# *Time-dependent transport through electron systems strongly or weakly coupled to quantum wires*

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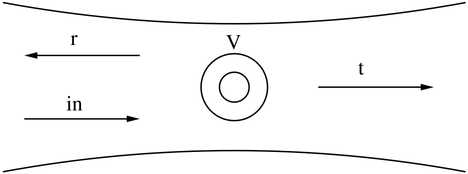
http://hartree.raunvis.hi.is/~vidar/Rann/Fyrirlestrar/MiaoLi_t.pdf

MiaoLi, October, 2008

# Lippmann-Schwinger scattering formalism

## Asymptotic regions




In scattering out

$$\left[-H_0(B)+E\right]\psi_{\rm E} = V_{\rm sc}\psi_{\rm E}$$

$$\psi_{\rm E} = \psi_{\rm in} + \psi_{\rm sc}$$

## T-matrix

$$T_{nn'}(q\omega, p\nu) = V^{\rm sc}_{nn'}(q\omega, p\nu) + \sum_{m'} \int \frac{dk}{2\pi} \frac{d\omega'}{2\pi} V^{\rm sc}_{nm'}(q\omega, k\omega') G_0^{m'}(k\omega') T_{m'n'}(k\omega', p\nu)$$

$$\left[\mathbf{1} - \mathbf{G}_0 \mathbf{V}_{\rm sc}\right] \mathbf{T} = \mathbf{V}_{\rm sc}$$

## Conductance

$$\mathbf{t} = \mathbf{1} - \alpha \mathbf{T}$$

$$G = \frac{2e^2}{h} \mathrm{Tr}[\mathbf{t}^\dagger \mathbf{t}]$$

## Wave functions

$$\psi_{\rm E} = \left(\mathbf{1} + \mathbf{G}_0 \mathbf{T}\right) \psi_{\rm in}$$

# Time-dependent transport

## Pulse propagation

- Static potential
- Elastic scattering
- G. Thorgilsson et al., PRB 76, 195314 (2007)

## Periodic potential

- Inelastic scattering
- Kristinn Torfason

## Current modulation

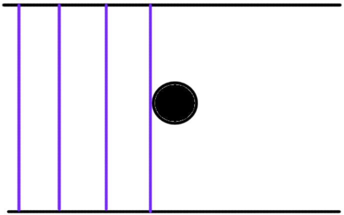
- Pulsed potential → current modulation, inelastic
- VG et al., PRB 77, 035329 (2008)

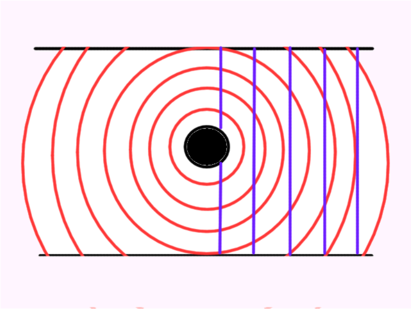
## Sudden switch-on → transients

- Non-equilibrium Green functions (NEGF)
  - Transients
  - V. Moldoveanu et al., PRB 76, 085330 (2007)
  - V. Moldoveanu et al., PRB 76, 165308 (2007)
- Generalized master equation (GME)
  - Transients → steady state
  - Geometrical effects
  - V. Moldoveanu et al., (arXiv:0807.4015) (2008)

# Propagation of a wave packet

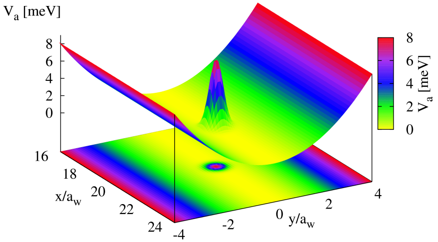
$$\Psi(x, y, t) = \Psi_0(x, y, t) + \Psi_{\rm sc}(x, y, t).$$



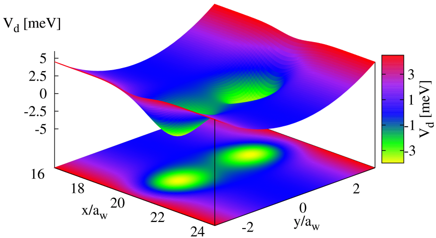


# Static potentials

## Antidot

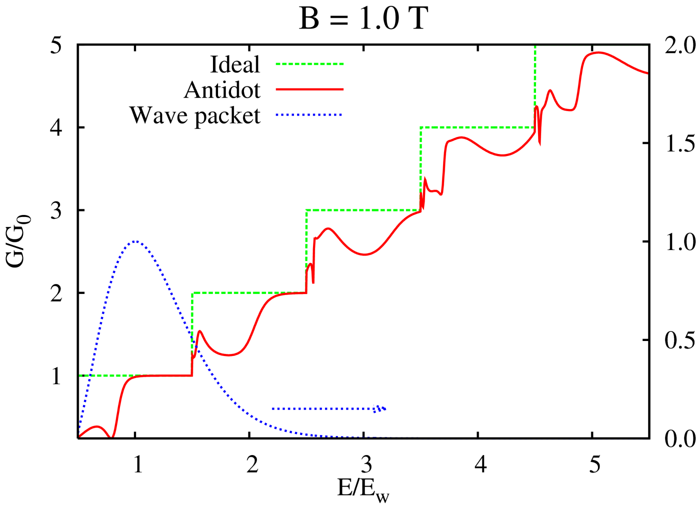



## Parallel double dot

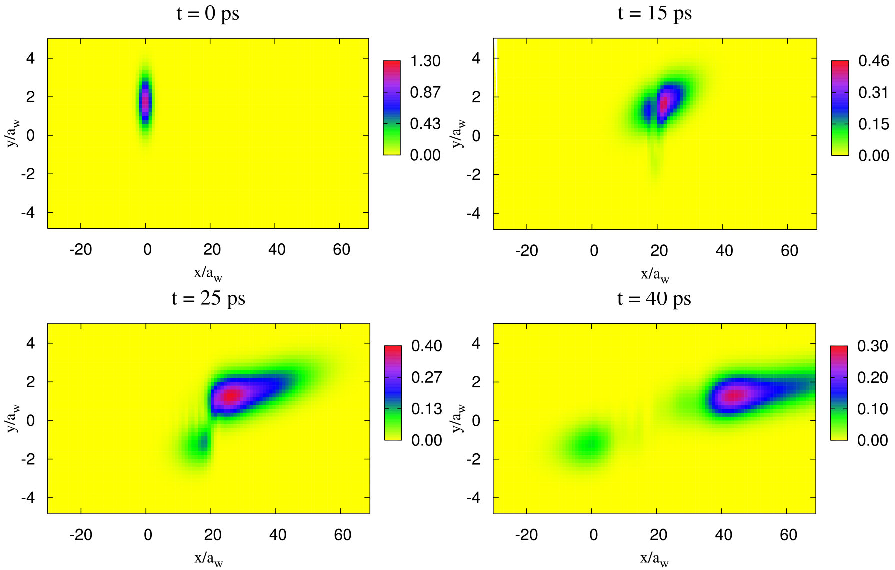


# Antidot

## Static conductance – wave packet

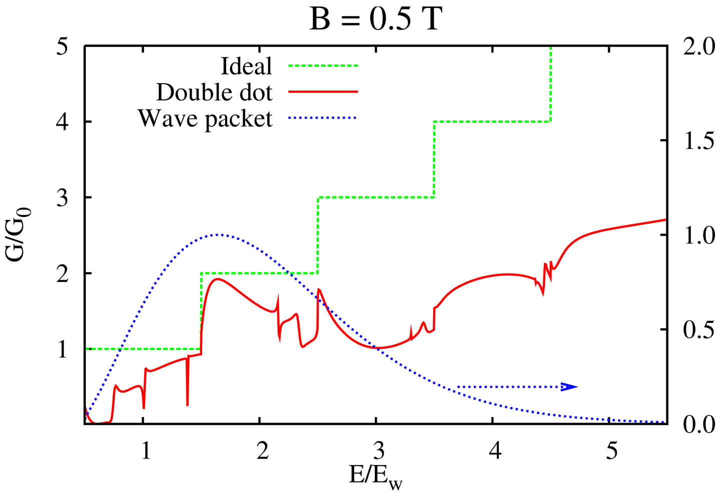


# Antidot, $B = 1.0$ T

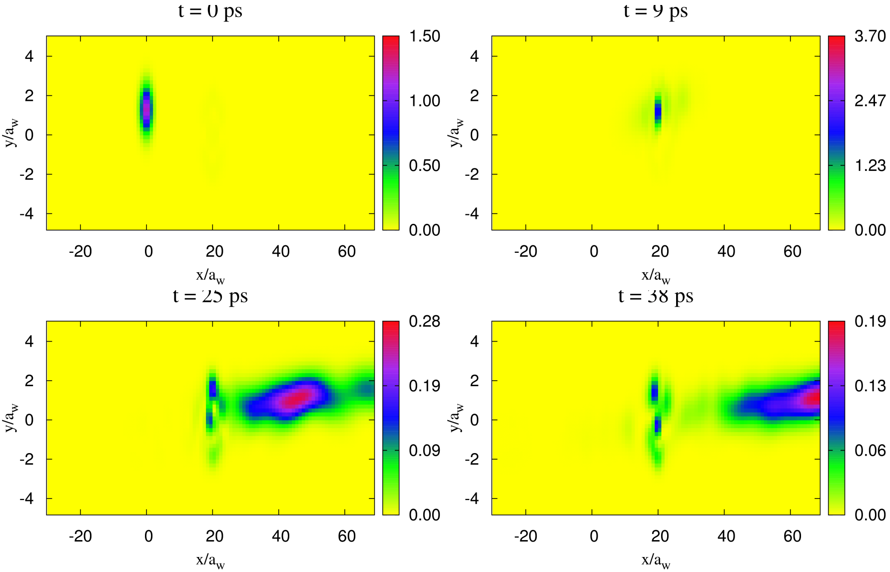


# Parallel double dot

## Static conductance – wave packet

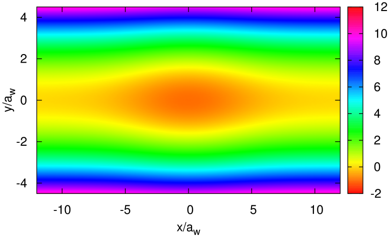


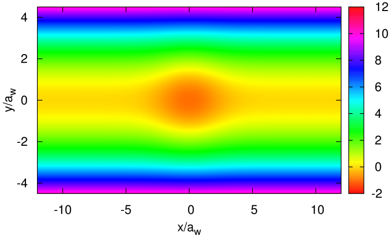
# Parallel double dot, $B = 0.5$ T



# Current modulation

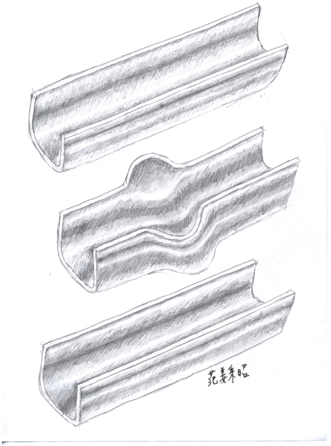
$$V_{\rm sc}(\mathbf{r},t) = V_0 e^{-\beta r^2} e^{-\gamma t} \cos(\Omega t),$$ view at $t = 0$:



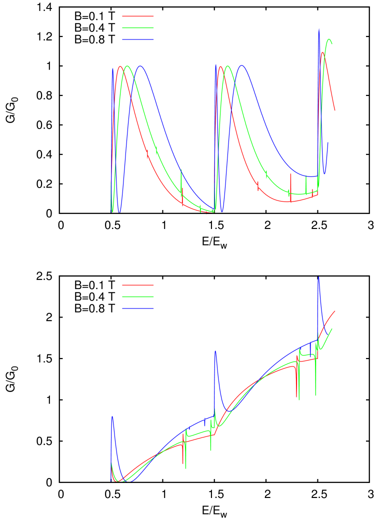

$V_0 = \pm 1.0$ meV, $\Omega = 0.2\Omega_w$, $\gamma = 1.0\Omega_w^2$, $\beta = 1$ or $4 \times 10^{-4}$ nm$^{-2}$, $\longrightarrow$ one smooth flash

## Smooth well-like pulse



$\beta = 1 \times 10^{-4}\ \mathrm{nm}^{-2}, \qquad \beta = 4 \times 10^{-4}\ \mathrm{nm}^{-2}$

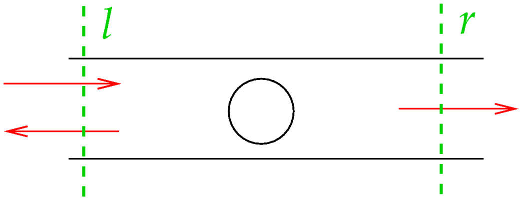
## Static conductance



Left and right current of state $\alpha$

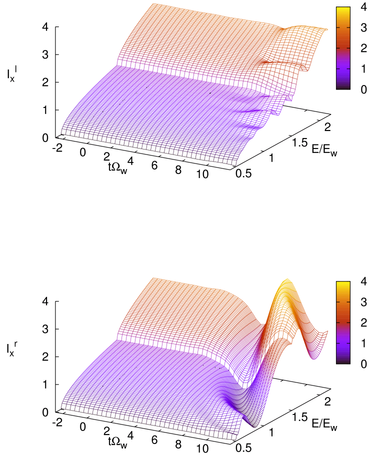
$$(I_\alpha^{r,l}(t))_x = \frac{\hbar}{m^*}\Re\left\{\int_{-\infty}^{\infty} dy\, (\Psi_\alpha^{r,l})^* D_x \Psi_\alpha^{r,l}\right\}$$

with $\hbar D_x = (p_x + (e/c)A_x) = \hbar(-i\partial_x - y/l^2)$

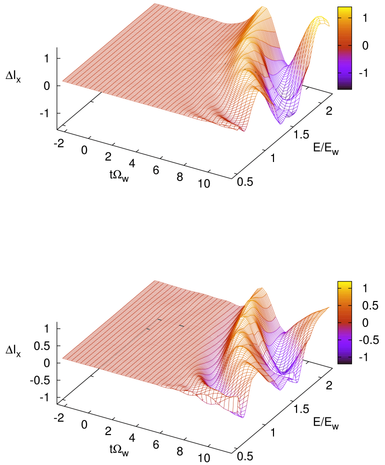



- Contributions from any point in sc-region for all earlier times
- Calculate for state $\alpha$ at Fermi energy
- Inelastic, any outstate possible, evanescent states explicitly in $G$

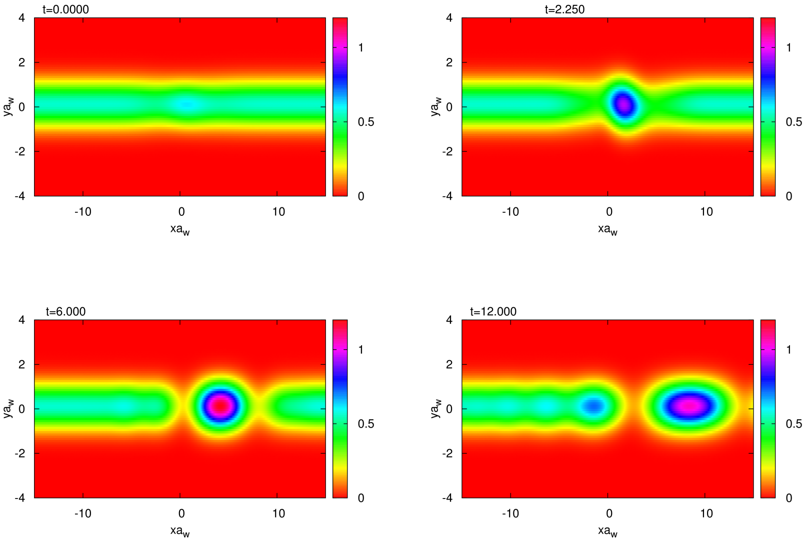
## $I_x^l$ and $I_x^r$, $B = 0.1$ T, $V_0 = -1$ meV



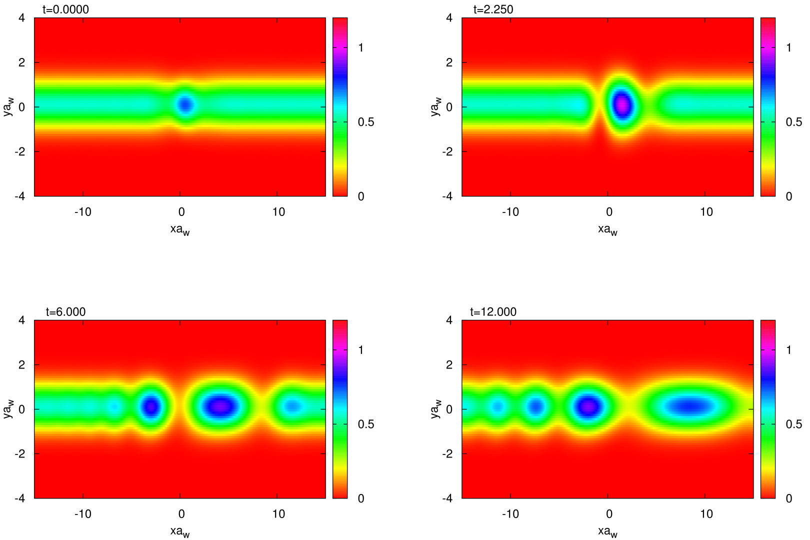

## $I_x^l - I_x^r$, $\beta = 1 \times 10^{-4}$ nm$^{-2}$, $\beta = 4 \times 10^{-4}$ nm$^{-2}$



## $|\Psi|^2$, $B = 0.1$ T, $V_0 = -1$ meV, $\beta = 1 \times 10^{-4}$ nm$^{-2}$, $E = 0.75 E_w$

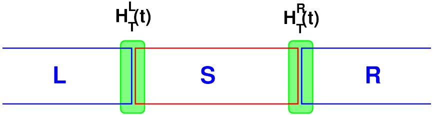


$|\Psi|^2$, $B = 0.1$ T, $V_0 = -1$ meV, $\beta = 4 \times 10^{-4}$ nm$^{-2}$, $E = 0.75 E_w$



# Generalized Master Equation Approach

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




Liouville-von Neumann equation

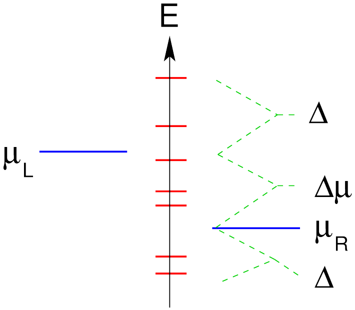
$$\dot{W}(t) = -\frac{i}{\hbar}[H(t), W(t)] = -i\mathcal{L}W(t)$$

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

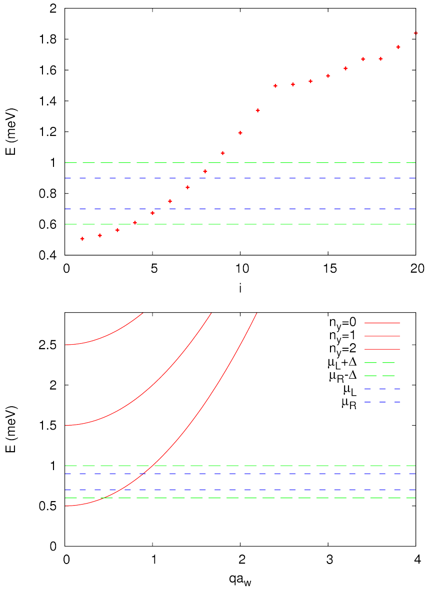
$$\langle Q_\mathrm{S}(t)\rangle = \mathrm{Tr}\{W(t)Q_\mathrm{S}\} = \mathrm{Tr}_\mathrm{S}\{[\mathrm{Tr}_\mathrm{L}\mathrm{Tr}_\mathrm{R}W(t)]Q_\mathrm{S}\} = \mathrm{Tr}_\mathrm{S}\{\rho(t)Q_\mathrm{S}\}$$

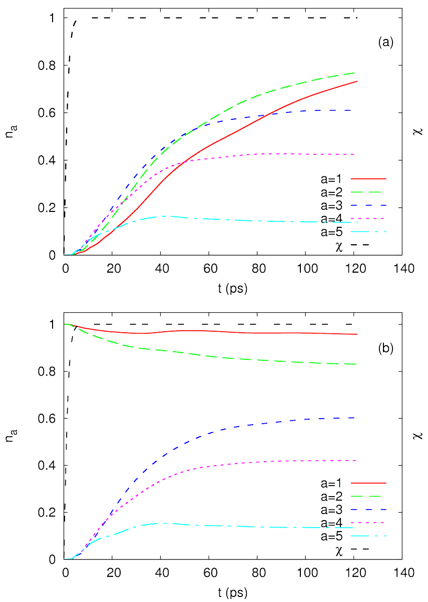
$$\dot{\rho}(t) = -i\mathcal{L}_{\text{eff}}(t)\rho(t) + \int_0^t dt' K(t,t')\rho(t)$$

- Integrodifferential equation
  Volterra type
- Life-times, decay rates
- Memory effects, non-Markovian
- Infinite order...
- Finite bias
- Many-body effects

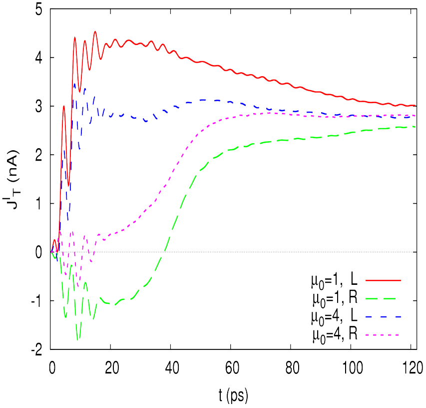



$$T^{L,R}_{a,k} = \int_{A_{L,R}} d\mathbf{r}\, d\mathbf{r}' \left(\Psi^{L,R}_k(\mathbf{r}')\right)^* \Psi^S_a(\mathbf{r}) g^{L,R}(\mathbf{r},\mathbf{r}') + h.c.$$

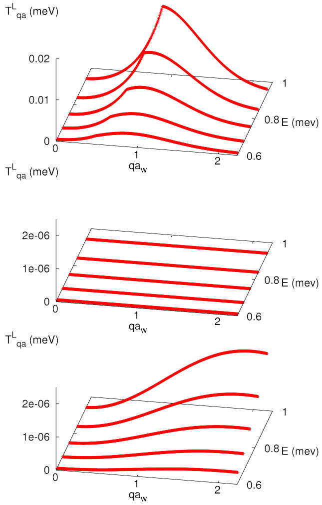

E (meV)
i
$n_y$=0
$n_y$=1
$n_y$=2
$\mu_L+\Delta$
$\mu_R-\Delta$
$\mu_L$
$\mu_R$
$qa_w$

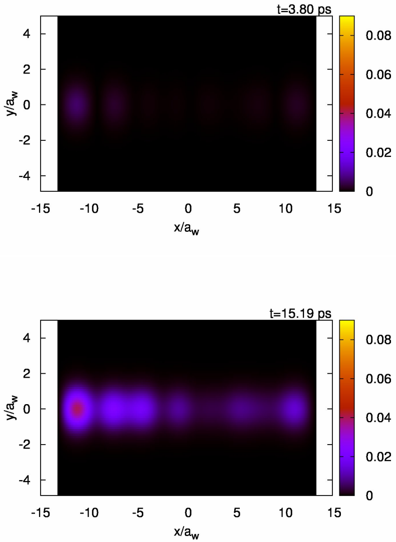

(a)
$n_a$
$\chi$
a=1
a=2
a=3
a=4
a=5
$\chi$
t (ps)
(b)

## Total current



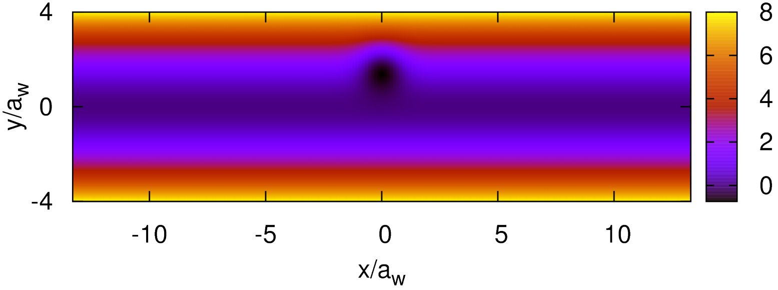

## Coupling



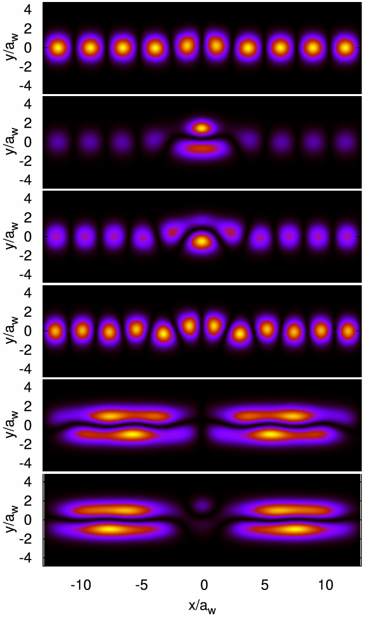


t=3.80 ps
t=30.38 ps
t=15.19 ps
t=60.00 ps
y/a_w
x/a_w
4
2
0
-2
-4
-15
-10
-5
0
5
10
15
0.08
0.06
0.04
0.02
0

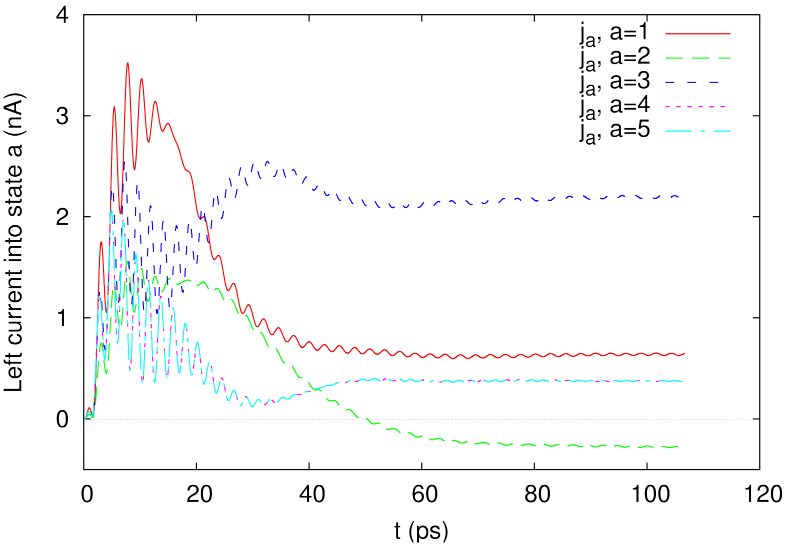
# System with an off-centered Gaussian well



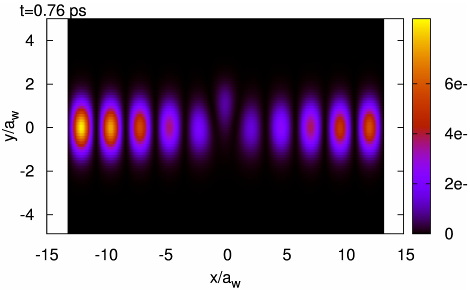
# Relevant eigenstates

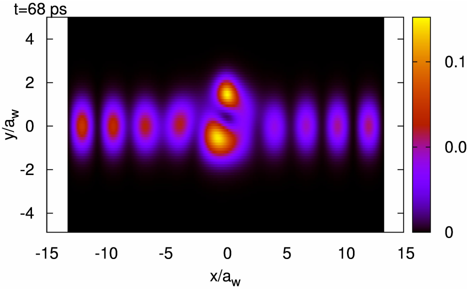


# Partial left current into state $a$

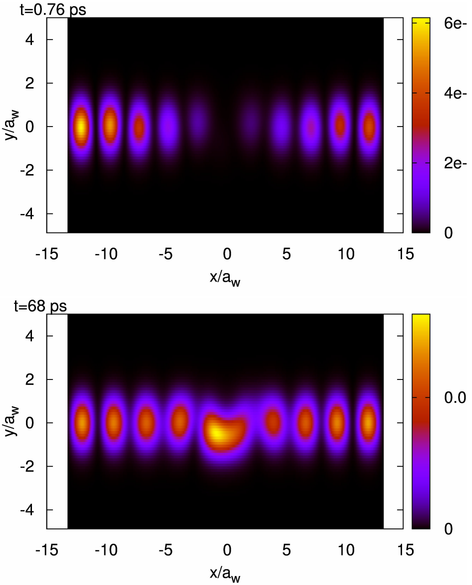


# Time-dependent charge density



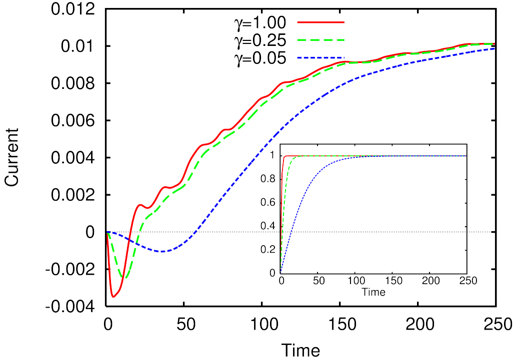



# ... off-centered hill



# Speed of coupling

- Steady state is independent of speed of coupling
- Proven by Cornean et al., arXiv:0708.3931 (2008)
- Calculated by Moldoveanu et al., arXiv:0807.4015 (2008) for a lattice model

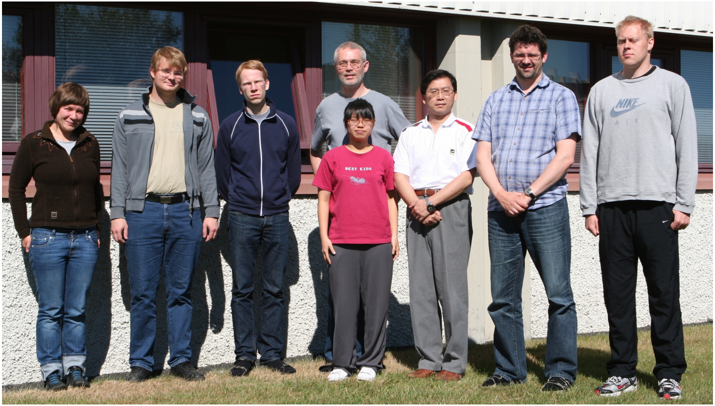


# Summary

- 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

# Cooperation

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| Gunnar Þorgilsson | Kristinn Torfason | Ómar Valsson |
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| Wing Wa Yu | Andrei Manolescu | Valeriu Moldoveanu |