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

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Coulomb interaction

$$\dot{\rho}_{\rm S}(t) = \frac{i}{\hbar}\left[H_{\rm S}, \rho_{\rm S}(t)\right] - \frac{1}{\hbar^2}{\rm Tr}_{\rm res}\left\{\left[H_{\rm T}(t'), \int_0^t dt' \left[U_0(t-t')H_{\rm T}(t')U_0^+(t-t') , e^{-i(t-t')H_{\rm S}/\hbar}\rho_{\rm S}(t')e^{+i(t-t')H_{\rm S}/\hbar}\right]\right]\right\}$$

can be rewritten as

$$\dot{\rho}_{\rm S}(t) = \frac{i}{\hbar}\left[H_{\rm S}, \rho_{\rm S}(t)\right] - \frac{\chi(t)}{\hbar^2}\int_0^t dt'\ \chi(t') \sum_{l=\{L,R\}} \int dq\ K[t, t', q, l; \rho_{\rm S}(t')]$$

with the kernel given by

$$
\begin{aligned}
K[t,&t', q, l; \rho_{\rm S}(t')] \\
&= \Big\{ \big[\mathcal{T}^{l}(q), U_{\rm S}^{+}(t-t')\mathcal{T}^{*l}(q)\rho_{\rm S}(t')U_{\rm S}(t-t') \big] e^{-i(t-t')\epsilon^{l}(q)/\hbar} \\
&+ \big[U_{\rm S}^{+}(t-t')\rho_{\rm S}(t')\mathcal{T}^{l}(q)U_{\rm S}(t-t'), \mathcal{T}^{*l}(q) \big] e^{+i(t-t')\epsilon^{l}(q)/\hbar} \Big\} \big(1 - f\left(\epsilon^{l}(q)\right)\big) \\
&+ \Big\{ \big[U_{\rm S}^{+}(t-t')\rho_{\rm S}(t')\mathcal{T}^{*l}(q)U_{\rm S}(t-t'), \mathcal{T}^{l}(q) \big] e^{-i(t-t')\epsilon^{l}(q)/\hbar} \\
&+ \big[\mathcal{T}^{*l}(q), U_{\rm S}^{+}(t-t')\mathcal{T}^{l}(q)\rho_{\rm S}(t')U_{\rm S}(t-t') \big] e^{+i(t-t')\epsilon^{l}(q)/\hbar} \Big\} f\left(\epsilon^{l}(q)\right)
\end{aligned}
$$

With the Coulomb interaction we had

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

Diagonalization brings

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

and with

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

we can transform the GME to the new interacting basis in which $\tilde{H}_\mathrm{S} = \mathcal{V}^\dagger H_\mathrm{S} \mathcal{V}$ is diagonal

Diagonalize H_S $\rightarrow$ transform GME unitarily $\rightarrow$ truncate ρ_S and $\{|\mu)\}$, truncation is not possible before transformation

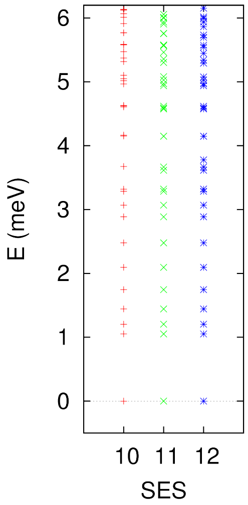
Operators can be represented in either basis and transformed between them

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

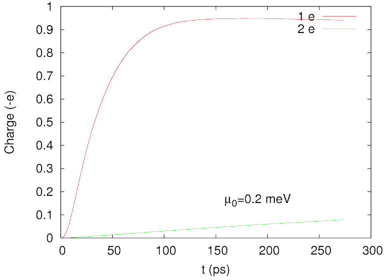
Finite quantum wire

Many-electron spectra

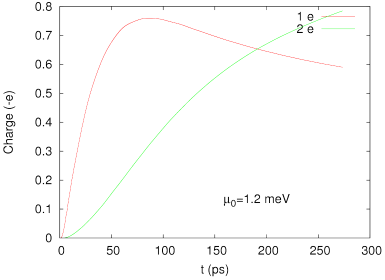
- $L_x = 300$ nm
- Parabolic confinement in y-direction, $\hbar\Omega_0 = 1.0$ meV
- Hard walls at $x = \pm L_x/2$
- $B = 1.0$ T
- GaAs parameters



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



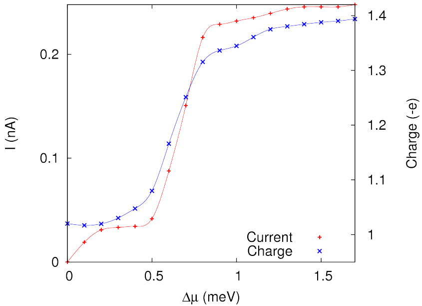
$\Delta\mu = \mu_L - \mu_R = 1.2$ meV

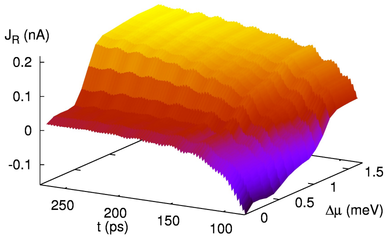


Finite parabolic wire, Total charge

$B = 1.0$ T, $L_x = 300$ nm, $\hbar\Omega_0 = 1.0$ meV

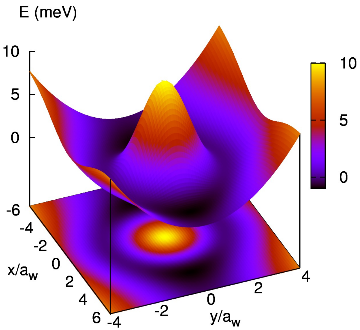
Total charge and current

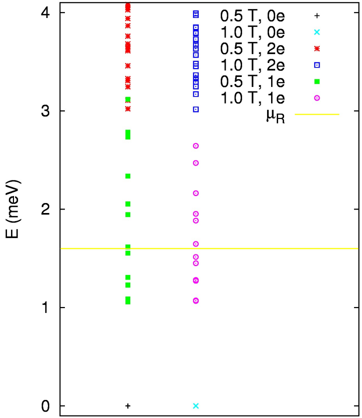




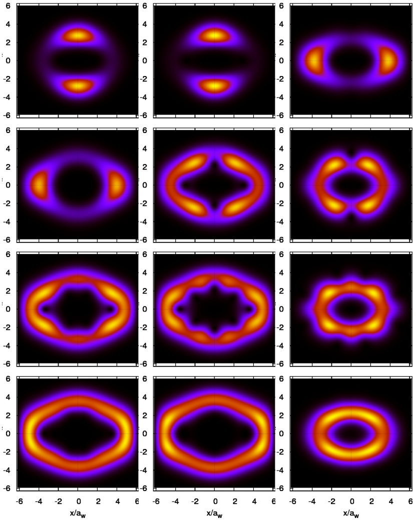
Coulomb blocking

Embedded ring

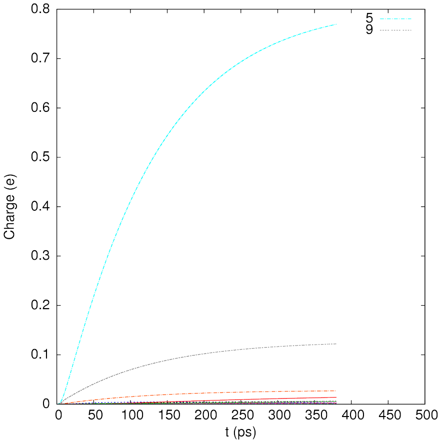




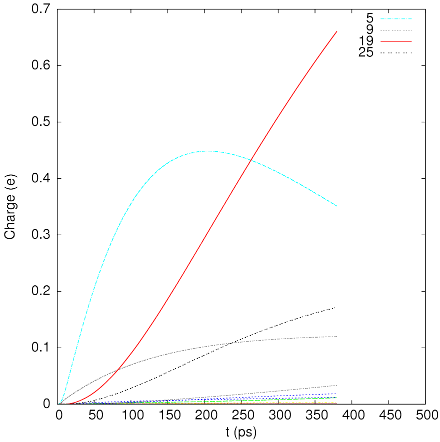
SES-probabilities



Coulomb interaction enhances occupation!

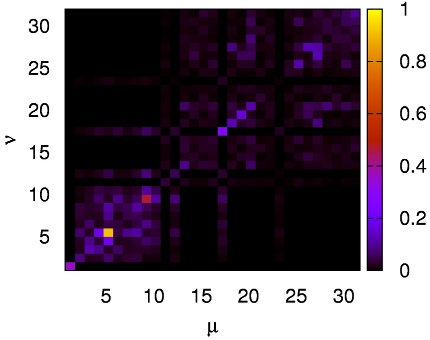


No interaction

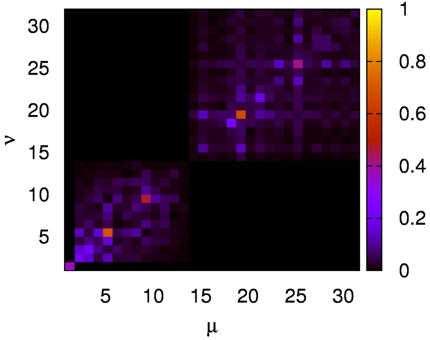


Interaction

Correlation enhanced by Coulomb interaction

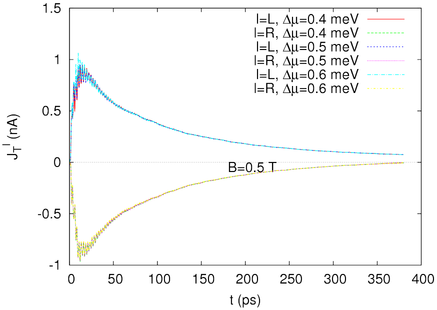


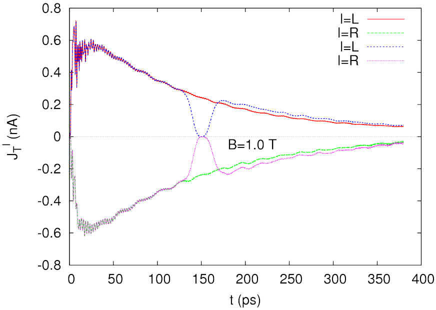
No interaction



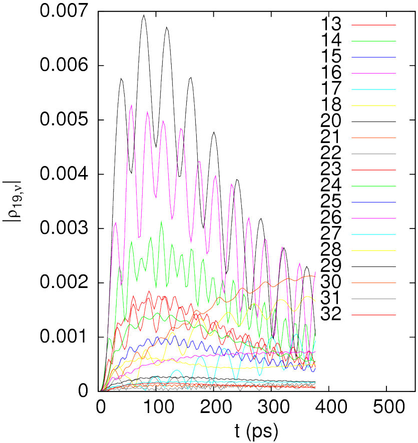
Interaction

Current oscillations

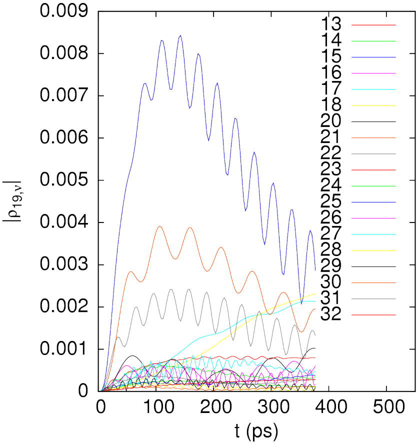




Correlation oscillations

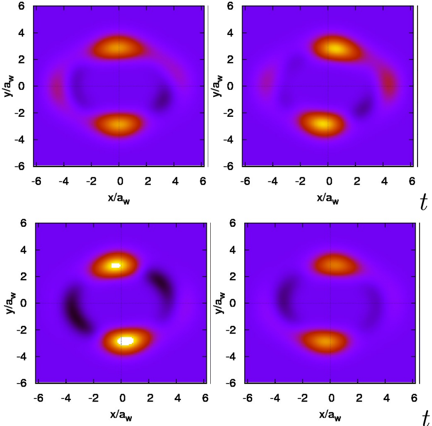


$B = 0.5$ T



$B = 1.0$ 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
- System extensions possible

Step-wise introduction of complexity – step-wise truncation of Fock spaces

References

- Transient charging: VM, AM, CST, VG, Phys. Rev. B81, 155442 (2010)
- Experimental systems: VM, AM, VG, Phys. Rev. B80, 205325 (2009)
- Correlations effects: VG, CST, OJ, VM, AM, Phys. Rev. B81, 205319 (2010)
- Dynamic cross correlation: VM, AM, VG, Phys. Rev. B82, 085311 (2010),