Tunneling current through insulating barrier

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INNOVATIVE ECONOMY
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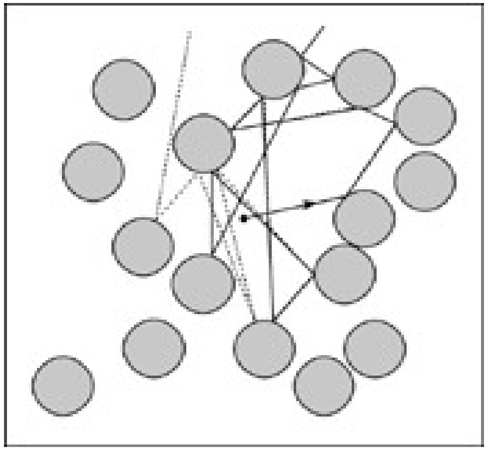
Motivation

Resistivity is often first measured, the last understood...

What is current?

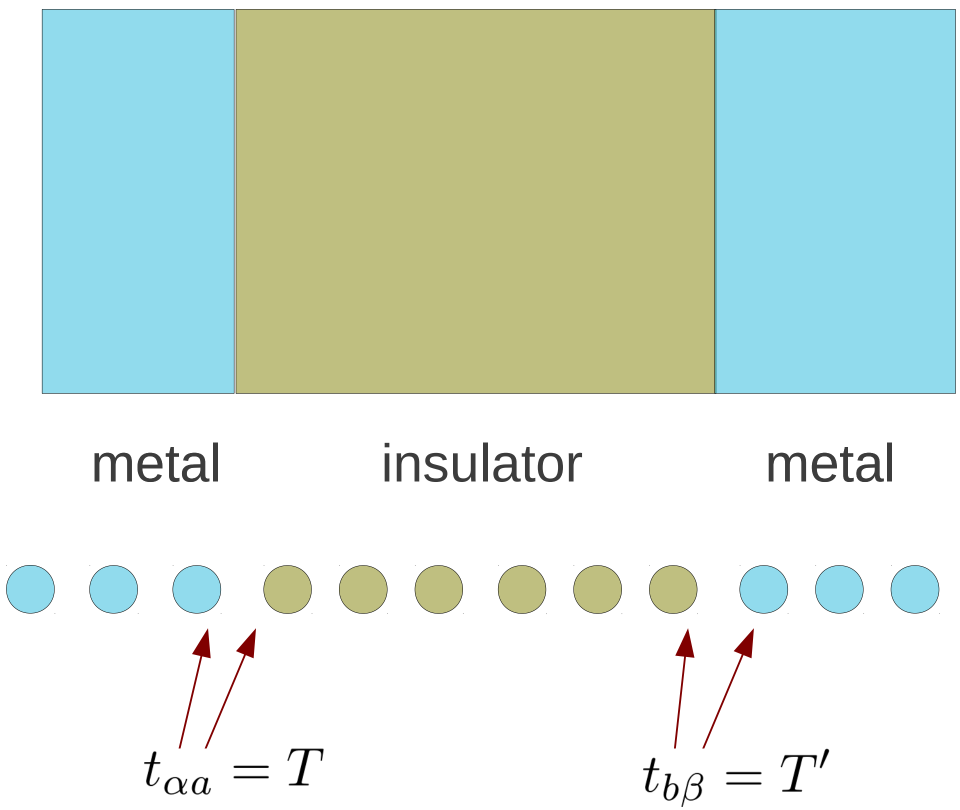
Lorentz model of electric current flow

No stationary state



electric field

Problem



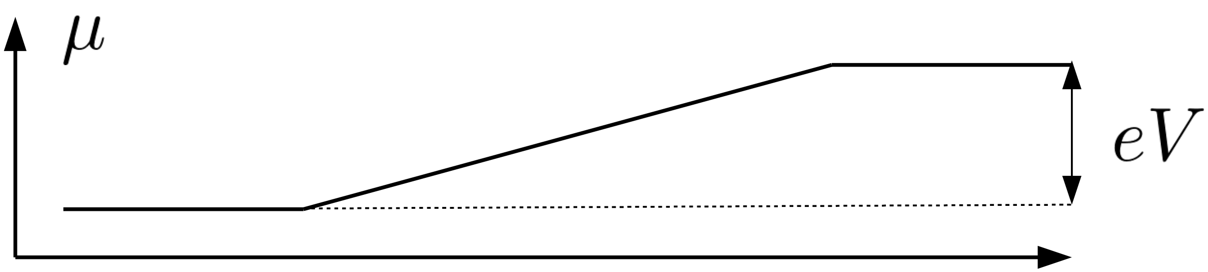
Grand canonical Hamiltonian:

$$H = \sum_{ij} t_{ij} a_i^\dagger a_j - \sum_i \mu_i a_i^\dagger a_i$$

lattice sites

chemical potential

1D

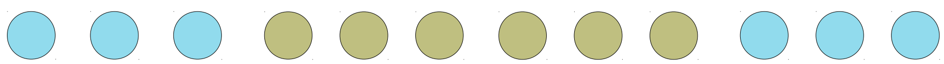


Electric current?

Method

C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, J.Phys.C 4, 916 (1971)

For $t \leq t_0$ no hopping between metal and insulator:

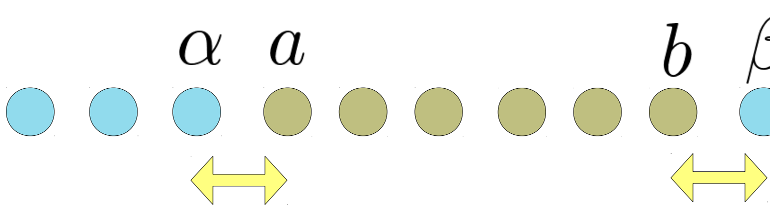


metal insulator metal

$$H(t \leq t_0) = \sum_{ij} t^0_{ij} a^\dagger_i a_j - \sum_i \mu_i a^\dagger_i a_i$$

Equilibrium quantum statistical physics

At time t_0 hopping turned on:



$$H(t > t_0) = H(t_0) + (T a^\dagger_\alpha a_a + T' a^\dagger_\beta a_b + h.c.)$$

Nonequilibrium, nonstationary situation

But limit $t_0 \to -\infty$, stationary state

Equilibrium case: $t \leq t_0$

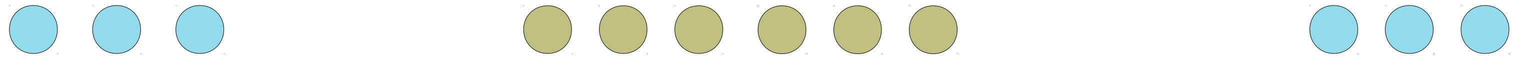
Grand canonical partition function (thermodynamics):

$$\Xi = \sum_{N,\gamma_N} \langle \gamma_N | e^{-\beta H(t_0)} | \gamma_N \rangle$$

number of particles

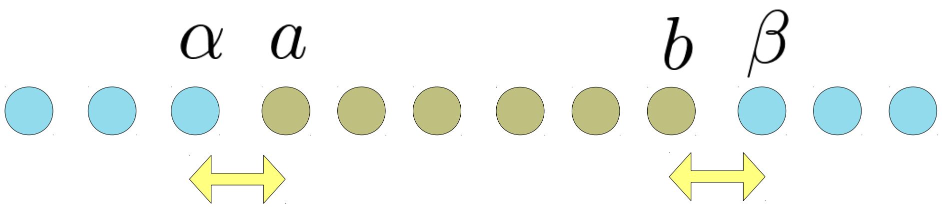
N-particle quantum states

Effectively three separate systems:



μ chemical potential grows $\mu + eV$

Current in the system: $t > t_0$



Operator calculating number of particles in the left metal

$$\hat{N}_L = \sum_{i \leq \alpha} a_i^\dagger a_i$$

$$|\gamma_N(t)\rangle = U(t, t_0)|\gamma_N(t_0)\rangle$$

$$\hat{N}_L(t) = U(t_0, t)\hat{N}_L U(t, t_0)$$

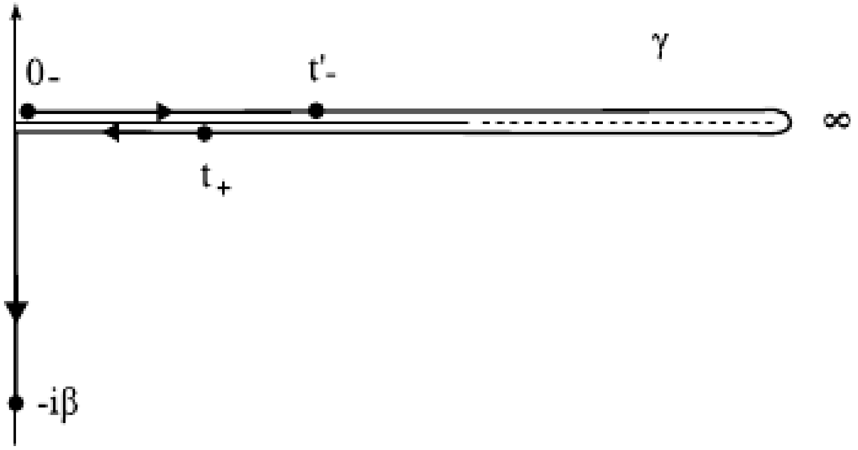
Current

$$J = e\frac{i}{\hbar}T\langle[a_\alpha^\dagger(t), a_a(t)]\rangle_{\text{eq}}$$

Non-equilibrium Green function

$$G_{ij}(t,t') = -i\langle T_c \hat{a}_i(t)\hat{a}_j^\dagger(t')\rangle_{\text{eq}}$$

$$e^{-\beta H(t_0)}\hat{a}_i(t)\hat{a}_j^\dagger(t') = e^{-\beta H(t_0)}U(t_0,t)\hat{a}_i U(t,t_0)U(t_0,t')\hat{a}_j^\dagger U(t',t_0)$$



$$U(t,t_0)U(t_0,t') = U(t,t') = U(t,\infty)U(\infty,t')$$

time ordering on Keldysh contour

$$T_c\hat{a}_i(t)\hat{a}_j^\dagger(t') = \begin{cases} \hat{a}_i(t)\hat{a}_j^\dagger(t') & \text{for} \quad t >_c t' \\ -\hat{a}_j^\dagger(t')\hat{a}_i(t) & \text{for} \quad t <_c t' \end{cases}$$

Green function for system with perturbation

$$H(t) = H_0 + H_1(t) \qquad H_1(t \leq t_0) = 0$$

For H_0 :
$$G_{0,ij}(t,t') = -i\langle T_c \hat{a}_i(t)\hat{a}_j^\dagger(t')\rangle_{\mathrm{eq}}$$

Hamiltonian in time evolution

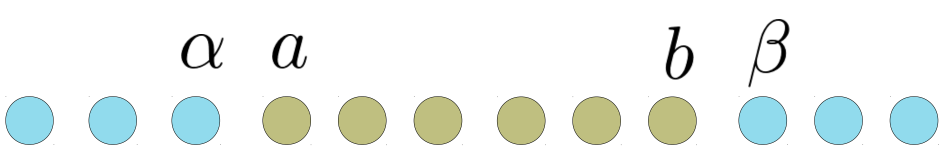
For H :
$$G_{ij}(t,t') = -i\langle T_c \hat{a}_i(t)\hat{a}_j^\dagger(t')\rangle_{\mathrm{eq}}$$

Keldysh-Kadanoff-Baym equation:

$$G = G_0 + G_0 \Sigma G$$

equilibrium!

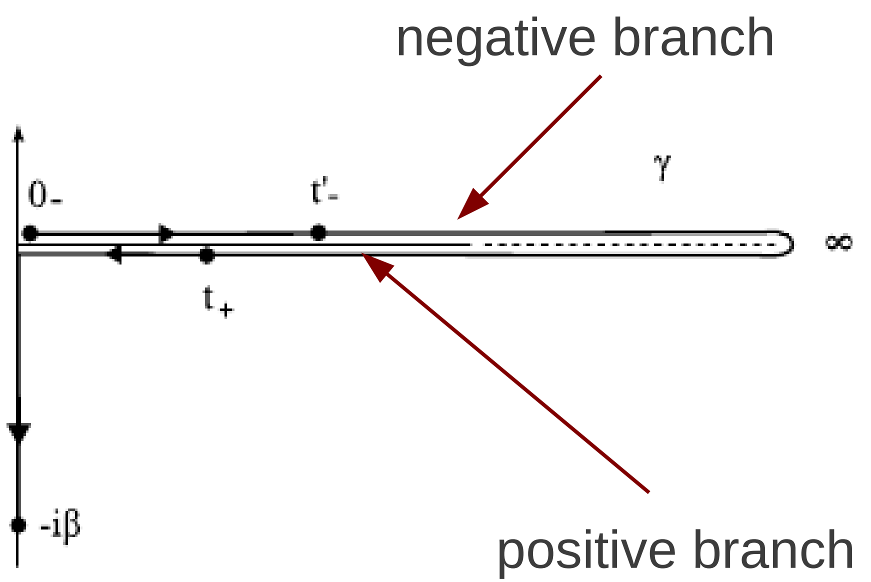
$$\Sigma(t,t')_{ij} = \delta_c(t,t')\big(T\delta_{i\alpha}\delta_{aj} + T\delta_{ia}\delta_{\alpha j} + T'\delta_{i\beta}\delta_{bj} + T\delta_{ib}\delta_{\beta j}\big)$$



Keldysh-Kadanoff-Baym equation in practice

Nonequilibrium Green function

$$G_{ij}(t,t')$$



Four possibilities

$$t_+, t'_-$$
$$t_+, t'_+$$
$$t_-, t'_-$$
$$t_-, t'_+$$

yield four different physical (real times) Green functions.

Keldysh-Kadanoff-Baym equation => four equations for physical Green functions

$$G = G_0 + G_0 \Sigma G$$

In Fourier transform four algebraic equations

=> non-equilibrium Green function

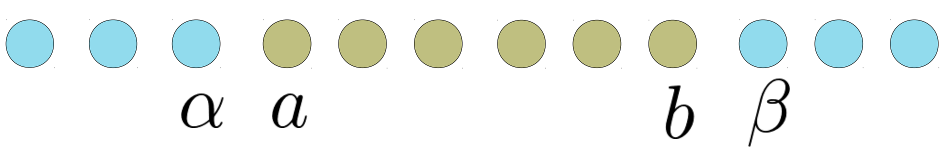
Current

Assumptions:
- stationary state
- zero temperature
- density of states in the insulator in the range of energy is strictly zero

advanced retarded

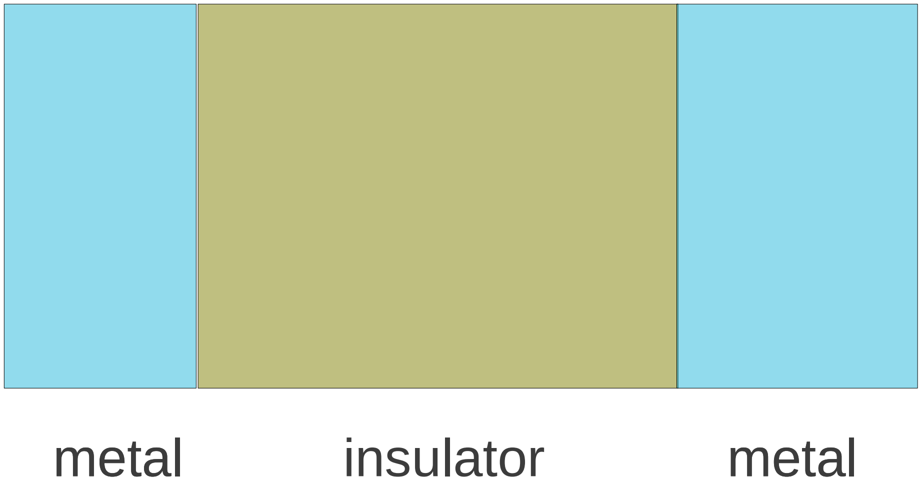
$$J = -\frac{(2\pi)^2 e T^2 T'^2}{\hbar} \int_{\mu}^{\mu+eV} \frac{d\omega}{2\pi} G_{ba}^{A}(\omega) G_{ab}^{R}(\omega) \rho_{\alpha}(\omega) \rho_{\beta}(\omega)$$

density of states



Current:
- built up from contribution of states with energy between
- depends not on momentum, but energy

Perspective – include interactions



Grand canonical Hamiltonian:

$$H = \sum_{ij} t_{ij} a_i^\dagger a_j - \sum_i \mu_i a_i^\dagger a_i$$

Extension:

$$H = \sum_{i,j} \sum_{\sigma=\uparrow,\downarrow} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - \sum_i \sum_{\sigma=\uparrow,\downarrow} \mu_i \hat{n}_{i\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

The main point: density of states for inhomogeneous equilibrium system (real space DMFT)