Non-stationary scattering theory

Pető jános

Current operator

- Operators for scattered electrons expressed in terms of operators for incident electrons
- Floquet scattering matrix
- Takeing into account the change of electron energy during scattering (several $\hbar\Omega_0$ quanta)
- $b_\alpha(E) = \sum_{n=-\infty}^{\infty} \sum_{\beta=1}^{N_r} S_{\alpha\beta}^F (E, E_n) a_\beta(E_n)$
- $b_\alpha^+(E) = \sum_{n=-\infty}^{\infty} \sum_{\beta=1}^{N_r} {S_{\alpha\beta}^F}^* (E, E_n) a_\alpha^+(E_n)$
- Above equations together with unitarity provide right anti-commutation relations (b-operators similar to a-operators)

Current operator

- We assume: periodicity in time varying of scattering properties causes periodic current
- Frequency representation:
- $I_\alpha(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} I_\alpha(\omega)$
- $I_\alpha(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} I_\alpha(t)$ (Fourier transformation)
- Current operator expressed in terms of a, b operators:
- $I_\alpha(t) = \frac{e}{h} \iint dE dE' e^{i\frac{E-E'}{\hbar}t} \{b_\alpha^+(E) b_\alpha(E') - a_\alpha^+(E) a_\alpha(E')\}$

Current operator

- Using this equation, we calculate:
- $I_\alpha(\omega) = e\int_0^\infty dE\{b_\alpha^+(E)b_\alpha(E+\hbar\omega) - a_\alpha^+(E)a_\alpha(E+\hbar\omega)\}$

AC current

- Substituting the equations for a,b operators into the equation for current (expressed above)
- Calculate current spectrum: $I_\alpha(\omega) = \langle \widehat{I_\alpha}(\omega) \rangle$
- $I_\alpha(\omega) = \sum_{l=-\infty}^{\infty} 2\pi\delta(\omega - l\Omega_0)\, I_{\alpha,l}$
- $I_{\alpha,l} = \frac{e}{h}\int_0^\infty dE \left\{\sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} {S_{\alpha\beta}^F}^*(E, E_n)S_{\alpha\beta}^F(E_l, E_n)f_\beta(E_n) - \delta_{l0}f_\alpha(E)\right\}$
- This can be rewritten ($E_n \to E, n \to -n$) :
- $I_{\alpha,l} = \frac{e}{h}\int_0^\infty dE \sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} {S_{\alpha\beta}^F}^*(E_n, E)S_{\alpha\beta}^F(E_{l+n}, E)\{f_\beta(E) - f_\alpha(E_n)\}$
- The above equation is convenient in case of slow variation

AC current

- Using these equations we can arrive at the time-dependent current:
- $I_\alpha(t) = \sum_{l=-\infty}^{\infty} e^{-il\Omega_0 t}\, I_{\alpha,l}$
- This is periodic in time: $I_\alpha(t) = I_\alpha\left(t + \frac{2\pi}{\Omega_0}\right)$

DC current

- $I_\alpha(t)$ has a time-independent part
- Only exists under special conditions
- We use l=0
- $I_{\alpha,0} = \frac{e}{h}\int_0^\infty dE \left\{\sum_{n=-\infty}^{\infty}\sum_{\beta=1}^{N_r}\left|S_{\alpha\beta}^F(E,E_n)\right|^2 f_\beta(E_n) - f_\alpha(E)\right\}$
- DC current is subject to conservation law: $\sum_{\alpha=0}^{N_r} I_{\alpha,0} = 0$
- $I_{\alpha,0} = \frac{e}{h}\int_0^\infty dE \sum_{n=-\infty}^{\infty}\sum_{\beta=1}^{N_r}\left|S_{\alpha\beta}^F(E_n,E)\right|^2 \{f_\beta(E) - f_\alpha(E_n)\}$
- From this equation we can see that (for $\hbar\Omega_0 \ll \mu$) only electrons close to the Fermi energy contribute to the current
- Energy window is defined by the maximum of: $\hbar\Omega_0, \left|eV_{\alpha\beta}\right|, k_B T_\alpha$

DC current

- $I_{\alpha,0} = \frac{e}{h} \int_0^\infty dE \sum_{n=-\infty}^{\infty} \sum_{\beta=1}^{N_r} \left\{ \left| S_{\alpha\beta}^F(E_n, E) \right|^2 f_\beta(E) - \left| S_{\beta\alpha}^F(E_n, E) \right|^2 f_\alpha(E) \right\}$
- DC current in lead α as the difference of two electron flows
- First term: electrons from various leads β scatter into lead α
- Second term: electrons from lead α scatter into leads β
- All the above written equations are equivalent

Adiabatic approximation for the Floquet scattering matrix

- One needs to solve the non-stationary Schrödinger equation
- Stationary scattering matrix S has $N_r \times N_r$ elements, while S^F has more, $N_r \times N_r \times (2n_{max}+1)^2$ (n_{max}: max. number of $\hbar\Omega_0$ quanta)
- If $\delta U \ll \hbar\Omega_0$, then $n_{max} = 1$, if $\delta U \gg \hbar\Omega_0$, then $n_{max} \gg 1$
- Multi-photon processes are important, if scatterer parameters vary slowly
- When $\Omega_0 \to 0$, the scatterer should not feel dynamic to scattered electrons, but there are principal differences between stationary and non-stationary scatterers

Adiabatic approximation for the Floquet scattering matrix
Frozen scattering matrix

- Stationary scattering matrix S depends on p_i parameters varied periodically in time
- $S(t, E) = S(\{p(t)\}, E) = S(t + \tau, E), \tau = \frac{2\pi}{\Omega_0}$
- We fix all paramters at $t = t_0$ and $S(t_0, E)$ describes this scatterer
- Treating every t moment like this defines the frozen scattering matrix (t is a parameter)
- At $\Omega_0 \to 0$ there exists some relation between the frozen and Floquet scattering matrices
- $S^F = \sum_{q=0}^{\infty} (\hbar\Omega_0)^q \, S^{F(q)}$ adiabatic expansion

Adiabatic approximation for the Floquet scattering matrix
Zeroth order approximation

- q=0, $S^{F(0)}$ only depends on initial E energy (initial=final energy)
- $S^F_{\alpha\beta}(E_n, E)$ describes electron energy change:
  $\Psi^{(out)}_{E_n,\alpha} \sim S^F_{\alpha\beta}(E_n, E)\Psi^{(in)}_{E,\beta}; \Psi^{(in)}_{E,\beta} \sim e^{-i\frac{Et}{\hbar}}; \Psi^{(out)}_{E_n,\alpha} \sim e^{-i\frac{E_n t}{\hbar}} = e^{-i\frac{Et}{\hbar}} e^{-in\Omega_0 t}$
- $\Psi^{(out)}_{E,\alpha} \sim S_{\alpha\beta}(E_n, E)\Psi^{(in)}_{E,\beta}$ with the frozen scattering matrix
- Fourier expansion: $S(t, E) = \sum_{n=-\infty}^{\infty} e^{-in\Omega_0 t} S_n(E)$
- Floquet scattering matrix elements=Fourier coefficients of frozen scattering matrix
- $S^{F(0)}(E_n, E) = S_n(E)$
- $S^{F(0)}(E, E_n) = S_{-n}(E)$

Adiabatic approximation for the Floquet scattering matrix
First order approximation

- q=1, $E \neq E_n$, simplest generalization of zeroth order would be the above written equations with $S\left(\frac{E+E_n}{2}\right)$ frozen scattering matrix, but this is not unitary!
- We have to introduce additional term: $\hbar\Omega_0 A_n(E)$, where $A_n(E)$ is Fourier transform of $A(t,E)$
- $\hbar\Omega_0 S^{F(1)}(E_n, E) = \frac{n\hbar\Omega_0}{2}\frac{\partial S_n(E)}{\partial E} + \hbar\Omega_0 A_n(E)$
- $\hbar\Omega_0 S^{F(1)}(E, E_n) = \frac{n\hbar\Omega_0}{2}\frac{\partial S_{-n}(E)}{\partial E} + \hbar\Omega_0 A_{-n}(E)$
- These equations point out the actual expansion parameter: $\varpi = \frac{\hbar\Omega_0}{\delta E} \ll 1$ (adiabacity parameter)
- δE: characteristic energy scale where stationary scattering matrix changes significantly

Anomalous scattering matrix

- The A matrix can not be expressed explicitly in terms of the frozen scattering matrix
- $S^F_{\alpha\beta}(E_n,E) = S_{\alpha\beta,n}(E) + \frac{n\hbar\Omega_0}{2}\frac{\partial S_{\alpha\beta,n}(E)}{\partial E} + \hbar\Omega_0 A_{\alpha\beta,n}(E) + \mathcal{O}(\varpi^2)$
- Using the unitarity of the Floquet matrix:
- $\sum_{n=-\infty}^{\infty}\sum_{\alpha=1}^{N_r}\left\{S^*_{\alpha\gamma,n-m}(E) + \frac{(n+m)\hbar\Omega_0}{2}\frac{\partial S^*_{\alpha\gamma,n-m}(E)}{\partial E} + \hbar\Omega_0 A^*_{\alpha\gamma,n-m}(E)\right\}\left\{S_{\alpha\beta,n}(E) + \frac{n\hbar\Omega_0}{2}\frac{\partial S_{\alpha\beta,n}(E)}{\partial E} + \hbar\Omega_0 A_{\alpha\beta,n}(E)\right\} = \delta_{\beta\gamma}\delta_{m0}$
- S(t,E) is unitary and we omit terms of order Ω_0^2

Anomalous scattering matrix

- $\sum_{n=-\infty}^{\infty}\sum_{\alpha=1}^{N_r}\left\{S_{\alpha\beta,n}(E)\left(n-\frac{n-m}{2}\right)\frac{\partial S^*_{\alpha\gamma,n-m}(E)}{\partial E}+\frac{n}{2}\frac{\partial S_{\alpha\beta,n}(E)}{\partial E}S^*_{\alpha\gamma,n-m}(E)+\left[S_{\alpha\beta,n}(E)A^*_{\alpha\gamma,n-m}(E)+A_{\alpha\beta,n}(E)S^*_{\alpha\gamma,n-m}(E)\right]\right\}=0$
- We use inverse Fourier transformation and arrive at the following:
- $\frac{i}{\Omega_0}\frac{\partial S^+}{\partial E}\frac{\partial S}{\partial t}+\frac{i}{2\Omega_0}\left\{\frac{\partial^2 S^+}{\partial t\partial E}S+S^+\frac{\partial^2 S}{\partial t\partial E}\right\}+A^+S+S^+A=0$
- We can simplify using: $\frac{\partial^2 S^+S}{\partial t\partial E}=0$
- $\hbar\Omega_0[S^+(t,E)A(t,E)+A^+(t,E)S(t,E)]=\frac{1}{2}P\{S^+(t,E),S(t,E)\}$
- P is the Poisson-bracket of the two matrices
- P is self-adjoint and traceless

Anomalous scattering matrix

- Symmetry conditions
- $S(t, E, H, \{\varphi\}) = S(-t, E, H, \{-\varphi\}) \Rightarrow A(t, E, H, \{\varphi\}) = - A(-t, E, H, \{-\varphi\})$
- $S_n(E, H, \{\varphi\}) = S_{-n}(E, H, \{-\varphi\}) \Rightarrow A_n(E, H, \{\varphi\}) = -A_{-n}(E, H, \{-\varphi\})$
- $A_{\alpha\beta}(t, E, H, \{\varphi\}) = -A_{\beta\alpha}(t, E, -H, \{\varphi\})$
- $S_{\alpha\beta}(t, E, H, \{\varphi\}) = S_{\beta\alpha}(t, E, -H, \{\varphi\})$