Time-dependent magnetotransport in semiconductor nanostructures via the generalized master equation

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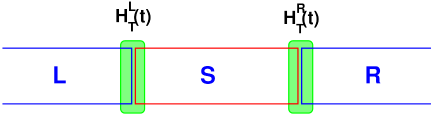
Generalized Master Equation Approach

- 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 $\rho(t) = \mathrm{Tr_L}\mathrm{Tr_R}\{W(t)\}$



Liouville-von Neumann equation

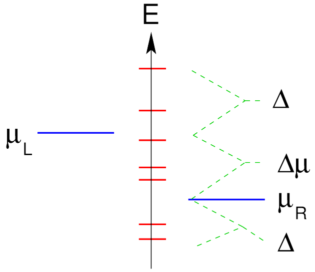
$$\dot{W}(t) = -\frac{i}{\hbar}[H(t), W(t)]$$

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

$$\langle A(t)\rangle = \mathrm{Tr}\{W(t)A\} = \mathrm{Tr_S}\{[\mathrm{Tr_L}\mathrm{Tr_R}\,W(t)]A\} = \mathrm{Tr_S}\{\rho(t)A\}$$

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H_{\mathrm{S}}, \rho(t)] + \int_0^t dt' \mathcal{K}[t, t'; \rho(t')]$$

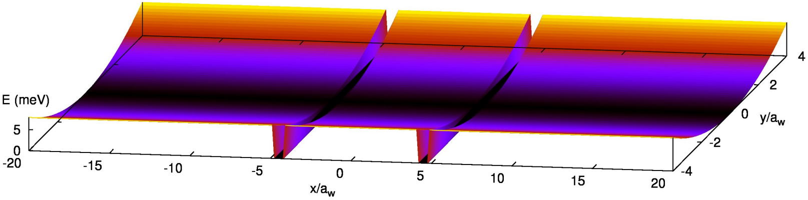
- Integro-differential equation
- Life-times, decay rates
- Memory effects, non-Markovian
- Infinite order, (approx. in kernel)
- Finite bias
- Magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$
- Correlation effects
- No assumption about equilibrium in leads after coupling

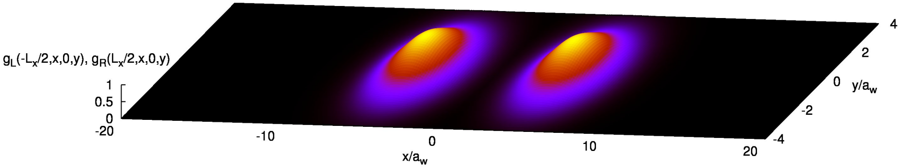


SES: $a \in \{1, 2, 3, \cdots, N_{\mathrm{SES}}\}$
MES: $|i_1^\mu, i_2^\mu, i_3^\mu, \cdots, i_{N_{\mathrm{SES}}}^\mu\rangle = |\mu\rangle$
$i_a^\mu \in \{0, 1\}$

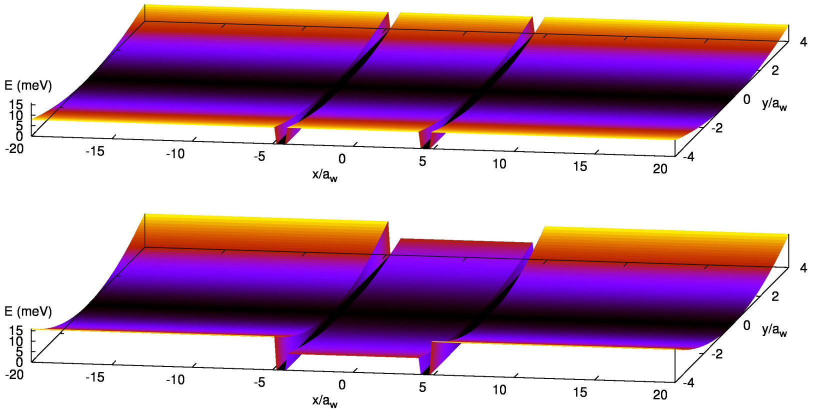
Coupling of leads

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

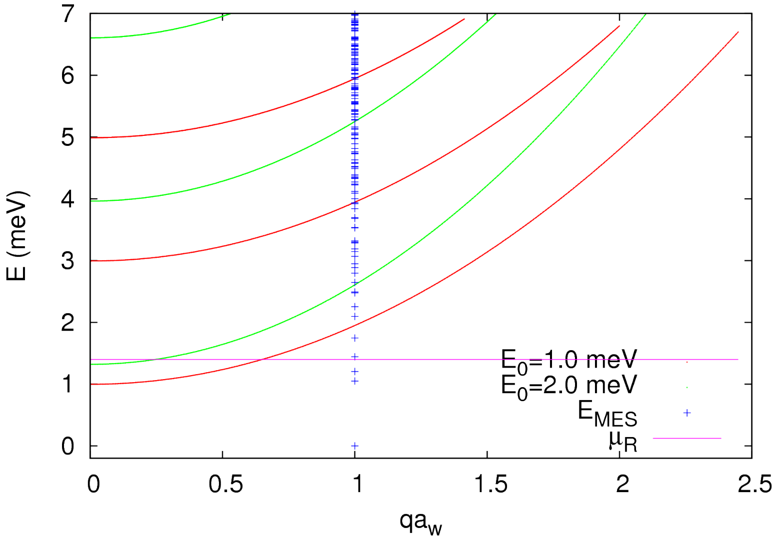




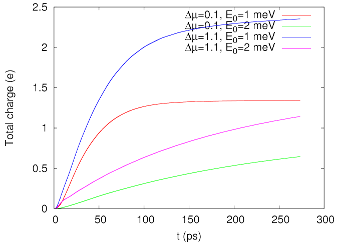
Width of leads, broad ↔ narrow

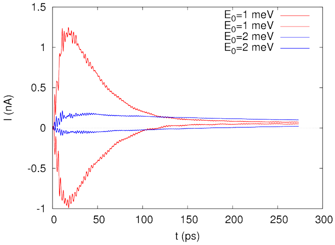


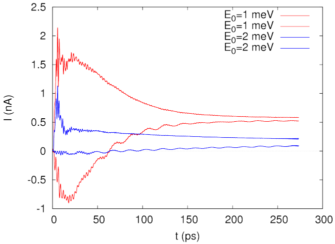
Energy spectra, leads (SES), system (MES), $B = 1.0$ T



Total charge and current







System empty at $t = 0$

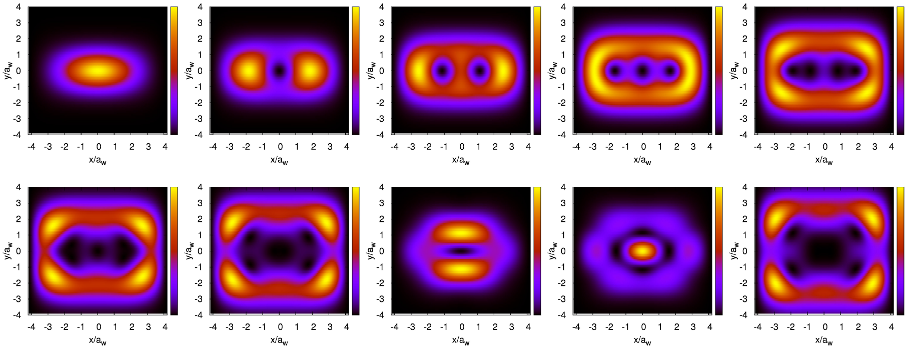
Charging, transient

Steady state

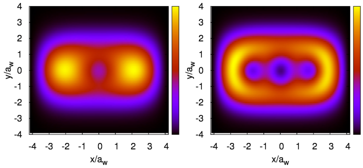
$B = 1.0$ T

$\Delta\mu = 0.1$ or 1.1 meV

10 lowest SES in the closed system, $B = 1.0$ T



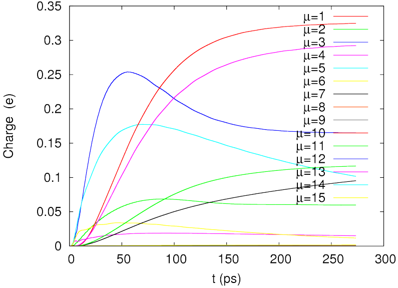
MES charge density at $t = 200$ ps, $\Delta\mu = 0.6$ meV, open system

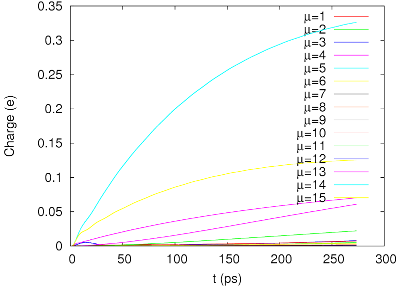


Broad, $E_0 = 1$ meV

Narrow, $E_0 = 2$ meV

Partial charge in each MES





Broad leads

$|01.00000000\rangle$

$|01.10000000\rangle$

$|01.01000000\rangle$

$\dots$

Narrow leads

$|00.10000000\rangle$

$|00.11000000\rangle$

$|00.10100000\rangle$

$\dots$

Occupied excited MES's, μ_R : .

Summary

- GME
- Magnetotransport
- Weak coupling
- Geometry, leads, system
- Bias
- Many-electron formalism
- Coulomb interaction

- Fortran 2003
- OpenMP parallelization
- Linux
- U of I Research Fund
- Equipment Fund of IS
- Research Fund of IS
- NCTS at NTHU, HsinChu

For background see: New Journal of Physics 11, 113007 (2009)