The Landauer-Büttiker formalism to transport phenomena in mesoscopic conducting systems

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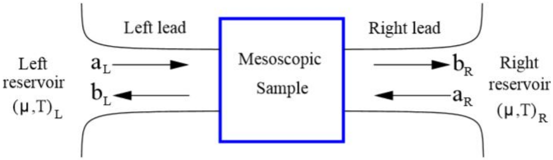
Content

Motivation

Describing transport phenomena in mesoscopic conducting systems

Scope

- a confined mesoscopic system coupled to thermal e^- reservoirs
- leads with one conducting sub-band
- low temperature: the phase coherence length (L_ϕ) » size of the sample (L)
- quantum mechanical scattering problem of e^--s



The scattering matrix

- incident electron $\Psi^{(in)} \rightarrow \Psi^{(out)}$ scattered electron
- solution for the $\psi_\alpha^{(in)}$ orthonormal basis $\rightarrow$ scattering state for an arbitrary initial state
- both wave functions can be expanded on a full orthonormal basis: $\left\{\psi_\alpha^{(in)}\right\}, \left\{\psi_\beta^{(out)}\right\}$

$$\Psi^{(in)} = \sum_\alpha a_\alpha \psi_\alpha^{(in)} \qquad \Psi^{(out)} = \sum_\beta b_\beta \psi_\beta^{(out)}$$

- Problem: find b_β if the set of a_α is known

The scattering matrix

Method

1. Expanding the initial state into a series of $\psi_\alpha^{(in)}$
2. Expanding the scattered state

$$\Psi^{(out)} = \sum_\alpha \Psi_\alpha^{(out)} \qquad (\text{due to } \Psi_\alpha^{(in)} = a_\alpha \psi_\alpha^{(in)})$$

$$\Psi_\alpha^{(out)} = a_\alpha \sum_\beta S_{\beta\alpha} \psi_\beta^{(out)}$$

3. Solution

$$\Psi^{(out)} = \sum_\alpha a_\alpha \sum_\beta S_{\beta\alpha} \psi_\beta^{(out)} \equiv \sum_\beta b_\beta \psi_\beta^{(out)}$$

$$\Downarrow$$

$$b_\beta = \sum_\alpha S_{\beta\alpha} a_\alpha$$

$$\hat{b} = \hat{S} \hat{a}$$

4. $S_{\beta\alpha}$: QM-amplitude to pass from $\psi_\alpha^{(in)}$ to $\psi_\beta^{(out)}$

Properties - Unitarity

The particle number (flow) conservation implies the unitarity of $\hat{S}$

$$\hat{S}^\dagger \hat{S} = \hat{S}\hat{S}^\dagger = \hat{I}$$

Proof - normalized wave function

$$\int d^3r |\Psi^{(in)}|^2 = \int d^3r \sum_\alpha a_\alpha \psi_\alpha^{(in)} \left(\sum_\beta a_\beta^* \psi_\beta^{(in)} \right)^*$$

$$= \sum_\alpha \sum_\beta a_\alpha a_\beta^* \int d^3r \psi_\alpha^{(in)} \left(\psi_\beta^{(in)} \right)^* = \sum_\alpha \sum_\beta a_\alpha a_\beta^* \delta_{\alpha\beta}$$

$$= \sum_\alpha |a_\alpha|^2 = \hat{a}^\dagger \hat{a} = 1$$

$$\hat{b}^\dagger \hat{b} = \hat{a}^\dagger \hat{S}^\dagger \hat{S} \hat{a} = \hat{a}^\dagger \hat{a}$$

Properties - Micro-reversibility

The time-reversal symmetry implies

$$\hat{S} = \hat{S}^T \Rightarrow S_{\alpha\beta} = S_{\beta\alpha}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \quad \rightarrow \quad i\hbar\frac{\partial(\Psi^*)}{\partial(-t)} = H(\Psi^*)$$

$$(\Psi^{out}(-t))^* = \left(\sum_\beta b_\beta \psi_\beta^{(out)}(-t)\right)^* = \sum_\beta b_\beta^* \psi_\beta^{(in)}(t)$$

$$\left(\Psi^{in}(-t)\right)^* = \left(\sum_\alpha a_\alpha \psi_\alpha^{(in)}(-t)\right)^* = \sum_\alpha a_\alpha^* \psi_\alpha^{(out)}(t)$$

$$\Downarrow$$

$$\hat{a} = \hat{S}^{-1}\hat{b}, \quad \hat{a}^* = \hat{S}\hat{b}^*$$

Properties - Micro-reversibility

$$\left.\begin{array}{r}\hat{S}^{\dagger}\hat{S}=\hat{I}\\ \hat{S}^{-1}\hat{S}=\hat{I}\end{array}\right\} \Rightarrow \hat{S}^{\dagger}=\hat{S}^{-1}, \hat{S}^{*}=\hat{S}^{-1} \Rightarrow \hat{S}=\hat{S}^{T}$$

Magnetic field - H

- In addition to the time and momentum reversal, one needs to inverse the direction of the magnetic field, $H \rightarrow -H$

$$\hat{S}(H)=\hat{S}(-H)^{T}$$

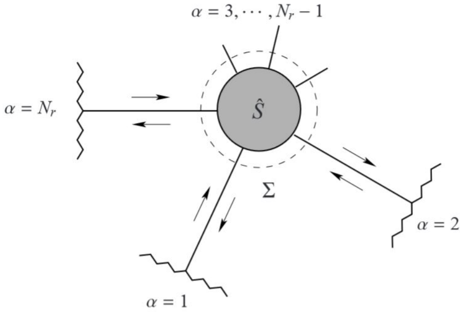
$$\Downarrow$$

$$S_{\alpha\beta}(H)=S_{\beta\alpha}(-H)$$

Current operator

Application of scattering matrices

- single-electron approximation $\rightarrow$ interaction is described by $U_{eff}(t, \mathbf{r})$
- incident and outgoing e^- flows through the surface $\sum$
- elastic, energy conserving scattering $\Rightarrow L_\phi >> L$



Current operator

Reservoirs and leads

- N_r macroscopic contacts as electron reservoirs:
  $T_\alpha, \mu_\alpha \rightarrow$ Fermi-distribution

$$f_\alpha(E) = \frac{1}{1+e^{\frac{E-\mu_\alpha}{k_B T_\alpha}}}$$

- Leads:
  - the eigenwave-functions are the basis functions for the scattering matrix

$$H_\alpha = \frac{1}{2m^*} p_{x_\alpha}^2 + \frac{1}{2m^*} p_{\perp_\alpha}^2 + U(\mathbf{r}_\perp)$$

  - assuming one conducting sub-band
  - the solution is the product of transverse and longitudinal terms

Current operator

Second quantization

- operators creating/annihilating particles in quantum states
- $\hat{a}^{\dagger}_{\alpha}(E)/\hat{a}_{\alpha}(E) \rightarrow \psi^{(in)}_{\alpha}(E)/\sqrt{v_{\alpha}(E)}$
- $\hat{b}^{\dagger}_{\alpha}(E)/\hat{b}_{\alpha}(E) \rightarrow \psi^{(out)}_{\alpha}(E)/\sqrt{v_{\alpha}(E)}$

$$\hat{a}^{\dagger}_{\alpha}(E)\hat{a}_{\beta}(E') + \hat{a}_{\beta}(E')\hat{a}^{\dagger}_{\alpha}(E) = \delta_{\alpha\beta}\delta(E - E')$$
$$\hat{b}^{\dagger}_{\alpha}(E)\hat{b}_{\beta}(E') + \hat{b}_{\beta}(E')\hat{b}^{\dagger}_{\alpha}(E) = \delta_{\alpha\beta}\delta(E - E')$$

$$\hat{\Psi}_{\alpha}(t,\mathbf{r}) = \frac{1}{\sqrt{h}}\int_0^{\infty} dE\ e^{-i\frac{E}{\hbar}t}\left\{\hat{a}_{\alpha}(E)\frac{\psi^{(in)}_{\alpha}(E,\mathbf{r})}{\sqrt{v_{\alpha}(E)}} + \hat{b}_{\alpha}(E)\frac{\psi^{(out)}_{\alpha}(E,\mathbf{r})}{\sqrt{v_{\alpha}(E)}}\right\}$$
$$\hat{\Psi}^{\dagger}_{\alpha}(t,\mathbf{r}) = \frac{1}{\sqrt{h}}\int_0^{\infty} dE\ e^{i\frac{E}{\hbar}t}\left\{\hat{a}^{\dagger}_{\alpha}(E)\frac{\psi^{(in)*}_{\alpha}(E,\mathbf{r})}{\sqrt{v_{\alpha}(E)}} + \hat{b}^{\dagger}_{\alpha}(E)\frac{\psi^{(out)*}_{\alpha}(E,\mathbf{r})}{\sqrt{v_{\alpha}(E)}}\right\}$$

Current operator

$$\hat{I}_\alpha(t,x) = \frac{i\hbar e}{2m}\int dr_\perp \left\{ \frac{\partial \hat{\Psi}_\alpha\dagger(t,\mathbf{r})}{\partial x}\hat{\Psi}_\alpha(t,\mathbf{r}) - \hat{\Psi}_\alpha\dagger(t,\mathbf{r})\frac{\partial \hat{\Psi}_\alpha(t,\mathbf{r})}{\partial x} \right\}$$

- The basis wave functions

$$\psi^{(in)}(E,\mathbf{r}) = \xi_E(r_\perp)e^{-ik(E)x}$$
$$\psi^{(out)}(E,\mathbf{r}) = \xi_E(r_\perp)e^{ik(E)x}$$

- Much smaller bias than the Fermi-energy, μ_0

$$|E - E'| << E \sim \mu_0$$

$$\Downarrow$$

$$\hat{I}_\alpha(t) = \int\int dE\, dE' e^{i\frac{E-E'}{\hbar}t} \left\{ \hat{b}^\dagger_\alpha(E)\hat{b}_\alpha(E') - \hat{a}^\dagger_\alpha(E)\hat{a}_\alpha(E') \right\}$$

Measurable current - $\langle \hat{I}_\alpha \rangle$

Propagating from reservoir - $\hat{a}^\dagger_\alpha(E)/\hat{a}_\alpha(E)$

- equilibrium in the reservoirs
- quantum-statistical average $\Rightarrow$ Fermi-distribution

$$\langle \hat{a}^\dagger_\alpha(E)\hat{a}_\beta(E')\rangle = \delta_{\alpha\beta}\delta(E-E')f_\alpha(E)$$
$$\langle \hat{a}_\alpha(E)\hat{a}^\dagger_\beta(E')\rangle = \delta_{\alpha\beta}\delta(E-E')\left\{1-f_\alpha(E)\right\}$$

Scattered particles - $\hat{b}^\dagger_\alpha(E)/\hat{b}_\alpha(E)$

- non-equilibrium particles
- calculate them from the in-coming particle operators

$$\hat{\Psi}^{(in)} = \sum_{\alpha=1}^{N_r} \hat{a}_\alpha \frac{\psi^{(in)}_\alpha}{\sqrt{v_\alpha}} \qquad \hat{\Psi}^{(out)} = \sum_{\beta=1}^{N_r} \hat{b}_\beta \frac{\psi^{(out)}_\beta}{\sqrt{v_\beta}}$$

$$\Downarrow$$

$$\hat{b}_\alpha = \sum_{\beta=1}^{N_r} S_{\alpha\beta}\hat{a}_\beta \qquad \hat{b}^\dagger_\alpha = \sum_{\beta=1}^{N_r} S^*_{\alpha\beta}\hat{a}^\dagger_\beta$$

DC current and the distribution functions

Scope

- under the DC bias: $\Delta V_{\alpha\beta} = V_\alpha - V_\beta$
- the chemical potentials: $\mu_\alpha = \mu_0 + eV_\alpha$
- energy: $E = E_{kin} + E_{pot}$ is conserved (in the stationary case)

Distribution functions

- Averaging:

$$\langle \hat{a}^\dagger_\alpha(E)\hat{a}_\alpha(E')\rangle = \delta(E-E')f^{(in)}_\alpha(E)$$
$$\langle \hat{b}^\dagger_\alpha(E)\hat{b}_\alpha(E')\rangle = \delta(E-E')f^{(out)}_\alpha(E)$$

- Average number of e$^-$-s: $\frac{dE}{h} f^{(in/out)}_\alpha(E)$
- For in-coming electrons: $f^{(in)}_\alpha(E) = f_\alpha(E)$

$$I_\alpha = \frac{e}{h}\int dE \left\{ f^{(out)}_\alpha(E) - f^{(in)}_\alpha(E) \right\}$$

Distribution for scattered electrons - $f_\alpha^{(out)}(E)$

$$\delta(E-E')f_\alpha^{(out)}(E) \equiv \langle \hat{b}_\alpha^\dagger(E)\hat{b}_\alpha(E')\rangle =$$
$$= \sum_{\beta=1}^{N_r}\sum_{\gamma=1}^{N_r} S_{\alpha\beta}^*(E)S_{\alpha\gamma}(E')\langle \hat{a}_\beta^\dagger(E)\hat{a}_\gamma(E')\rangle =$$
$$= \sum_{\beta=1}^{N_r}\sum_{\gamma=1}^{N_r} S_{\alpha\beta}^*(E)S_{\alpha\gamma}(E')\delta(E-E')\delta_{\beta\gamma}f_\beta(E)$$

$$\Downarrow$$

$$f_\alpha^{(out)}(E) = \sum_{\beta=1}^{N_r} |S_{\alpha\beta}(E)|^2 f_\beta(E)$$

$$I_\alpha = \frac{e}{h}\int dE \sum_{\beta=1}^{N_r} |S_{\alpha\beta}(E)|^2 \left\{f_\beta(E) - f_\alpha(E)\right\}$$

DC current conservation

Current conservation

- Electrical charge continuity equation:

$$\mathrm{div}\mathbf{j} + \frac{\partial \rho}{\partial t} = 0$$

- $\int$ it over the volume enclosed by the surface $\sum$

$$\sum_{\alpha=1}^{N_r} I_\alpha(t) + \frac{\partial Q}{\partial t} = 0$$

- $\Rightarrow$ both in stationary and non-stationary case:

$$\sum_{\alpha=1}^{N_r} I_\alpha = 0$$

DC current conservation

Does I_α satisfy the conservation law?

- The unitarity of the scattering matrix:

$$\hat{S}^\dagger \hat{S} = \hat{I} \Rightarrow \sum_{\alpha=1}^{N_r} \left|S_{\alpha\beta}(E)\right|^2 = 1$$

- Substituting back:

$$\sum_{\alpha=1}^{N_r} I_\alpha = \frac{e}{h}\int dE \sum_{\alpha=1}^{N_r}\sum_{\beta=1}^{N_r} \left|S_{\alpha\beta}(E)\right|^2 \left\{f_\beta(E) - f_\alpha(E)\right\} =$$

$$= \frac{e}{h}\int dE \left\{\sum_{\beta=1}^{N_r} f_\beta(E) \sum_{\alpha=1}^{N_r} \left|S_{\alpha\beta}(E)\right|^2 - \sum_{\alpha=1}^{N_r} f_\alpha(E) \sum_{\beta=1}^{N_r} \left|S_{\alpha\beta}(E)\right|^2\right\} =$$

$$= \frac{e}{h}\int dE \left\{\sum_{\beta=1}^{N_r} f_\beta(E) - \sum_{\alpha=1}^{N_r} f_\alpha(E)\right\} = 0$$

Summary

- Derivation of the scattering matrix method
- Problem of transport phenomena in macroscopic sample
- Definition of current operator in 2^{nd} quantization
- Measurable current for DC bias
- DC current conservation

Thank you for your attention!