Nano- és mikro feladatok modellezése az EQuUs keretrendszerrel.

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Non-equilibrium Green's function theory

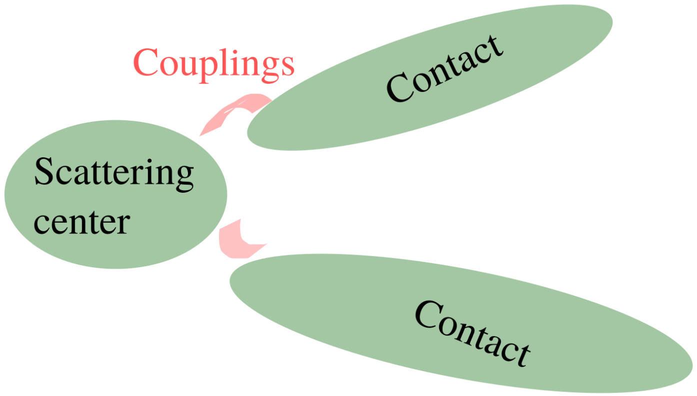
- expectation value of operator A in Heisenberg picture:

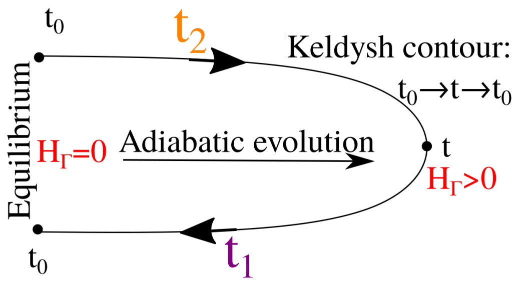
$$\langle A(t)\rangle = \mathrm{Tr}\left[\rho_0 A(t)_H\right]$$

$$A(t)_H = e^{\mathrm{i}\int_{t_0}^{t} \mathrm{d}t' H(t')} A e^{-\mathrm{i}\int_{t_0}^{t} \mathrm{d}t' H(t')}$$

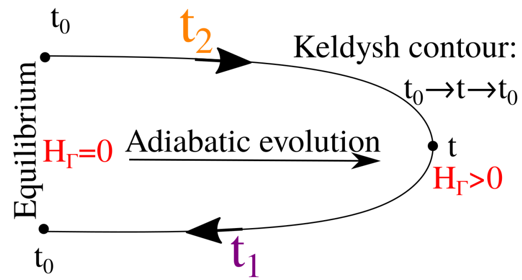
- Hamiltonian: $H(t) = H_0 + H_\Gamma(t)$
- Coupling is adiabatically turned on
- $e^{\mathrm{i}H_0 t}$ can be evaluated analytically/numerically $\left(a_n^\dagger(t)_{H_0} = e^{\frac{\mathrm{i}}{\hbar}E_n t} a_n^\dagger\right)$
- Interaction picture:

$$A(t)_H = e^{-\mathrm{i}\int_{t}^{t_0} \mathrm{d}t_1 H_\Gamma(t_1)} A(t)_{H_0} e^{-\mathrm{i}\int_{t_0}^{t} \mathrm{d}t_2 H_\Gamma(t_2)}$$





Evaluate the Green's functions

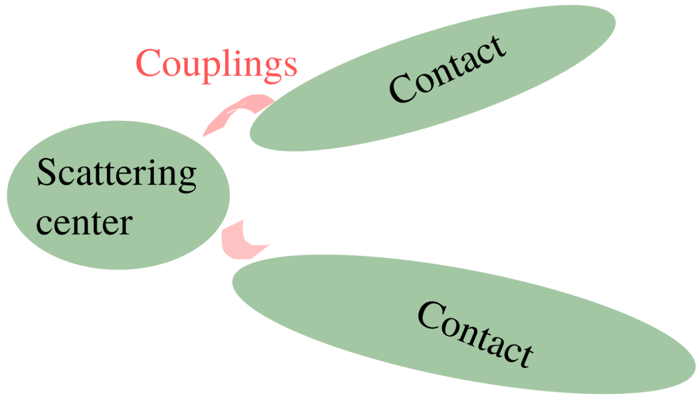


- Lesser Green's function: $A = G^<(t_1, t_2) = -\mathrm{i}\langle \Psi_H^\dagger(t_2)\Psi_H(t_1)\rangle$

$$G^<(t,t') = -\mathrm{i}\langle T_C \left[S_C^H \Psi_{H_0}^\dagger(t')\Psi_{H_0}(t) \right]\rangle$$

$$S_C^H = \exp\left[-\mathrm{i}\int_C \mathrm{d}\tau H_\Gamma(\tau) \right]$$

- T_C: contour-ordering operator



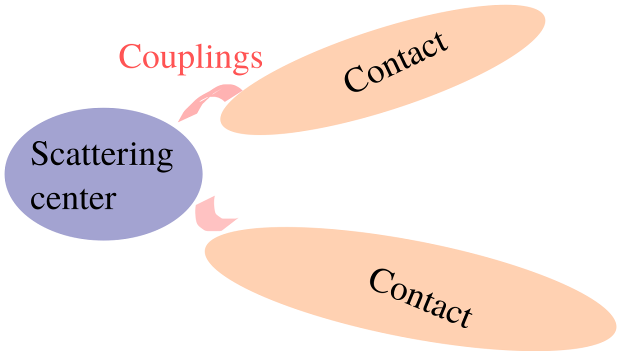
$G^<(t_1, t_2)$ **can be calculated using Wick's theorem** and

- (a) evaluate the Dyson equation
- (b) evaluate the perturbation series: diagrammatic technique.

Diagrammatic technique

Capable to describe Coulomb blockade transport regime

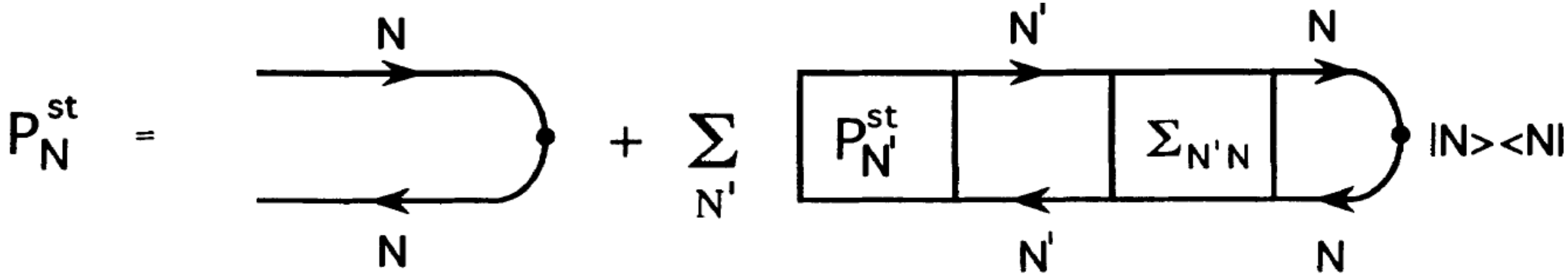
H. Schoeller, G. Schön, PRB **50**, 18436 (1994)



- Hamiltonian of the uncoupled system:
  $$H_0 = H_{central} + E_C\left(\hat{N} - n_x\right)^2 + \sum H_{contact}$$
- E_C: the charging energy
- $$H_\Gamma = \sum_{r=L,R}^{contacts} \sum_{kln}^{states} \left(T_{kl}^{rn} a_{krn}^\dagger c_{ln} e^{-\mathrm{i}\hat{\phi}} + h.c.\right)$$
- $[\hat{\phi}, \hat{N}] = \mathrm{i}$: canonically conjugated pairs
- $e^{\pm\mathrm{i}\hat{\phi}}$ changes the occupation number N by ± 1.
- approximation: $\hat{N}$ is independent of c_{ln}
- Perturbation series in $H_\Gamma \Rightarrow$ Feynman diagrams of the individual processes.

Reduced density matrix of the central region (QD)

- H_Γ tunneling changes the probability P_N of the state $A = |N\rangle\langle N|$ of the quantum dot.
- Dyson equation for the operator $A = |N\rangle\langle N|$:



- Time derivation $\Rightarrow$ Master equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} P_N(t) = \sum_{N' \neq N} \int_{t_0}^{t} \mathrm{d}t' \left[P_{N'}(t')\Sigma_{N',N}(t',t) - P_N(t')\Sigma_{N,N'}(t',t) \right]$$

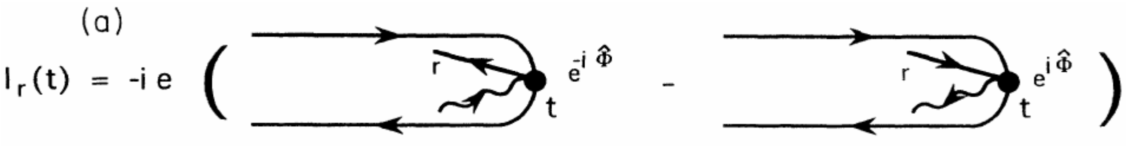
- Self energy $\Sigma_{N,N'}$ is a sum of irreducible diagrams
- Stationary solution: $\frac{\mathrm{d}}{\mathrm{d}t} P_N^{st}(t) = 0$ is independent of the initial $P_N(t_0 = -\infty)$
- Stationary state of the QD can be described by a mixed state of states $|N\rangle$ by probabilities P_N^{st}.

Example for diagrammatic rules: current through the contact r

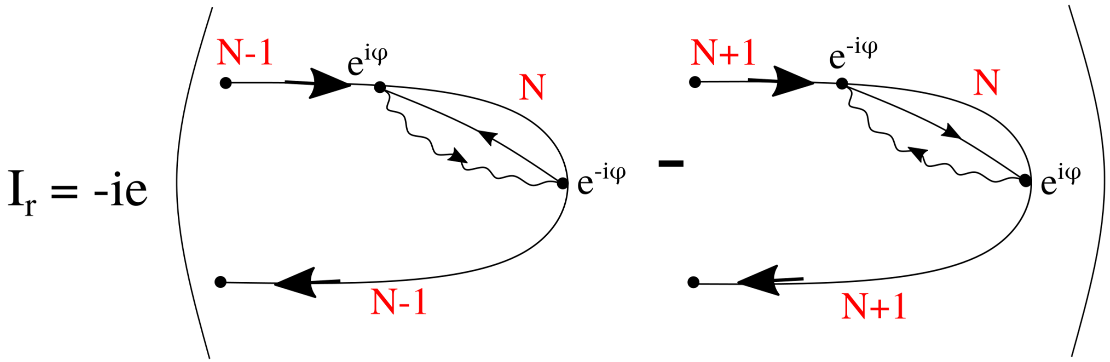
- $I_r = e\frac{\mathrm{d}}{\mathrm{d}t}\langle N_r\rangle = \mathrm{i}e\langle [H, N_r]\rangle$ (H is the full Hamiltonian)

$$I_r = -\mathrm{i}e \sum_{kln}^{states} \left(T_{kl}^{rn} \langle a_{krn}^{\dagger} c_{ln} e^{-\mathrm{i}\hat{\phi}} \rangle - c.c. \right)$$

- Current operator:



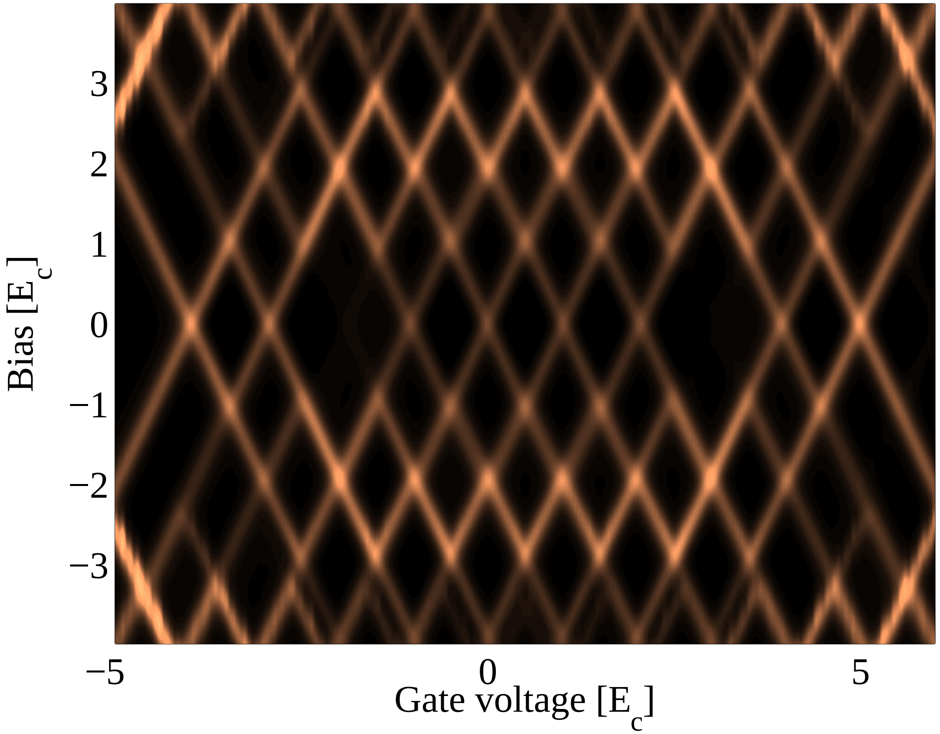
- expectation value of the current operator:



- Vertices $e^{\pm\mathrm{i}\hat{\phi}}$ are paired via contact ($\longrightarrow$) and central region ($\leadsto$) propagators using Wick's theorem

Transport through graphene QD

- Differential conductance vs bias voltage and doping gate voltage



- I. Weymann, J. Barnas, S. Krompiewsky, PRB **92**, 045427 (2015):
- central region: rectangle shaped graphene with Coulomb interaction (~ 100 sites)
- within the diamonds the current is suppressed due to the charginf energy

Motivation to do this

- Starightforward to generalize for normal-superconducting hybrid structures
- modeling nonequlibrium processes in multiterminal structures:
- unconventional Andreev interferometers
- π-Josephson transition etc.
- Cooper-pair splitting process
- Combined with EQuUs it can be used for arbitrary geometry

Acknowledgement

- NKFIH within the Quantum Technology National Excellence Program (Project No. 2017-1.2.1-NKP-2017-00001)

NEMZETI KUTATÁSI, FEJLESZTÉSI ÉS INNOVÁCIÓS HIVATAL

AZ INNOVÁCIÓ LENDÜLETE

AZ NKFI ALAPBÓL MEGVALÓSULÓ PROJEKT

- OTKA PD123927, K123894 and K108676

Non-equilibrium Green's function approach

EQuUs is a suitable tool to perform efficient numerical analisys to study non-equilibrium quantum processes in nano- and micro scaled systems in the tight-binding framework. To this end EQuUs makes use of the Keldysh non-equilibrium Green's function approach.

Variety of built-in functionalities

EQuUs supports the research work with numerous bult-in functionalities:

- inclusion of magnetic vector potentials
- various preprogrammed lattice types
- support of superconducting systems
- inclusion of external electric potential
- instant access to all the calculated data and other metadata during the scripting
- calculation of the equilibrium and non-equilibrium charge currents.
- calculate the spectral density function
- transforming direct space Hamiltonians into Fourier Hamiltonians
- etc.

Automatic Testing: backward compatibility

EQuUs contains an automatic self testing tool. All new developments can be validated, while the previous functionalities can be also tested. Thus, the compatibility of older versions of EQuUs is assured.

WEB documentation for detail-oriented users

The functionalities of EQuUs are thoroughly documented via the Doxygen tool. Since the documentation is prodeced automatically, it is always up to date. Thus, the student can find the needed functionalities of EQuUs on ther own.

Portability to many hardwares

EQuUs can be run on traditional desktops or laptops. High performance calculations can be done on CPU, GPU or MIC clusters.

Application Programing Interface: varsetile problem solving

Instead of the input file driven approach, one can chose specific set of functionalities of EQuUs according to the given research problem.
EQuUs provides two abstraction levels to access (i) low level functionalities (like calculating the group velocities of the modes, etc.) (ii) and to combine these basic functionalities in order to solve complex problems.

Efficient numerical methods

The EQuUs MKL component provides enhanced numerical efficiency (compared to MATLAB or Octave) to calculate elements of the inverse of a large sparse matrices via the Intel PARDISO solver.

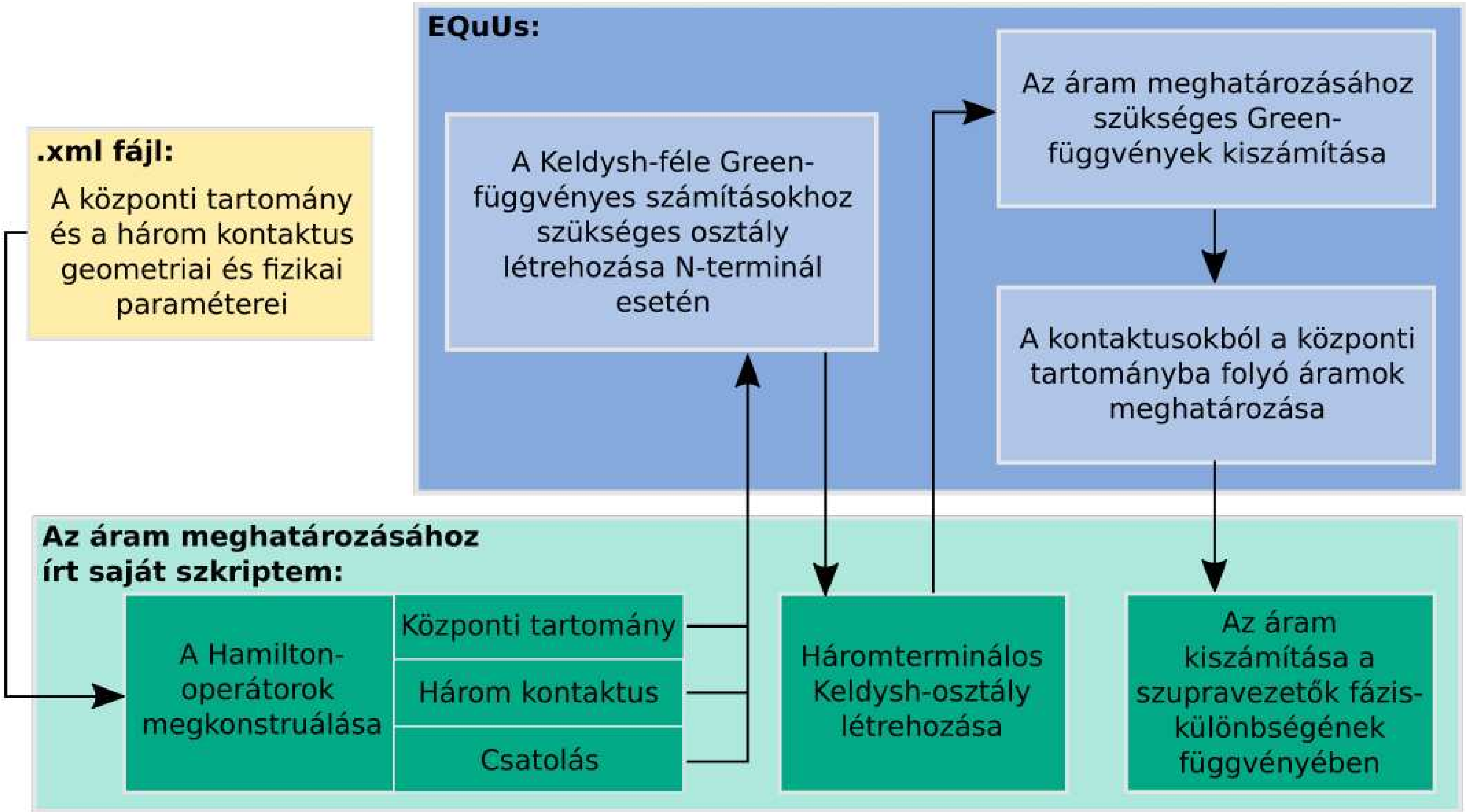
Eötvös Quantum Utilities (EQuUs)

- 1 mondatban:

Időfüggetlen egyensúlyi és nemegyensúlyi Green-függvényes technikák nano- és mikro méretű minták tight binding minták kvantumos modellezése

- **Jelenleg aktív** 15203 **kódsort tartalmaz**
- **Automatikus ön-tesztesztelési eljárás** (minden mérföldkő hibátlanul teljesíti, minden új funkcionalitásnál bővül a teszteljárás)
- **Webes dokumentáció az elérhető API szintű funkcionalitásokról** (algoritmusok, adatstruktúrák)

Diákok vs EQuUs



- A diákok elérhetik és kombinálhatják a bonyolult funkcionalitásokat
- Lerövidül az idő, mialatt a diákok bekapcsolódhatnak egy-egy kutatási projektekbe