Time-dependent transport through quantum nanostructures

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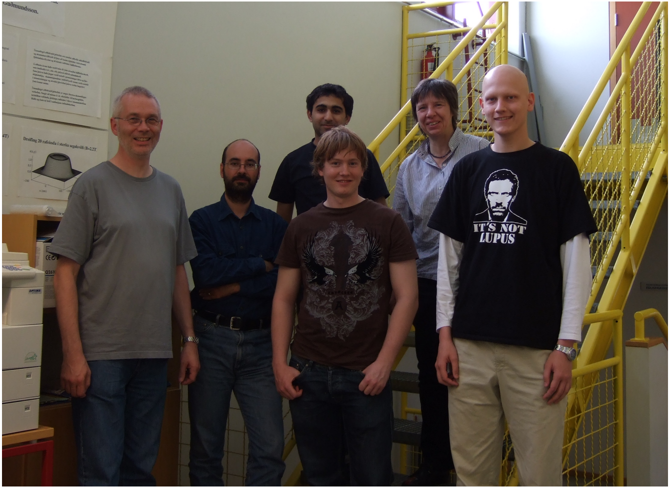
Cooperation



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Content

Background - Motivation

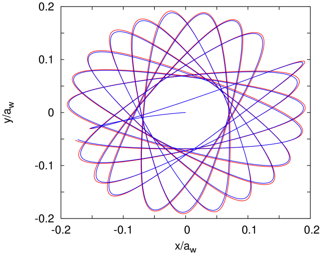
- Closed systems
- t-dependence
- Open systems
- Scattering formalism for transport
- Nonequilibrium Green functions
- t-dependent scattering
- Geometry

Generalized Master Equation

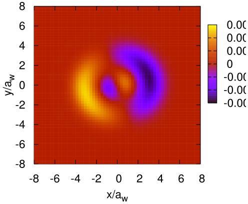
- Finite Quantum wire
- Semi-infinite leads
- Band structure, geometry
- Bias, coupling
- Magnetic field
- New development
- Experiments

Closed dot, dipole excitation

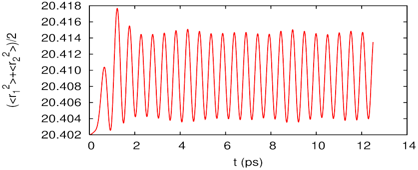
Center of mass



Induced density, $(t = 12.5$ ps, 5000 steps)



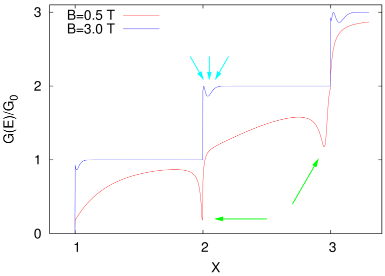
$(\langle r_\downarrow^2\rangle + \langle r_\uparrow^2\rangle)/2$



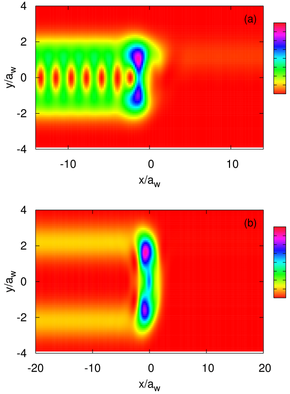
- $i\hbar d_t \rho(t) = [H + V(t), \rho(t)]$
- DFT + magnetic field
- No energy flows into internal modes
- Kohn's theorem

Magnetotransport

Open quantum dot, scattering formalism: $\mathbf{T} = \mathbf{V}_{sc} + \mathbf{G}_0\mathbf{V}_{sc}\mathbf{T}$

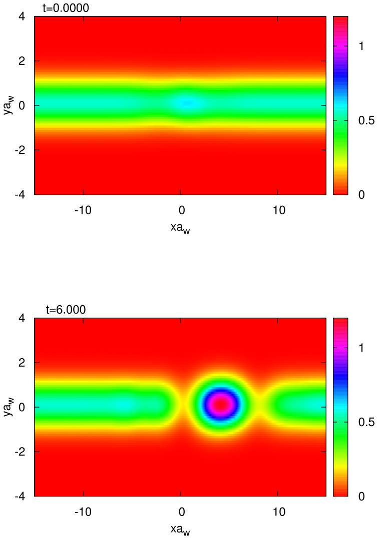


$B = 0.5$ T, $B = 1.2$ T



- Quantization, with or without B, symmetry breaking
- Lorentz force $\rightarrow$ electrons bypass dot at high B

Extension to the time-domain, current modulation



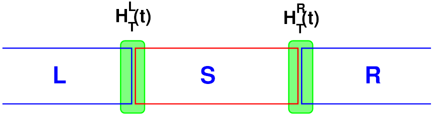
“Zwischengedanken”

- Bias?
- Strong - weak coupling?
- Many-electron formalism?
- Interaction?
- Non-equilibrium $\longrightarrow$ density operator ρ

- Phys. Rev. B70, 245308 (2004)
- Phys. Rev. B71, 235302 (2005)
- Phys. Rev. B76, 195314 (2007)
- Phys. Rev. B77, 035329 (2008)

Generalized Master Equation Approach

- Weak coupling to leads
- Variable coupling to leads, (coupled at $t = 0$)
- Many-electron formalism
- Origin in quantum optics
- Projection on the system
- Reduced statistical operator $\rho(t) = \mathrm{Tr_L Tr_R}\{W(t)\}$



Liouville-von Neumann equation

$$\dot{W}(t) = -\frac{i}{\hbar}[H(t), W(t)] = -i\mathcal{L}W(t)$$

$$H = H_\mathrm{S} + H_\mathrm{L} + H_\mathrm{R} + H_\mathrm{T}^\mathrm{L} + H_\mathrm{T}^\mathrm{R}$$

$$\langle A(t)\rangle = \mathrm{Tr}\{W(t)A\} = \mathrm{Tr_S}\{[\mathrm{Tr_L Tr_R}\,W(t)]A\} = \mathrm{Tr_S}\{\rho(t)A\}$$

$$H(t) = \sum_a E_a d_a^\dagger d_a + \sum_{q,l=\mathrm{L,R}} \epsilon^l(q) c_{ql}^\dagger c_{ql} + H_\mathrm{T}(t)$$

$$H_\mathrm{T}^l(t) = \chi^l(t) \sum_{q,a} \left\{ T_{qa}^l c_{ql}^\dagger d_a + (T_{qa}^l)^* d_a^\dagger c_{ql} \right\}$$

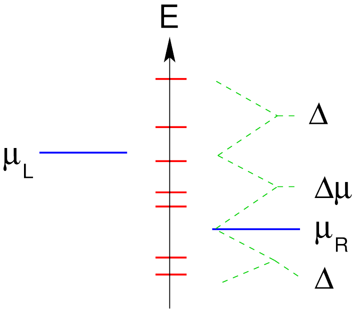
$$T \exp\left\{ -i \int_s^t ds' \mathcal{Q}\mathcal{L}(s')\mathcal{Q} \right\} = \exp\{-i\mathcal{Q}\mathcal{L}_0\mathcal{Q}(t-s)\}(1+\mathcal{R})$$

$$i\hbar\dot{\rho} = \mathcal{L}_S\rho(t) + \frac{1}{i\hbar}\mathrm{Tr}_{LR}\left\{ \mathcal{L}_T(t) \int_0^t ds e^{-i(t-s)\mathcal{L}_0} \mathcal{L}_T(s)\rho_L\rho_R\rho(s) \right\}$$

$$\mathcal{P} + \mathcal{Q} = 1, \quad \mathcal{P} = \rho_L\rho_R\mathrm{Tr}_{LR}$$

$$\dot{\rho}(t) = -i\mathcal{L}_{\text{eff}}(t)\rho(t) + \int_0^t dt'\mathcal{K}(t,t')\rho(t')$$

- Integrodifferential equation Volterra type
- Life-times, decay rates
- Memory effects, non-Markovian
- Infinite order. . . ,(but approximation)
- Finite bias
- Many-body effects
- No assumption about equilibrium in leads after coupling



$$\dot{\rho}(t) = -\frac{i}{\hbar}[H_\mathrm{S}, \rho(t)] - \frac{1}{\hbar^2} \sum_{l=\mathrm{L,R}} \int dq\, \chi^l(t)([\mathcal{T}^l, \Omega_{ql}(t)] + h.c.)$$

$$\Omega_{ql}(t) = e^{-\frac{i}{\hbar}tH_\mathrm{S}} \int_0^t ds\, \chi^l(s)\Pi_{ql}(s)e^{\frac{i}{\hbar}(s-t)\varepsilon^l(q)}e^{\frac{i}{\hbar}tH_\mathrm{S}}$$

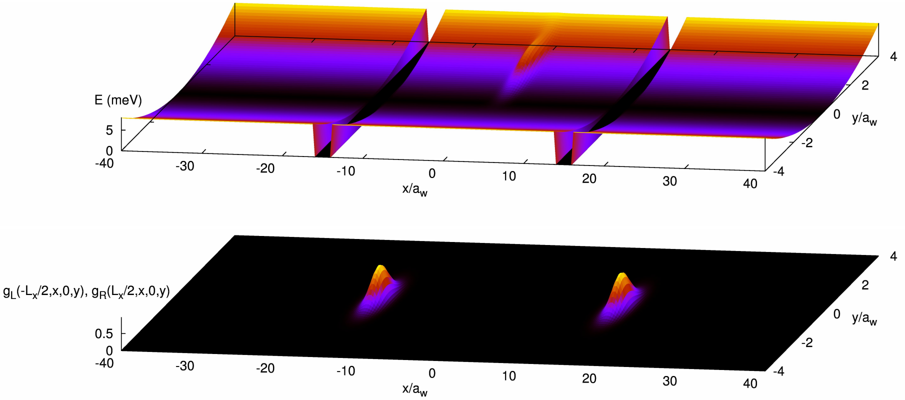
$$\Pi_{ql}(s) = e^{\frac{i}{\hbar}sH_\mathrm{S}}\left(\mathcal{T}^{l\dagger}\rho(s)(1-f^l) - \rho(s)\mathcal{T}^{l\dagger}f^l\right)e^{-\frac{i}{\hbar}sH_\mathrm{S}}$$

$$\mathcal{T}^l(q) = \sum_{\alpha,\beta} \mathcal{T}^l_{\alpha\beta}(q)|\alpha\rangle\langle\beta|, \quad \mathcal{T}^l_{\alpha\beta}(q) = \sum_a T^l_{aq}\langle\alpha|d^\dagger_a|\beta\rangle$$

$$|\mu\rangle = |\underbrace{1,1,....1}_{N_0\,\text{states}}, i^\mu_{N_0+1}, ..., i^\mu_{N_\mathrm{max}}, 0, 0, ...\rangle$$

Coupling of leads

$$T_{a,k}^{L,R} = \int_{A_{L,R}} d\mathbf{r}\, d\mathbf{r}' \left(\Psi_k^{L,R}(\mathbf{r}')\right)^* \Psi_a^S(\mathbf{r}) g^{L,R}(\mathbf{r},\mathbf{r}') + h.c.$$



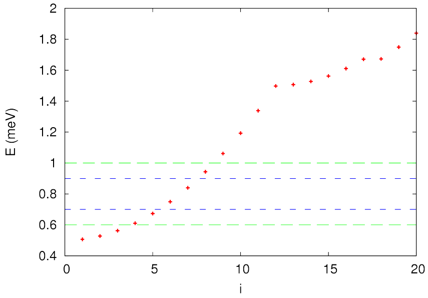
Measurable quantities

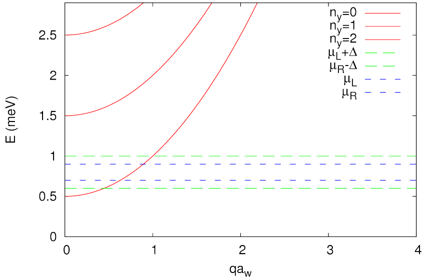
Total charge: $Q_{\rm S} = e\sum_a d_a^\dagger d_a$

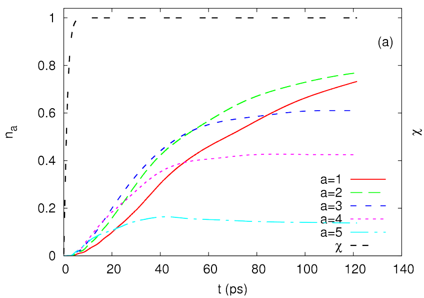
$$\begin{aligned}\langle Q_{\rm S}(t)\rangle &= {\rm Tr}\{W(t)Q_{\rm S}\} = {\rm Tr}_{\rm S}\{[{\rm Tr}_{\rm LR}W(t)]Q_{\rm S}\}\\ &= {\rm Tr}_{\rm S}\{\rho(t)Q_{\rm S}\} = e\sum_{a,\mu} i_a^\mu\,\langle\mu|\rho(t)|\mu\rangle\end{aligned}$$

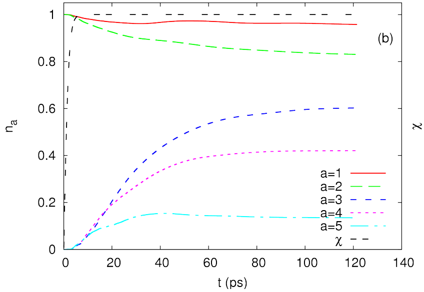
$$\langle Q_{\rm S}(\mathbf{r},t)\rangle = e\sum_{ab}\sum_{\mu\nu}\Psi_a^*(\mathbf{r})\Psi_b(\mathbf{r})\rho_{\mu\nu}(t)\langle\nu|d_a^\dagger d_b|\mu\rangle$$

$$\Delta\langle J_{\rm T}(t)\rangle = \langle J_{\rm T}^{\rm L}(t)\rangle - \langle J_{\rm T}^{\rm R}(t)\rangle = \frac{d\langle Q_{\rm S}(t)\rangle}{dt} = e\sum_a\sum_\mu i_a^\mu\,\langle\mu|\dot\rho(t)|\mu\rangle$$

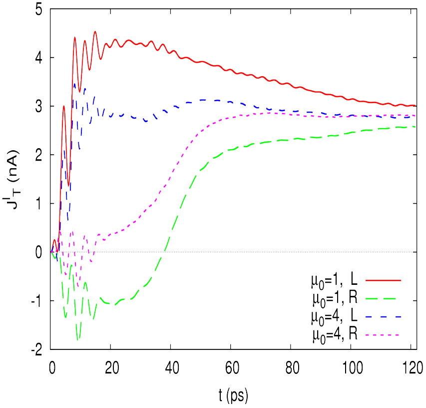

E (meV)
i


E (meV)
qa_w
n_y=0
n_y=1
n_y=2
μ_L+Δ
μ_R-Δ
μ_L
μ_R

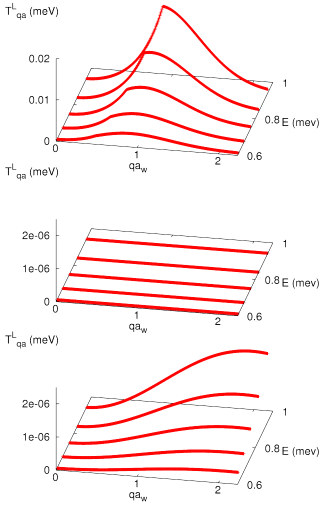

(a)
n_a
χ
t (ps)
a=1
a=2
a=3
a=4
a=5
χ

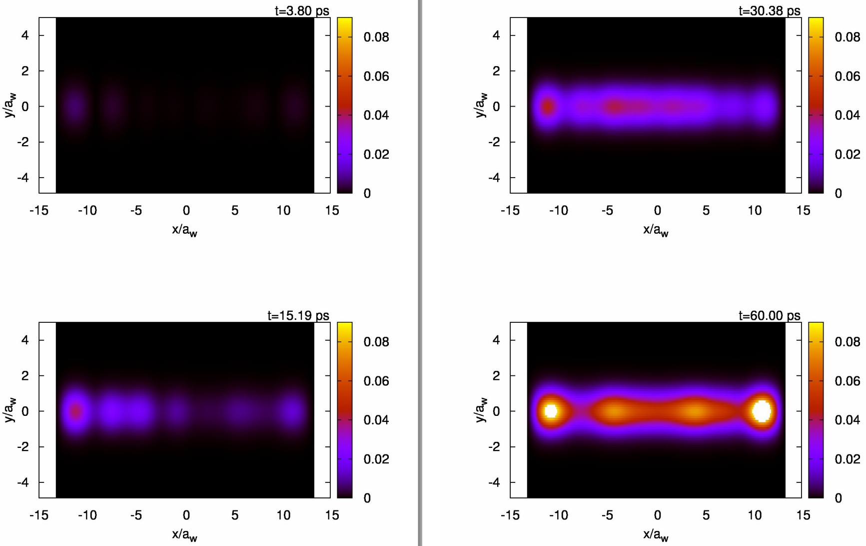

(b)
n_a
χ
t (ps)
a=1
a=2
a=3
a=4
a=5
χ

Total current

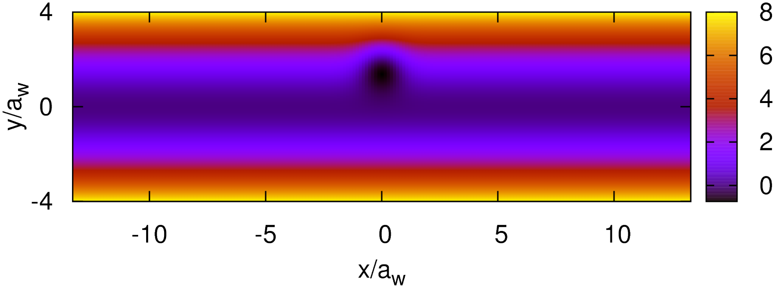


Coupling

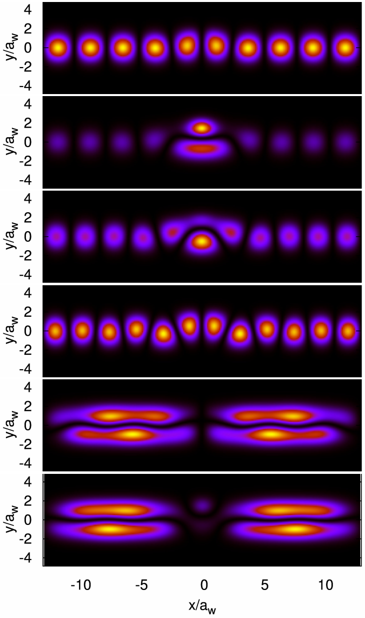



t=3.80 ps
t=30.38 ps
t=15.19 ps
t=60.00 ps
y/a_w
x/a_w
4
2
0
-2
-4
-15
-10
-5
0
5
10
15
0.08
0.06
0.04
0.02
0

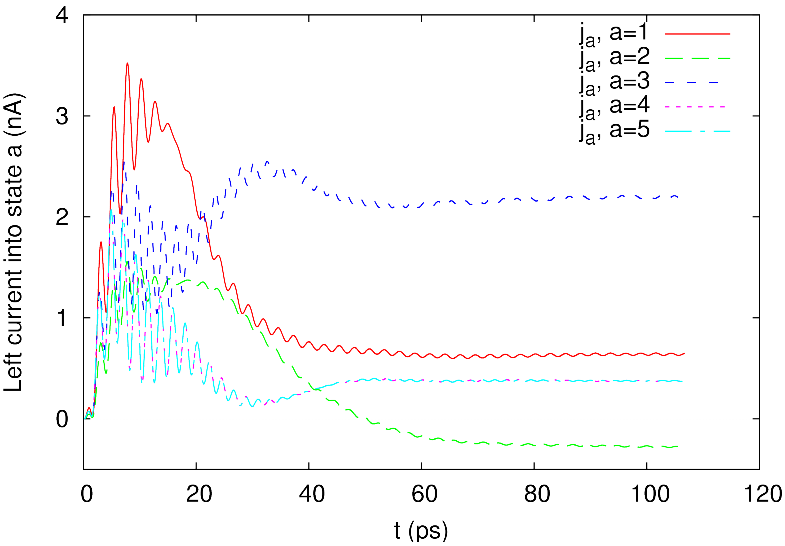
System with an off-centered Gaussian well



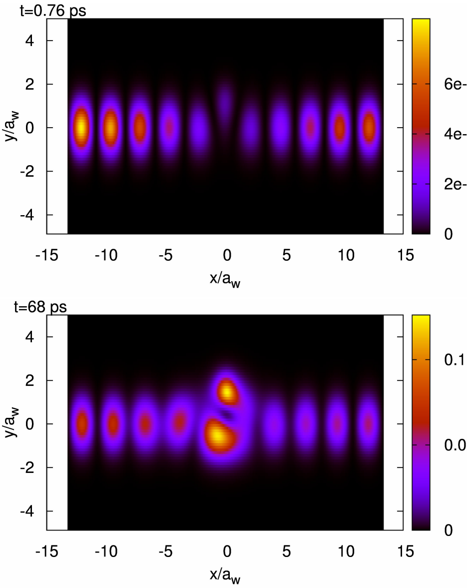
Relevant eigenstates



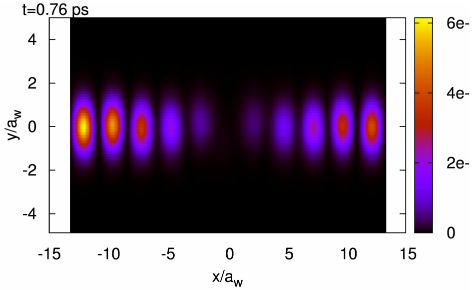
Partial left current into state a

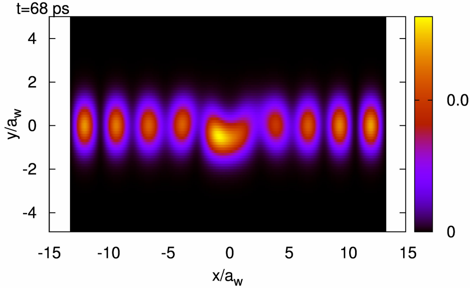


Time-dependent charge density



… off-centered hill





Unpublished new results

Magnetic field

- In central system, finite quantum wire
- In semi-infinite leads

Coulomb interaction

- Coupling to leads $\rightarrow$ correlation in the system
- Mean-field approach would destroy correlations
- Mean-field approach would make $H_{\rm S}$ t-dependent
- Full Coulomb interaction in a limited section of Fock-space

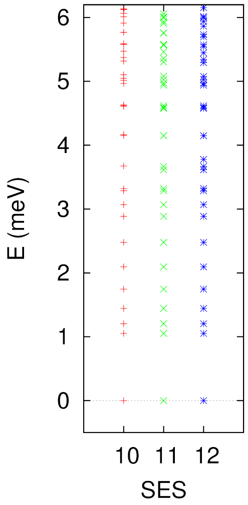
$$\hat{H}_{\mathrm{S}} = \sum_a E_a \hat{d}_a \hat{d}_a^\dagger + \frac{1}{2} \sum_{abcd} (ab|V|cd) \hat{d}_a^\dagger \hat{d}_b^\dagger \hat{d}_d \hat{d}_c$$

$$|\mu) = U|\mu\rangle, \quad U^\dagger|\mu) = |\mu\rangle$$

$$\tilde{\mathcal{T}}^l(q) = U^\dagger \mathcal{T}^l(q)\, U, \quad (\tilde{\mathcal{T}}^l(q))^* = U^\dagger (\mathcal{T}^l(q))^*\, U$$

Diagonalize $\hat{H}_{\mathrm{S}}$, transform GME, truncate ρ and $\{|\mu)\}$

Many-electron spectra

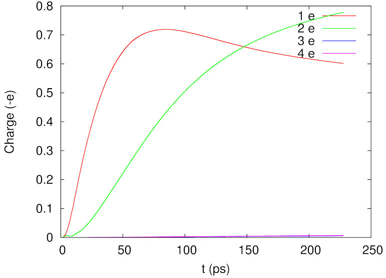


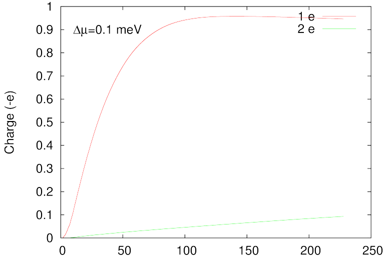
Short broad wire

- $L_x = 200$ nm
- Parabolic confinement in y-direction, $\hbar\Omega_0 = 1.0$ meV
- $B = 1.0$ T
- GaAs parameters

Interacting ↔ non-interacting

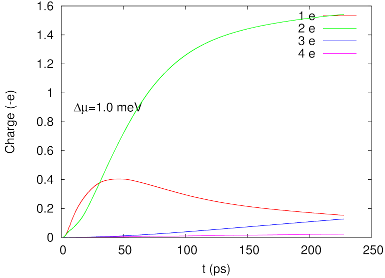
$\mu_L = 1.7$ meV and $\mu_R = 1.5$ meV

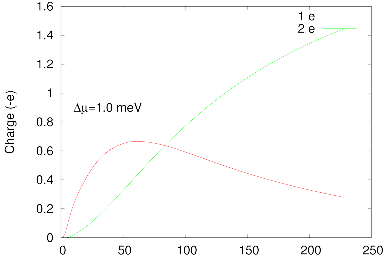




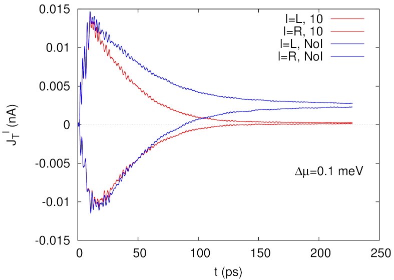
Interacting ↔ non-interacting

$\mu_L = 2.6$ meV and $\mu_R = 2.4$ meV

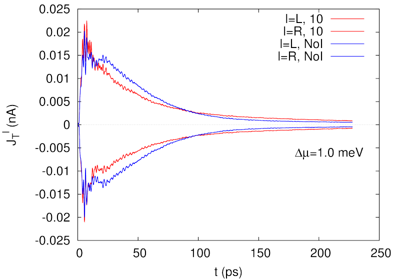




$\mu_L = 1.7$ meV $\mu_R = 1.5$ meV

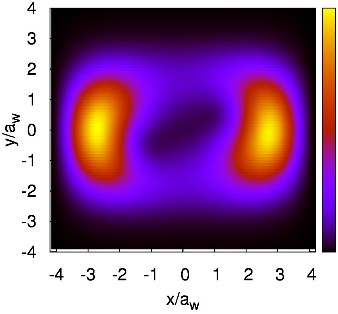


$\mu_L = 2.6$ meV $\mu_R = 2.4$ meV



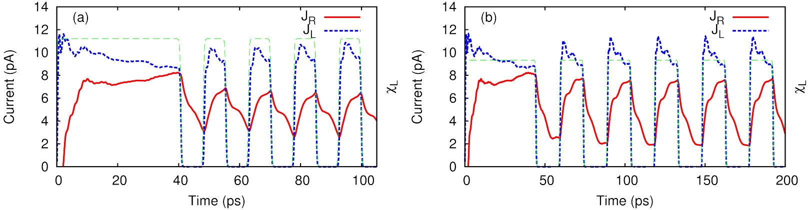
Charge density

$\mu_L = 2.6$ meV $\mu_R = 2.4$ meV, $t = 6$ ps, and 61 ps



Experiments

- B. Naser, D. K. Ferry, J. Heeren, J. L. Reno, and J. P. Bird, Appl. Phys. Lett. 89, 083103 (2006), Appl. Phys. Lett. 90, 043103 (2007).
- W-T Lai, D. M. T. Kuo, and P-W Li, Physica E 41, 886 (2009).



Valeriu Moldoveanu et al, (arXiv:0909.0815).

Summary

- Initial steps taken for t-dependent transport
- Lippmann-Schwinger scattering formalism
  - Periodic
  - Aperiodic, pulses
  - Current modulation
  - Coulomb interaction
- NEGF - formalism

- GME-formalism
  - Bias
  - Many-electron formalism
  - Coulomb interaction
  - General model
- Analytical + numerical
- FORTRAN 2003 + parallelization
- Experimental systems

- Valeriu Moldoveanu et al, 2009 New J. Phys. 11 073019
- V. Gudmundsson et al, http://arxiv.org/abs/0903.3491

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