Beyond the linear regime: Real-time TDDFT prediction of electron dynamics far from equilibrium.
Electronic transport with TDDFT

Bias between L and R is turned on: $U(t)$ for large $t$.
Electronic transport with TDDFT

• How to deal with time-dependent external fields?
• Is the steady state unique?
• After switching on, does one always reach a steady state?

Questions:

Bias between L and R is turned on: $U(t)$ for large $t$

[Diagram of a system with leads L and R, and a central region, illustrating the electronic transport with TDDFT]
Electronic transport with TDDFT

(E. Runge, EKUC, PRL 52, 997 (1984))

\[
(\mu) [((\mu,\mu) \Phi (r,\mu))^2 + \frac{\mu}{\mu} \Phi \int + (\mu) \Lambda = (\mu) [((\mu,\mu) \Phi)^2 \Lambda 

+ \frac{\mu}{\mu} \Phi \int \Lambda = (\mu) \Phi \int \Lambda

\]
Electronic transport with TDDFT

TDKS equation
Effective TDKS Equation for the central (molecular) region only

Note: So far, no approximation has been made.

Memory term: $C \leftarrow L$ and $C \leftarrow R$ charge injection

Source term: $I \leftarrow C$ and $I \leftarrow R$ charge injection

\[ (0) \Phi(0, t) C^R + (0) \Phi(0, t) C^L + \int_0^t \Phi(H(t, t') C^R + C^L R^L + C^R L^L) dt \]

Efficient TDKS Equation for the central (molecular) region only

\[ (1) \Phi(1) C \leftarrow H = (1) \Phi \frac{\partial}{\partial t} \]


Numerical examples for non-interacting electrons

Recovering the Landauer steady state

Steady state coincides with Landauer formula

Fermi energy $E_F = 0.3$ a.u.

Time evolution of current in response to bias switched on at time $t = 0$.
Can there be more than one steady state?
Multi-stability in TDHF and TDDFT for one-site Anderson model

Is there always a steady state?
No steady state in two-site Anderson model
ELECTRON PUMP Device which generates a net current between two electrodes with no static bias by applying a time-dependent potential in the device region: Pumping through carbon nanotubes by surface acoustic waves on piezoelectric surfaces (Leek et al., PRB 77, 256802 (2005)).

Experimental realization: Pumping through carbon nanotubes (with no static bias) by applying a time-dependent potential in the device region.
Archimedes' screw: patent 200 B.C.

Pumping through a square barrier (of height 0.5 a.u.) using a travelling wave in device region

\[ U(x,t) = U_0 \sin(kx - \omega t) \quad (k = 1.6 \text{ a.u., } \omega = 0.2 \text{ a.u., Fermi energy } = 0.3 \text{ a.u.}) \]
Current flows in direction opposite to sound wave
Current goes in direction opposite to the external field.