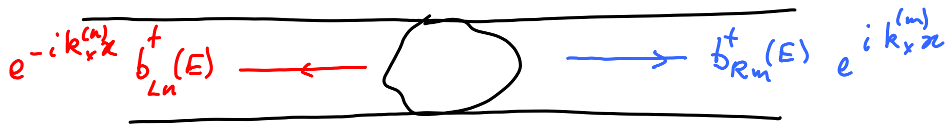
1.3.4 Scattering in Operator Formalism (SOF)

30.6.10 SOF1



$$k_x^{(n)} = \sqrt{2m(E-E_n(x))}$$

Basis for outgoing states in left, right waveguides:

$$\{ b_{\alpha l \sigma}(E), b^\dagger_{\alpha' l' \sigma'}(E) \} = \delta_{\alpha\alpha'}\,\delta_{ll'}\,\delta_{\sigma\sigma'}\,\delta(E-E') \qquad (1)$$

$$\{ b, b' \} = \{ b^\dagger, b'^\dagger \} = 0 \qquad (2)$$

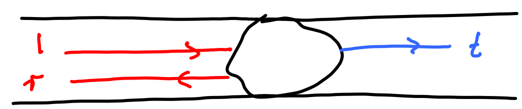
$\alpha = L, R \quad l = \text{mode index}, \ \sigma = \uparrow,\downarrow = \text{spin}$

These plane waves do not form a basis throughout full scattering region, only represent asymptotic expressions for outgoing states

Scattering state basis:

SOF2

Incident from left, scattered to right:



In left waveguide:

$$\Psi_{Ln}(x_L, y_L, z_L) = \frac{1}{\sqrt{2\pi\hbar v_n(E)}}\,\Phi_n(y_L,z_L)\,e^{ik_x^{(n)}x_L} \qquad (1)$$

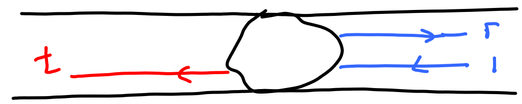
$$+ \sum_{n'} \frac{1}{\sqrt{2\pi\hbar v_{n'}(E)}}\, r_{n'n}(E)\,\Phi_{n'}(y_L,z_L)\,e^{-ik_x^{(n')}x_L}$$

In right waveguide:

$$\Psi_{Ln}(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m(E)}}\, t_{mn}(E)\,\Phi_m(y_R,z_R)\,e^{-ik_x^{(m)}x_R} \qquad (2)$$

Similarly: (SOF3)

Incident from right, scattered to left:



In right waveguide:

$$\Psi_{Rm}(x_R, y_R, z_R) = \frac{1}{\sqrt{2\pi\hbar v_m(E)}}\, \Phi_m(y_R, z_R)\, e^{ik_x^{(m)} x_R} \qquad (1)$$

$$+ \sum_{m'} \frac{1}{\sqrt{2\pi\hbar v_{m'}(E)}}\, r_{m'm}(E)\, \Phi_{m'}(y_R, z_R)\, e^{-ik_x^{(m')} x_R}$$

In left waveguide:

$$\Psi_{Rm}(x_L, y_L, z_L) = \sum_n \frac{1}{\sqrt{2\pi\hbar v_n(E)}}\, t_{m'm}(E)\, \Phi_n(y_L, z_L)\, e^{-ik_x^{(n)} x_L} \qquad (2)$$

(SOF4)

$\psi_{Ln}(x,y,z)$ form complete basis, with associated operators $a^\dagger_{Ln}(E)$ $\left(a_{Ln}(E)\right)$ which create (annihilate) electrons originating in left reservoir

$\psi_{Rn}(x,y,z)$ form complete basis, with associated operators $a^\dagger_{Rn}(E)$ $\left(a_{Rn}(E)\right)$ which create (annihilate) electrons originating in right reservoir

Anticommutators:

$$\{a_{\alpha\ell\sigma}(E),\, a^\dagger_{\alpha'\ell'\sigma'}(E')\} = \delta_{\alpha\alpha'}\,\delta_{\ell\ell'}\,\delta_{\sigma\sigma'}\,\delta(E-E') \qquad (1a)$$

$$\{a_{\alpha\ell\sigma}(E),\, a_{\alpha'\ell'\sigma'}(E')\} = 0 \qquad (1b)$$

$$\{a^\dagger_{\alpha\ell\sigma}(E),\, a^\dagger_{\alpha'\ell'\sigma'}(E')\} = 0 \qquad (1c)$$

The a, a^+ and b, b^+ both form a complete set of single-particle operators. Thus, they are linearly related: (SOF5)

scattering matrix

$$b_{\alpha l \sigma}(E) = \sum_{\alpha'=L,R} \sum_{l'} S_{\alpha l, \alpha' l'}(E)\, a_{\alpha' l' \sigma}(E) \quad (1)$$

$$b^+_{\alpha l \sigma}(E) = \sum_{\alpha'=L,R} \sum_{l'} S^*_{\alpha l', \alpha' l}(E)\, a^+_{\alpha' l' \sigma}(E) \quad (2)$$

for $\alpha = L, R$, $l = n, m$

Quantum-mechanical averages:

Fermi function of $\alpha = L/R$ lead

$$\langle a^+_{\alpha l \sigma}(E)\, a_{\alpha' l' \sigma'}(E') \rangle = \delta_{\alpha\alpha'} \delta_{ll'} \delta_{\sigma\sigma'} \delta(E - E')\, f_\alpha(E) \quad (3)$$

$$\langle a a \rangle = \langle a^+ a^+ \rangle = 0 \quad (4)$$

Field operators which annihilate/create electron with spin σ at $\bar{x}, t$: (SOF6)

In left waveguide: incident outgoing (1)

$$\hat{\Psi}_\sigma(\vec{r}, t) = \int dE\, e^{-iEt/\hbar} \sum_n \frac{\Phi_n(y_L, z_L)}{\sqrt{2\pi\hbar v_n(E)}} \left[\hat{a}_{Ln\sigma} e^{ik_x^{(n)} x_L} + \hat{b}_{Ln\sigma} e^{-ik_x^{(n)} x_L} \right]$$

In right waveguide: incident outgoing (2)

$$\hat{\Psi}_\sigma(\vec{r}, t) = \int dE\, e^{-iEt/\hbar} \sum_m \frac{\Phi_m(y_R, z_R)}{\sqrt{2\pi\hbar v_m(E)}} \left[\hat{a}_{Rm\sigma} e^{-ik_x^{(m)} x_R} + \hat{b}_{Rm\sigma} e^{+ik_x^{(m)} x_R} \right]$$

(3)

Current: in left guide:

$$\hat{I}(x_L, t) = \frac{\hbar e}{2im} \sum_\sigma \int dy_L \int dz_L \left[\hat{\Psi}^+_\sigma \frac{\partial}{\partial x_L} \hat{\Psi}_\sigma - \left(\frac{\partial}{\partial x_L} \hat{\Psi}^+ \right) \Psi_\sigma \right](x_L)$$

To find time-averaged current, use trick: SOF 7

Suppose all quantities are periodic in time with period $\mathcal{T} \to \infty$

Exponent $e^{-iEt/\hbar}$ must then be periodic, $\Longrightarrow$

replace $E \longrightarrow 2\pi q \hbar/\mathcal{T}$ with $q \in \mathbb{Z}$ (1)

$$\Rightarrow \quad \int dE \to \frac{2\pi\hbar}{\mathcal{T}} \sum_E \quad (2a), \qquad \delta(E-E') \longrightarrow \frac{\mathcal{T}}{2\pi\hbar}\,\delta_{EE'} \quad (2b)$$

means: $\sum_q$ with $E = 2\pi q\hbar/\mathcal{T}$ means: $\delta_{qq'}$

and time-average:

$$\left\langle e^{i(E-E')t/\hbar}\right\rangle_t = \frac{1}{\mathcal{T}}\int_0^{\mathcal{T}} dt\, e^{i2\pi(q-q')t/\mathcal{T}} \quad (3)$$

$$= \left\{ \begin{array}{ll} 1 & \text{if } q = q' \\ \left(e^{i2\pi(q-q')}-1\right) = 0 & \text{if } q \neq q' \end{array} \right\} = \delta_{qq'} \equiv \delta_{EE'} \quad (4)$$

Time-averaged current: SOF 8

$$\left\langle \hat{I}(x_L,t)\right\rangle_t \overset{(6.2)}{=} \frac{e\hbar}{2im}\int dy_L \int dz_L \sum_\sigma \left\{ \left\langle \psi_\sigma^\dagger \frac{\partial}{\partial x_L}\psi_\sigma \right\rangle_t - \left\langle \frac{\partial}{\partial x_L}\psi_\sigma^\dagger\, \psi_\sigma\right\rangle_t \right\} \quad (1)$$

$$= \underbrace{\int dE \int dE'}_{\substack{(7.2a) \\ \left(\frac{2\pi\hbar}{\mathcal{T}}\right)^2 \sum_E \cancel{\sum_{E'}}}} \left\langle \underbrace{e^{i(E-E')t}}_{\substack{(7.4) \\ \cancel{\delta_{EE'}}}} \right\rangle_t \overbrace{\int dy_L \int dz_L \sum_{n\sigma} \frac{\Phi_n^*(y_L,z_L)}{\sqrt{2\pi\hbar\, \cancel{v_n(E)}}} \sum_{n'} \frac{\Phi_{n'}(y_L,z_L)}{\sqrt{2\pi\hbar\, \cancel{v_{n'}(E')}}}}^{\delta_{nn'} \text{ (orthogonality)}} \quad (2a)$$

$$\times \left\{ \left[\hat{a}^\dagger_{Ln\sigma} e^{-ik_x^{(n)}x_L} + \hat{b}^\dagger_{Ln\sigma} e^{+ik_x^{(n)}x_L}\right] e \overbrace{\frac{\hbar k_x^{(n)}}{m}}^{\cancel{v_{n'}(E')}} \left[\hat{a}_{Ln'\sigma} e^{ik_x^{(n)}x_L} - \hat{b}_{Ln'\sigma} e^{-ik_x^{(n')}x_L} \right] \right. \quad (2b)$$

$$\left. - \left[-\hat{a}^\dagger_{Ln\sigma} e^{-ik_x^{(n)}x_L} + \hat{b}^\dagger_{Ln\sigma} e^{+ik_x^{(n)}x_L}\right] e \overbrace{\frac{\hbar k_x^{(n)}}{m}}^{\cancel{v_n(E)}} \left[\hat{a}_{Ln'\sigma} e^{ik_x^{(n)}x_L} + \hat{b}_{Ln'\sigma} e^{-ik_x^{(n')}x_L} \right] \right\} \quad (2c)$$

SF09

In (7.2b+c): $a^\dagger a$ and $b^\dagger b$ survive, $a^\dagger b$ and $b^\dagger a$ drop out:

$$\langle I\rangle_t = \frac{G_Q}{e}\left(\frac{2\pi\hbar}{T}\right)^2 \underbrace{\frac{1}{2_s}\sum_\sigma}_{\text{average over spin}}\sum_n\sum_E \Big[\underbrace{a^\dagger_{Ln\sigma}(E)\,a_{Ln\sigma}(E)}_{} - \underbrace{b^\dagger_{Ln\sigma}(E)\,b_{Ln\sigma}(E)}_{}\Big] \qquad (1)$$

$G_Q = \frac{2_s e^2}{2\pi\hbar}$

Interpretation: (total # of particles moving to right) − (total # of particles moving to left)

Eliminate b for a using (5.1),(5.2):

$$b_{\alpha l\sigma}(E) = \sum_{\alpha'=L,R}\sum_{l'} S_{\alpha l,\alpha' l'}(E)\, a_{\alpha' l'\sigma}(E) \qquad (5.1)$$

$$\langle \hat I\rangle_t = \frac{G_Q}{e}\left(\frac{2\pi\hbar}{T}\right)^2 \frac{1}{2_s}\sum_\sigma\sum_n\sum_E\sum_{\alpha\alpha'}\sum_{ll'} a^\dagger_{\alpha l\sigma}(E)\, a_{\alpha' l'\sigma}(E) \qquad (2)$$

$$\times\Big[\delta_{\alpha L}\delta_{\alpha' L}\delta_{ln}\delta_{l'n} - S^*_{Ln,\alpha l}(E)\, S_{Ln,\alpha' l'}(E)\Big] \qquad (3)$$

SF010

Now perform QM average, using (5.3):

$$\langle a^\dagger_{\alpha l\sigma}(E)\, a_{\alpha' l'\sigma'}(\epsilon)\rangle = \delta_{\alpha\alpha'}\delta_{ll'}\delta_{\sigma\sigma'}\underbrace{\delta(E-\epsilon)}_{(7.2b)\, =\, \left(\frac{T}{2\pi\hbar}\right)\underbrace{\delta_{EE}}_{=1}}\, f_\alpha(E) \qquad (5.3)$$

$$\boxed{(SM3.2)\quad S = \begin{pmatrix}\hat S_{LL} & \hat S_{LR}\\ \hat S_{RL} & \hat S_{RR}\end{pmatrix} = \begin{pmatrix}\hat r & \hat t'\\ \hat t & \hat r'\end{pmatrix}}$$

$$\langle\langle \hat I\rangle_t\rangle_{QM} = G_Q \underbrace{\frac{2\pi\hbar}{T}\sum_E}_{\int dE} \underbrace{\frac{1}{2_s}\sum_\sigma}_{=1}\Big[\cancel{\sum_l} f_L(E)$$

$$-\Big(\underbrace{f_L(E)\sum_{ln}\underbrace{S^*_{Ln,Ll}(E)}_{\hat r^*_{nl}=\hat r^\dagger_{ln}}\underbrace{S_{Ln,Ll}(E)}_{\hat r_{nl}}}_{} + \underbrace{f_R(E)\sum_{ln}\underbrace{S^*_{Ln,Rl}(E)}_{\hat t'^*_{nl}=\hat t'^\dagger_{ln}}\underbrace{S_{Ln,Rl}(E)}_{\hat t'_{nl}}}_{}\Big)\Big]$$

$$\sum_l(\hat r^\dagger\hat r)_{ll} = \cancel{\sum_l 1} - \underbrace{\sum_l(\hat t^\dagger t)_{ll}}_{=\sum_p T_p} \qquad \sum_l(\hat t'^\dagger t')_{ll} = \sum_p T_p$$

$$\boxed{\langle\langle \hat I\rangle_t\rangle_{QM} = \frac{G_Q}{e}\int_0^\infty dE\,\sum_p T_p(E)\,[f_L(E) - f_R(E)] = \text{Landauer!}\ (SM12.4)}$$