# *Time-dependent transport in quantum wires*

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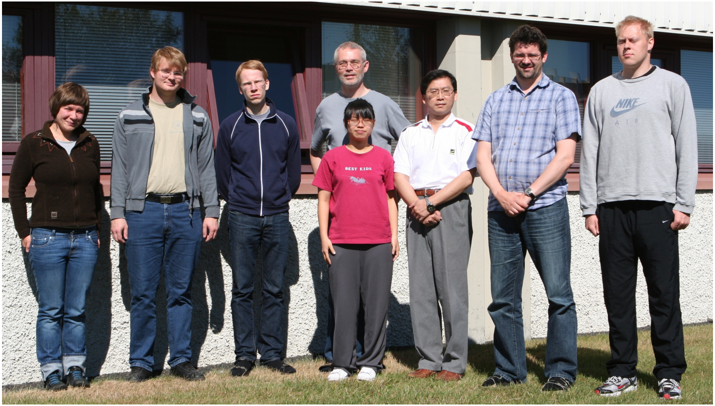
# Cooperation

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# Content

## Background

- Closed systems
- t-dependence
- Open systems
- Scattering formalism for transport

## GME

- Finite Quantum wire
- Semi-infinite leads
- Band structure
- Magnetic field

# Closed system - strong excitation

## Ground state

- Confined closed system of several 2D electrons
- General shape, ring, circular, elliptic, square, triangular dot …
- External constant perpendicular magnetic field

## Time evolution

- Weak → strong perturbation, general shape in time and space
- Nonequilibrium evolution
- Non-adiabatic
- No dissipation

## Grid-free LSDA

- Y.C. Zheng and J. Almlöf, Chem. Phys. Lett. 214, 397 (1993)
- G. Berghold, J. Hutter, and M. Parrinello, Theor. Chem. Acc. 99, 344 (1998)
- K.R. Glaesemann and M.S. Gordon, J. Chem. Phys. 110, 6580 (1999)

# Ground state

$$H|\alpha) = \left(H_0 + H_\sigma + V_\phi + H_{\rm int}\right)|\alpha) = \varepsilon_\alpha|\alpha),$$

$$V_\phi(\mathbf{r}) = \frac{1}{2}m^*\omega_0 r^2 \sum_{p=1}^{p_{\max}} \alpha_p \cos\left(p\varphi\right) + V_0 \exp\left(-\gamma r^2\right),$$

$H_0$ includes $\mathbf{B} = B\hat{\mathbf{z}}$ and $V_{\rm conf}(r) = m^*\omega_0^2 r^2/2$

Zeeman energy: $H_\sigma = \pm(1/2)g^*\mu_B B$

Length scale: $l = \sqrt{\hbar c/(eB)} \longrightarrow a = l\sqrt{\omega_c/\Omega}$

Energy scale: $\hbar\omega_c = \hbar eB/(m^* c) \longrightarrow \hbar\Omega = \hbar\sqrt{\omega_c^2 + 4\omega_0^2}$

Density: $n = n_\uparrow + n_\downarrow \longrightarrow \tilde{\nu}(\mathbf{r}) = 2\pi a^2 n(\mathbf{r})$ effective filling factor

Polarization: $\zeta(\mathbf{r}) = [n_\uparrow(\mathbf{r}) - n_\downarrow(\mathbf{r})]/n(\mathbf{r})$

# DFT - ground state

## Change of variables

$$V_{xc,\sigma}(\mathbf{r},B) = \frac{\partial}{\partial n_\sigma}(n\epsilon_{xc}[n_\uparrow,n_\downarrow,B])|_{n_\sigma=n_\sigma(\mathbf{r})},$$

$$\Downarrow$$

$$V_{xc,\uparrow} = \frac{\partial}{\partial\tilde{\nu}}(\tilde{\nu}\epsilon_{xc}) + (1-\zeta)\frac{\partial}{\partial\zeta}\epsilon_{xc}$$
$$V_{xc,\downarrow} = \frac{\partial}{\partial\tilde{\nu}}(\tilde{\nu}\epsilon_{xc}) - (1+\zeta)\frac{\partial}{\partial\zeta}\epsilon_{xc}$$

## Functionals and parametrization

- M. Koskinen, et al., Phys. Rev. Lett. 79, 1389 (1997)
- U. von Barth and B. Holm, Phys. Rev. B 54, 8411 (1996)
- B. Tanatar and D.M. Ceperley, Phys. Rev. B 39, 5005 (1989)

# Grid-free LSDA

## Use a basis

$$|\alpha) = \sum_\beta c_{\alpha\beta}|\beta\rangle, \quad \psi_\alpha(\mathbf{r}) = \sum_\beta c_{\alpha\beta}\phi_\beta(\mathbf{r})$$

$$\langle\alpha|\tilde{\nu}|\beta\rangle = \sum_{p,q} \rho_{qp} \int d\mathbf{r}\ \phi_\alpha^*(\mathbf{r})\phi_p^*(\mathbf{r})\phi_q(\mathbf{r})\phi_\beta(\mathbf{r})$$

$$\rho_{qp} = \sum_\gamma f(\varepsilon_\gamma - \mu)\, c_{\gamma p}^* c_{\gamma q}$$

$$\langle\alpha|\zeta|\beta\rangle = \sum_\gamma \langle\alpha|(\tilde{\nu}_\uparrow - \tilde{\nu}_\downarrow)|\gamma\rangle\langle\gamma|\tilde{\nu}^{-1}|\beta\rangle$$

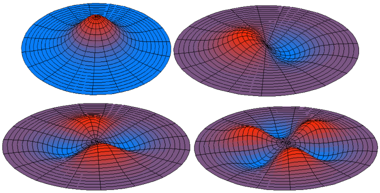
$$\tilde{\nu} = \mathbf{U}\ \mathbf{diag}(\lambda_1, \cdots, \lambda_n)\mathbf{U}^+$$

$$\mathbf{f}[\tilde{\nu}] = \mathbf{U}\ \mathbf{diag}\left(f(\lambda_1), \cdots, f(\lambda_n)\right)\mathbf{U}^+.$$

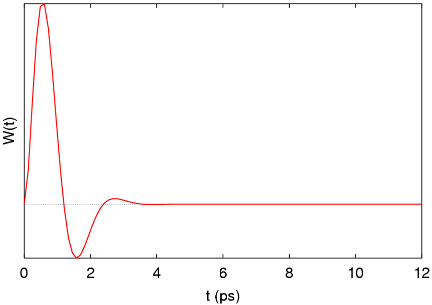
# Time evolution

At $t = t_0$: $H(t) \rightarrow H + W(t)$

$$W(t) = V_t r^{|N_p|} \cos(N_p\phi) \exp(-sr^2 - \Gamma t) \sin(\omega_1 t) \sin(\omega t) \theta(\pi - \omega_1 t)$$



- $N_p = 0, \pm 1, \pm 2, \pm 3$
- $s = 0$, $\Gamma = 2$ THz
- $\omega = 4$ THz, $\omega_1 = 1$ THz



## Nonequilibrium evolution

$$i\hbar d_t\rho(t) = [H + W(t), \rho(t)].$$

$$\begin{aligned} i\hbar\dot{T}(t) &= H(t)T(t) \\ -i\hbar\dot{T}^+(t) &= T^+(t)H(t) \end{aligned}$$

$$\rho(t+\Delta t) = T(\Delta t)\rho(t)T^+(\Delta t)$$

Crank-Nicholson + iteration

$$\left\{1 + \frac{i\Delta t}{2\hbar}H[\rho; t+\Delta t]\right\} T(\Delta t) \approx \left\{1 - \frac{i\Delta t}{2\hbar}H[\rho; t]\right\}$$

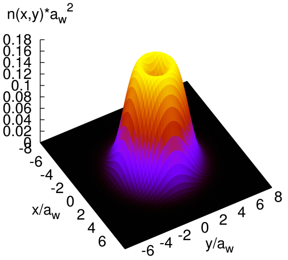
# Technical implementation

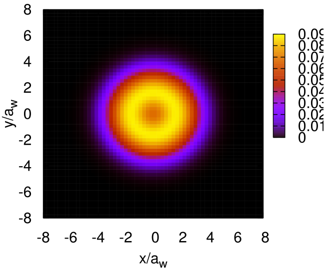
- Fock-Darwin basis $\{\phi_\alpha\} \rightarrow$
- Analytical matrix elements
- Grid-free LSDA, compact "small" matrices
- Complicated LSDA potentials $\rightarrow$ complicated functions of $\tilde{\nu}$ $\rightarrow$ heavy matrix multiplication
- F95 $\rightarrow$ easy parallelization on multicore machines


- Phys. Rev. B67, 161301(R) (2003)
- Phys. Rev. B68, 165343 (2003)
- Physica E 27, 278 (2005)

# Circular quantum dot

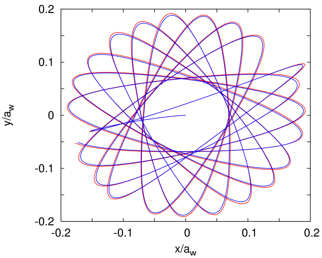
- Circular dot
- $N = 6$
- $B = 0.6$ T
- $T = 4$ K



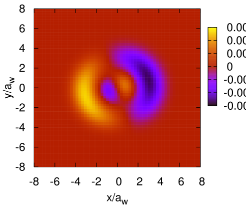



# Dipole excitation

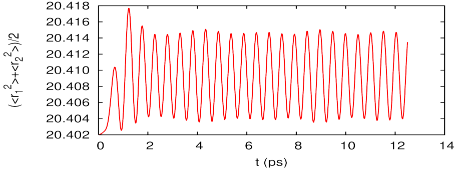
## Center of mass




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



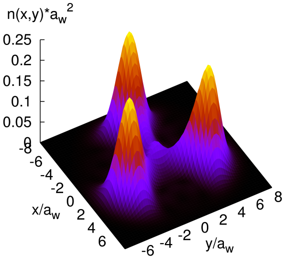

$(\langle r_\downarrow^2\rangle + \langle r_\uparrow^2\rangle)/2$

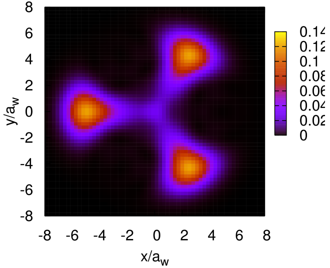



- No energy flows into internal modes
- Kohn's theorem

# Triangular quantum dot

- Triangular dot, $\alpha_3 = 0.7$
- $N = 6$
- $B = 0.6$ T
- $T = 1$ K

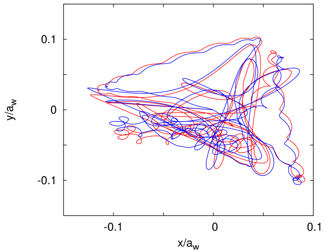


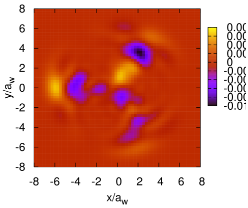

- Kohn's theorem does not hold
- Energy will flow into internal modes, transient time?

# Dipole excitation

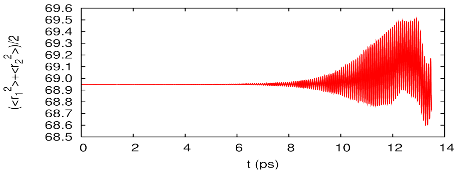
## Center of mass




## Induced density, ($t = 13.5$ ps, 9000 steps)



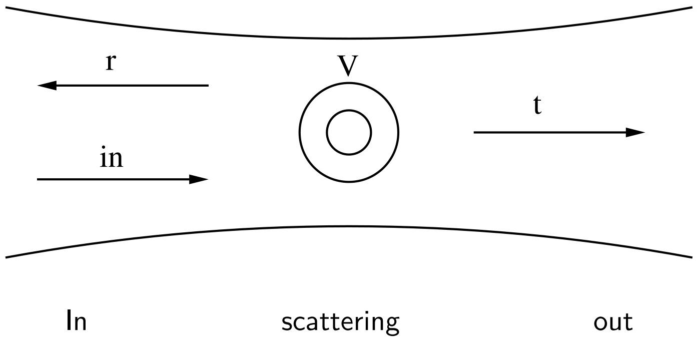

$(\langle r_\downarrow^2 \rangle + \langle r_\uparrow^2 \rangle)/2$




- Energy pumped into relative modes
- long transient time
- Spin modes

# Connection to leads - Scattering formalism

## Lippmann-Schwinger



# External magnetic field, $\mathbf{B} \neq 0$

## Asymptotic regions, free parabolic wire, perpendicular magnetic field

$$H_0 = \frac{\hbar^2}{2m^*}\left[-i\boldsymbol{\nabla} - \frac{eB}{\hbar c}y\hat{\boldsymbol{x}}\right]^2 + V_{\rm c}(y)$$

$$\psi^+(x,y,k_n) = e^{ik_n x}\phi_n(y-y_0)$$

$$E = \left(n+\frac{1}{2}\right)\hbar\Omega_w + \mathcal{K}_n(k_n)$$

$$\Omega_w = \sqrt{\omega_c^2+\Omega_0^2}, \quad y_0 = k_n a_w^2\frac{\omega_c}{\Omega_w}, \quad \omega_c = \frac{eB}{m^*c}$$

$$\mathcal{K}_n(k_n) = \frac{(k_n a_w)^2}{2}\left(\frac{\hbar^2\Omega_0^2}{\hbar\Omega_w}\right), \quad a_w^2\Omega_w = \frac{\hbar}{m^*}$$

## Green function → T-matrix

$$\tilde{T}_{nn'}(q,p) = \tilde{V}_{nn'}(q,p) + \sum_{m'} \int \frac{dka_w}{2\pi} \tilde{V}_{nm'}(q,k) G_E^{m'}(k) \tilde{T}_{nm'}(k,p).$$

## Wavefunctions

$$\psi_E(x,y) = e^{ik_n x}\phi_n(k_n,y) + \sum_m \int \frac{dqa_w}{2\pi} e^{iqx} G_E^m(q) \tilde{T}_{mn}(q,k_n)\phi_m(q,y)$$

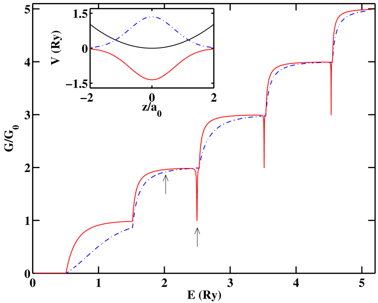
## Transmission amplitudes

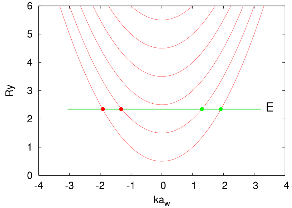
$$t_{nm}(E) = \delta_{nm} - \frac{i\sqrt{(k_m/k_n)}}{2(k_m a_w)} \tilde{T}_{nm}(k_n,k_m)$$

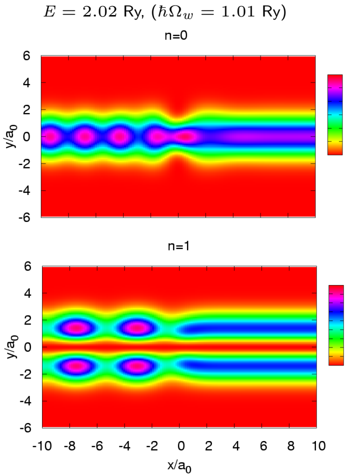
## Conductance

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

# B=0, simple Gaussian hill or well

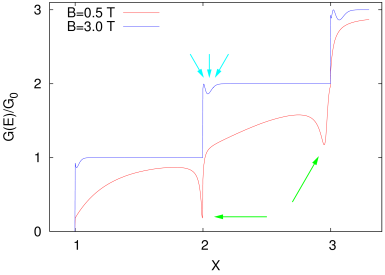


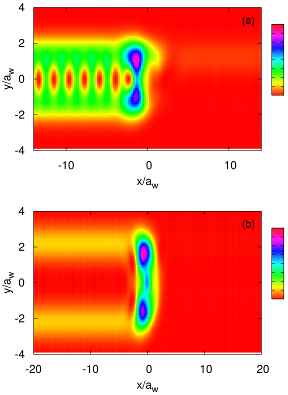
# Magnetic field, $B \neq 0$

Small open quantum dot or well,




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

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



# L-S $\longrightarrow$ t-domain

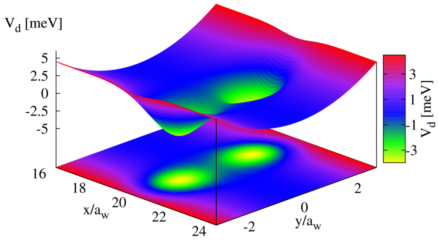
$$T_{nn'}(q\omega, p\nu) = V^{\rm sc}_{nn'}(q\omega, p\nu) + \sum_{m'} \int \frac{dk}{2\pi}\frac{d\omega'}{2\pi} V^{\rm sc}_{nm'}(q\omega, k\omega')\, G_0^{m'}(k\omega')\, T_{m'n'}(k\omega', p\nu)$$

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

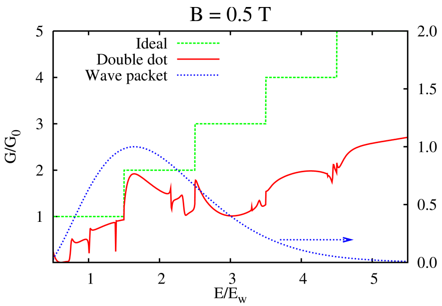
$$\psi_{\rm E} = \left(\mathbf{1} + \mathbf{G}_0\mathbf{T}\right)\psi_{\rm in}$$

# Static potentials

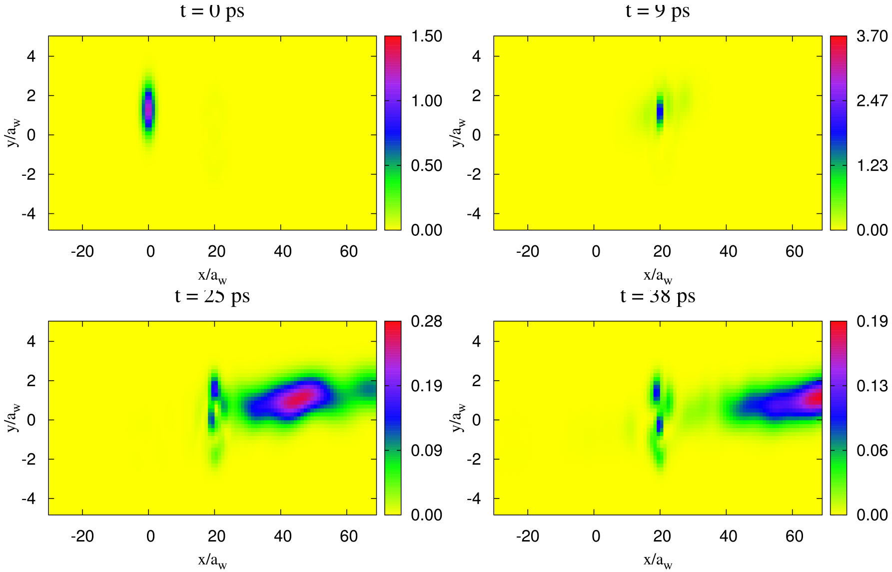
## Parallel double dot




## Conductance

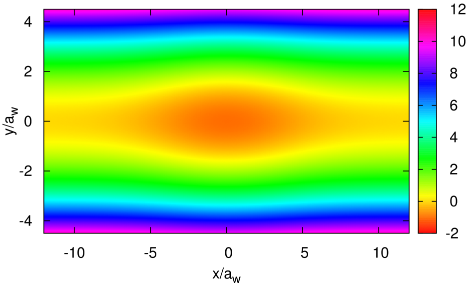


# Parallel double dot, $B = 0.5$ T



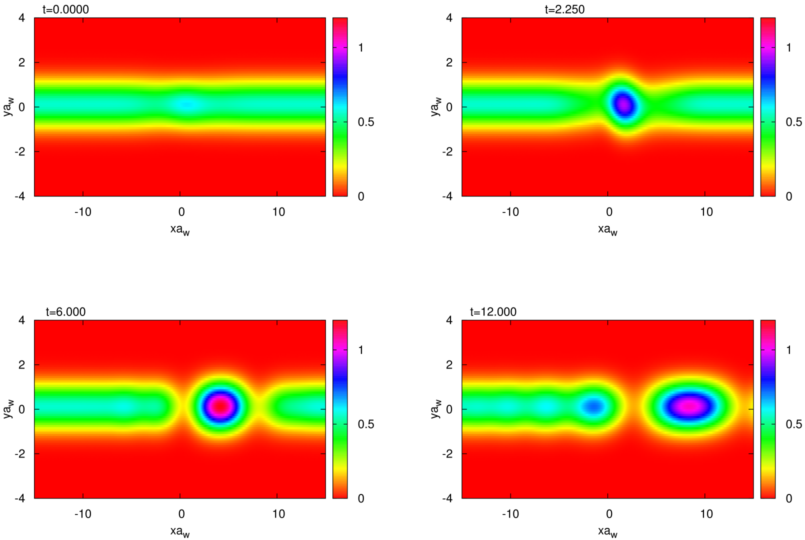
# Current modulation

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

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



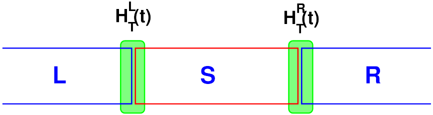
# “Zwischengedanken”

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


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

# 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

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

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

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

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

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

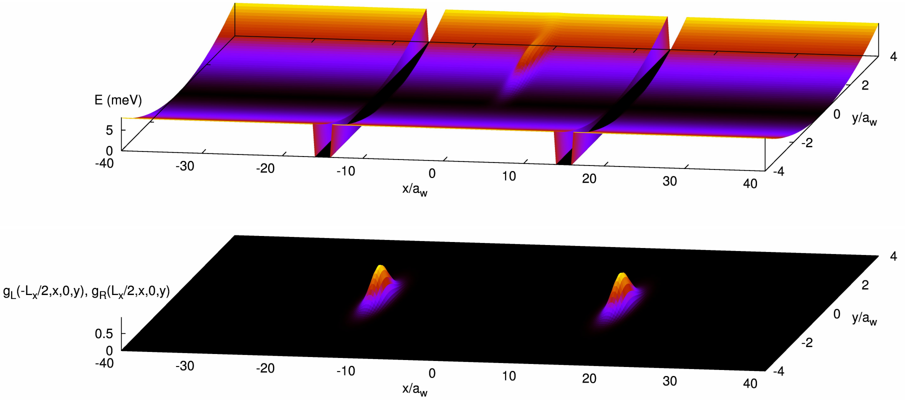
$$T \exp\left\{ -\frac{i}{\hbar} \int_s^t ds' \, Q\mathcal{L}(s') Q \right\} = \exp\{Q\mathcal{L}_0 Q\}(1 + \mathcal{R})$$

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

$$P + Q = 1$$

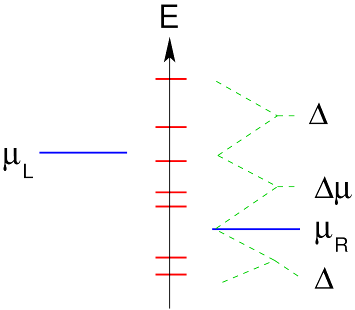
# Coupling of leads

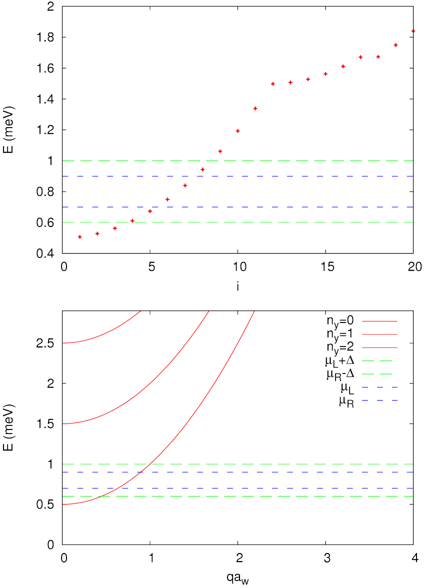
$$T_{a,k}^{L,R} = \int_{A_{L,R}} d\mathbf{r}\, d\mathbf{r}' \left(\Psi_k^{L,R}(\mathbf{r}')\right)^* \Psi_a^S(\mathbf{r}) g^{L,R}(\mathbf{r},\mathbf{r}') + h.c.$$

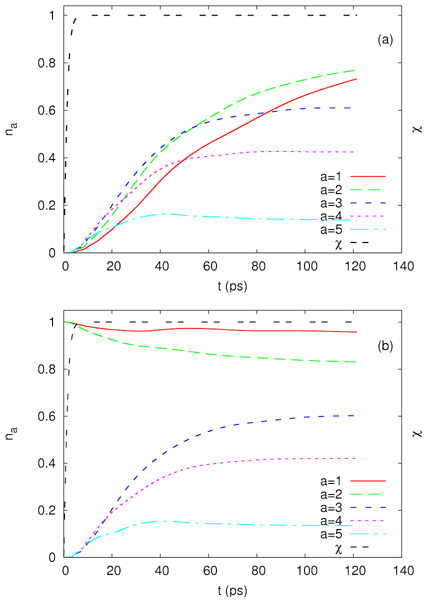


$$\dot{\rho}(t) = -i\mathcal{L}_{\text{eff}}(t)\rho(t) + \int_0^t dt' K(t,t')\rho(t)$$

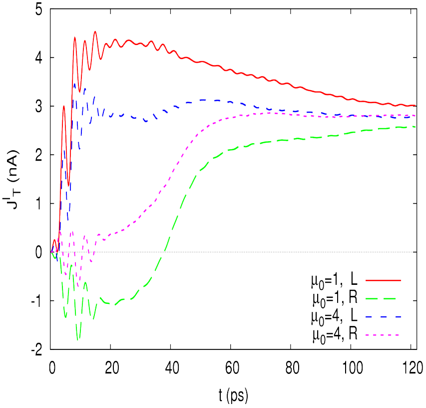
- Integrodifferential equation Volterra type
- Life-times, decay rates
- Memory effects, non-Markovian
- Infinite order...,(but approximation)
- Finite bias
- Many-body effects
- No assumption about equilibrium in leads after coupling



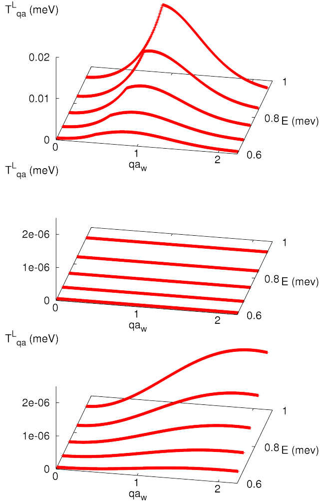

E (meV)
i
$n_y$=0
$n_y$=1
$n_y$=2
$\mu_L$+Δ
$\mu_R$-Δ
$\mu_L$
$\mu_R$
$qa_w$

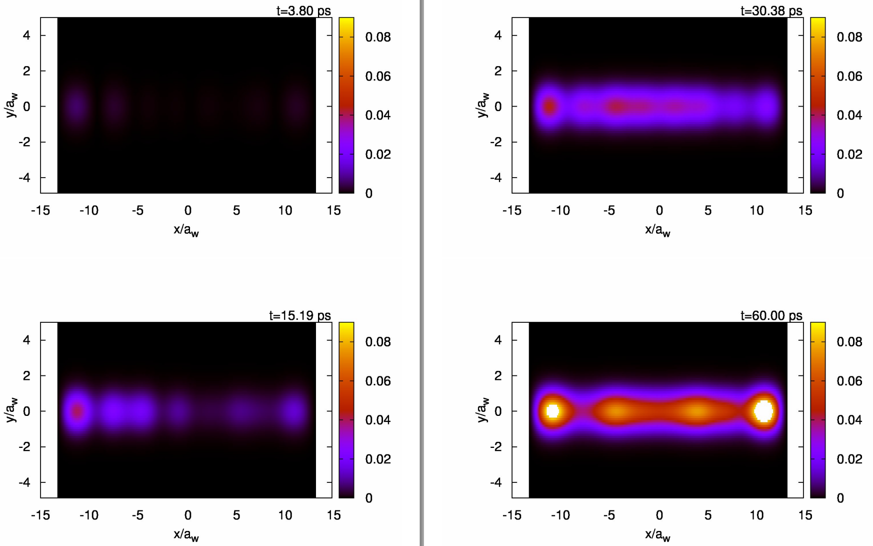

(a)
(b)
$n_a$
χ
t (ps)
a=1
a=2
a=3
a=4
a=5
χ

# Total current

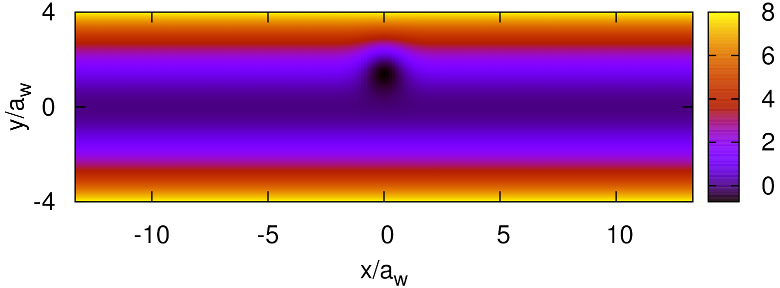



# Coupling

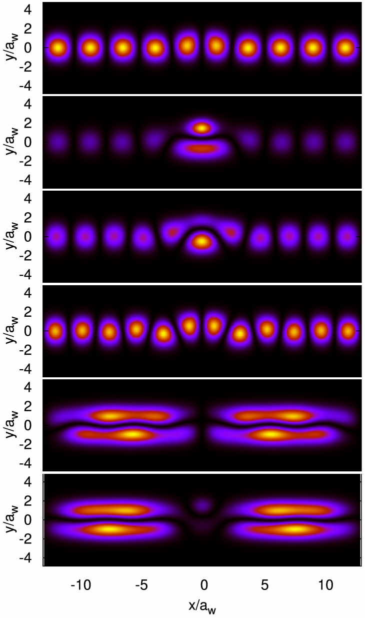



t=3.80 ps
t=30.38 ps
t=15.19 ps
t=60.00 ps
y/a_w
x/a_w
-15 -10 -5 0 5 10 15
4 2 0 -2 -4
0 0.02 0.04 0.06 0.08

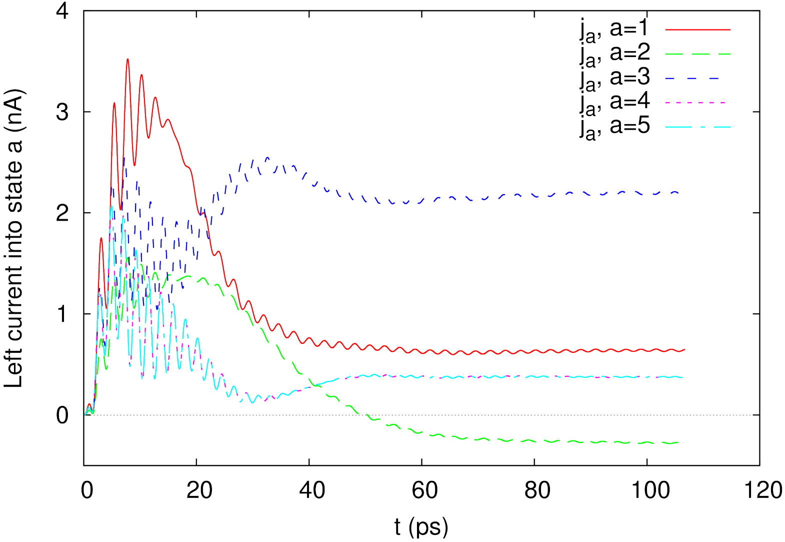
# System with an off-centered Gaussian well



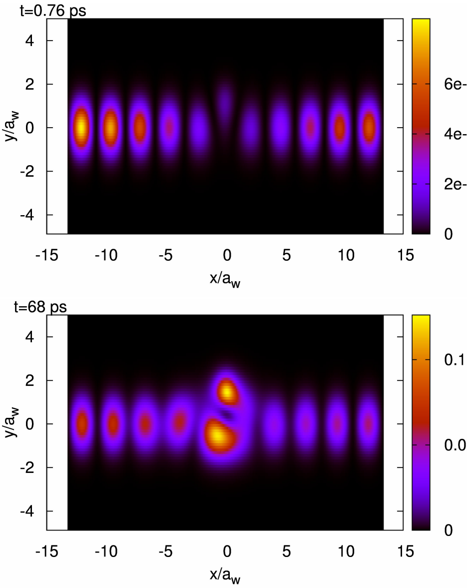
# Relevant eigenstates



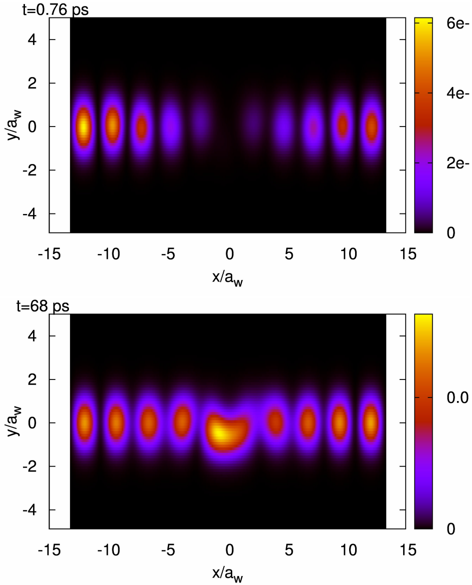
# Partial left current into state $a$



# Time-dependent charge density



# ... off-centered hill



# 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

- http://arxiv.org/abs/0807.4015
- http://arxiv.org/abs/0903.3491

# Funding + external help

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