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

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Choice of method

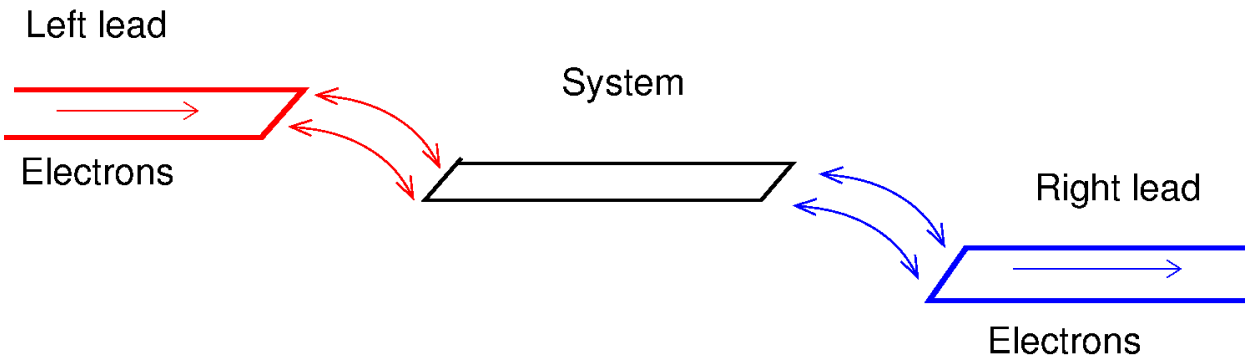
- Lippmann-Schwinger scattering formalism
- R-matrix scattering formalism
- Non-equilibrium Green's functions (NEGF)
- Generalized master equation (GME)

Here, I shall detail the construction of a transport model based on the GME with computational implementation in mind

Model

For $t < 0$ in equilibrium

$$H_{\mathrm{S}} + H_{\mathrm{Coul}}, \quad H_{\mathrm{L}}, \quad H_{\mathrm{R}}$$



Coupled at $t = 0$

$$H_{\mathrm{S}} + H_{\mathrm{Coul}} + H_{\mathrm{L}} + H_{\mathrm{R}} + H_{\mathrm{T}}(t)$$

Central system

- Variable electron number
- Coulomb interaction
- Complex geometry + magnetic field

$$\Downarrow$$

- Many-body theory
- Exact diagonalization
- Grid-free $\rightarrow$ functional basis

Single-electron states $\rightarrow$ construction of many-electron states

Single-electron basis for a finite system

Consider, for example, finite parabolic quantum wire with Hamiltonian

$$h_{\mathrm{S}} = -\frac{\hbar^2}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + \frac{1}{2}m\Omega_0^2 y^2 + V(x,y)$$

Landau gauge $\mathbf{A} = (-By, 0)$

$$h_{\mathrm{S}} = -\frac{\hbar^2}{2m}\left(\nabla^2 - \frac{2i}{l^2}y\partial_x - \frac{y^2}{l^4}\right) + \frac{1}{2}m\Omega_0^2 y^2 + V(x,y)$$

with $l^2 = (c\hbar/(eB))$ and boundary conditions for wavefunctions $\psi(\pm L/2, y) = 0$, and $\psi(x, y \to \pm\infty) = 0$

The Schrödinger equation will not be separable

Possible basis $\psi^0_{n_x n_y}(x,y) = \varphi^0_{n_x}(x)\phi^0_{n_y}(y)$ with

$$\phi^0_{n_y}(y) = \frac{e^{-\frac{y^2}{2a_w}}}{\sqrt{2^{n_y}\sqrt{\pi}n_y!a_w}} H_{n_y}\left(\frac{y}{a_w}\right)$$

$$\varphi^0_{n_x}(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{n_x\pi x}{L}\right), & n_x = 1,3,5,\cdots \\ \sqrt{\frac{2}{L}}\sin\left(\frac{n_x\pi x}{L}\right), & n_x = 2,4,6,\cdots \end{cases}$$

where $l^2\omega_c = a_w^2\Omega_w = \hbar/m$, $\Omega_w = \sqrt{\Omega_0^2 + \omega_c^2}$, and $\omega_c = eB/(mc)$

Diagonalization

The basis is the eigenstates of h_{S} if V and the $y\partial_x$-term were neglected, we call that Hamiltonian h_0 with eigenvalues $E^0_{n_x n_y}$

Expand the eigenstates of h_{S} in the basis

$$\psi_a(x,y) = \sum_{n_x n_y}^{\infty} C_{a,n_x n_y} \varphi^0_{n_x}(x) \phi^0_{n_y}(y)$$

Use the notation $|a)$ and here $|n_x n_y\rangle$

$$|a) = \sum_{n_x n_y}^{\infty} C_{a,n_x n_y} |n_x n_y\rangle$$

for the states

The equation

$$h_{\mathrm{S}}|a) = E_a|a)$$

can be solved by using

$$\langle m_x m_y|h_{\mathrm{S}}|a) = \langle m_x m_y|E_a|a)$$

and using the state expansion to obtain

$$\sum_{n_x n_y}^{\infty} \left\{\langle m_x m_y|h_0|n_x n_y\rangle + \langle m_x m_y|h_{\mathrm{S}} - h_0|n_x n_y\rangle\right\} C_{a,n_x n_y} = E_a C_{a,m_x m_y}$$

or

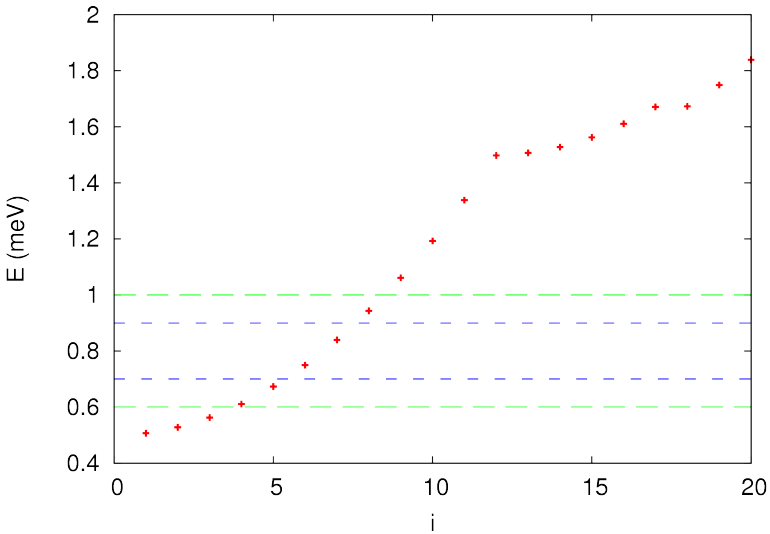
$$\sum_{n_x n_y}^{\infty} \left\{E^0_{n_x n_y}\delta_{n_x n_y,m_x m_y} + \langle m_x m_y|h_{\mathrm{S}} - h_0|n_x n_y\rangle\right\} C_{a,n_x n_y} = E_a C_{a,m_x m_y}$$

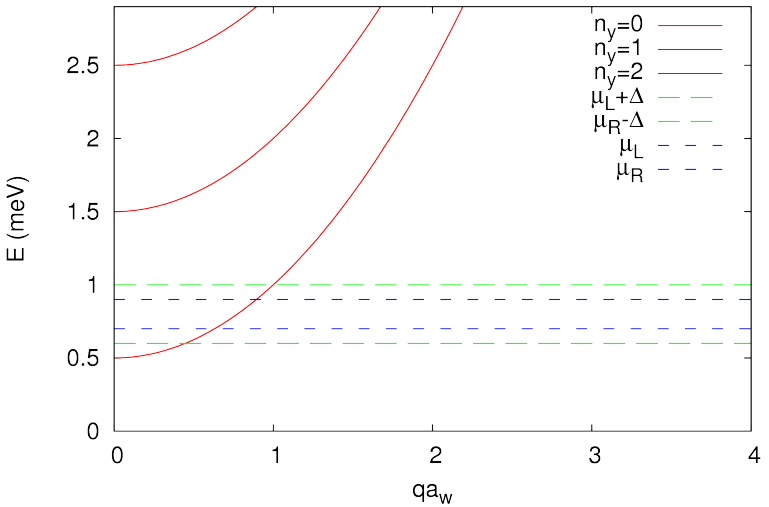
An eigenvalue problem giving the eigenspectrum E_a, and the eigenvectors supply the expansion coefficients $C_{a,n_x n_y}$

We truncate the eigenvalue equation and obtain eigenstates and spectrum with high accuracy beyond any simple finite order perturbation expansion!

The single-electron states in the semi-infinite leads can also be found by similar methods giving $|nq)^l$ and E^l_{nq}, with $l = L, R$ and q a continuous quantum number representing the momentum

In external magnetic field spectrum of the leads can be found by analytically integrating the eigenvalue equation over q in the complex plane, and solving numerically the n-part for the band index n





Many-electron basis $\{|\mu\rangle\}$

Select N_{SES} single-electron states, (for ex. the lowest ones...) and build $N_{\mathrm{MES}} = 2^{N_{\mathrm{SES}}}$ many-electron states in Fock space

$$|\mu\rangle = |i_1^\mu, i_2^\mu, i_3^\mu, \cdots, i_{N_{\mathrm{SES}}}^\mu\rangle, \quad i_a^\mu = \{0,1\}, \text{Fermions}$$

Creation and annihilation operators

$$\text{Creation operator:} \quad d_d^\dagger |\cdots, i_d^\mu, \cdots\rangle = (1 - i_d^\mu)(-1)^{\gamma_d^\mu} |\cdots, (i_d^\mu + 1), \cdots\rangle$$

$$\text{Annihilation operator:} \quad d_d |\cdots, i_d^\mu, \cdots\rangle = i_d^\mu (-1)^{\gamma_d^\mu} |\cdots, (i_d^\mu - 1), \cdots\rangle$$

$$\gamma_d^\mu = \sum_{s=1}^{d-1} i_s^\mu$$

Introduction of the field operator

$$\psi(\mathbf{r}) = \sum_a \psi_a(\mathbf{r})\, d$$

with the many-electron Hamiltonian

$$\begin{aligned} H &= \int d\mathbf{r}\; \psi^\dagger(\mathbf{r})(h_{\mathrm{S}} + h_{\mathrm{Coul}})\psi(\mathbf{r}) \\ &= \sum_a E_a\, d_a^\dagger d_a + \sum_{abcd} (ab|\, V_{\mathrm{Coul}}|cd)\, d_a^\dagger d_b^\dagger d_d\, d_c \end{aligned}$$

where

$$(ab|\, V_{\mathrm{Coul}}|cd) = \int d\mathbf{r}\, d\mathbf{r}'\; \psi_a^*(\mathbf{r})\psi_b^*(\mathbf{r}')\, V_{\mathrm{Coul}}(|\mathbf{r}-\mathbf{r}'|)\psi_c(\mathbf{r}')\psi_d(\mathbf{r})$$

and

$$V_{\mathrm{Coul}}(|\mathbf{r}-\mathbf{r}'|) = \frac{e^2}{\kappa\sqrt{(x-x')^2 + (y-y')^2 + \eta^2}}, \quad \eta \to 0^+$$

For numerical evaluation

$$(ab|\,V_{\rm Coul}|cd) = \int d\mathbf{r}\;\psi_a^*(\mathbf{r})I_{bc}(\mathbf{r})\psi_d(\mathbf{r})$$

with

$$I_{bc}(\mathbf{r}) = \int d\mathbf{r}'\;\psi_b^*(\mathbf{r}')\,V_{\rm Coul}(|\mathbf{r}-\mathbf{r}'|)\psi_c(\mathbf{r}')$$

Practical points

We need spectra and states for any number of electrons $0 - N_{\rm SES}$

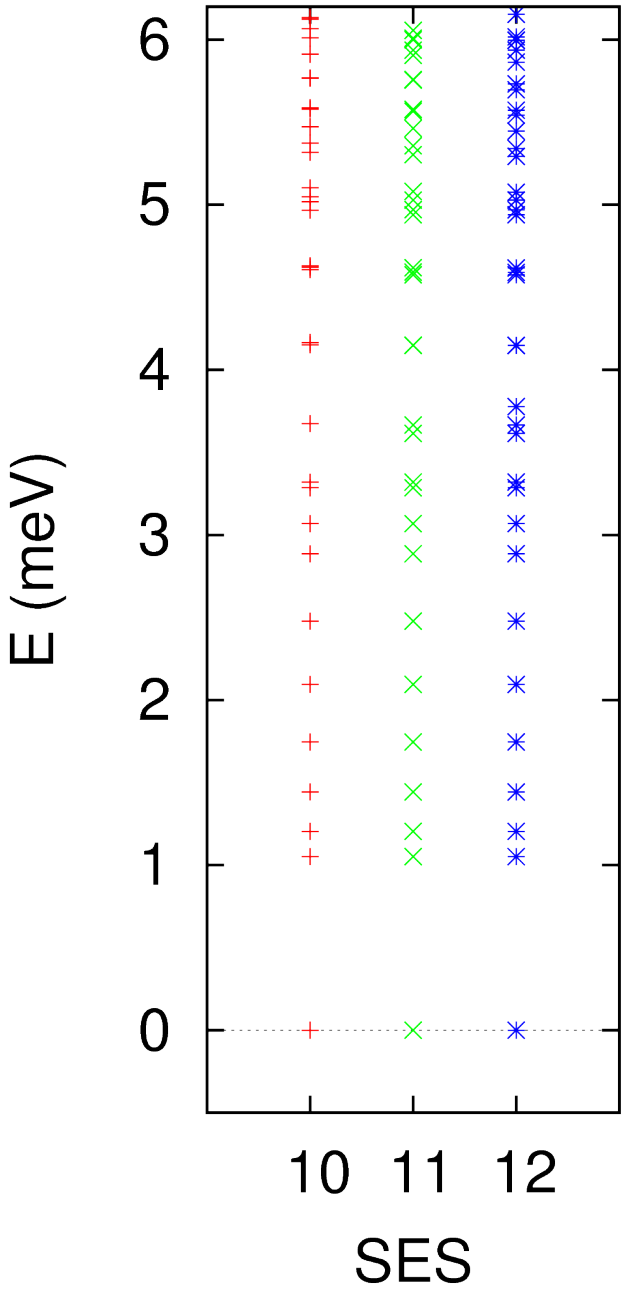
- We need all binary vectors $|\mu\rangle = |i_1^\mu, i_2^\mu, i_3^\mu, \cdots, i_{N_{\rm SES}}^\mu\rangle$
- Label them $\mu =$ binary value of $i_1^\mu\, i_2^\mu\, i_3^\mu \cdots i_{N_{\rm SES}}^\mu$
- Need $c_a|\mu\rangle$ and $c_a^\dagger|\mu\rangle$
- Need $\langle\mu|d_a^\dagger d_b^\dagger d_d\, d_c|\nu\rangle$, fast but copious integer evaluations

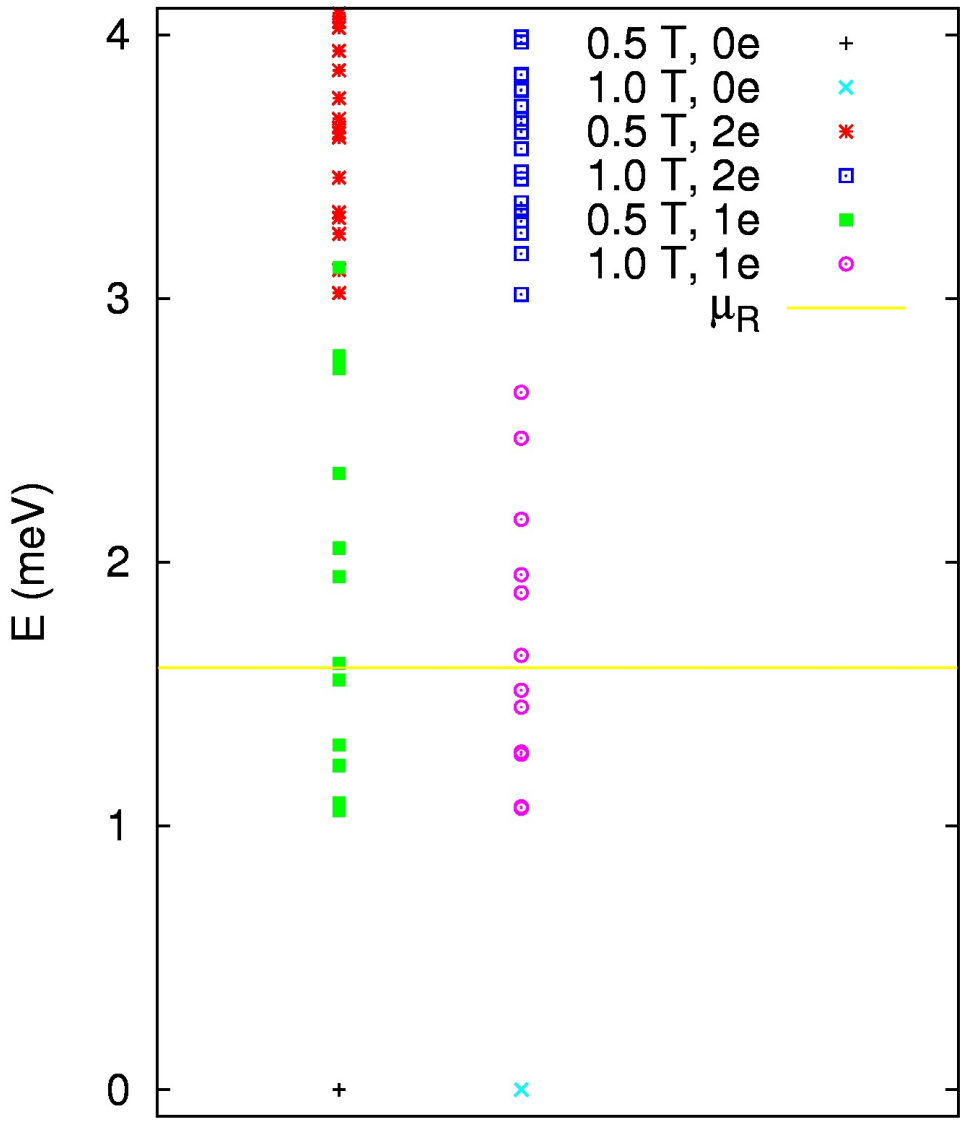
Build matrix elements $\langle\mu|H|\nu\rangle$ diagonalize $\rightarrow$ energy spectrum $\tilde{E}_\mu$ and states $|\mu)$ that are equivalent to an expansion over all possible Slater determinants, (here an expansion over all possible Fock states)

Unitary transformation between the noninteracting and the interacting basis is the matrix of eigenvectors

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

The methods is called "Exact numerical diagonalization" or "Configuration interaction"


E (meV)
0
1
2
3
4
5
6
10
11
12
SES


E (meV)
0
1
2
3
4
0.5 T, 0e
1.0 T, 0e
0.5 T, 2e
1.0 T, 2e
0.5 T, 1e
1.0 T, 1e
μR

Play with transformations

$$\sum_a E_a d_a^\dagger d_a = \sum_{\mu\nu a} E_a |\mu\rangle\langle\mu| d_a^\dagger d_a |\nu\rangle\langle\nu| = \sum_\mu \left\{ \sum_a E_a i_a^\mu \right\} |\mu\rangle\langle\mu| = \sum_\mu E_\mu |\mu\rangle\langle\mu|$$

or

$$\sum_a E_a d_a^\dagger d_a = \sum_{\mu\nu a} E_a |\mu)(\mu| d_a^\dagger d_a |\nu)(\nu| = \sum_\mu |\mu) \left\{ \sum_a E_a (\mu| d_a^\dagger d_a |\mu) \right\} (\mu|$$

$$= \sum_\mu |\mu) \left\{ \sum_a E_a (\mu| N_a |\mu) \right\} (\mu| = \sum_\mu |\mu\rangle \mathcal{V} \left\{ \sum_a E_a \langle\mu| \mathcal{V}^+ N_a \mathcal{V} |\mu\rangle \right\} \langle\mu| \mathcal{V}^+$$

$$= \mathcal{V} \left[\sum_\mu |\mu\rangle \left\{ \sum_a E_a \langle\mu| \tilde{N}_a |\mu\rangle \right\} \langle\mu| \right] \mathcal{V}^+ = \mathcal{V} \left[\sum_\mu |\mu\rangle \tilde{E}_\mu \langle\mu| \right] \mathcal{V}^+$$

$$= \sum_\mu |\mu) \tilde{E}_\mu (\mu|$$

References

- Details about a single-electron properties of a finite quantum wire, Líney Halla Kristinsdóttir, “Finite wire in a magnetic field with a Gauss potential”, `http://hartree.raunvis.hi.is/~vidar/Nam/TE/Verkefni/LHK.pdf`
- Inofficial, but very valuable: Daniela Pfannkuche, “Aspects of Coulomb Interaction in Semiconductor Nanostructures”, `http://hartree.raunvis.hi.is/~vidar/Rann/habil_DP.pdf`
- In contrast, a good text with programs about mean-field interacting electrons on a ring, Sigríður Sif Gylfadóttir, “Electrons on a ring”, `http://hartree.raunvis.hi.is/~vidar/Nam/TE/Verkefni/SSG.pdf`