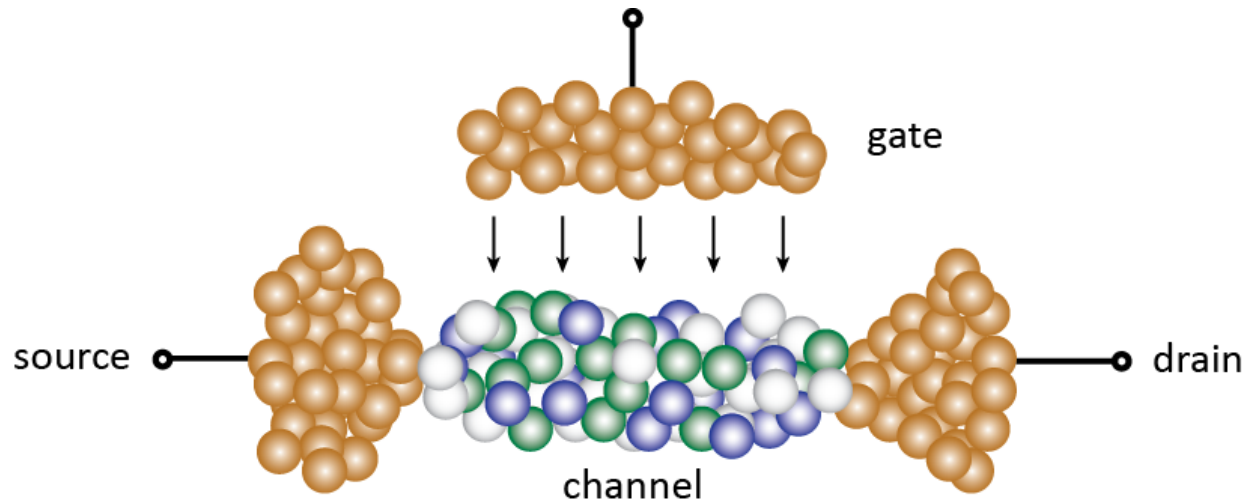


Quantum transport in nanojunctions with time-varying components

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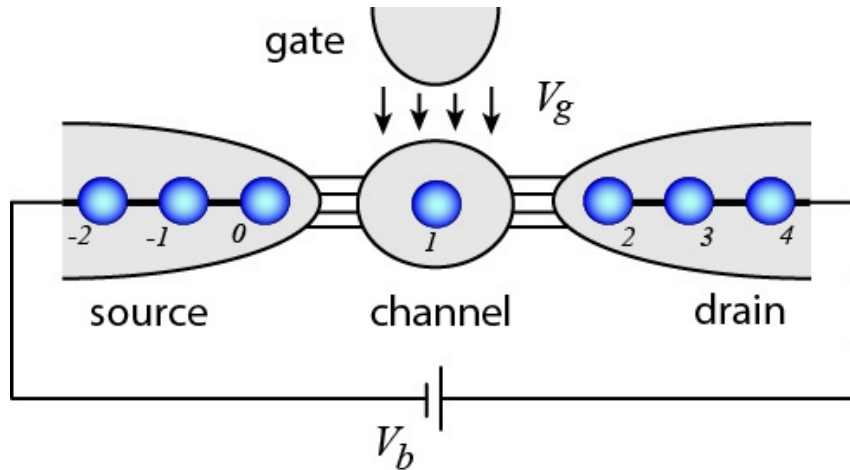
Electronics at the nanoscale:



Nanoscale device with a source-channel-drain configuration

- Channel can be a molecule, quantum dot, impurity, graphene nanoribbon
- Electrons propagate from the source to the drain
- Presence of time-varying components such as a time-dependent gate voltage, temperature gradient, incident laser, incoming electromagnetic signal, mechanical deformations
- Current is dynamic: transient regime, long-time regime
- Theory: quantum + many-body + nonequilibrium

Single-site channel with a time-varying gate:



Gate exerts a time-dependent potential on the channel

Step-function gate is switched on at $t = 0$

Chemical potentials:

$$\mu_L = E_F = 0 \quad \mu_R = E_F - V_b$$

Temperatures: $T^L = T^R = 300$ K

Current flowing out of the left lead:

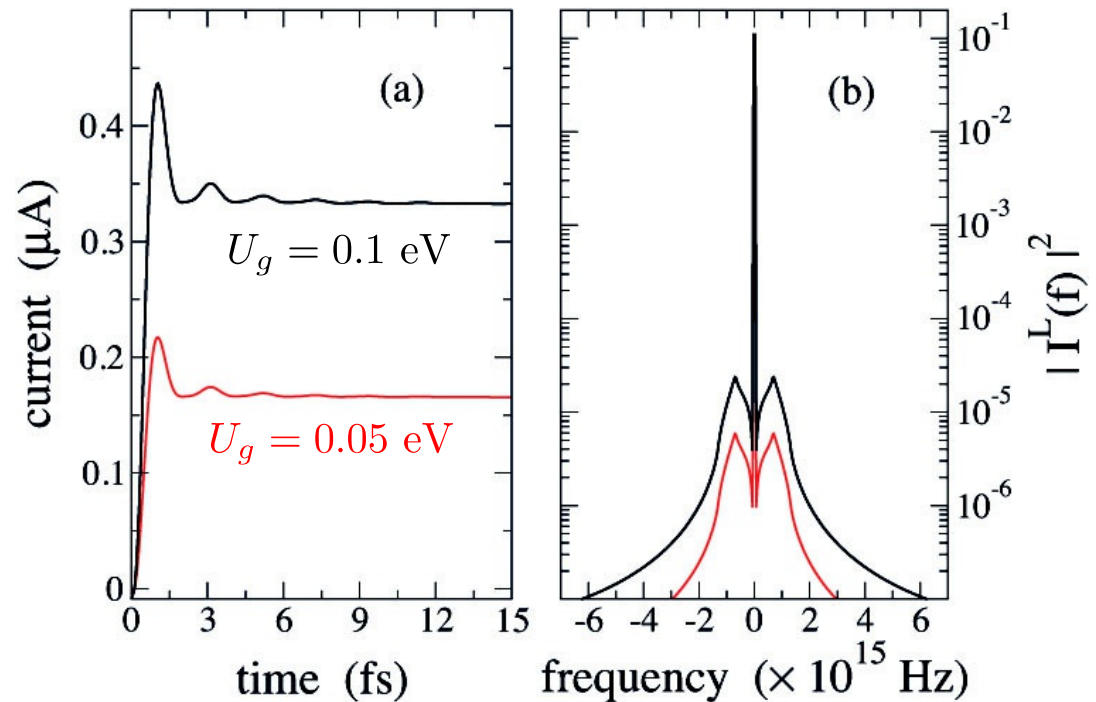
No source-drain bias voltage: $V_b = 0$

Current response to the gate:

- not instantaneous
- overshoots
- oscillates
- eventually settles down to a steady value

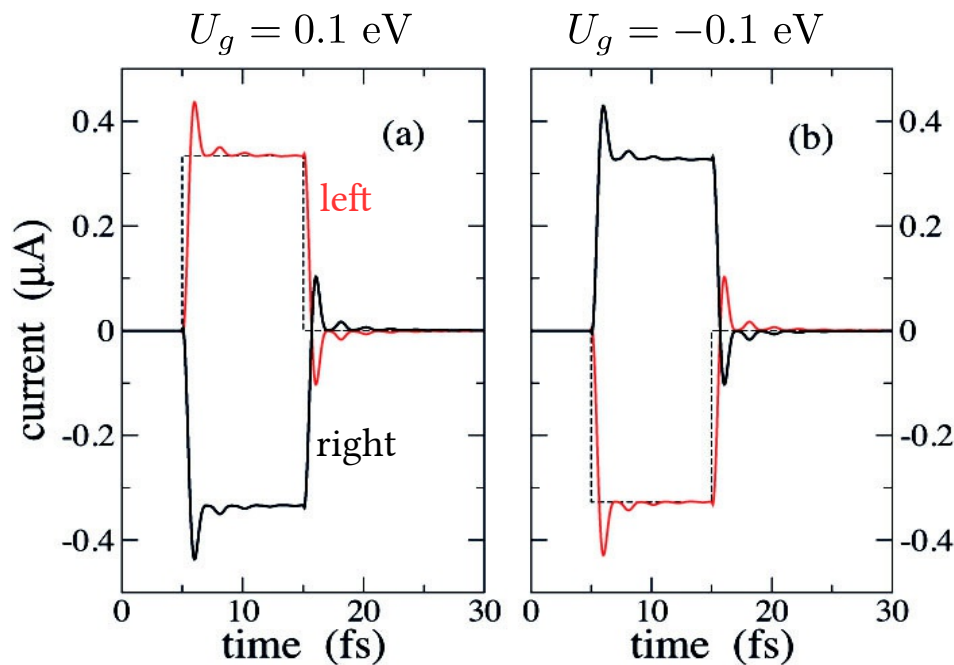
Frequency spectrum:

- dc component
- transient oscillation at $f = 0.7 \times 10^{15}$ Hz



ECC, Int. J. Mod. Phys. B 31, 1750105 (2017)

Current when the gate potential is a pulse:



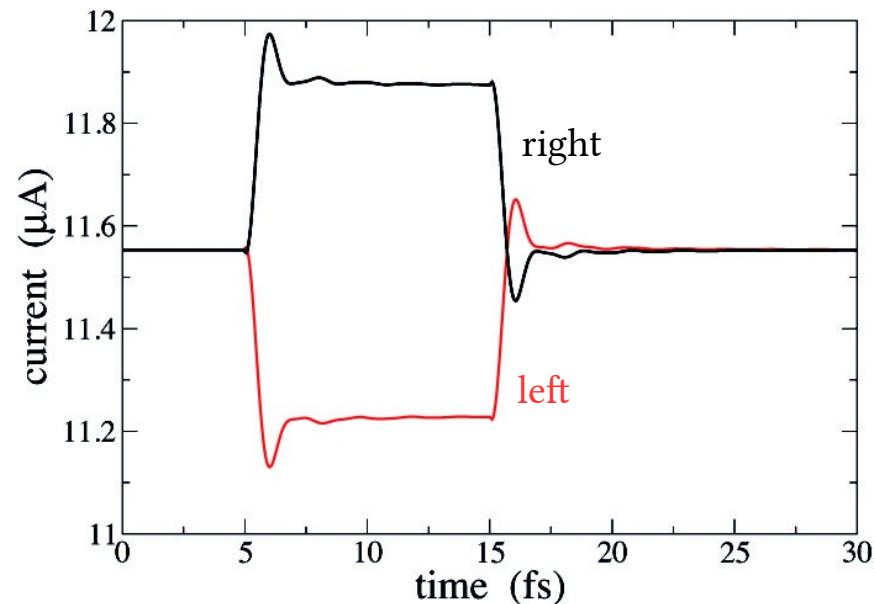
No source-drain bias voltage: $V_b = 0$

Gate potential pulse from 5 fs to 15 fs

Direction of current flow reverses with the sign of the gate potential

No net current in the channel:

- continuity equation



Bias voltage: $V_b = 0.3 \text{ eV}$

Pulse gate potential: $U_g = -0.1 \text{ eV}$

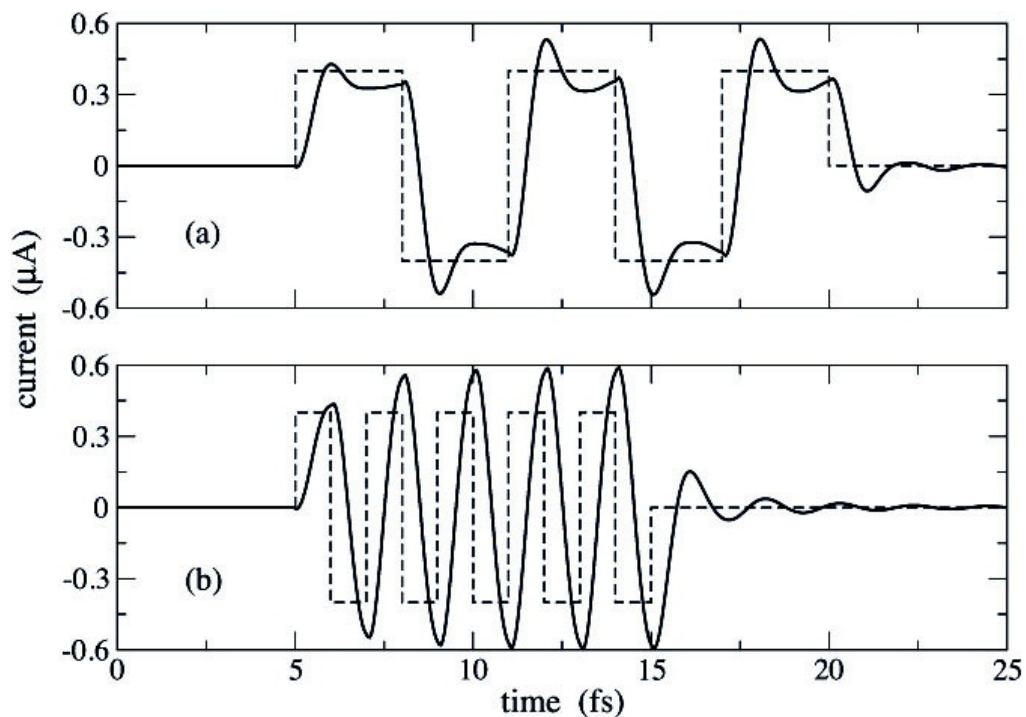
Right current is amplified

Left current is attenuated

Steady value is the same as the Landauer formula value

ECC, Int. J. Mod. Phys. B **31**, 1750105 (2017)

Potential pulses and ramps:



3 fs
pulses

Gate potential: $U_g = \pm 0.3$ eV

No source-drain bias potential:

$$V_b = 0$$

Current flowing into the right lead

$$I^R(t)$$

1 fs
pulses

varying the ramp width

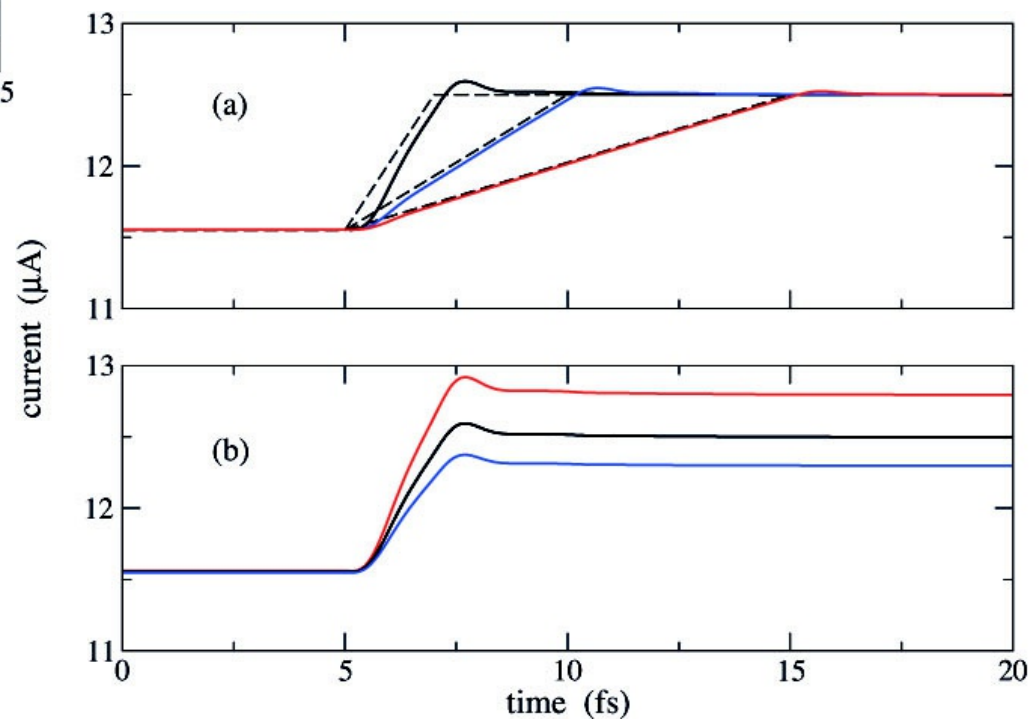
source-drain bias potential: $V_b = 0.3$ eV

varying the leads-channel coupling

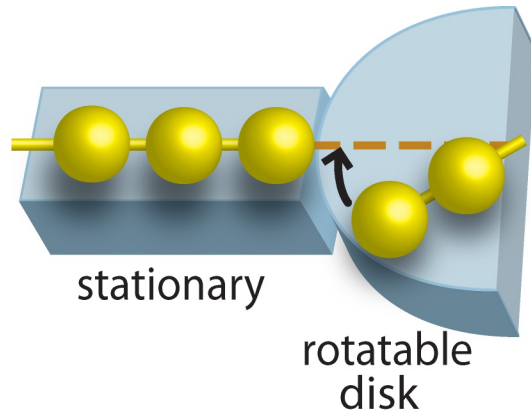
$$v^{LC} = v^{RC} = 1.8 \text{ eV}$$

$$v^{LC} = v^{RC} = 2.0 \text{ eV}$$

$$v^{LC} = v^{RC} = 2.2 \text{ eV}$$

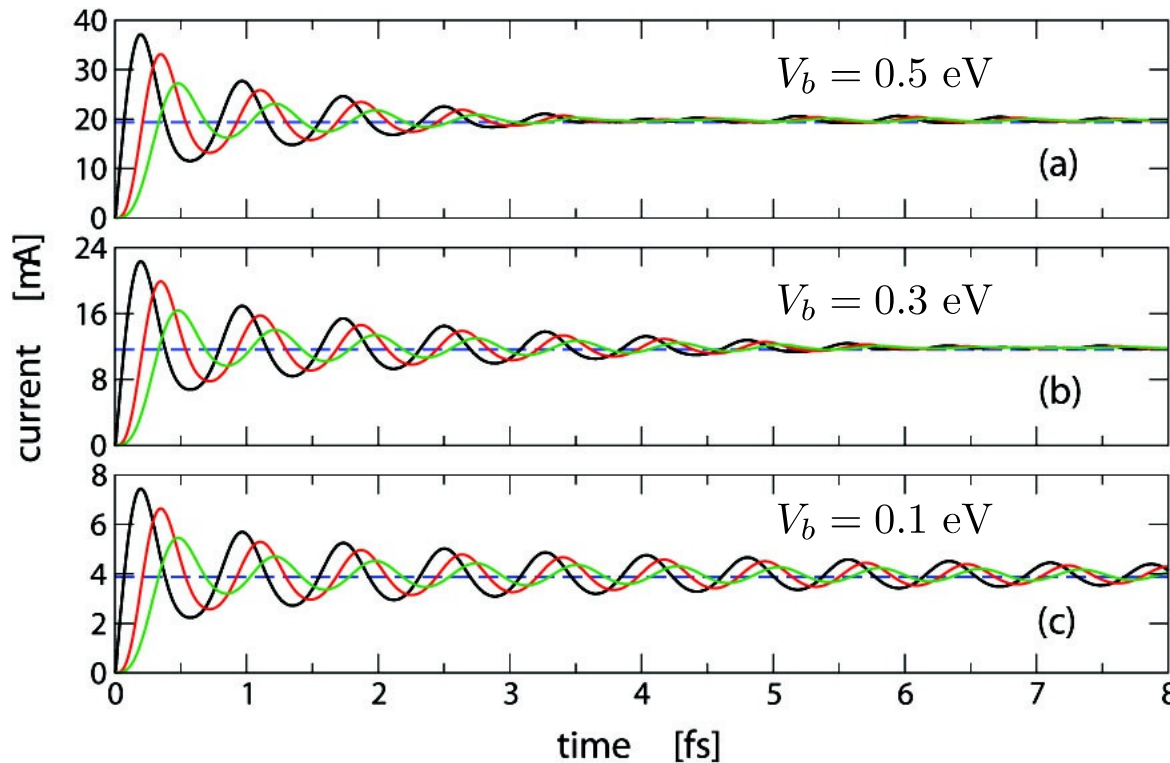


Nanoswitch:



Coupling between the two leads varies with time

- step function switch-on
- gradual
- modulated



Switch-on speeds:

Step function

Slow

Slowest

Form of the slow switch-on:

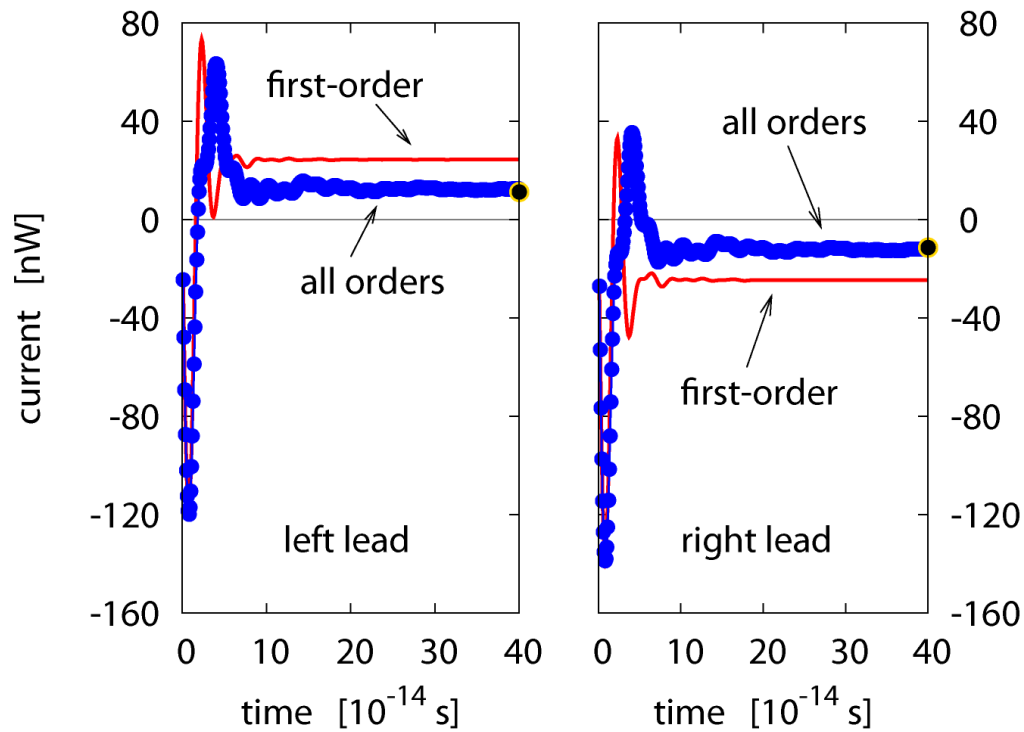
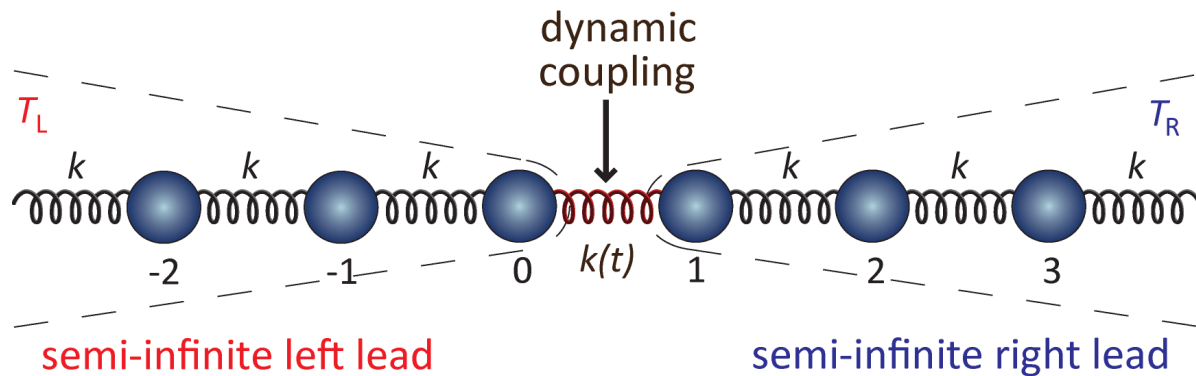
$$v^{\text{LR}}(t) = v^{\text{LR}} \tanh \omega_d t$$

Power-law fit to the current:

$$I(t) = I_0 \left(\frac{t}{t_0} \right)^{-\alpha} \sin(\omega t + \phi) + I_0$$

ECC and G. Liang, J. Appl. Phys. **110**, 083704 (2011)

Thermal switch (phonon transport):



Heat bath temperatures:

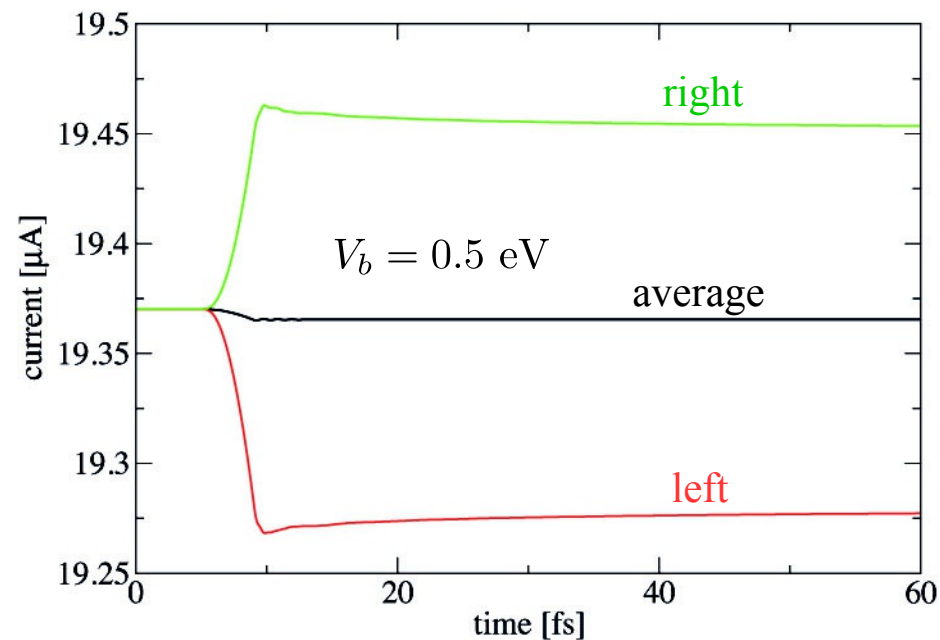
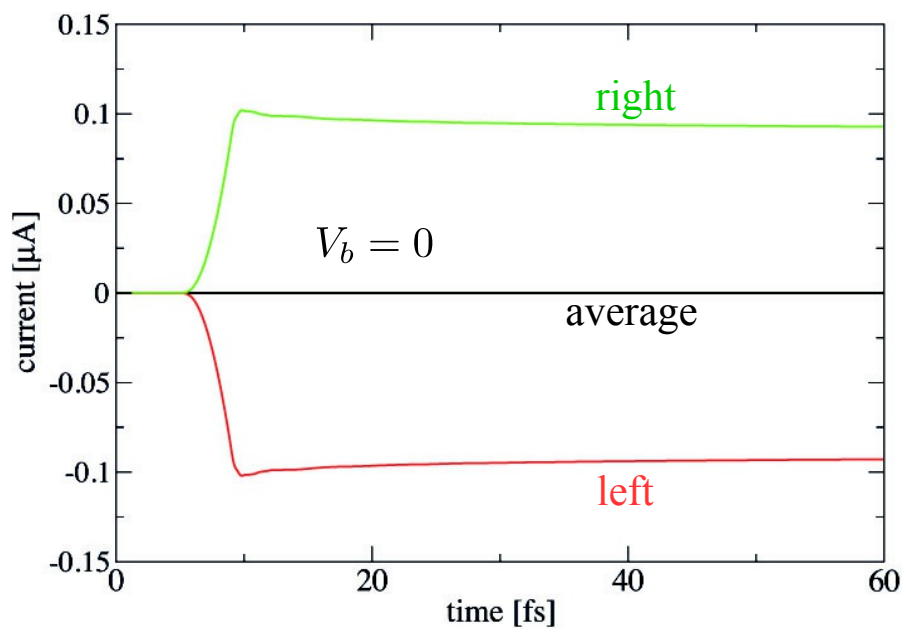
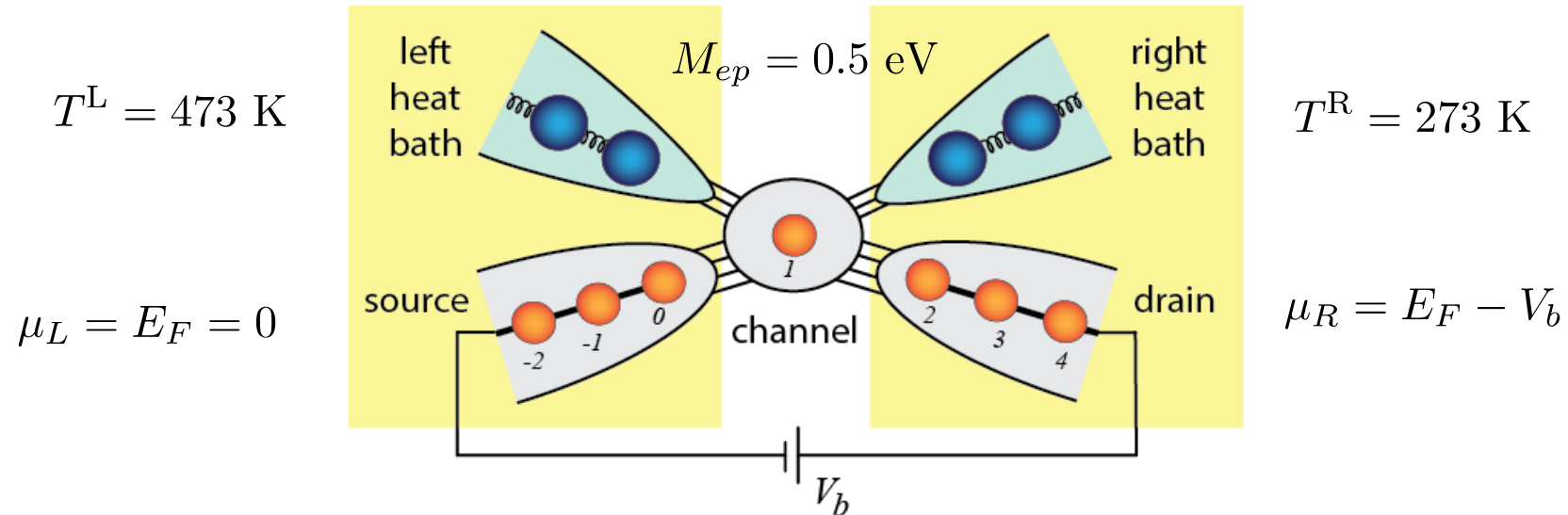
$$T^L = 310 \text{ K}$$

$$T^R = 290 \text{ K}$$

Oscillations in phonon transport
is 10 times slower than in
electron transport

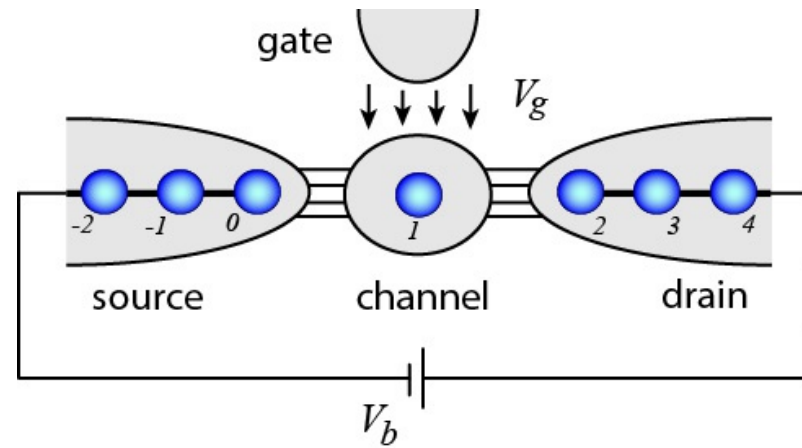
ECC and J.-S. Wang, Phys. Rev. B **81**, 052302 (2010)
ECC and J.-S. Wang, Phys. Rev. E **82**, 021116 (2010)

With electron-phonon interactions:



ECC, F.A. Bayocboc, and C.M. Laurio, AIP Conf. Proc. **1871**, 030003 (2017)

Calculating the time-dependent current: An example



Left Lead Hamiltonian:

$$H^L = \sum_k \varepsilon_k^L a_k^\dagger a_k + \sum_{kj} v_{kj}^L (a_k^\dagger a_j + a_j^\dagger a_k)$$

Right Lead Hamiltonian:

$$H^R = \sum_k \varepsilon_k^R b_k^\dagger b_k + \sum_{kj} v_{kj}^R (b_k^\dagger b_j + b_j^\dagger b_k)$$

Center Hamiltonian:

$$H_0^C = \varepsilon_1^C c_1^\dagger c_1$$

$$H_t^C = U(t) c_1^\dagger c_1 \quad U(t) = -q V_g(t)$$

$$H^C = H_0^C + H_t^C$$

Couplings:

$$H^{LC} = v_{01}^{LC} (a_0^\dagger c_1 + c_1^\dagger a_0)$$

$$H^{RC} = v_{21}^{RC} (c_1^\dagger b_2 + b_2^\dagger c_1)$$

$$\text{Total Hamiltonian: } H = H^L + H^R + H_0^C + H^{LC} + H^{RC} + H_t^C$$

E.C. Cuansing, Int. J. Mod. Phys. B 31, 17501015 (2017).

Current from electron flow and electron energy flow:

Current out of the Left Lead:

$$I^L(t) = \left\langle -q \frac{dN^L}{dt} \right\rangle = -\frac{iq}{\hbar} \langle [H, N^L] \rangle = 2q \operatorname{Re} \left[v_{01}^{\text{LC}} G_{10}^{\text{CL},<}(t, t) \right]$$

Current into the Right Lead:

$$I^R(t) = \left\langle q \frac{dN^R}{dt} \right\rangle = \frac{iq}{\hbar} \langle [H, N^R] \rangle = -2q \operatorname{Re} \left[v_{21}^{\text{RC}} G_{12}^{\text{CR},<}(t, t) \right]$$

positive current \longrightarrow flowing to the right

Lesser Nonequilibrium Green's Functions:

$$G_{10}^{\text{CL},<}(t_1, t_2) = \frac{i}{\hbar} \langle a_0^\dagger(t_2) c_1(t_1) \rangle \quad G_{12}^{\text{CR},<}(t_1, t_2) = \frac{i}{\hbar} \langle b_2^\dagger(t_2) c_1(t_1) \rangle$$

Electronic Energy Current out of the Left Lead:

$$Q^L(t) = \left\langle \frac{dH^L}{dt} \right\rangle = 2 \operatorname{Re} \left[(\varepsilon_0^L v_{01}^{\text{LC}} + v_{00}^L v_{01}^{\text{LC}}) G_{10}^{\text{CL},<}(t, t) \right]$$

Electronic Energy Current into the Right Lead:

$$Q^R(t) = \left\langle \frac{dH^R}{dt} \right\rangle = -2 \operatorname{Re} \left[(\varepsilon_2^R v_{21}^{\text{RC}} + v_{22}^R v_{21}^{\text{RC}}) G_{12}^{\text{CR},<}(t, t) \right]$$

Nonequilibrium Green's Functions:

Perturbing Hamiltonian: $H_t^C = U(t) c_1^\dagger c_1$

Contour-Ordered Green's Function:

$$G_{10}^{\text{CL}}(\tau_1, \tau_2) = -\frac{i}{\hbar} \left\langle T_c c_1(\tau_1) a_0^\dagger(\tau_2) \right\rangle = -\frac{i}{\hbar} \left\langle T_c e^{-\frac{i}{\hbar} \int_c H_t^C d\tau'} c_1(\tau_1) a_0^\dagger(\tau_2) \right\rangle_0$$

Keldysh contour

$$= G_{10,0}^{\text{CL}}(\tau_1, \tau_2) + \int_c d\tau' G_{11,0}^{\text{CC}}(\tau_1, \tau') U(\tau') G_{10}^{\text{CL}}(\tau', \tau_2)$$

Use analytic continuation and Langreth's theorem:

Retarded CL Nonequilibrium Green's Function:

$$G_{10}^{\text{CL},r}(t_1, t_2) = G_{10,0}^{\text{CL},r}(t_1, t_2) + \int_0^t dt' G_{11,0}^{\text{CC},r}(t_1, t') U(t') G_{10}^{\text{CL},r}(t', t_2)$$

Advanced CL Nonequilibrium Green's Function:

$$G_{10}^{\text{CL},a}(t_1, t_2) = G_{10,0}^{\text{CL},a}(t_1, t_2) + \int_0^t dt' G_{11,0}^{\text{CC},a}(t_1, t') U(t') G_{10}^{\text{CL},a}(t', t_2)$$

Lesser CL Nonequilibrium Green's Function:

$$G_{10}^{\text{CL},<}(t_1, t_2) = G_{10,0}^{\text{CL},<}(t_1, t_2) + \int_0^t dt' G_{11}^{\text{CC},r}(t_1, t') U(t') G_{10,0}^{\text{CL},<}(t', t_2)$$

$$+ \int_0^t dt' G_{11,0}^{\text{CC},<}(t_1, t') U(t') G_{10}^{\text{CL},a}(t', t_2)$$

$$+ \int_0^t dt' \int_0^t dt'' G_{11}^{\text{CC},r}(t_1, t') U(t') G_{11,0}^{\text{CC},<}(t', t'') U(t'') G_{10}^{\text{CL},a}(t'', t_2)$$

Nonequilibrium Green's Functions: CC terms

CC Contour-Ordered Green's Function:

$$\begin{aligned} G_{11}^{\text{CC}}(\tau_1, \tau_2) &= -\frac{i}{\hbar} \left\langle T_c c_1(\tau_1) c_1^\dagger(\tau_2) \right\rangle = -\frac{i}{\hbar} \left\langle T_c e^{-\frac{i}{\hbar} \int_c H_t^{\text{C}} d\tau'} c_1(\tau_1) c_1^\dagger(\tau_2) \right\rangle_0 \\ &= G_{11,0}^{\text{CC}}(\tau_1, \tau_2) + \int_c d\tau' G_{11,0}^{\text{CC}}(\tau_1, \tau') U(\tau') G_{11}^{\text{CC}}(\tau', \tau_2) \end{aligned}$$

Retarded CC Nonequilibrium Green's Function:

$$G_{11}^{\text{CC},r}(t_1, t_2) = G_{11,0}^{\text{CC},r}(t_1, t_2) + \int_0^t dt' G_{11,0}^{\text{CC},r}(t_1, t') U(t') G_{11}^{\text{CC},r}(t', t_2)$$

Advanced CC Nonequilibrium Green's Function:

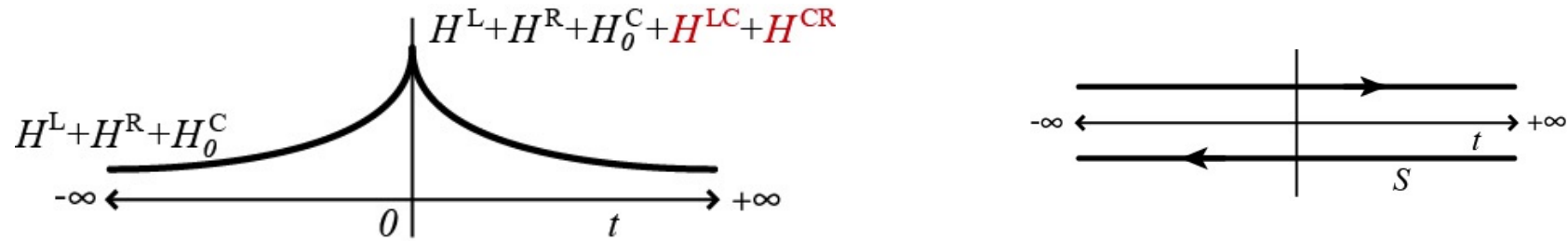
$$G_{11}^{\text{CC},a}(t_1, t_2) = G_{11,0}^{\text{CC},a}(t_1, t_2) + \int_0^t dt' G_{11,0}^{\text{CC},a}(t_1, t') U(t') G_{11}^{\text{CC},a}(t', t_2)$$

Lesser CC Nonequilibrium Green's Function:

$$\begin{aligned} G_{11}^{\text{CC},<}(t_1, t_2) &= G_{11,0}^{\text{CC},<}(t_1, t_2) + \int_0^t dt' G_{11}^{\text{CC},r}(t_1, t') U(t') G_{11,0}^{\text{CC},<}(t', t_2) \\ &\quad + \int_0^t dt' G_{11,0}^{\text{CC},<}(t_1, t') U(t') G_{11}^{\text{CC},a}(t', t_2) \\ &\quad + \int_0^t dt' \int_0^t dt'' G_{11}^{\text{CC},r}(t_1, t') U(t') G_{11,0}^{\text{CC},<}(t', t'') U(t'') G_{11}^{\text{CC},a}(t'', t_2) \end{aligned}$$

Steady-State Green's Functions

Adiabatic switch-on of the leads-channel coupling:



Steady-State Contour-Ordered Green's Function:

$$G_{11,0}^{CC}(\tau_1, \tau_2) = -\frac{i}{\hbar} \left\langle T_c c_1(\tau_1) c_1^\dagger(\tau_2) \right\rangle_0 = -\frac{i}{\hbar} \left\langle T_c e^{-\frac{i}{\hbar} \int_c d\tau' (H^{LC}(\tau') + H^{RC}(\tau'))} c_1(\tau_1) c_1^\dagger(\tau_2) \right\rangle_\infty$$

$$= g_{11}^C(\tau_1, \tau_2) + \int_c d\tau' \int_c d\tau'' g_{11}^C(\tau_1, \tau') \Sigma_{11}^C(\tau', \tau'') G_{11,0}^{CC}(\tau'', \tau_2)$$

$$\text{Self-Energy: } \Sigma_{11}^C(\tau', \tau'') = v_{10}^{CL} g_{00}^L(\tau', \tau'') v_{01}^{LC} + v_{12}^{CR} g_{22}^R(\tau', \tau'') v_{21}^{RC}$$

Analytic continuation and Langreth's theorem + Fourier transform:

$$\text{Retarded: } G_{11,0}^{CC,r}(E) = \left[(E + i\eta) - \varepsilon_1^C - \Sigma_{11}^{C,r}(E) \right]^{-1}$$

$$\text{Advanced: } G_{11,0}^{CC,a}(E) = \left[G_{11,0}^{CC,r}(E) \right]^*$$

$$\text{Lesser: } G_{11,0}^{CC,<}(E) = G_{11,0}^{CC,r}(E) \Sigma_{11}^{C,<}(E) G_{11,0}^{CC,a}(E)$$

Haug and Jauho, Quantum Kinetics in Transport and Optics of Semiconductors

CL Steady-State Green's Functions:

CL Steady-State Green's Functions:

Retarded: $G_{10,0}^{\text{CL},r}(E) = G_{11,0}^{\text{CC},r}(E) v_{10}^{\text{CL}} g_{00}^{\text{L},r}(E)$

Advanced: $G_{10,0}^{\text{CL},a}(E) = \left[G_{10,0}^{\text{CL},r}(E) \right]^*$

Lesser: $G_{10,0}^{\text{CL},<}(E) = G_{11,0}^{\text{CC},r}(E) v_{10}^{\text{CL}} g_{00}^{\text{L},<}(E) + G_{11,0}^{\text{CC},r}(E) \Sigma_{11}^{\text{C},<}(E) G_{10,0}^{\text{CL},a}(E)$

Equilibrium Green's Functions of the Leads:

Can be determined from the Equation of Motion of a Free Lead:

Retarded Equilibrium Green's Function:

$$g^r(E) = \frac{2}{v^2} ((E + i\eta) - \varepsilon) \pm i \frac{2}{v^2} \sqrt{v^2 - (\varepsilon - E)^2} \quad -v \leq \varepsilon - E \leq v$$

Advanced Equilibrium Green's Function:

$$g^a(E) = (g^r(E))^*$$

Lesser Equilibrium Green's Function:

$$g^<(E) = -f_{FD}(E) (g^r(E) - g^a(E)) \quad f_{FD}(E) = \left(e^{(E-\mu)/k_B T} + 1 \right)^{-1}$$

Summary: How to calculate the time-dependent current

1. Equilibrium Green's Functions of the Free Leads in E-Space:

$$g_{00}^{L,r}, g_{00}^{L,a}, g_{00}^{L,<} \quad g_{22}^{R,r}, g_{22}^{R,a}, g_{22}^{R,<}$$

2. Steady-State Green's Functions in E-Space:

$$G_{11,0}^{CC,r}, G_{11,0}^{CC,a}, G_{11,0}^{CC,<} \quad G_{10,0}^{CL,r}, G_{10,0}^{CL,a}, G_{10,0}^{CL,<} \quad G_{12,0}^{CR,r}, G_{12,0}^{CR,a}, G_{12,0}^{CR,<}$$

3. Fourier transforms of the Steady-State Green's Functions into t-Space

4. Nonequilibrium Green's Functions in t-Space:

$$G_{11}^{CC,r}, G_{11}^{CC,a}, G_{11}^{CC,<} \quad G_{10}^{CL,r}, G_{10}^{CL,a}, G_{10}^{CL,<} \quad G_{12}^{CR,r}, G_{12}^{CR,a}, G_{12}^{CR,<}$$

5. Left and Right current:

$$I^L(t) = 2q \operatorname{Re} \left[v_{01}^{LC} G_{10}^{CL,<}(t, t) \right] \quad I^R(t) = -2q \operatorname{Re} \left[v_{21}^{RC} G_{12}^{CR,<}(t, t) \right]$$

Thank you for
your attention!

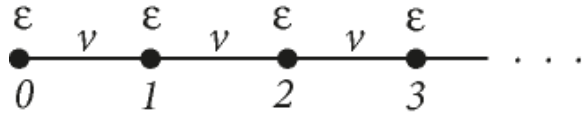


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Hanoi, Vietnam, 20-24 November 2017

Calculating the equilibrium Green's function of a free lead:



$$H = \sum_k \varepsilon_k a_k^\dagger a_k + \sum_{kj} v_{kj} (a_k^\dagger a_j + a_j^\dagger a_k)$$

Equation of motion of electrons in the lead:

$$(H - E)g = -I$$

$$\begin{pmatrix} \varepsilon - E & v & 0 & 0 & \cdots \\ v & \varepsilon - E & v & 0 & \\ 0 & v & \varepsilon - E & v & \\ 0 & 0 & v & \varepsilon - E & \\ \vdots & & & & \ddots \end{pmatrix} \begin{pmatrix} g_{00} & g_{01} & g_{02} & \cdots \\ g_{10} & g_{11} & g_{12} & \\ g_{20} & g_{21} & g_{22} & \\ g_{30} & g_{31} & g_{32} & \\ \vdots & & & \ddots \end{pmatrix} = - \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \\ 0 & 0 & 1 & 0 & \\ 0 & 0 & 0 & 1 & \\ \vdots & & & & \ddots \end{pmatrix}$$

$$(\varepsilon - E)g_{00} + v g_{10} = -1$$

$$v g_{00} + (\varepsilon - E)g_{10} + v g_{20} = 0$$

Ansatz: $g_{mn} = c\lambda^{|m-n|}$

$$\lambda = e^{\pm iq} \quad \cos q = \frac{\varepsilon - E}{v} \quad \sin q = \frac{\sqrt{v^2 - (\varepsilon - E)^2}}{v} \quad c = -\frac{2}{v} e^{\pm iq}$$

we get: $g_{mn} = -\frac{2}{v} e^{\pm iq(|m-n|-1)}$

$$g_{00} = \frac{2}{v^2} (E - \varepsilon) \pm \frac{2i}{v^2} \sqrt{v^2 - (\varepsilon - E)^2}$$

Solving the iterative equation for the retarded NEGF:

Retarded Nonequilibrium Green's Function:

$$G_{10}^{\text{RL},r}(t_1, t_2) = G_{10,0}^{\text{RL},r}(t_1, t_2) + \int_0^t dt' G_{10,0}^{\text{RL},r}(t_1, t') v_{01}^{\text{LR}}(t') G_{10}^{\text{RL},r}(t', t_2)$$

In the form:

$$f(t_a, t_b) = f_0(t_a, t_b) + \int_{t_1}^{t_N} f_0(t_a, t') v(t') f(t', t_b) dt'$$

Use numerical integration:

$$f(t_a, t_b) = f_0(t_a, t_b) + \Delta t \sum_{i=1}^N c_i f_0(t_a, t_i) v(t_i) f(t_i, t_b) \quad c_i = \text{numerical integration coefficient}$$

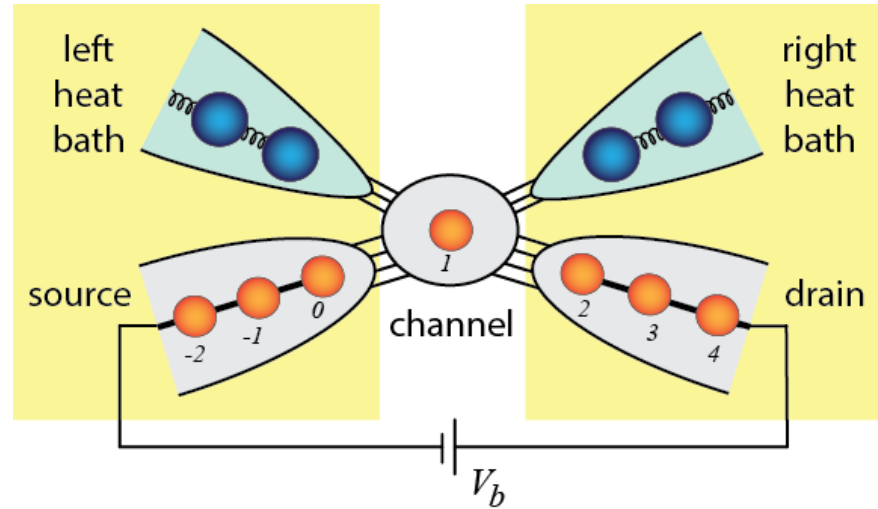
$$f(t_a, t_b) - \Delta t \sum_{i=1}^N c_i f_0(t_a, t_i) v(t_i) f(t_i, t_b) = f_0(t_a, t_b)$$

Construct the equivalent matrix equation: $Ax = b$

$$\begin{pmatrix} 1 - \Delta t c_1 f_0(t_1, t_1) v(t_1) & -\Delta t c_2 f_0(t_1, t_2) v(t_2) & \cdots \\ -\Delta t c_1 f_0(t_2, t_1) v(t_1) & 1 - \Delta t c_2 f_0(t_2, t_2) v(t_2) & \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} f(t_1, t_b) \\ f(t_2, t_b) \\ \vdots \end{pmatrix} = \begin{pmatrix} f_0(t_1, t_b) \\ f_0(t_2, t_b) \\ \vdots \end{pmatrix}$$

which can be solved by taking the inverse: $x = A^{-1}b$

With electron-phonon interactions:



Electron part: $H_e = H_e^L + H_e^R + H_{e,0}^C + H_e^{LC} + H_e^{RC}$ $H_{e,0}^C = \varepsilon_{e,1}^C c_1^\dagger c_1$

Phonon part:

Heat baths: $H_p^L = \sum_k \varepsilon_{p,k}^L q_k^\dagger q_k + \sum_{jk} v_{p,jk}^L q_j^\dagger q_k$ Couplings: $H_p^{LC} = v_{p,01}^{LC} (q_0^\dagger p_1 + p_1^\dagger q_0)$
 $H_p^R = \sum_k \varepsilon_{p,k}^R r_k^\dagger r_k + \sum_{jk} v_{p,jk}^R r_j^\dagger r_k$ $H_p^{RC} = v_{p,21}^{RC} (r_2^\dagger p_1 + p_1^\dagger r_0)$

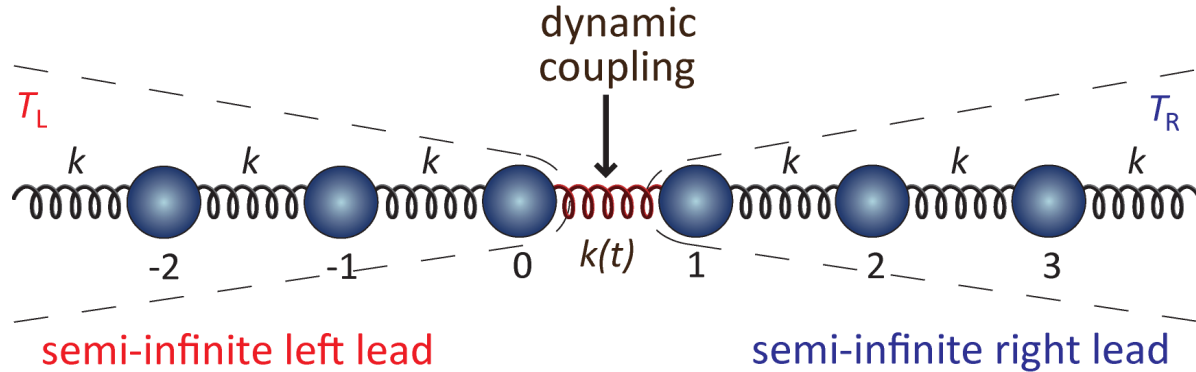
Channel: $H_p^C = \varepsilon_{p,1}^C p_1^\dagger p_1$

Phonon Hamiltonian: $H_p = H_p^L + H_p^R + H_p^C + H_p^{LC} + H_p^{RC}$

Electron-Phonon Interaction: $H_{ep}^C = M_{ep}(t) (p_1^\dagger + p_1) c_1^\dagger c_1$

Total Hamiltonian: $H = H_e + H_p + H_{ep}^C$

Thermal switch:



Hamiltonian for the left and right leads:

$$H^\alpha = \frac{1}{2} \sum_i \dot{u}_i^\alpha \dot{u}_i^\alpha + \frac{1}{2} \sum_{ij} u_i^\alpha K_{ij}^\alpha u_j^\alpha \quad \alpha = L, R \quad u_i = \sqrt{m_i} x_i$$

Coupling between the leads:

$$H^{\text{LR}}(t) = \sum_{ij} u_i^{\text{L}} V_{ij}^{\text{LR}} u_j^{\text{R}}$$

Total Hamiltonian of the system: $H = H^{\text{L}} + H^{\text{R}} + H^{\text{LR}}(t)$