Time-dependent transport through quantum nanostructures

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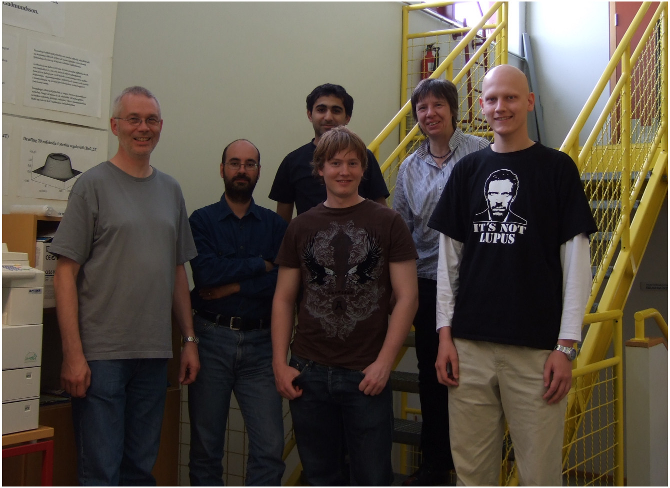
http://hartree.raunvis.hi.is/~vidar/Rann/Fyrirlestrar/Nice0610.pdf

Cooperation



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Background - Motivation

Closed systems

- 2D electronic systems
- Quantum dots, wires
- Magnetic field
- FIR absorption
- Raman scattering
- Magnetization
- Coulomb interaction
- Geometry effects
- Time-dependence

Open systems

- Broad quantum wires
- Semi-infinite leads
- Band structure, geometry
- Embedded subsystems
- Lippmann-Schwinger formalism
- Non Equilibrium Greens's functions
- No interaction
- Time-dependent systems
- Weak or strong coupling

Content

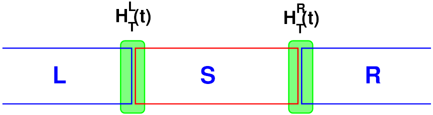
Time-dependent transport

- Generalized Master Equation (GME)
- Implementation
- Bias, Many-Electron States (MES)
- Transient effects
- Geometrical effects, resonances
- Coulomb interaction
- Correlation effects

- New Journal of Physics 11, 073019 (2009), and 113007 (2009)
- Phys. Rev. B81, 155442 (2010), and 205319 (2010)

Open System – 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 $\rho(t) = \mathrm{Tr}_\mathrm{L}\mathrm{Tr}_\mathrm{R}\{W(t)\}$



Liouville-von Neumann equation

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

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

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

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

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

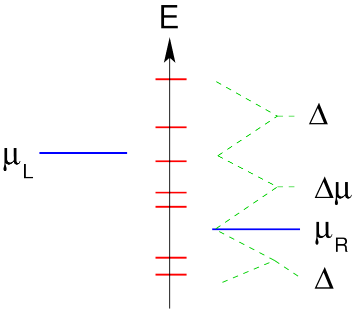
$$T \exp\left\{-i \int_s^t ds' \mathcal{QL}(s')\mathcal{Q}\right\} = \exp\{-i\mathcal{QL}_0\mathcal{Q}(t-s)\}(1+\mathcal{R})$$

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

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

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

- Integro-differential equation
- Life-times, decay rates
- Memory effects, non-Markovian
- Infinite order. . . ,(but approximation)
- Finite bias: $\Delta\mu = \mu_L - \mu_R$
- Many-body effects
- No assumption about equilibrium in leads after coupling



Relevant states

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

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

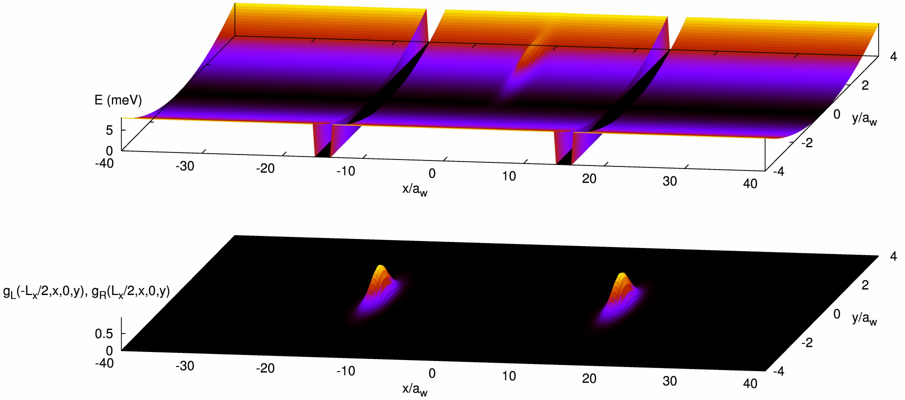
$$\Pi_{ql}(s) = e^{\frac{i}{\hbar}sH_{\mathrm{S}}} \left(\mathcal{T}^{l\dagger}\rho(s)(1-f^l) - \rho(s)\mathcal{T}^{l\dagger}f^l\right) e^{-\frac{i}{\hbar}sH_{\mathrm{S}}}$$

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

$$|\mu\rangle = |\underbrace{1, 1, ...1}_{N_0\ \text{states}}, i^\mu_{N_0+1}, ..., i^\mu_{N_{\max}}, 0, 0, ...\rangle, \quad N_{\mathrm{MES}} = 2^{N_{\mathrm{SES}}}$$

Coupling of leads

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



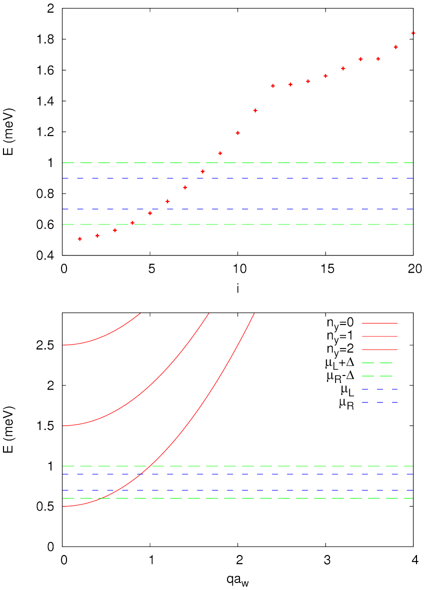
Measurable quantities

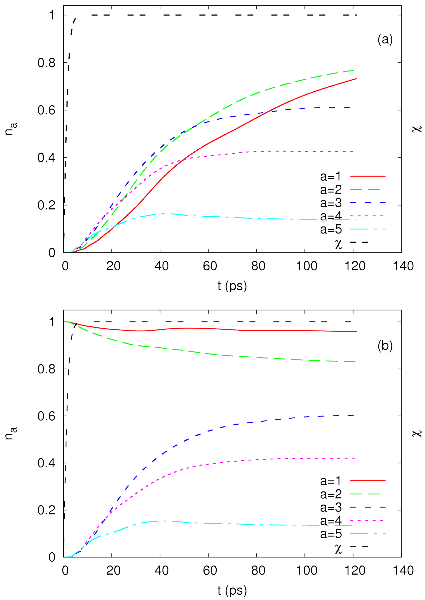
Total charge: $Q_{\rm S} = e\sum_a d_a^\dagger d_a$

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

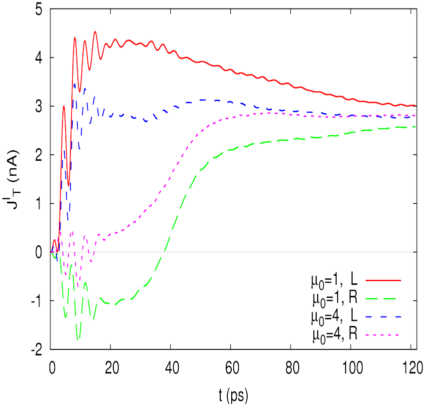
$$\langle Q_{\rm S}(\mathbf{r},t)\rangle = e\sum_{ab}\sum_{\mu\nu}\Psi_a^*(\mathbf{r})\Psi_b(\mathbf{r})\rho_{\mu\nu}(t)\langle\nu|d_a^\dagger d_b|\mu\rangle$$

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

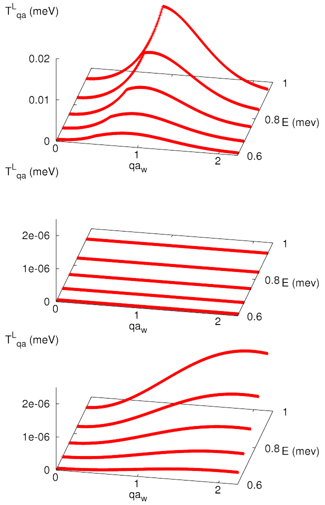

E (meV)
i
E (meV)
qa_w
n_y=0
n_y=1
n_y=2
μ_L+Δ
μ_R-Δ
μ_L
μ_R

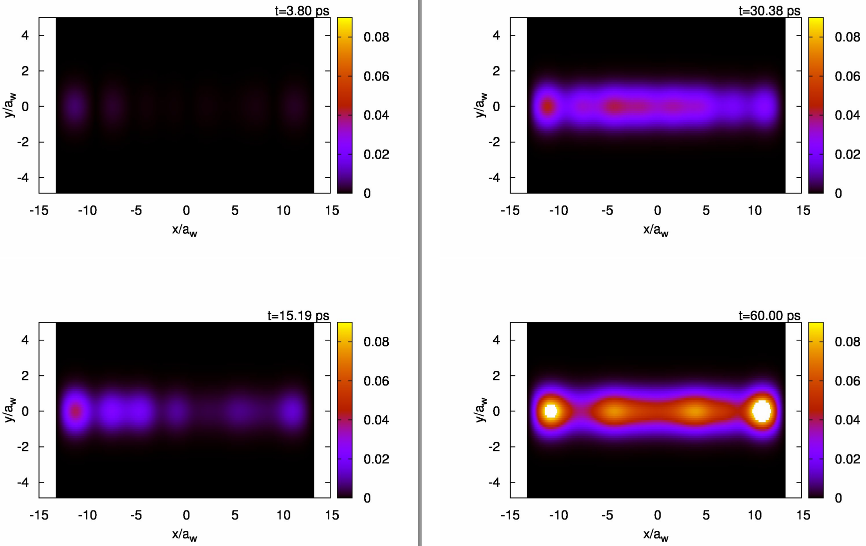

(a)
n_a
χ
t (ps)
a=1
a=2
a=3
a=4
a=5
χ
(b)
n_a
χ
t (ps)
a=1
a=2
a=3
a=4
a=5
χ

Total current

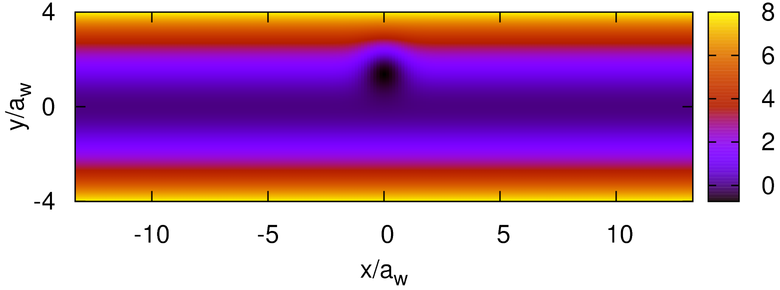


Coupling

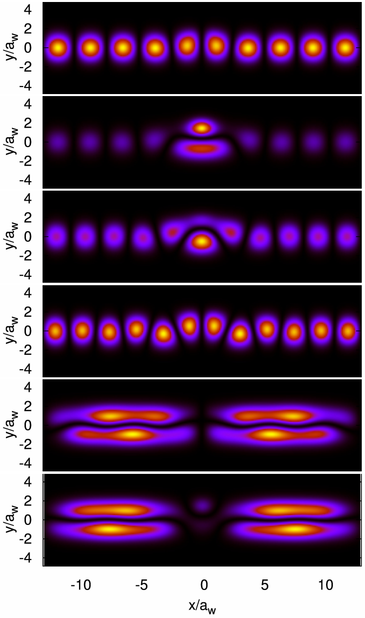



t=3.80 ps
t=30.38 ps
t=15.19 ps
t=60.00 ps
y/a_w
x/a_w
-15 -10 -5 0 5 10 15
4 2 0 -2 -4
0.08 0.06 0.04 0.02 0

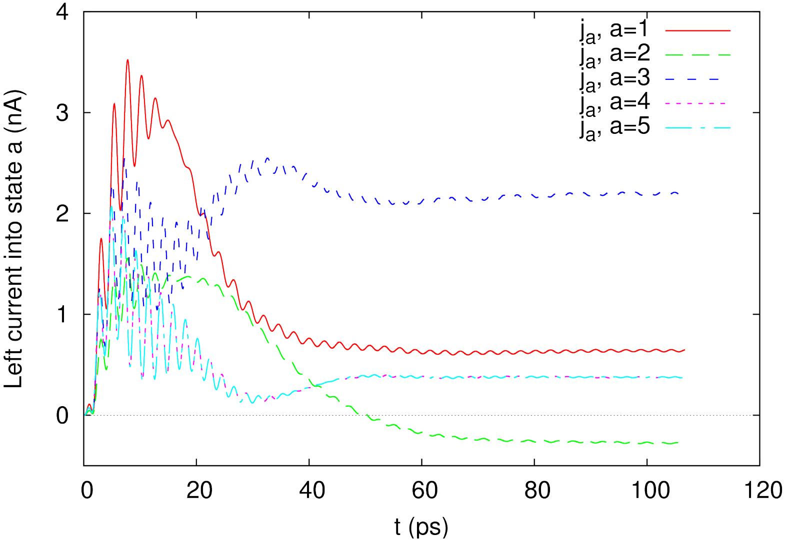
System with an off-centered Gaussian well



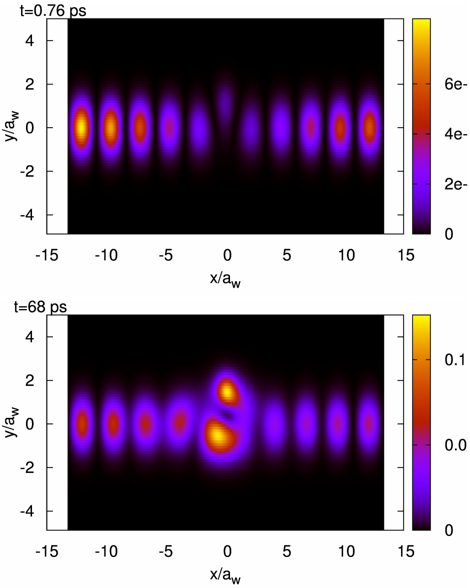
Relevant eigenstates



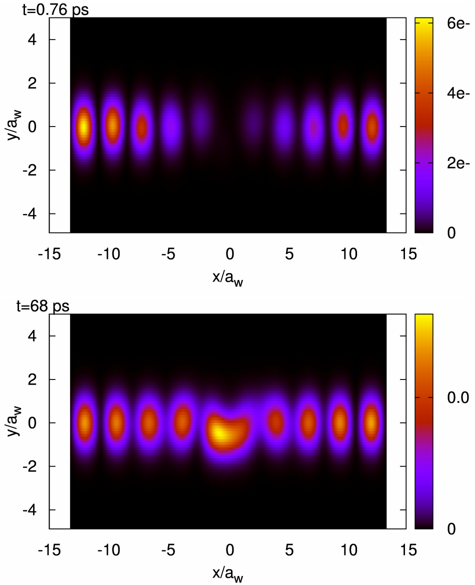
Partial left current into state a



Time-dependent charge density



... off-centered hill



Coulomb interaction

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, (exact diagonalization – configuration interaction)

$$H_{\rm S} = \sum_a E_a d_a d_a^\dagger + \frac{1}{2}\sum_{abcd} (ab|\, V_{\rm Coul} |cd)\, d_a^\dagger d_b^\dagger d_d d_c$$

$$|\mu) = \mathcal{V}|\mu\rangle, \quad \mathcal{V}^\dagger|\mu) = |\mu\rangle$$

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

$$\langle Q_s(t)\rangle_{\rm I} = {\rm Tr}_{\rm S}\{\rho(t)\, Q_s\} = {\rm Tr}_{\rm S}\{\tilde{\rho}(t)\, \tilde{Q}_s\} = {\rm Tr}_{\rm S}\{\tilde{\rho}(t)\mathcal{V}^\dagger\, Q_s \mathcal{V}\}$$

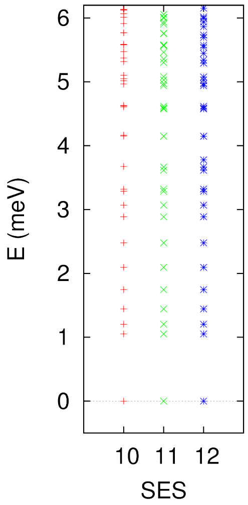
Diagonalize $H_{\rm S}$, transform GME, truncate ρ and $\{|\mu)\}$

- Phys. Rev. B81, 155442 (2010)
- Phys. Rev. B81, 205319 (2010)

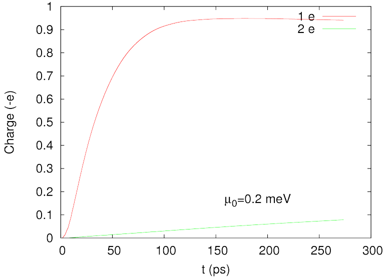
Finite quantum wire

Many-electron spectra

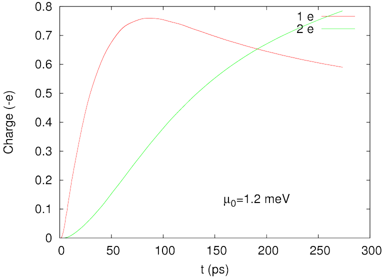
- $L_x = 300$ nm
- Parabolic confinement in y-direction, $\hbar\Omega_0 = 1.0$ meV
- Hard walls at $x = \pm L_x/2$
- $B = 1.0$ T
- GaAs parameters



$\Delta\mu = \mu_L - \mu_R = 0.2$ meV

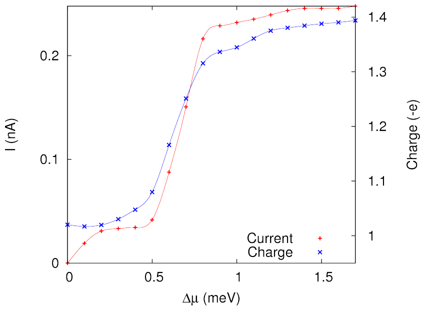


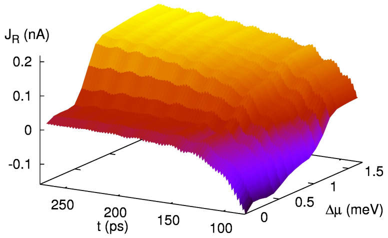
$\Delta\mu = \mu_L - \mu_R = 1.2$ meV



Finite parabolic wire, Total charge
$B = 1.0$ T, $L_x = 300$ nm, $\hbar\Omega_0 = 1.0$ meV

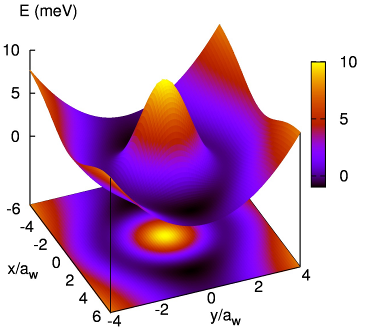
Total charge and current

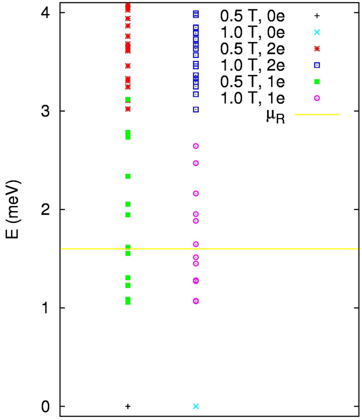




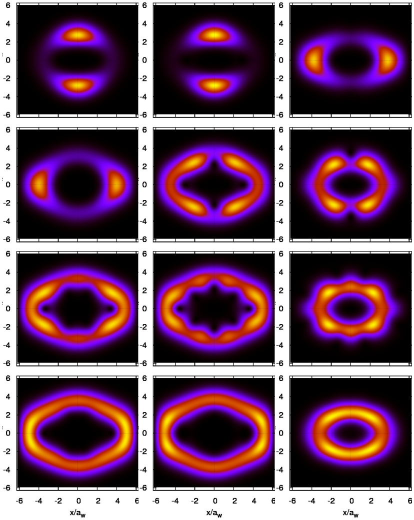
Coulomb blocking

Embedded ring

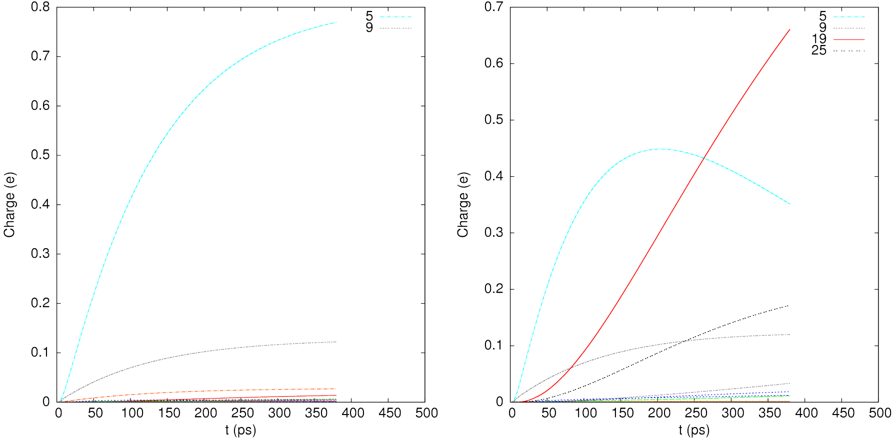




SES-probabilities

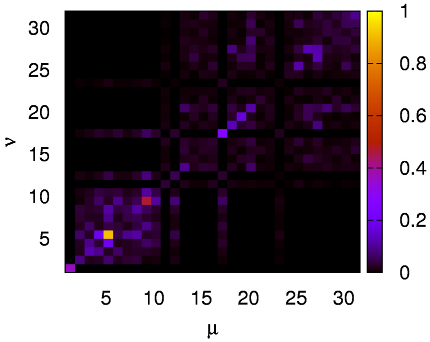


Coulomb interaction enhances occupation!

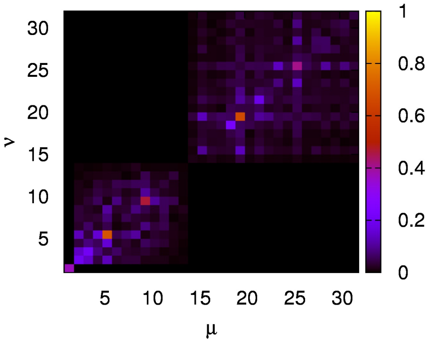


No interaction   Interaction

Correlation enhanced by Coulomb interaction

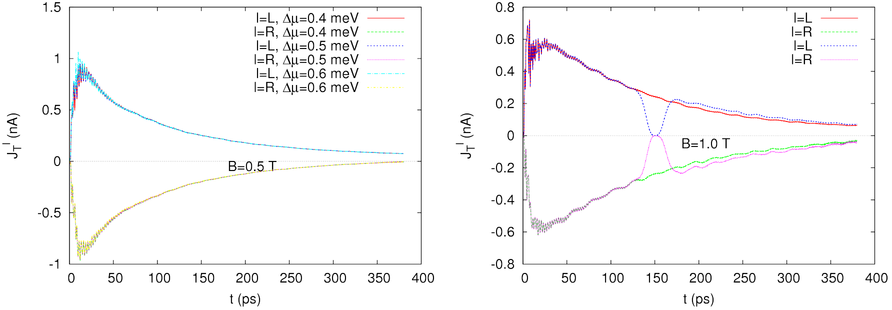


No interaction

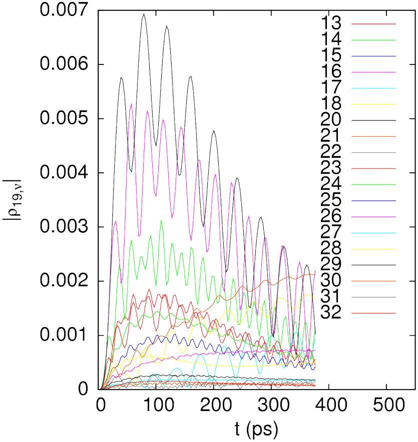


Interaction

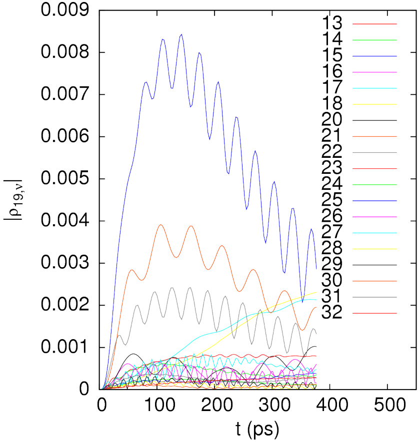
Current oscillations



Correlation oscillations



$B = 0.5$ T

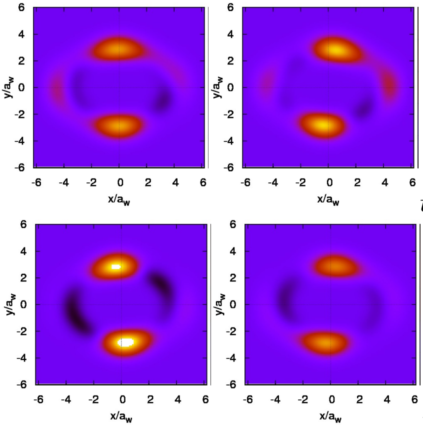


$B = 1.0$ T

Correlation oscillations

$t = 252.2$ ps

$t = 264.3$ ps



$t = 273, 4$ ps

$t = 282.5$ ps

$$n(\mathbf{r}, t) - n(\mathbf{r}, t - \delta t)$$
$$B = 1.0 \text{ T}$$

Summary

- GME-formalism
  - Bias
  - Weak coupling
  - Magnetic field
  - Many-electron formalism
  - General model
- Analytical + numerical
- Time-evolution, transients, steady state

- Coulomb interaction
  - Exact diagonalization
  - Coulomb blocking
  - Interaction enhances correlations
  - Correlation oscillations
- Geometry matters
- FORTRAN 2003 + parallelization

- Experimental systems: VM, AM, VG, Phys. Rev. B80, 205325 (2009)
- Correlations effects: VG, C-ST, OJ, VM, AM, Phys. Rev. B81, 205319 (2010)
- Cross correlation: VM, AM, VG, (arXiv:1005.3860), (2010)

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