Time-dependent transport through a nanostructure via the generalized master equation, III

Viðar Guðmundsson

Science Institute, University of Iceland

vidar@raunvis.hi.is

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Solution of the GME

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

where

$$\Omega_{ql}(t) = U_{\rm S}^\dagger(t)\int_{t_0}^{t} ds\, \chi^l(s)\Pi_{ql}(s)e^{i((s-t)/\hbar)\varepsilon^l(q)}\, U_{\rm S}(t),$$

$$\Pi_{ql}(s) = U_{\rm S}(s)\left(\mathcal{T}^{l\dagger}\rho(s)(1-f^l) - \rho(s)\mathcal{T}^{l\dagger}f^l\right) U_{\rm S}^\dagger(t),$$

with $U_{\rm S}(t) = e^{i(t/\hbar)H_{\rm S}}$, $f^l = f(\epsilon^l(q) - \mu_l)$

Solution

- Set time-grid $\rightarrow$ finite differences
- Set up initial matrix $\rho_{\mathrm{S}}(0)$
- Calculate the diagonal $U_{\mathrm{S}}(t)$
- Calculate the matrix $\Omega_{ql}(t)$
- Calculate $\rho_{\mathrm{S}}(t)$
- Calculate $\Pi_{ql}(s)$ and iterate $\rho_{\mathrm{S}}(t)$ within each time-step

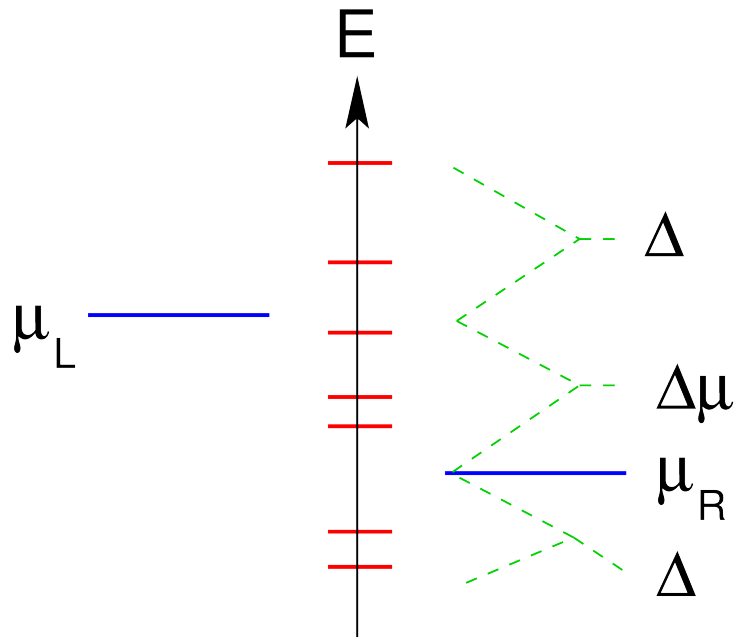
If we start with $N_{\mathrm{SES}} = 12 \rightarrow N_{\mathrm{MES}} = 4096$ we have to truncate $\rho_{\mathrm{S}}(t)$ to 32 or 64 lowest lying MES in energy due to many points needed for q-integration and time

Computational aspects

- We use Intel Fortran Compiler XE (ifort), FORTRAN 2008
- MKL - BLAS and LAPACK parallelized routines for matrix handeling
- BLAS: GEMM3M and GEMM instead of MATMUL for matrix multiplication
- OpenMP parallelization for shared memory machines
- Linux

Results for noninteracting system

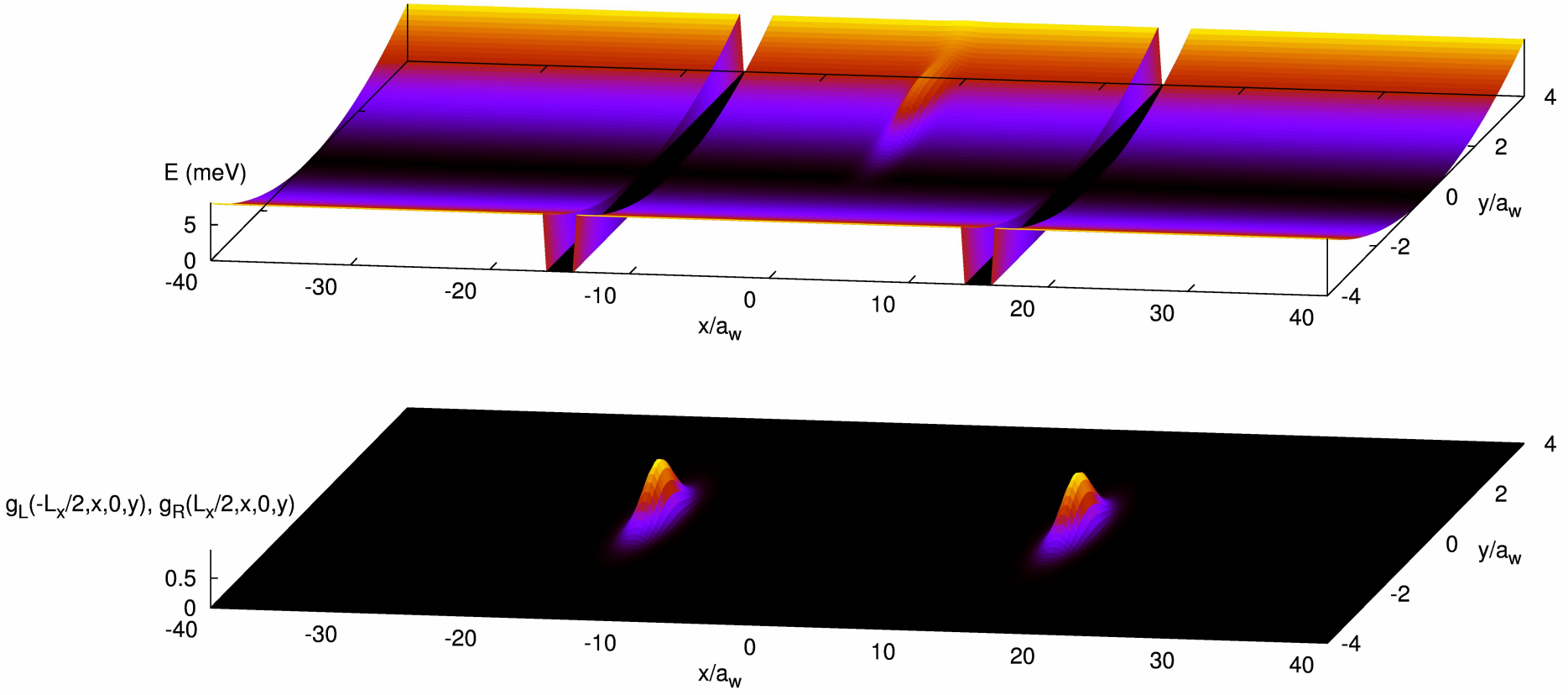
- Can we see geometry effects?
- GaAs parameters
- $L_x = 900$ nm
- Finite bias: $\Delta\mu = \mu_L - \mu_R$
- Parabolic finite quantum wire
- Confinement energy $\hbar\Omega_0 = 1.0$ meV
- Selection of relevant states
- No Coulomb interaction, but coupling to leads enforces correlation on electrons in the system



Relevant states

Coupling of semi-infinite parabolic leads

$$T_{a,k}^{L,R} = \int_{A_{L,R}} d\mathbf{r} d\mathbf{r}' \left(\psi_k^{L,R}(\mathbf{r}')\right)^* \psi_a^S(\mathbf{r}) g^{L,R}(\mathbf{r},\mathbf{r}')$$



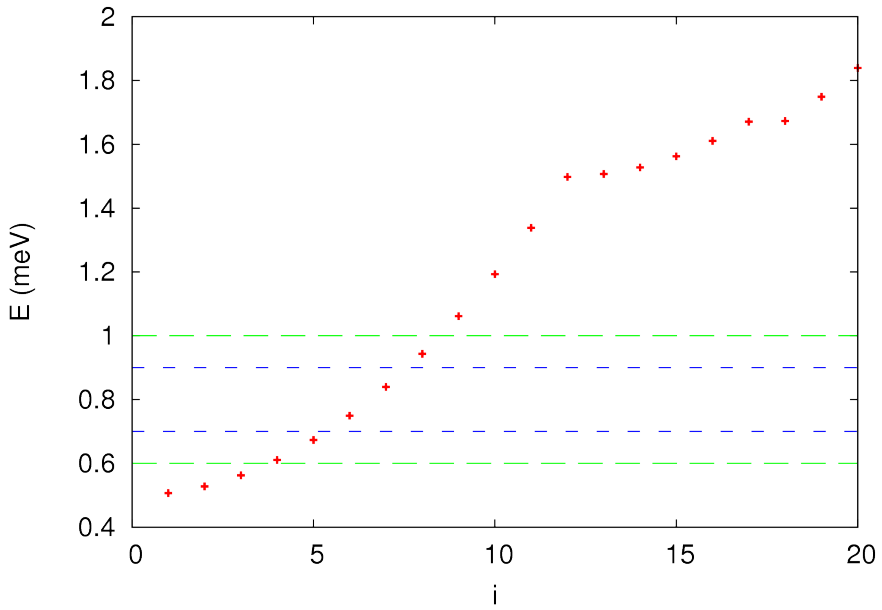
Measurable quantities

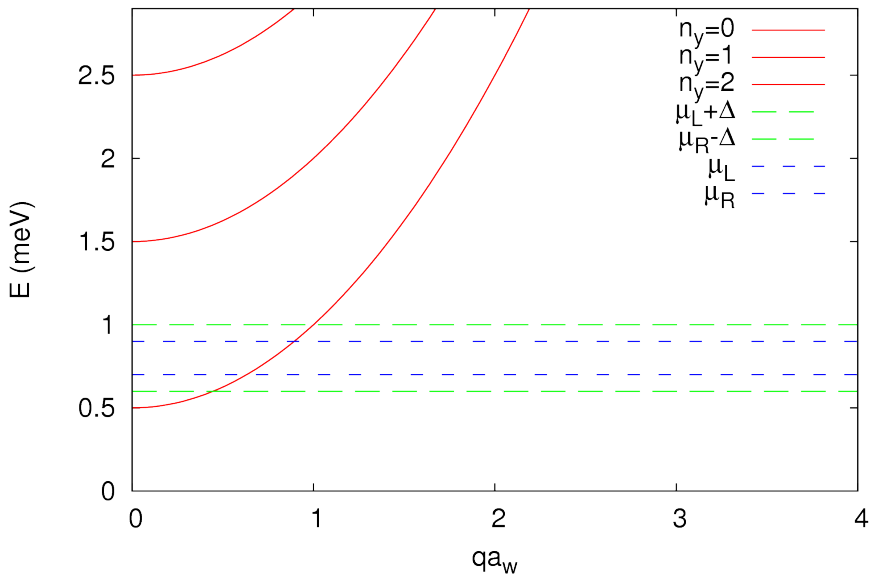
Total charge: $Q_{\rm S} = eN = e\sum_a d_a^\dagger d_a$

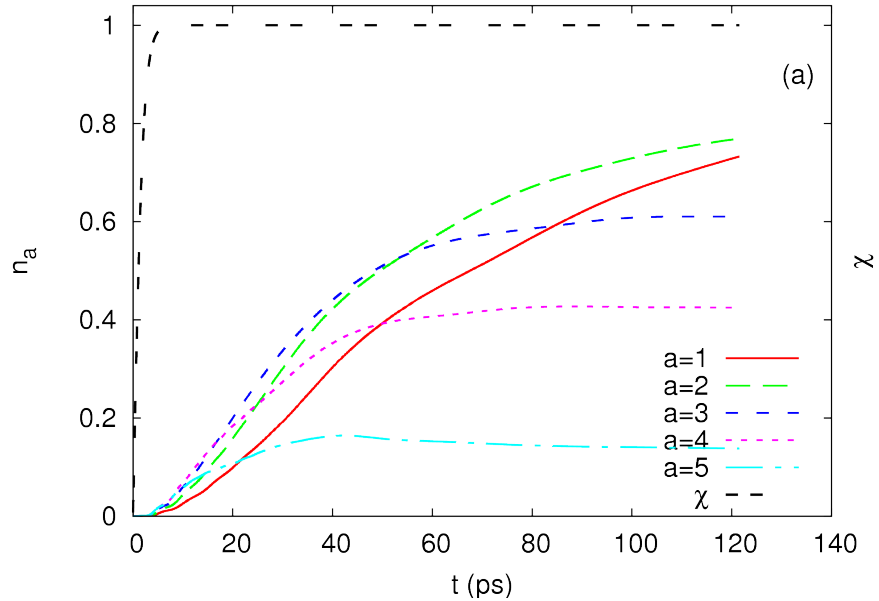
$$\begin{aligned}\langle Q_{\rm S}(t)\rangle &= {\rm Tr}\{\,W(t)\,Q_{\rm S}\} = {\rm Tr}_{\rm S}\{[{\rm Tr}_{\rm LR}\,W(t)]\,Q_{\rm S}\}\\ &= {\rm Tr}_{\rm S}\{\rho_{\rm S}(t)\,Q_{\rm S}\} = e\sum_{\mu\nu}\langle\mu|\rho_{\rm S}(t)|\nu\rangle\langle\nu|N|\mu\rangle\\ &= e\sum_{\mu\nu}\rho^{\rm S}_{\mu\nu}(t)\,N_{\nu\mu}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

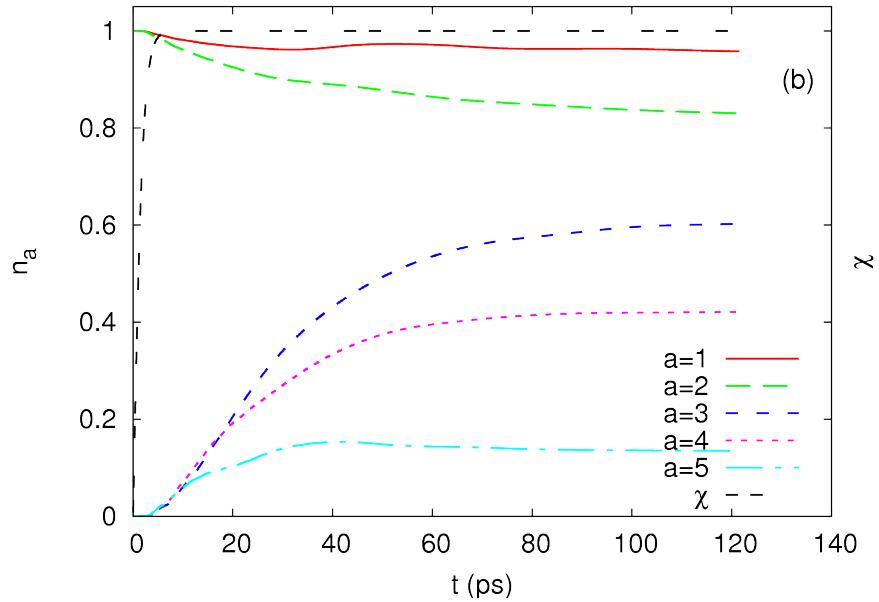
$$\langle Q_{\rm S}(\mathbf{r},t)\rangle = e\sum_{ab}\sum_{\mu\nu}\psi_a^*(\mathbf{r})\psi_b(\mathbf{r})\rho^{\rm S}_{\mu\nu}(t)\langle\nu|d_a^\dagger d_b|\mu\rangle$$

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


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

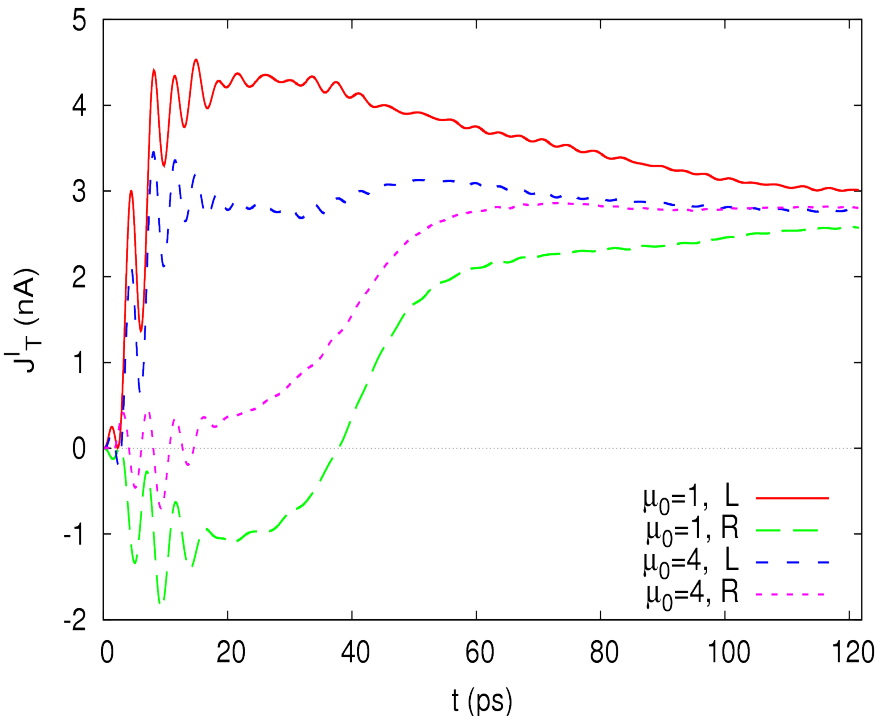

(a)
n_a
χ
t (ps)
a=1
a=2
a=3
a=4
a=5
χ


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

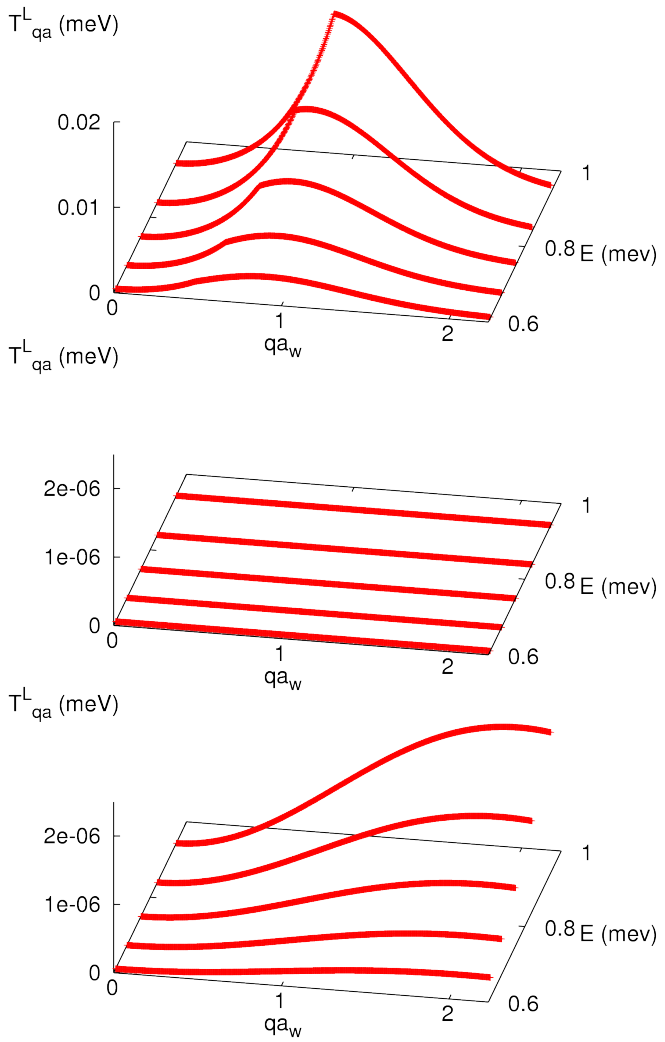
Total current

μ_0 the number of the initially occupied state, here

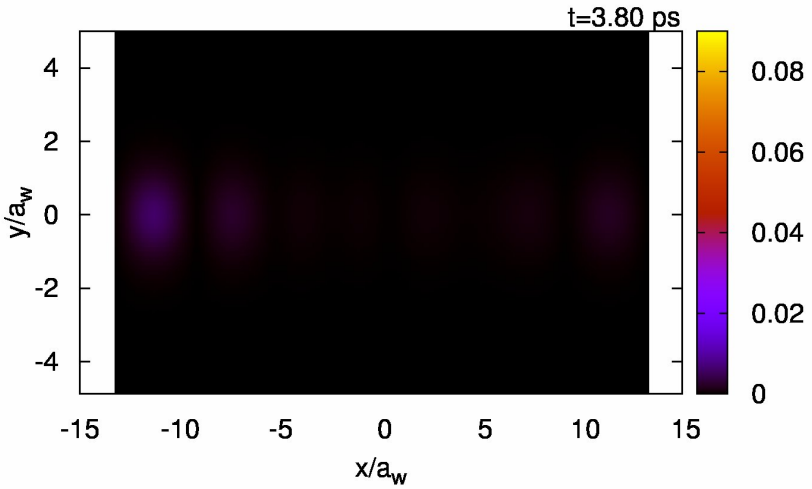
- $\mu_0 = 1$: vacuum state
- $\mu_0 = 1$: one electron

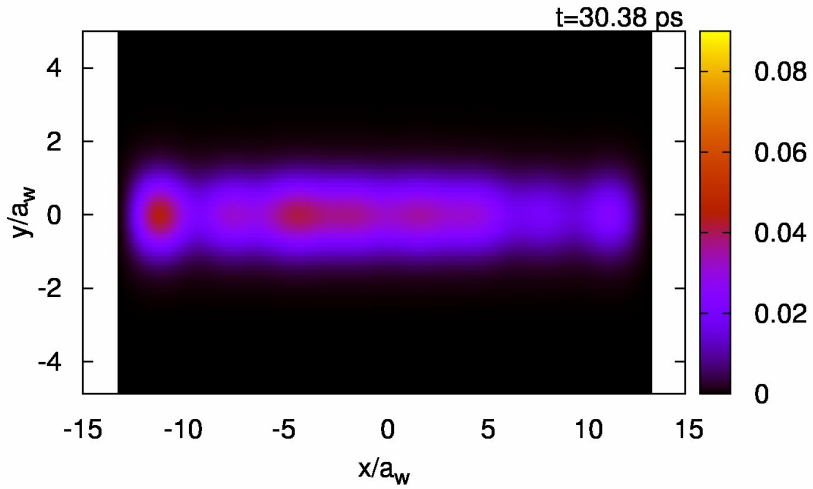


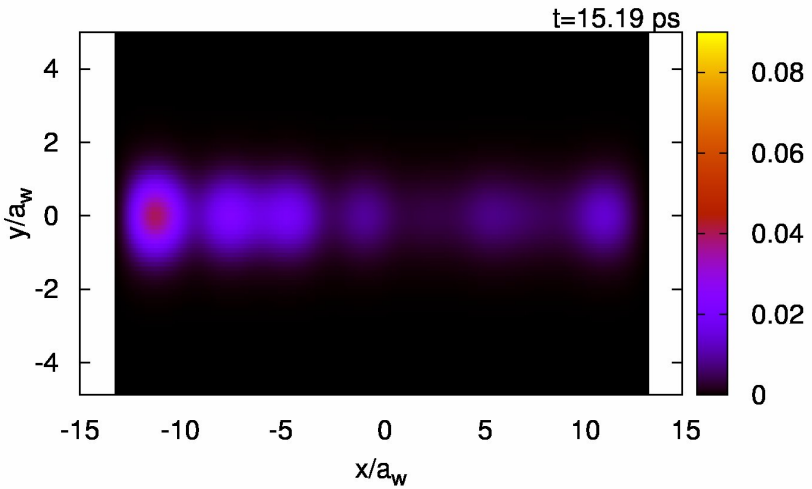
Coupling – selection rules

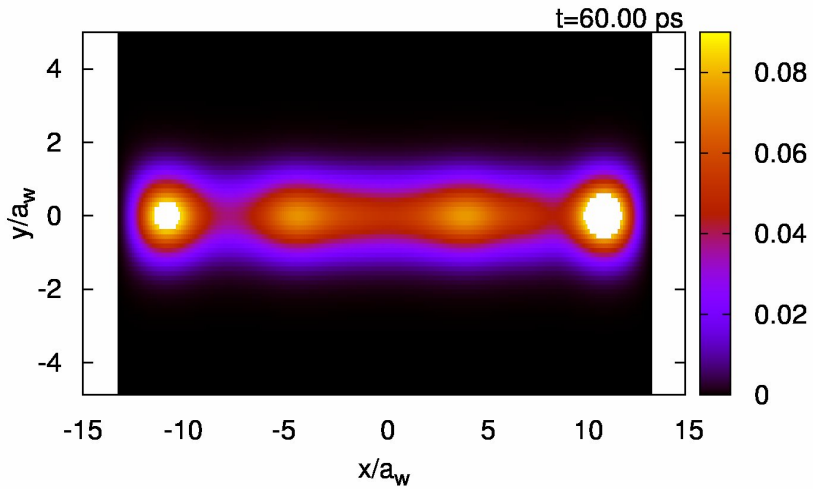


Time-dependent many-electron density

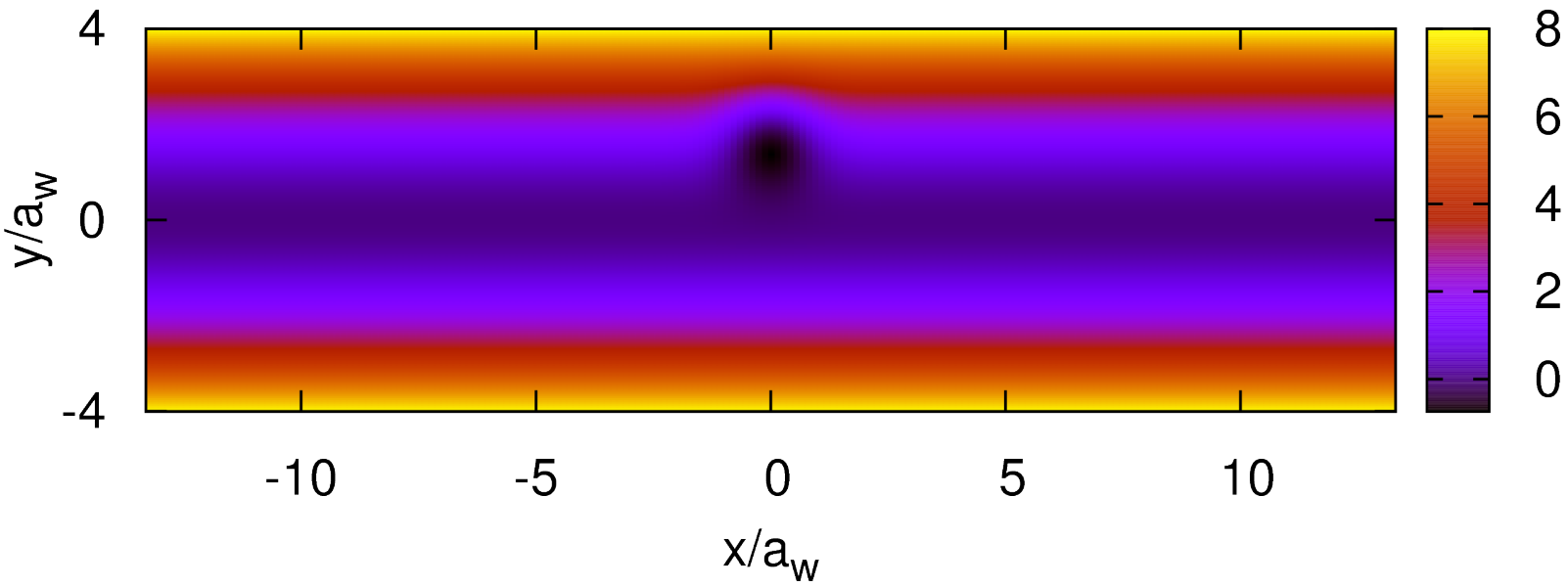




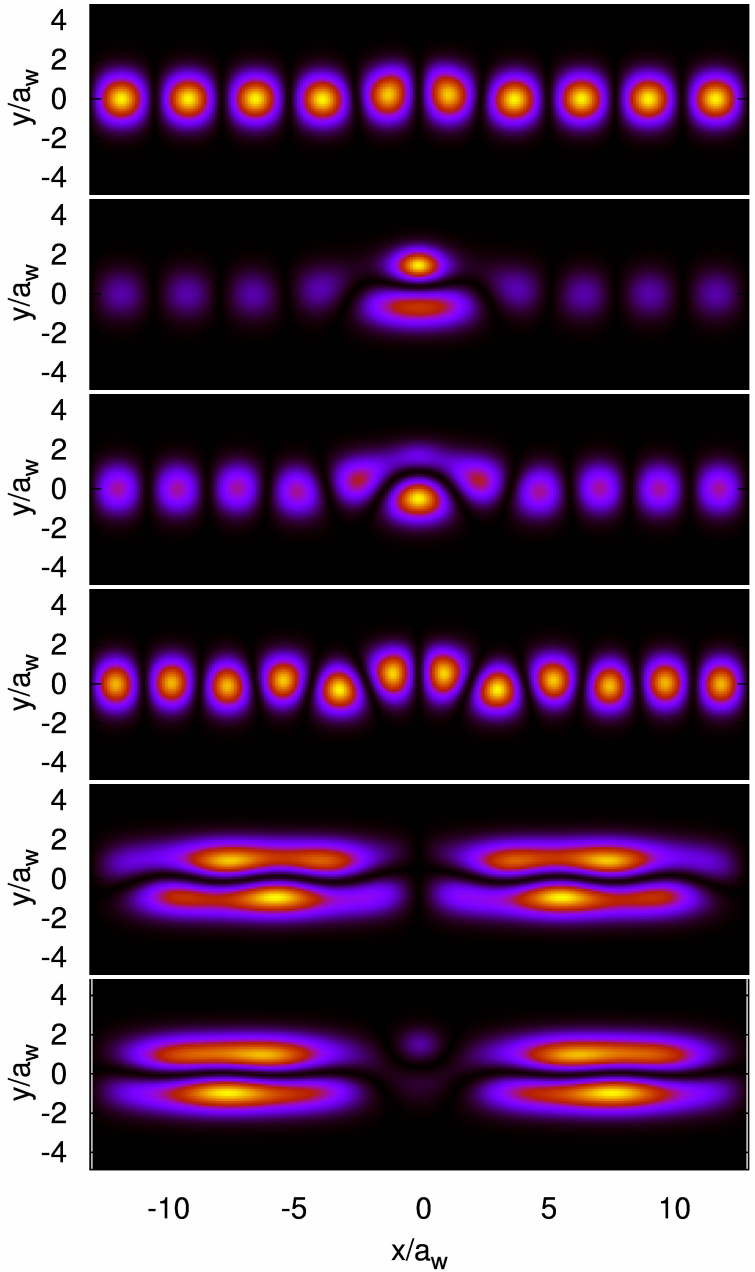




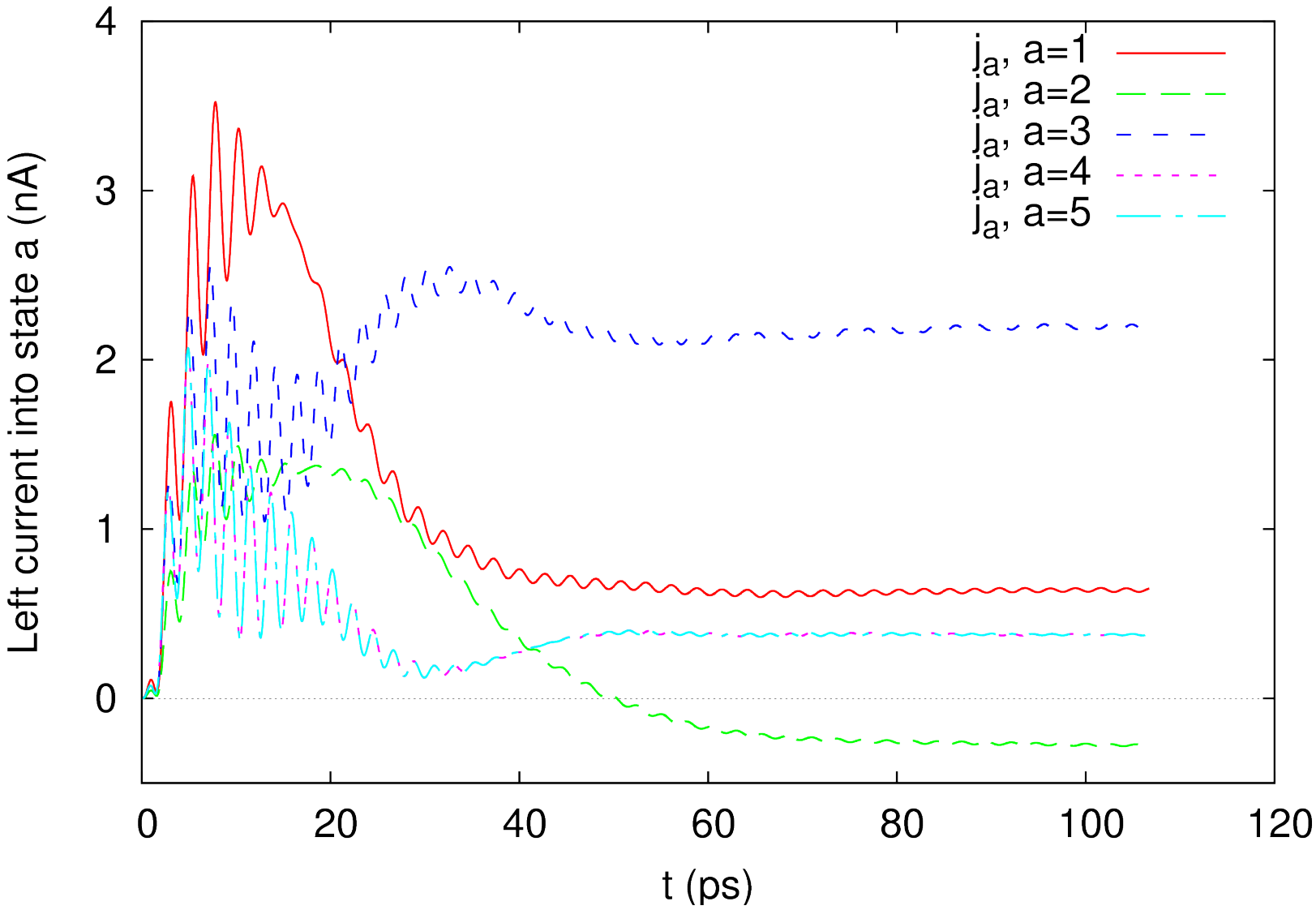
System with an off-centered Gaussian well



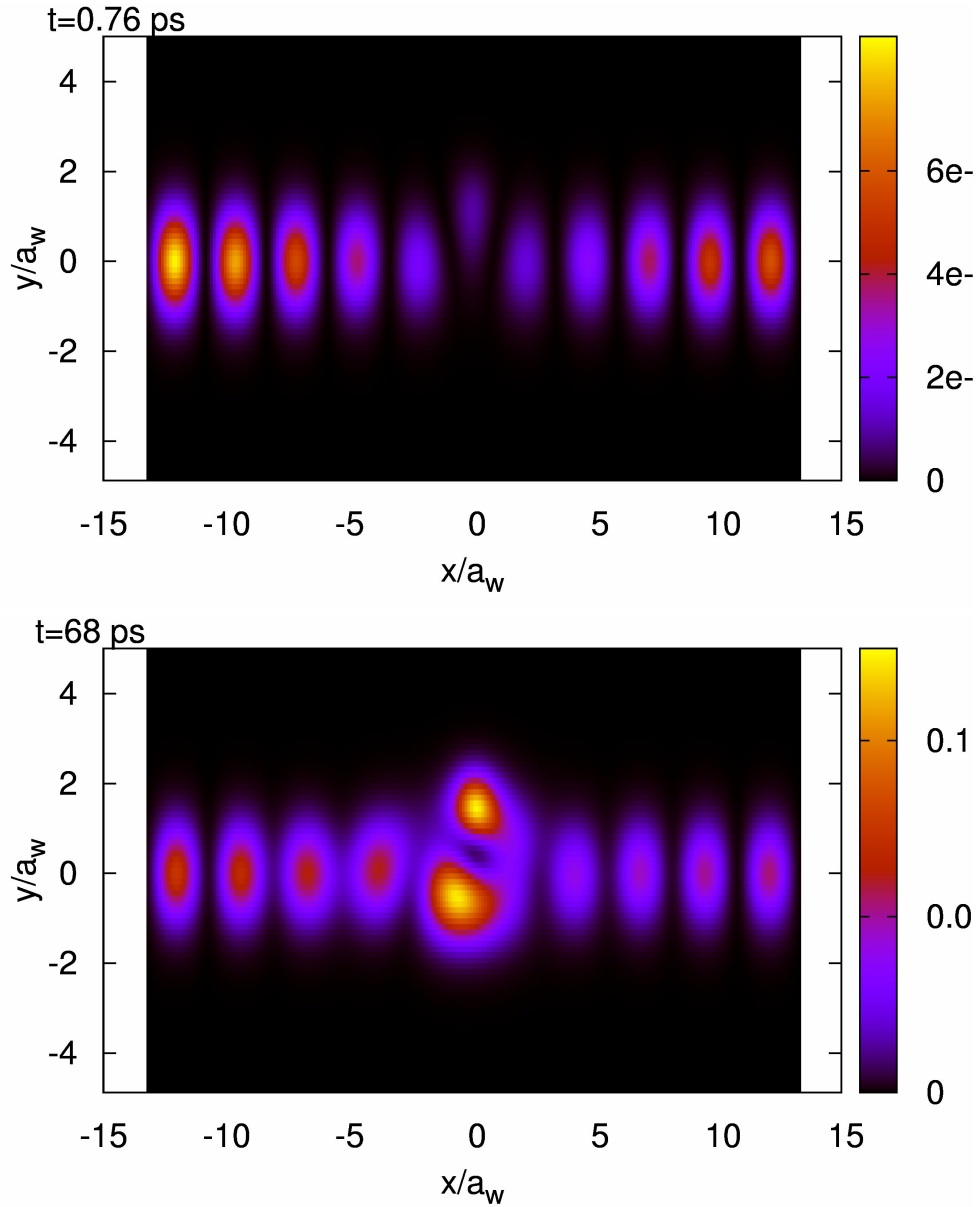
Relevant eigenstates



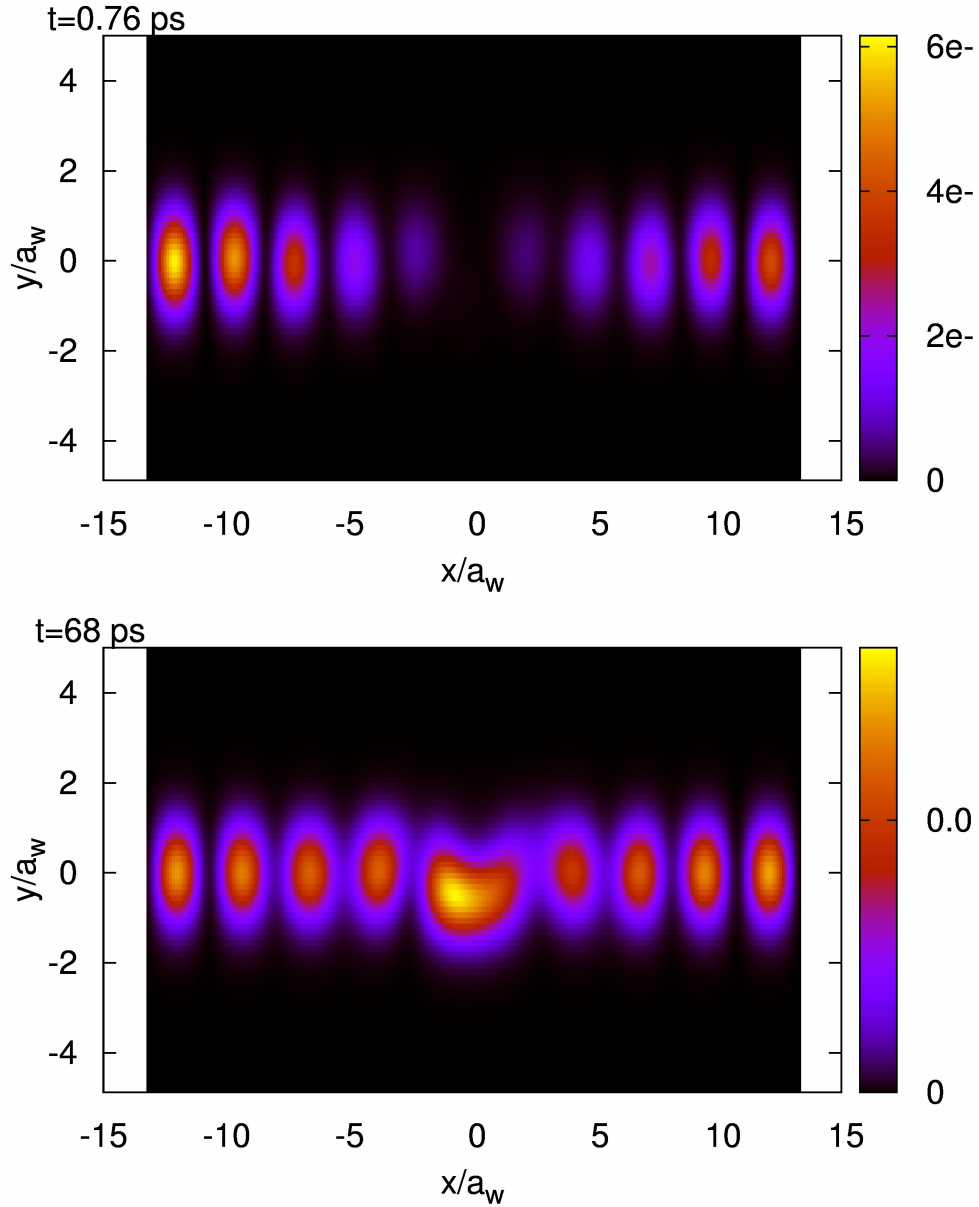
Partial left current into state a



Time-dependent charge density



... off-centered hill



We see time and geometrical effects

- Charging effects
- Bias seen in charge density
- Back scattering resonances in steady state
- Selection rules

References

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