in a form allowing for a solution to be found as the Lagrange multiplier a(x) is not known yet. The additional equation for the Lagrangian multiplier a(x) can be obtained if we require that the Kohn-Sham orbitals from the eq.(9) yield the required current I(x):

$$\frac{1}{2i}\sum_{i}n_{i}\int dydz\left(\psi_{i}^{*}(\mathbf{r})\partial_{x}\psi_{i}(\mathbf{r})-\psi_{i}(\mathbf{r})\partial_{x}\psi_{i}^{*}(\mathbf{r})\right)=I(x) .$$
(17)

The system of nonlinear equations (9, 17) are to be solved simultaneously and being combined together composes a set of Kohn-Sham equations for nanowire with direct current.

IV. SELF-CONSISTENT ABSORBING-EMITTING BOUNDARY CONDITIONS

Multiplying the eq. (9) from the left on the $n_i\psi_i(\mathbf{r})^*$, summing up over the Kohn-Sham orbitals and subtracting from the obtained equation its own complex conjugate yields the continuity equation:

$$\nabla \cdot \mathbf{j}(\mathbf{r}) = \partial_x(a(x)\rho(\mathbf{r})) . \tag{18}$$

After the integration of eq.(18) over the $\{y, z\}$ plane and substitution of the constraint for the current density eq.(3) into the equation the following first order differential equation for the Lagrange multiplier a(x) can be deduced:

$$\partial_x(a(x)\rho_{yz}(x) - I(x)) = 0, \qquad (19)$$

where we have introduced the quantity

$$\rho_{yz}(x) = \int dy dz \rho(\mathbf{r}) . \qquad (20)$$

The solution of the differential equation (19) depends upon the asymptotic behavior of the specified function for the current I(x). It is computationally convenient to assume the space-localized boundary conditions $(I(x), \rho_{yz}(x) \to 0, \text{ when } x \to \pm \infty)$. This space-localized boundary conditions yields zero integration constant for the differential equation (19) and we obtain the following expression for the Lagrange multiplier:

$$a(x) = -\frac{I_x}{\rho_{yz}(x)} \,. \tag{21}$$

With this choice of the Lagrange multiplier (21) we complete the Kohn-Sham equations with the current I in the self-consistent and closed form:

$$\left(-\frac{1}{2}\nabla + v(\mathbf{r}) + \int d\mathbf{r} \frac{\rho(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[\rho](\mathbf{r}) - \frac{1}{2i} \left[\frac{I(x)}{\rho_{yz}(x)}, \frac{\partial}{\partial x}\right]_{+}\right) \psi_i(\mathbf{r}) = E_i \psi_i(\mathbf{r}) .$$
(22)

Some aspects of eq.(22) deserve special discussion. Suppose that the constrained current starts at the left system boundary L and completely absorbed at the right system boundary R:

$$I(x) = I \ \theta(x - L)\theta(R - x) , \qquad (23)$$

where I is the steady current through the system and θ is the step function. Then one of the terms in the anticommutator imaginary potential becomes proportional to the derivative of the step function and yields the singular imaginary δ -function potential on the system boundaries:

$$\frac{Ii}{2\rho_{yz}(x)}(\delta(x-L) - \delta(x-R))$$

This absorbing-emitting imaginary boundary potential is optimized due to its selfconsistency. It depends upon the density and value of the input current and emits the current I at the left boundary and completely absorbs the same current at the right boundary.

V. CONCLUSIONS

In this paper, we have derived the set of Kohn-Sham equations for a nanowire with direct, steady current. Not restricted to the linear response, our approach uses a constrained minimization of the total energy with a subsidiary condition for the current density to formulate the Kohn-Sham equation with direct current. The subsidiary condition for the current density is maintained during the variation by a pointwise Lagrange multiplier. Being entirely based on the DFT, our method incudes electronic correlations into the transport calculations at the same level as they are taken into account into the corresponding exchange-correlation functionals.

APPENDIX A: FUNCTIONAL DERIVATIVES OF THE CONSTRAINT FUNC-TIONAL WITH RESPECT TO ORBITALS

In this Appendix we compute the functional derivative of the constraint functional. The constraint functional has the following form

$$\Lambda[\psi_i, \psi_i^*] = \int dx a(x) \left(\int dy \, dz \, j_x(\mathbf{r}) - I_x \right) \,, \tag{A1}$$

with

$$j_x(\mathbf{r}) = \frac{1}{2i} \sum_i n_i \left(\psi_i^*(\mathbf{r}) \partial_x \psi_i(\mathbf{r}) - \psi_i(\mathbf{r}) \partial_x \psi_i^*(\mathbf{r}) \right)$$
(A2)

The direct variation of the constraint functional with respect to the $\psi^*(\mathbf{r})$ yields:

$$\frac{\delta\Lambda[\psi]}{\delta\psi_i^*(\mathbf{r})} = \frac{1}{2i} \int d\mathbf{r}' a(x') \frac{\delta}{\delta\psi^*(\mathbf{r})} \sum_k n_k \left\{ \psi_k^*(\mathbf{r}') \partial_x \psi_k(\mathbf{r}') - \psi_k(\mathbf{r}') \partial_x \psi_k^*(\mathbf{r}') \right\}$$

$$= \frac{1}{2i} a(x) \partial_x \psi_i(\mathbf{r}) - \frac{1}{2i} \frac{\delta}{\delta\psi_i^*(\mathbf{r})} \int d\mathbf{r}' \ a(x') \sum_k n_k \psi_k(\mathbf{r}') \nabla\psi_k^*(\mathbf{r}')$$

$$= \frac{1}{2i} a(x) \partial_x \psi_i(\mathbf{r}) - \frac{1}{2i} \frac{\delta}{\delta\psi_i^*(\mathbf{r})} \int d\mathbf{r}' \ \partial_x \left\{ \sum_k n_k a(x') \psi_k(\mathbf{r}') \psi_k^*(\mathbf{r}') \right\}$$

$$+ \frac{1}{2i} \frac{\delta}{\delta\psi_i^*(\mathbf{r})} \int d\mathbf{r}' \ \sum_k n_k \psi_k^*(\mathbf{r}') \partial_x \left\{ a(x') \psi_k(\mathbf{r}') \right\}$$

$$= \frac{1}{2i} a(x) \partial_x \psi_i(\mathbf{r}) + \frac{1}{2i} \partial_x \left\{ a(x) \psi_i(\mathbf{r}) \right\} = \frac{1}{2i} [a(x), \partial_x]_+ \psi_x(\mathbf{r})$$

APPENDIX B: DIFFERENTIATION OF THE CONSTRAINED FUNCTIONAL WITH RESPECT TO AN OCCUPATION NUMBER n_i

In this appendix the technical details of the direct differentiation of the constraint functional (A1) is presented.

$$\frac{\partial}{\partial n_i} \Lambda[\psi_i, \psi_i^*] = \frac{\partial}{\partial n_i} \int dx a(x) \int dy \, dz \, j_x(\mathbf{r}) = \int dx a(x) j_{ix}(x) + \frac{1}{2i} \int dx a(x) \int dy \, dz \, \sum_k n_k \frac{\partial}{\partial n_i} \left(\psi_k^*(\mathbf{r}) \partial_x \psi_k(\mathbf{r}) - \psi_k(\mathbf{r}) \partial_x \psi_k^*(\mathbf{r})\right) (B1)$$

Here we have introduced the new quantity which is the current through the orbital i integrated over the plane $\{y, z\}$:

$$j_{ix}(x) = \frac{1}{2i} \int dy \, dz \, \left(\psi_i^*(\mathbf{r})\partial_x\psi_i(\mathbf{r}) - \psi_i(\mathbf{r})\partial_x\psi_i^*(\mathbf{r})\right)$$

Then

$$\frac{\partial}{\partial n_{i}}\Lambda[\psi_{i},\psi_{i}^{*}] = \int dxa(x)j_{ix}(x) + \frac{1}{2i}\sum_{k}n_{k}\int d\mathbf{r}a(x)\left(\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}\partial_{x}\psi_{k}(\mathbf{r}) - \frac{\partial\psi_{k}(\mathbf{r})}{\partial n_{i}}\partial_{x}\psi_{k}^{*}(\mathbf{r})\right) + \frac{1}{2i}\sum_{k}n_{k}\int d\mathbf{r}a(x)\left(\psi_{k}^{*}(\mathbf{r})\partial_{x}\frac{\partial\psi_{k}(\mathbf{r})}{\partial n_{i}} - \psi_{k}(\mathbf{r})\partial_{x}\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}\right) \\
= \int dxa(x)j_{ix}(x) + \frac{1}{2i}\sum_{k}n_{k}\int d\mathbf{r}a(x)\left(\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}\partial_{x}\psi_{k}(\mathbf{r}) - \frac{\partial\psi_{k}(\mathbf{r})}{\partial n_{i}}\partial_{x}\psi_{k}^{*}(\mathbf{r})\right) + \frac{1}{2i}\sum_{k}n_{k}\int d\mathbf{r}\left(\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}\partial_{x}(a(x)\psi_{k}(\mathbf{r})) - \frac{\partial\psi_{k}(\mathbf{r})}{\partial n_{i}}\partial_{x}(a(x)\psi_{k}^{*}(\mathbf{r}))\right) = \int dxa(x)j_{ix}(x) + \frac{1}{2i}\left[\sum_{k}n_{k}\int d\mathbf{r}\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}[\partial_{x},a(x)]_{+}\psi_{k}(\mathbf{r}) - c.c.\right] = \frac{1}{2i}\int d\mathbf{r}a(x)\left(\psi_{i}^{*}(\mathbf{r})\partial_{x}\psi_{i}(\mathbf{r}) - \psi_{i}(\mathbf{r})\partial_{x}\psi_{i}^{*}(\mathbf{r})\right) + \frac{1}{2i}\left[\sum_{k}n_{k}\int d\mathbf{r}\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}[\partial_{x},a(x)]_{+}\psi_{k}(\mathbf{r}) - c.c.\right] = \frac{1}{2i}\int d\mathbf{r}\psi_{i}^{*}(\mathbf{r})[\partial_{x},a(x)]_{+}\psi_{i}(\mathbf{r}) + \frac{1}{2i}\left[\sum_{k}n_{k}\int d\mathbf{r}\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}[\partial_{x},a(x)]_{+}\psi_{k}(\mathbf{r}) - c.c.\right] = \frac{1}{2i}\int d\mathbf{r}\psi_{i}^{*}(\mathbf{r})[\partial_{x},a(x)]_{+}\psi_{i}(\mathbf{r}) + \frac{1}{2i}\left[\sum_{k}n_{k}\int d\mathbf{r}\frac{\partial\psi_{k}^{*}(\mathbf{r})}{\partial n_{i}}[\partial_{x},a(x)]_{+}\psi_{k}(\mathbf{r}) - c.c.\right]$$
(B2)

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