Steady-state quantum transport from a (TD)DFT perspective

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Outline

Molecular Electronics Steady-state approach to electron transport Steady-state transport with DFT for model systems Summary



- Molecular electronics
- Steady-state approach to transport
 - Landauer + static DFT for steady state transport
 - TDDFT approach to (steady-state) transport
- Steady-state transport with DFT for model systems
 - Derivative discontinuity in static DFT
 - A simple impurity model and finite-temperature functionals
 - Kondo effect from (TD)DFT point of view
 - XC bias by reverse engineering
- Summary

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Molecular Electronics

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Molecules as electronic devices

in 1974, Aviram and Ratner (Chem. Phys. Lett. **29**, 277 (1974)) suggested the use of individual molecules as rectifiers (i.e. a device which allows current to pass only for bias voltages larger than a threshold value)



Idea: part of molecule acts as donor, other part as acceptor

Why Molecular Electronics?

- ultimate limit of miniaturization in electronics (higher packing density, ...)
- times for electron transit through molecules smaller than typical operation times of semiconductor-based transistors
- chemically tailor molecular devices according to desired functionality

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Experimental techniques for single-molecule transport

mechanically controlled break junction technique (MCBJ)



open a nanoscale gap between two gold electrodes by mechanical bending, put molecule in solution on junction, hope that a molecule bridges the gap

Experimental techniques for single-molecule transport

Reed et al (Science 278, 252 (1997)):

first current measurements through single molecules using MCBJ



Experimental techniques for single-molecule transport

• Scanning tunneling microscopy (STM)



from webpage of J.C. Cuevas



from F. Pump et al, Appl. Phys. **93**, 335 (2008)

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Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

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Landauer steady-state approach to electron transport

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

Standard approach: Landauer formalism plus static DFT



Starting point: Hamiltonian of static DFT in localized basis, define retarded Green function

$$\begin{bmatrix} (E+i\eta)1 - \begin{pmatrix} H_{LL} & H_{LC} & 0\\ H_{CL} & H_{CC} & H_{CR}\\ 0 & H_{RC} & H_{RR} \end{pmatrix} \end{bmatrix} \begin{pmatrix} G_{LL} & G_{LC} & G_{LR}\\ G_{CL} & G_{CC} & G_{CR}\\ G_{RL} & G_{RC} & G_{RR} \end{pmatrix} = 1$$

note: no direct hopping between left and right leads

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

Standard approach: Landauer formalism plus static DFT

project on central region

$$G_{CC}(E) = ((E + i\eta)1_{CC} - H_{CC} - \Sigma_L(E) - \Sigma_R(E))^{-1}$$

embedding self-energy for lead $\boldsymbol{\alpha}$

$$\Sigma_{\alpha}(E) = H_{C\alpha} \left((E + i\eta) \mathbf{1}_{\alpha} - H_{\alpha\alpha} \right)^{-1} H_{\alpha C}$$

Landauer formula for steady-state current

$$I(V) = \frac{2e}{h} \int dE \ T(E, V) \left(f_{\beta}(E - eV_L) - f_{\beta}(E - eV_R) \right)$$

with bias $V = V_L - V_R$ and transmission function

$$T(E,V) = \operatorname{Tr} \left\{ \Gamma_L G_{CC} \Gamma_R G_{CC} \right\} \qquad \Gamma_\alpha = i (\Sigma_\alpha - \Sigma_\alpha^{\dagger})$$

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

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Standard approach: Landauer formalism plus static DFT

Schematic idea of Landauer approach



Zero-bias conductance in Landauer formalism

$$\frac{G}{G_0} = \frac{dI}{dV}\Big|_{V=0} = -\int dE \ T(E) \frac{\partial f_\beta(E)}{\partial E} \qquad G_0 = \frac{2e^2}{h}$$

in zero-temperature limit: $\frac{G}{G_0} = T(E_F)$

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

Example for application of Landauer formalism

Chrysazine molecule attached to gold leads Ref.:

A. Zacarias, E.K.U. Gross, Theor. Chem. Acc. 125, 535 (2010)



Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

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Landauer + static DFT

- Landauer + static DFT (DFT-NEGF) widely used for ab-initio transport
- inclusion of phonons possible: inelastic transport spectroscopies
- extension to thermal transport: thermal electron currents by Landauer-like formula

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

Critique of the Landauer approach

Empirical finding: currents through single (esp. organic) molecules often differ from experimental ones by 2-3 orders of magnitude Basic assumptions behind Landauer:

- A stationary current always develops
- The stationary state is uniquely determined by the bias

Theoretical weaknesses:

- Landauer formalism valid for non-interacting electrons
- Static DFT is a ground state theory and therefore in principle not suited to describe systems in a non-equilibrium situation → even if exact effective KS potential of static DFT could be used, predictions of Landauer might still be incorrect!

→ use time-dependent DFT which is exact in principle. Furthermore, it allows to study *time-dependent* transport phenomena (transients, AC bias, interaction with laser, etc.,),

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

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Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

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Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

TDDFT for transport: general idea

- start from contacted system L-C-R in the ground state (or in thermal equilibrium)
- at some time t_0 switch on the bias and follow time evolution
- for DC bias: expect evolution towards a steady state

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

Steady-state transport in TDDFT

assume KS system evolves towards steady state \longrightarrow steady-state current in TDDFT (G. Stefanucci et al, in Molecular and Nano Electronics: Analysis, Design, and Simulation, ed. by J. Seminario, (Elsevier, 2007))

Landauer-like formula for steady-state current

$$= -\int \frac{\mathrm{d}E}{2\pi} T(E, V) \left(f_{\beta}(E + V_L + \delta V_{xc,L}) - f_{\beta}(E + V_R + \delta V_{xc,R}) \right)$$

with
$$\delta V_{xc,\alpha} = \lim_{t\to\infty} \lim_{\mathbf{r}\to s_{\alpha}\infty} (V_{xc}(\mathbf{r},t) - V_{xc}(\mathbf{r},0))$$
 where $s_L = -1$ and $s_R = +1$

<u>note:</u> in general, standard Landauer formula has to be augmented by xc contribution $\delta V_{xc,\alpha}$ to the bias

Landauer + static DFT for steady-state transport TDDFT approach to (steady-state) transport

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Steady-state transport in TDDFT (cont.)

zero-bias conductance

$$\frac{G}{G_0} = -(1 + Q_{xc}) \int dE \ T(E) \frac{\partial f_\beta(E)}{\partial E}$$

with dynamical xc corrections Q_{xc}

see also:

M. Koentopp, K. Burke, F. Evers, PRB **73**, 121403(R) (2006) N. Sai, M. Zwolack, G. Vignale, M. Di Ventra, PRL **94**, 186810 (2005)

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Steady-state transport with DFT for model systems

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Derivative discontinuity in static DFT

total energy as function of (fractional) particle number is a series of straight lines (Perdew et al, PRL **49**, 1691 (1982))

 $E(N+\omega)$



derivative discontinuity

$$\Delta = I(N) - A(N)$$

I(N): ionization potential A(N): electron affinity

N : integer number of electrons

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Derivative discontinuity in static DFT (cont.)

for given external potential $v(\mathbf{r})$, extend HK ground state energy functional to non-integer particle numbers:

derivative discontinuity

$$\Delta = \lim_{\omega \to 0} \left(\frac{\delta E_v[n]}{\delta n(\mathbf{r})} \bigg|_{N+\omega} - \frac{\delta E_v[n]}{\delta n(\mathbf{r})} \bigg|_{N-\omega} \right) = \Delta_{KS} + \Delta_{xc}$$

KS discontinuity $\Delta_{KS} = \varepsilon_{LUMO} - \varepsilon_{HOMO}$

xc contribution to discontinuity:

$$\Delta_{xc} = \lim_{\omega \to 0} \left(\frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})} \bigg|_{N+\omega} - \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})} \bigg|_{N-\omega} \right)$$

<u>note</u>: for traditional functionals (LDA, GGA): $\Delta_{xc} = 0 !!$

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Simple impurity model for transport



one interacting impurity (level), on-site interaction U (charging energy of level), non-interacting leads, hopping V in leads and hopping V_{Link} from leads to impurity, on-site energy ε_0 at impurity, assume local KS potential only non-vanishing at impurity interested in case of weak links $|V_{\text{Link}}| < |V|$ and in wide-band limit: $|V_{\text{Link}}| \to \infty$, $|V| \to \infty$ such that $\Gamma_{\alpha} = (V_{\text{link}})^2/|V| = const$

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Self-consistency condition for steady state density

Landauer approach:

assume for biased system there exists steady state with density n at impurity \longrightarrow self-consistency condition for n

$$n = 2 \sum_{\alpha=L,R} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f_{\beta}(\omega - V_{\alpha}) \Gamma_{\alpha}(\omega - G_{\alpha}) |G(\omega)|^{2}$$
$$G(\omega) = [\omega - v_{KS}(n) - \Sigma_{L}(\omega - V_{L}) - \Sigma_{R}(\omega - V_{R})]^{-1}$$
$$v_{KS}(n) = \varepsilon_{0} + v_{Hxc}(n)$$

 V_{α} : bias in lead α $f_{\beta}(\omega)$: Fermi function at inverse temperature β Σ_{α} : embedding self energy for lead α (= $-\frac{i}{2}\Gamma_{\alpha}$ in wide-band limit)

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Landauer formula for steady state current

$$I = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} T(\omega) \left[f_{\beta}(\omega - V_L) - f_{\beta}(\omega - V_R) \right]$$

with transmission function

$$T(\omega) = \operatorname{Tr} \left\{ \Gamma_L(\omega - V_L) G(\omega) \Gamma_R(\omega - V_R) G^*(\omega) \right\}$$

 \longrightarrow zero-bias conductance:

$$G/G_0 = -\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} T(\omega) \frac{\partial f_{\beta}(\omega)}{\partial \omega}$$

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Single-site model to construct finite temperature functional



4 states in Fock space: $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$ calculate density $n(v_0 - \mu) = n(\tilde{v}_0)$ invert analytically $\longrightarrow \tilde{v}_0(n)$

non-interacting KS system: density $n_s(\tilde{v}_s)$ invert analytically $\longrightarrow \tilde{v}_s(n_s)$

Hartree-xc potential:

$$v_{Hxc}(n) = \tilde{v}_s(n) - \tilde{v}_0(n)$$

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Spectral function and smoothening

Spectral function of single-site model

$$A^{SSM}(\omega) = \lim_{\eta \to 0} \left[\frac{n}{2} L_{2\eta}(\omega - v_0 - U) + \left(1 - \frac{n}{2} \right) L_{2\eta}(\omega - v_0) \right]$$

with Lorentzian
$$L_{\delta}(\omega) = rac{\delta}{\omega^2 + \left(rac{\delta}{2}
ight)^2}$$

smoothen peaks by replacing $\eta\to\gamma/2,$ the WBL emb. self energy

Spectral function of "smoothened" single-site model

$$A^{SSM-sm}(\omega) = \frac{n}{2}L_{\gamma}(\omega - v_0 - U) + \left(1 - \frac{n}{2}\right)L_{\gamma}(\omega - v_0)$$

often derived from EOM for Coulomb blockade regime

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Hartree-xc potential from reverse engineering

density from spectral function

$$n(\tilde{v}_0) = 2 \int \frac{\mathrm{d}\omega}{2\pi} f_\beta(\omega) A(\omega)$$

invert $n(\tilde{v}_0)\longrightarrow \tilde{v}_0(n);$ same for non-interacting density $n_s(\tilde{v}_s)\longrightarrow \tilde{v}_s(n_s)$

Hartree-xc potential

$$v_{\text{Hxc}}(n) = \tilde{v}_s(n) - \tilde{v}_0(n)$$

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Hartree-xc potential for (smoothened) single-site model

Hartree-xc potential for different temperatures and U=10 (energies in units of γ)



derivative "discontinuity" (better: step feature) emerges naturally in the zero-temperature limit

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Kondo effect: what TDDFT has to say

This work (finite temperature, TDDFT):

• Stefanucci, Kurth, PRL 107, 216401 (2011)

Related work (zero temperature, DFT/Landauer):

- Bergfield, Liu, Burke, Stafford, PRL 108, 066801 (2012)
- Tröster, Schmitteckert, Evers, PRB 85, 115409 (2012)

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Finite temperature conductance with Landauer



exact data from: Izumida, Sakai, J. Phys. Soc. Jpn., 2005

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Finite temperature conductance with Landauer

two ways to understand T = 0 result:

• Meir-Wingreen formula for conductance:

$$\frac{G}{G_0} = \gamma^2 |\mathcal{G}(\mu)|^2 \frac{\gamma - \operatorname{Im} \Sigma(\mu)}{\gamma}$$

with many-body GF $\mathcal{G}(\omega)$ at impurity and self energy Σ at Fermi energy: $\operatorname{Im} \Sigma(\mu) = 0 \longrightarrow$ can describe conductance by a KS potential $v_s = v_0 + \operatorname{Re}\Sigma(\mu)$

• Friedel sum rule (Langreth):

conductance determined by density n_0 on dot: $G = G(n_0)$ if KS potential gives good density \longrightarrow good conductance

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Finite temperature conductance with Landauer

Warning: KS density of states is *always* a simple Lorentzian, i.e., it has nothing to do with the exact DOS of the model!

However: due to discontinuity, the peak of the Lorentzian is pinned to Fermi energy (like the many-body resonance for the exact DOS) leading to conductance G_0

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Finite temperature conductance with Landauer

<u>note</u>: at particle-hole symmetric point $v_0 = -U/2$ our approximation gives *exact* KS potential for all temperatures



for finite *T*: Landauer does not give correct conductance although static KS potential is exact!

exact results from T.A. Costi, PRL (2000)

difference between Landauer and exact results due to dynamical xc corrections!

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XC bias by reverse engineering

Reference:

• P. Schmitteckert, M. Dzierzawa, P. Schwab, Phys. Chem. Chem. Phys. **15**, 5477 (2013)

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IRL model: xc bias by reverse engineering

Interacting resonant level model: two 1-d leads connected to one interacting site: $\hat{H}=\hat{H}_L+\hat{H}_R+\hat{H}_{LR}$

$$\hat{H}_{LR} = -V_{\text{link}}(\hat{c}^{\dagger}\hat{c}_{L,1} + \hat{c}^{\dagger}\hat{c}_{R,1} + H.c.) + U(\hat{n} - 1/2)(\hat{n}_{L,1} + \hat{n}_{R,1} - 1)$$

Numerically exact solution (for finite leads) with td-DMRG \rightarrow reverse engineering to obtain exact TD KS potential

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IRL model: xc bias by reverse engineering (cont.)

external potential, exact KS potential, and KS potential in adiabatic approximation in the IRLM close to impurity



Adiabatic approximation (obtained from condition that ground state gives density n(T)) completely misses the bias renormalization due to dynamical xc effects

Summary

- Landauer + static DFT: the de-facto standard approach to ab-initio steady-state transport, BUT: in principle incomplete
- Landauer + static DFT can be exact in zero-bias limit, but only under special circumstances (e.g. when Friedel sum rule applies, at T=0)
- TDDFT approach to transport in principle ok
- in steady state TDDFT leads to a Landauer-like formula for the current but includes xc corrections to the bias
- adiabatic approximation fails to capture dynamical xc corrections