Non-stationary scattering theory

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October, 2015.

Motivation

- The non-stationary scatterer can change an energy of incident electrons
- We will compare two method for solving of a non-stationary problem.
- The first method is the perturbation theory **with weak potential**
- The second one, the Floquet theorem is applied **for periodic in time potentials with arbitrary strength**
- We will define the **Floquet scattering matrix** what decribe energy change, and examine some of its properties.

Schrödinger equations with periodic in time potential

The Schrödinger equation: $$i\hbar \frac{\partial \Psi(t,\vec{r})}{\partial t} = H(t,\vec{r})\,\Psi(t,\vec{r})$$

Where the Hamiltonian: $$H(t,\vec{r}) = H_0(\vec{r}) + V(t,\vec{r})$$

We suppose that: $$H_0(\vec{r})\,\psi_n(\vec{r}) = E_n\psi_n(\vec{r})$$

$$\Psi_n(t,\vec{r}) = e^{-\frac{iE_n t}{\hbar}}\psi_n(\vec{r})$$

Solving by two method

Perturbation theory

Floquet theorem

Perturbation theory

Let the time-dependent potential is small: $V(t,\vec{r}) \to 0$

We are looking for the solution as

$$\Psi(t,\vec{r}) = \sum_n a_n(t)\,\Psi_n(t,\vec{r})$$

Substituting to Schrödinger equation:

$$i\hbar \sum_n \Psi_n(t,\vec{r})\,\frac{da_n(t)}{dt} = \sum_n a_n(t)\,V(t,\vec{r})\,\Psi_n(t,\vec{r})$$

Multiply both parts of this equation with $\Psi_k^*(t,\vec{r})$ and integrate over space. Using the orthogonality of the eigenfunctions of the Hamiltonian,

$$\int d^3r\,\psi_k^*(\vec{r})\,\psi_n(\vec{r}) = \delta_{n,k}$$

This way we get an equation for the coefficients a_k:

$$\boxed{i\hbar\,\frac{da_k(t)}{dt} = \sum_n V_{kn}(t)\,a_n(t)}$$

Perturbation theory

$$i\hbar \frac{da_k(t)}{dt} = \sum_n V_{kn}(t)\, a_n(t)$$

Where:

$$V_{kn}(t) = \int d^3r\, \psi_k^*(\vec{r})\, V(t,\vec{r})\, \psi_n(\vec{r})\, e^{i\frac{E_k - E_n}{\hbar}t}$$

We will use an upper index (m) to show an initial state

$$\Psi^{(m)}(t=0,\vec{r}) = \Psi_m(t=0,\vec{r}) \Rightarrow \begin{cases} a_m^{(m)}(0) = 1\,, \\ a_n^{(m)}(0) = 0\,, \quad n \neq m \end{cases}$$

$$a_m^{(m)}(t) \;= 1 + a_m^{(m,1)}(t)\,,$$

$$a_n^{(m)}(t) \;= 0 + a_n^{(m,1)}(t)\,, \quad n \neq m$$

Perturbation theory

$$a_m^{(m)}(t) = 1 + a_m^{(m,1)}(t)\,,$$

$$a_n^{(m)}(t) = 0 + a_n^{(m,1)}(t)\,, \quad n \neq m$$

Substituting previous equations into $\Psi(t,\vec{r}) = \sum_n a_n(t)\,\Psi_n(t,\vec{r})$ and keeping only linear terms in V we find:

$$i\hbar \frac{da_k^{(m,1)}(t)}{dt} = V_{km}(t)$$

This equation can be integrated out:

$$a_k^{(m,1)}(t) = -\frac{i}{\hbar}\int_0^t dt'\, V_{km}(t')$$

$|a_k^{(m)}(t)|^2$ defines a probability to observe a particle in the state $\Psi_k(t,\vec{r})$ with energy E_k at time t. Note at initial time $t = 0$ the particle was in the state with energy E_m.

Perturbation theory

Example

Let the potential periodoic in time:

$$V(t,\vec{r}) = U(t)\,R(\vec{r})$$

Where

$$U(t) = 2U\cos(\Omega_0 t)$$

We can solve the previous integral:

$$a_k^{(m,1)}(t) = -UR_{km}\left(\frac{e^{i(\omega_{km}-\Omega_0)t}-1}{\hbar(\omega_{km}-\Omega_0)} + \frac{e^{i(\omega_{km}+\Omega_0)t}-1}{\hbar(\omega_{km}+\Omega_0)}\right)$$

Where:

$$R_{km} = \int d^3r\psi_k^*(\vec{r})R(\vec{r})\psi_n(\vec{r}) \qquad \hbar\omega_{km} = E_k - E_m$$

The perturbation theory is correct if the absolute value of $a_{k\neq m}^{(m)}(t)$ is small compared to unity:

$$\frac{V_{km}}{\hbar(\omega_{km}\pm\Omega_0)} \sim \frac{UR_{km}}{\hbar(\omega_{km}\pm\Omega_0)} \ll 1$$

Perturbation theory

Example

Substituting to the previous equations,

$$\Psi^{(m)}(t,\vec{r}) \;=\; e^{-i\frac{E_m}{\hbar}t}\sum_n \psi_n(\vec{r})\left\{\delta_{nm} - \frac{UR_{nm}\left(e^{-i\Omega_0 t} - e^{-i\omega_{nm}t}\right)}{\hbar(\omega_{nm}-\Omega_0)} - \frac{UR_{nm}\left(e^{i\Omega_0 t} - e^{-i\omega_{nm}t}\right)}{\hbar(\omega_{nm}+\Omega_0)}\right\}$$

Floquet theorem

- The perturbation theory: $$\frac{V_{km}}{\hbar(\omega_{km} \pm \Omega_0)} \sim \frac{UR_{km}}{\hbar(\omega_{km} \pm \Omega_0)} \ll 1$$
- Floquet functions method: No restrictions! We can use any periodic in time potential.

Floquet theorem overcomes the restrictions and allows to consider an arbitrary but periodic in time potential

According to this theorem:

$$H(t,\vec{r}) = H(t+\mathfrak{T},\vec{r}) \Longrightarrow \begin{aligned} \Psi(t,\vec{r}) &= e^{-i\frac{E}{\hbar}t}\phi(t,\vec{r}) \\ \phi(t,\vec{r}) &= \phi(t+\mathfrak{T},\vec{r}) \end{aligned}$$

Floquet theorem

The outline of the proof of this theorem:

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

The two general solutions have to be proportional each other:

$$\Psi(t+\mathfrak{T}, \vec{r}) = C\,\Psi(t, \vec{r})$$

Since the wave function is normalized:

$$\int d^3r |\Psi(t, \vec{r})|^2 = 1$$

$$\int d^3r |\Psi(t+\mathfrak{T}, \vec{r})|^2 = |C|^2 \int d^3r |\Psi(t, \vec{r})|^2 = 1$$

We find:

$$|C|^2 = 1 \quad \Rightarrow \quad C = e^{-i\alpha}$$

Floquet theorem

Let us consider these equation below:

$$\Psi(t,\vec{r}) = e^{-i\frac{\alpha}{\mathfrak{T}}t}\phi(t,\vec{r})$$

$$\phi(t,\vec{r}) = \phi(t+\mathfrak{T},\vec{r})$$

Where $E = \hbar\alpha/\mathfrak{T}$

With these equation we can write:

$$\Psi(t+\mathfrak{T}) = e^{-i\frac{\alpha}{\mathfrak{T}}(t+\mathfrak{T})}\phi(t+\mathfrak{T}) = e^{-i\alpha}\left\{e^{-i\frac{\alpha}{\mathfrak{T}}t}\phi(t)\right\} = e^{-i\alpha}\Psi(t)$$

This is what we want to see, so the The Floquet theorem has proven

Floquet theorem

Next we expand a periodic in time function $\phi(t,\vec{r})$ into the Fourier series,

$$\phi(t,\vec{r}) = \sum_{q=-\infty}^{\infty} e^{-iq\Omega_0 t}\psi_q(\vec{r})$$

$$\psi_q(\vec{r}) = \int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}}\, e^{iq\Omega_0 t}\phi(t,\vec{r})$$

Where $\Omega_0 = 2\pi/\mathcal{T}$. Then the Floquet wave function becomes,

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

Floquet theorem

Example

We consider the Schrödinger equation with the same potential as in the previous example:

$$i\hbar\frac{\partial\Psi(t,\vec{r})}{\partial t} = \left\{H_0 + 2U\cos(\Omega_0 t)\right\}\Psi(t,\vec{r})$$

The solution:

$$\Psi(t,\vec{r}) = e^{-i\left\{\frac{E}{\hbar}t+\frac{2U}{\hbar\Omega_0}\sin(\Omega_0 t)\right\}}\psi_E(\vec{r})\,,$$

where we use the stationary problem's solution:

$$H_0\,\psi_E(\vec{r}) = E\,\psi_E(\vec{r})$$

Next we use the following Fourier series:

$$e^{-i\alpha\sin(\Omega_0 t)} = \sum_{q=-\infty}^{\infty} e^{-iq\Omega_0 t}J_q(\alpha)$$

We get the next equation, what is reallay a Floquet wave function with $\psi_q(\vec{r}) = J_q(2U/\hbar\Omega_0)\psi_E(\vec{r})$

$$\Psi(t,\vec{r}) = e^{-i\frac{E}{\hbar}t}\sum_{q=-\infty}^{\infty} e^{-iq\Omega_0 t}J_q\left(\frac{2U}{\hbar\Omega_0}\right)\psi_E(\vec{r})$$

Floquet theorem

Example

Let the amplitude is small:

$$U/(\hbar\Omega_0) \ll 1$$

We expand the Bessel functions into the Tailor series in powers of a small
Parameter $\alpha = 2U/(\hbar\Omega_0)$

$$J_0(\alpha) \approx 1 - \alpha^2/4\,, \quad J_{\pm 1}(\alpha) \approx \pm\,\alpha/2\,, \quad J_{\pm|n|} \sim \pm\,\alpha^{|n|}, \quad |n| > 1$$

Then up to linear in U terms the solution becomes,

$$\Psi(t,\vec{r}) \approx e^{-i\frac{E}{\hbar}t}\psi_E(\vec{r})\left\{1 + \frac{Ue^{-i\Omega_0 t}}{\hbar\Omega_0} - \frac{Ue^{i\Omega_0 t}}{\hbar\Omega_0}\right\}$$

This equation is exactly what we get by perturbation theory with $R_{nm} = \delta_{nm}$ and $\psi_m(\vec{r}) = \psi_E(\vec{r})$

Floquet scattering matrix

- The main difference of a dynamic scatterer compared to a stationary one is that it can change an energy of incident electrons.

- The parameters of a scatterer vary periodically in time

- It is convenient to choose an energy E of an incident electron as the Floquet energy.

- The scattering matrix dependent on two energies, incident and scattered. It is referred to as *the Floquet scattering matrix* $\hat{S}_F$. The element $S_{F,\alpha\beta}(E_n, E)$ describes a process when an electron with energy E incident from the lead β is scattered into the lead α and its energy is changed to $E_n = E + n\hbar\Omega_0$

Floquet scattering matrix

Unitarity

Since the particle flow is conserved at scattering, the Floquet scattering matrix is unitary:

$$\sum_n \sum_{\alpha=1}^{N_r} S^*_{F,\alpha\beta}(E_n\,,\,E_m)\, S_{F,\alpha\gamma}(E_n\,,\,E) = \delta_{m0}\,\delta_{\beta\gamma}$$

$$\sum_n \sum_{\beta=1}^{N_r} S_{F,\gamma\beta}(E_m\,,\,E_n)\, S^*_{F,\alpha\beta}(E\,,\,E_n) = \delta_{m0}\,\delta_{\alpha\gamma}$$

Note the negative values, $E_n < 0$, correspond to the states localized on the scatterer. These states do not contribute to current.

Floquet scattering matrix

Micro-reversibility

- In the stationary case the Schrödinger equation remains invariant under $t \to -t$ if simultaneously to reverse a magnetic field direction and to replace the wave function by its complex conjugate.

- In the case of a dynamical scattering the time reversal can change a time dependent Hamiltonian. Let us assume that the Hamiltonian depends on N_p parameters $p_i(t)$, $i = 1, \ldots, N_p$, which are all periodic in time:

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

- The Hamiltonian remains invariant if in addition we change the signs of all the phases

$$\varphi_i \to -\varphi_i,\ \forall i$$

- Thus the micro-reversibility results in the following symmetry conditions:

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

Summary

- Dynamic scattering
- perturbation theory; **weak potential**
- Floquet theorem; **periodic in time potentials with arbitrary strength**
- **Floquet scattering matrix**

Thank you for your attention!