Floquet scattering matrix
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Beyond the adiabatic approximation

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Content

1. Reminder - Floquet scattering matrix
2. Floquet matrix in mixed representation
3. Time-dependent AC current
4. Point-like scattering potential
   - General consideration
   - Wave with unit amplitude - Incident from the left
   - Wave with unit amplitude - Incident from the right
   - Wave with unit amplitude - Incident from both side
5. Summary

Floquet theorem

Non-stationary scattering theory - Time periodic potential

$$i\hbar\frac{\partial\Psi(t,\vec{r})}{\partial t} = H(t,\vec{r})\Psi(t,\vec{r})$$
$$H(t,\vec{r}) = H_0(\vec{r}) + V(t,\vec{r})$$

Floquet theorem

- V is periodic in time $\rightarrow$ but! no restriction on the strength
- Time periodic Hamiltonian: $H(t,\vec{r}) = H(t+\tau,\vec{r})$
- The solution can be written as

$$\Psi(t,\vec{r}) = e^{-i\frac{E}{\hbar}t}\Phi(t,\vec{r})$$
$$\Phi(t,\vec{r}) = \Phi(t+\tau,\vec{r})$$

- After the Fourier-expansion of a time-periodic function

$$\Psi(t,\vec{r}) = e^{-i\frac{E}{\hbar}t}\sum_{q=-\infty}^{\infty} e^{-iq\Omega_0 t}\psi_q(\vec{r})$$

Floquet scattering matrix

Floquet scattering matrix

- The main difference to the stationary one: it can change the energy of incident electrons
- Time periodic Hamiltonian $\rightarrow$ the scattered electron's wave function is the Floquet function type with components corresponding to different energies
- E energy of the incident e^-: Floquet-energy
- Floquet scattering matrix: $\hat{S}_F$
- Scattering amplitudes $S_{F,\alpha\beta}(E_n, E)$: transition between states of the stationary Hamiltonian

Floquet scattering matrix

Properties

- Unitarity

$$\sum_n \sum_{\alpha=1}^{N_r} S^*_{F,\alpha\beta}(E_n, E_m) S_{F,\alpha\gamma}(E_n, E) = \delta_{m,0}\delta_{\beta,\gamma}$$

$$\sum_n \sum_{\beta=1}^{N_r} S_{F,\gamma\beta}(E_m, E_n) S^*_{F,\alpha\beta}(E, E_n) = \delta_{m,0}\delta_{\alpha,\gamma}$$

- Micro-reversibility
  - the Hamiltonian depends on N_p parameters: $p_i(t)$

$$p_i(t) = p_{i,0} + p_{i,1}\cos(\Omega_0 t + \phi_i)$$

$$\Downarrow$$

$$S_{F,\alpha\beta}(E, E_n; H, \{\phi\}) = S_{F,\beta\alpha}(E_n, E; -H, \{-\phi\})$$

Adiabatic approximation

The frozen scattering matrix

- Let $\hat{S}$ depend on several time periodic parameters: $\hat{S}(t,E) = \hat{S}(\{p(t)\};E), \qquad \hat{S}(t,E) = \hat{S}(t+\tau,E)$
- $\hat{S}(t)$ does not describe a scattering into a dynamic scatterer, $\hat{S}(t,E)$ is the frozen scattering matrix which stands for the scattering into a frozen state defined by the values of the parameters at time t
- Relation to the Floquet scattering matrix if $\Omega_0 \to 0$ (*adiabatic expansion*):

$$\varpi = \frac{\hbar\Omega_0}{\delta E} << 1, \qquad \hat{S}_F = \sum_{q=0}^{\infty} (\hbar\Omega_0)^q \hat{S}_F^{(q)}$$

First order approximation

- The initial energy E is different from the final one E_n
- Additional term $(\hbar\Omega_0 \hat{A}_n(E))$ in order to recover unitarity

$$\hbar\Omega_0 \hat{S}_F^{(1)}(E_n,E) = \frac{n\hbar\Omega_0}{2}\frac{\partial \hat{S}_n(E)}{\partial E} + \hbar\Omega_0 \hat{A}_n(E)$$

$$\hbar\Omega_0 \hat{S}_F^{(1)}(E,E_n) = \frac{n\hbar\Omega_0}{2}\frac{\partial \hat{S}_{-n}(E)}{\partial E} + \hbar\Omega_0 \hat{A}_{-n}(E)$$

The mixed representation

Mixed enery-time representation

- Let us introduce $\hat{S}_{in}(t,E)$ and $\hat{S}_{out}(E,t)$

$$\hat{S}_F(E_n,E) = \hat{S}_{in,n}(E) \equiv \int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}} e^{in\Omega_0 t} \hat{S}_{in}(t,E)$$

$$\hat{S}_F(E,E_n) = \hat{S}_{out,-n}(E) \equiv \int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}} e^{-in\Omega_0 t} \hat{S}_{out}(E,t)$$

- $\hat{S}_{in}(t,E)$: scattering amplitudes for incident e$^-$-s with energy E and leaving the scatterer at time t
- $\hat{S}_{out}(E,t)$: scattering amplitudes for incident e$^-$-s at time t and leaving the scatterer with energy E
- Consistent with the Heisenberg uncertainty

incident energy $E_m = E + m\hbar\Omega_0$ from the lead $\beta \to$ outgoing energy E in lead α

$|S_{out,\alpha\beta,-m}(E)|^2$

Properties

- Unitarity

$$\int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}} e^{in\Omega_0 t} \hat{S}_{in}^{\dagger}(t, E_m) \hat{S}_{in}(t, E) = \delta_{m,0} \hat{I}$$

$$\int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}} e^{in\Omega_0 t} \hat{S}_{out}(E_m, t) \hat{S}_{out}^{\dagger}(E, t) = \delta_{m,0} \hat{I}$$

- Micro-reversibility

$$\hat{S}_{in}(t, E; H, \{\phi\}) = \hat{S}_{out}^{T}(E, -t; -H, \{-\phi\})$$

- From the definition

$$\hat{S}_{in,n}(E) = \hat{S}_{out,n}(E_n)$$

that in time representation reads

$$\hat{S}_{in}(t, E) = \sum_{n=-\infty}^{\infty} \int_0^{\mathcal{T}} \frac{dt'}{\mathcal{T}} e^{in\Omega_0 (t'-t)} \hat{S}_{out}(E_n, t')$$

$$\hat{S}_{out}(E, t) = \sum_{n=-\infty}^{\infty} \int_0^{\mathcal{T}} \frac{dt'}{\mathcal{T}} e^{-in\Omega_0 (t'-t)} \hat{S}_{in}(t', E_n)$$

Time-dependent AC current

AC current in terms of $\hat{S}_{in}$

$$I_\alpha(t) = \frac{e}{h}\int_0^\infty dE \sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty}\{f_\beta(E) - f_\alpha(E_n)\}$$
$$\times \int_0^\tau \frac{dt'}{\tau} e^{in\Omega_0(t'-t)} S_{in,\alpha\beta}(t,E) S^*_{in,\alpha\beta}(t',E)$$

- Generalization: exclude the periodicity

$$\boxed{n\Omega_0 \to \omega} \qquad \boxed{\sum_{n=-\infty}^{\infty} \to \frac{\tau}{2\pi}\int_{-\infty}^{\infty} d\omega} \qquad \boxed{\int_0^\tau dt'\, e^{in\Omega_0 t'} \to \int_{-\infty}^{\infty} dt'\, e^{i\omega t'}}$$

$$\Downarrow$$

$$I_\alpha(t) = \frac{e}{h}\int dE \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \sum_{\beta=-1}^{N_r}[f_\beta(E) - f_\alpha(E+\hbar\omega)]$$
$$\times \int_{-\infty}^{\infty} dt'\, e^{i\omega(t-t')} S_{in,\alpha\beta}(t,E) S^*_{in,\alpha\beta}(t',E)$$

Point-like scattering potential

The point-like potential

- One-dimensional Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(t,x) \right] \Psi$$

with point-like potential $V(t,x)$,

$$V(t,x) = \delta(x) V(t)$$
$$V(t) = V_0 + 2V_1 \cos(\omega_0 t + \phi)$$

The solution

- According to the Floquet theorem the solution reads as

$$\Psi(t,x) = e^{-i\frac{E}{\hbar}t} \sum_{n=-\infty}^{\infty} e^{-in\Omega_0 t} \psi_n(x)$$

- Since $V(t,x) = 0$ except in $x = 0$, the general solution for a free particle

$$\psi_n(x) = \begin{cases} a_n^{(-)} e^{ik_n x} + b_n^{(-)} e^{-ik_n x}, & \text{if } x < 0 \\ a_n^{(+)} e^{ik_n x} + b_n^{(+)} e^{-ik_n x}, & \text{if } x > 0 \end{cases}$$

where $k_n = \sqrt{2m(E + n\hbar\Omega_0)}/\hbar$

Point-like scattering potential

Boundary conditions

$$\Psi(t, x=-0) = \Psi(t, x=+0)$$

$$\left.\frac{\partial \Psi(t,x)}{\partial x}\right|_{x=+0} - \left.\frac{\partial \Psi(t,x)}{\partial x}\right|_{x=-0} = \frac{2m}{\hbar} V(t)\Psi(t, x=0)$$

General solution in terms of incident and scattered waves

$$\psi_n(x) = \psi_n^{(in)}(x) + \psi_n^{(out)}(x)$$

where

$$\psi_n^{(in)}(x) = \begin{cases} a_n^{(-)} e^{ik_n x}, & x < 0 \\ b_n^{(+)} e^{-ik_n x}, & x > 0 \end{cases}$$

and

$$\psi_n^{(out)}(x) = \begin{cases} b_n^{(-)} e^{-ik_n x}, & x < 0 \\ a_n^{(+)} e^{ik_n x}, & x > 0 \end{cases}$$

$$\Psi(t,x) = \Psi^{(in)}(t,x) + \Psi^{(out)}(t,x)$$

Wave with unit amplitude - Incident from the left

Wave with unit amplitude

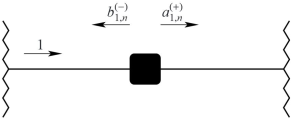
- Corresponds to a particle with energy E incident from the left

$$\Psi_1^{(in)}(t,x) = e^{-i\frac{E}{\hbar}t}\begin{cases} e^{ikx}, & x<0 \\ 0, & x>0 \end{cases}$$

- We find $a_{1,n}^{(-)} = \delta_{n,0}$ and $b_{1,n}^{(+)} = 0$
- Boundary conditions + collecting coefficients with $\sim e^{-i\frac{E+n\hbar\Omega_0}{\hbar}t}$ $\Rightarrow$ set of linear equations for $n = 0, \pm 1, \pm 2, \ldots$

$$\begin{cases} \delta_{n,0} + b_{1,n}^{(-)} = a_{1,n}^{(+)}, \\ (k_n + ip_0)a_{1,n}^{(+)} = k\delta_{n,0} - i(p_{+1}a_{1,n-1}^{(+)} + p_{-1}a_{1,n+1}^{(+)}) \end{cases}$$

where $p_0 = mV_0/\hbar^2$ and $p_{\pm 1} = mV_1 e^{\mp i\phi}/\hbar^2$ are the Fourier coefficients for $p(t) = mV(t)/\hbar^2$



Wave with unit amplitude - Incident from the left

Floquet scattering matrix elements

$$S^{(1)}_{F,11}(E_n, E) = S^{(1)}_{in,11,n}(E) = \sqrt{\frac{k_n}{k}}\, b^{(-)}_{1,n}$$

$$S^{(1)}_{F,21}(E_n, E) = S^{(1)}_{in,21,n}(E) = \sqrt{\frac{k_n}{k}}\, a^{(+)}_{1,n}$$

Approximation

- Solve the system of equations with accuracy to the first order in the parameter $\epsilon = \hbar\Omega_0/E$
- To the 1^{st} order in ϵ

$$k_n = k + \frac{n\Omega_0}{v} + \mathcal{O}(\epsilon^2), \qquad \sqrt{\frac{k_n}{k_{n\mp1}}} = 1 \pm \frac{\Omega_0}{2vk} + \mathcal{O}(\epsilon^2)$$

where $v = \hbar k/m$ is the velocity.

Wave with unit amplitude - Incident from the left

Approximation

- After the inverse Fourier transformation

$$\begin{cases} 1 + S^{(1)}_{in,11}(t,E) = S^{(1)}_{in,21}(t,E), \\ (k_n + ip(t))S^{(1)}_{in,21}(t,E) = k - \frac{i}{v}\frac{\partial S^{(1)}_{in,21}(t,E)}{\partial t} + \frac{1}{2vk}\frac{dp(t)}{dt}S^{(1)}_{in,21}(t,E) \end{cases}$$

- Solution via iteration in the terms containing time derivative
- Omitting such terms we arrive to

$$S^{(1)}_{11}(t,E) = \frac{-ip(t)}{k+ip(t)}, \qquad S^{(1)}_{21}(t,E) = \frac{k}{k+ip(t)}$$

First-order solution

- After substituting the zero-order solution

$$S^{(1)}_{in,11}(t,E) = \frac{-ip(t)}{k+ip(t)} - \frac{1}{2v}\frac{dp(t)}{dt}\frac{k-ip(t)}{[k+ip(t)]^3}$$

$$S^{(1)}_{in,21}(t,E) = \frac{k}{k+ip(t)} - \frac{1}{2v}\frac{dp(t)}{dt}\frac{k-ip(t)}{[k+ip(t)]^3}$$

Wave with unit amplitude - Incident from the left

First-order solution

- Based on the zero-order solution one can show

$$\frac{\partial^2 S_{11}^{(1)}(t,E)}{\partial t \partial E} = \frac{\partial^2 S_{21}^{(1)}(t,E)}{\partial t \partial E} = \frac{i}{\hbar v}\frac{dp(t)}{dt}\frac{k - ip(t)}{[k + ip(t)]^3}$$

- Therefore, the first-order solution can be rewritten as

$$S_{in,11}^{(1)}(t,E) = S_{11}^{(1)}(t,E) + \frac{i\hbar}{2}\frac{\partial^2 S_{11}^{(1)}(t,E)}{\partial t \partial E}$$
$$S_{in,21}^{(1)}(t,E) = S_{21}^{(1)}(t,E) + \frac{i\hbar}{2}\frac{\partial^2 S_{21}^{(1)}(t,E)}{\partial t \partial E}$$

Wave with unit amplitude - Incident from the right

Wave with unit amplitude

- Solving the same problem but with a particle incident from the right

$$\Psi_2^{(in)}(t,x) = e^{-i\frac{E}{\hbar}t}\begin{cases}0, & x<0\\ e^{-ikx}, & x>0\end{cases}$$

- We can calculate

$$S_{22}^{(1)}(t,E) = S_{11}^{(1)}(t,E), \quad S_{12}^{(1)}(t,E) = S_{21}^{(1)}(t,E),$$
$$S_{in,22}^{(1)}(t,E) = S_{in,11}^{(1)}(t,E), \quad S_{in,12}^{(1)}(t,E) = S_{in,21}^{(1)}(t,E),$$

Frozen scattering matrix

- Thus we get the following relation between the scattering matrix $\hat{S}_{in}^{(1)}(t,E)$ and the frozen scattering matrix $\hat{S}^{(1)}(t,E)$:

$$\hat{S}_{in}^{(1)}(t,E) = \hat{S}^{(1)}(t,E) + \frac{i\hbar}{2}\frac{\partial^2 S^{(1)}(t,E)}{\partial t \partial E}$$

with

$$\hat{S}^{(1)}(t,E) = \frac{1}{k+ip(t)}\begin{bmatrix}-ip(t) & k\\ k & -ip(t)\end{bmatrix}$$

Wave with unit amplitude

Consequences

- The solution is derived with the accuracy of order ϵ
- In the case under consideration the parameter ϵ coincides with the adiabaticity parameter $\epsilon \sim \varpi$
- Consequently, the anomalous scattering matrix is identically zero for a point-like scatterer

$$\hat{A}^{(1)}(t, E) = 0$$

Wave with unit amplitude - Incident from both side

Wave with unit amplitude - incident from both side

- Solving the same problem with incident waves from both side

$$\Psi^{(in)}(t,x) = e^{-i\frac{E}{\hbar}t} \begin{cases} a_0^{(-)} e^{ikx}, & x < 0 \\ b_0^{(+)} e^{-ikx}, & x > 0 \end{cases}$$

- Superposition principle: $\Psi^{(in)} = a_0^{(-)}\Psi_1^{(in)} + b_0^{(+)}\Psi_2^{(in)}$ and $\Psi^{(out)} = a_0^{(-)}\Psi_1^{(out)} + b_0^{(+)}\Psi_2^{(out)}$
- Based on earlier results we find:

$$\Psi^{(out)}(t,x) = e^{-i\frac{E}{\hbar}t} \sum_{n=-\infty}^{\infty} e^{-in\Omega_0 t} \begin{cases} b_n^{(-)} e^{-ik_n x}, & x < 0 \\ a_n^{(+)} e^{ik_n x}, & x > 0 \end{cases}$$

Vector-column representation

- Using

$$\hat{\Psi}_0^{(in)} = \begin{bmatrix} a_0^{(-)} \\ b_0^{(+)} \end{bmatrix}, \qquad \hat{\Psi}_n^{(out)} = \begin{bmatrix} b_n^{(-)} \\ a_n^{(+)} \end{bmatrix}$$

- The scattered wave

$$\hat{\Psi}_n^{(out)} = \sqrt{\frac{k}{k_n}}\hat{S}_F(E_n, E)\hat{\Psi}_0^{(in)}$$

Wave with unit amplitude - Incident from both side

Floquet function type incident waves

- The incident wave is Floquet type having side-bands with energies E_m

$$\Psi^{(in)}(t,x) = e^{-i\frac{E}{\hbar}t} \sum_{m=-\infty}^{\infty} e^{-im\Omega_0 t} \begin{cases} a_m^{(-)} e^{ik_m x}, & x < 0 \\ b_m^{(+)} e^{-ik_m x}, & x > 0 \end{cases}$$

- With the corresponding vector-columns

$$\hat{\Psi}_m^{(in)} = \begin{bmatrix} a_m^{(-)} \\ b_m^{(+)} \end{bmatrix}$$

- The scattered wave (using the superposition principle)

$$\hat{\Psi}_n^{(out)} = \sum_{m=-\infty}^{\infty} \sqrt{\frac{k_m}{k_n}} \hat{S}_F(E_n, E_m) \hat{\Psi}_m^{(in)}$$

Summary

- Review of the Floquet scattering matrix
- Floquet scattering matrix in mixed representation
- Definition of the time-dependent AC current
- Description of the problem with point-like scattering potential

Thank you for your attention!