1 Time-dependent perturbation theory

• One of the main tasks of quantum mechanics is the calculation of transition probabilities from a state $|n\rangle$ to another state $|m\rangle$. There transitions occur under the influence of a time-dependetn perturbation which, so to say, "shakes" the system and so assumes transition.

To caclcualte the change in $\psi(\mathbf{r},t)$ due to the action pf the perturbation $V(\mathbf{r},t)$, one needs to solve the time-independent SWE:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi(\mathbf{r},t) \tag{1}$$

where

$$\hat{H} = \hat{H}_0(\mathbf{r}) + \hat{V}(\mathbf{r},t) \tag{2}$$

operator for total energy of the system without perturbation

perturbing potential

In principle, this is a rather formidable problem and general predictions can only be made if the transition is caused by weak influences, i.e., weak potentials $V(\mathbf{r},t)$. These influences are trhen interpreted as perturbations.

• We first consider the unperturbed system:

$$i\hbar\frac{\partial\psi_n^0}{\partial t} = \hat{H}_0(\mathbf{r})\psi_n^0(\mathbf{r},t) \tag{3}$$

or

$$i\hbar\frac{\partial|n\rangle_0}{\partial t} = \hat{H}_0(\mathbf{r})|n\rangle_0 \tag{4}$$

The stationary part of the normalized wavefunction is assumed to satisfiy the eigenvalue equation

$$\hat{H}_0(\mathbf{r})|n\rangle_0 = E_n^{(0)}|n\rangle_0 \tag{5}$$

The time-dependent function $\psi_n(\mathbf{r},t)$, of the form

$$\psi_n^0(\mathbf{r},t) = e^{-iE_n^{(0)}t/\hbar}|n\rangle_0 \tag{6}$$

is then a solution of the unperturbed system.

• The wavefunctions $\psi_n^0(\mathbf{r},t)$ form an orthonormal and complete set of functions, and the solutions of our general problem can be written in terms of these functions, i.e.,

$$\psi(\mathbf{r},t) = \sum_n a_n(t)\psi_n^0(\mathbf{r},t) \tag{7}$$

$$= \sum_n a_n(t)e^{-iE_n^{(0)}t/\hbar}|n\rangle_0 \tag{8}$$

Inserting the above expression into the TDSE gives:

$$i\hbar\frac{\partial}{\partial t}\sum_n a_n(t)e^{-iE_n(0)t/\hbar}|n\rangle_0 = \left(\hat{H}_0(\mathbf{r}) + V(\mathbf{r},t)\right)\sum_n a_n(t)e^{-iE_n^{(0)}t/\hbar}|n\rangle_0 \tag{9}$$

or

$$i\hbar\sum_n\left\{\frac{\partial a_n}{\partial t}e^{-iE_n^{(0)}t/\hbar} - \frac{iE_n^{(0)}}{\hbar}a_n(t)e^{-iE_n^{(0)}t/\hbar}\right\}|n\rangle_0 =$$
$$= \sum_n a_n(t)e^{-iE_n^{(0)}t/\hbar}\left[\hat{H}_0(\mathbf{r}) + V(\mathbf{r},t)\right]|n\rangle_0 \tag{10}$$

Using

$$H_0(\mathbf{r})|n\rangle_0 = E_n^{(0)}|n\rangle_0 \tag{11}$$

gives

$$\sum_n i\hbar\frac{\partial a_n}{\partial t}e^{-iE_n^{(0)}t/\hbar}|n\rangle_0 + \sum_n E_n^{(0)}a_n(t)e^{-iE_n^{(0)}t/\hbar} =$$
$$= \sum_n a_n(t)E_n^{(0)}e^{-iE_n^{(0)}t/\hbar}|n\rangle_0 + \sum_n a_n(t)e^{-iE_n^{(0)}t/\hbar}V(\mathbf{r},t)|n\rangle_0 \tag{12}$$

or

$$\boxed{\sum_n i\hbar\frac{\partial a_n}{\partial t}e^{-iE_n^{(0)}t/\hbar}|n\rangle_0 = \sum_n a_n(t)e^{-iE_n^{(0)}t/\hbar}V(\mathbf{r},t)|n\rangle_0} \tag{13}$$

• We now employ the orthogonality of our basis set for the unperturbed problem. We multiply the above expression by $\psi_{m0}^*(\mathbf{r},t) = e^{iE_n^{(0)}t/\hbar}\,{}_0\langle m|$ and integrate over the internal variables to get:

$$\sum_n i\hbar\frac{\partial a_n}{\partial t}e^{i[E_m^{(0)}-E_n^{(0)}]t/\hbar}\underbrace{{}_0\langle m|n\rangle_0}_{\delta_{m,n}} = \sum_n a_n(t)e^{i[E_m^{(0)}-E_n^{(0)}]t/\hbar}\,{}_0\langle m|V|n\rangle_0 \tag{14}$$

where

$$\langle m|V(\mathbf{r},t)|n\rangle = \int d^3r\psi_m^{*(0)}(\mathbf{r})V(\mathbf{r},t)\psi_n^{(0)}(\mathbf{r}) \tag{15}$$

The Kroneker-delta on the LHS simplifies our expression, to get

$$i\hbar\frac{\partial a_m}{\partial t} = \sum_n a_n(t)e^{i\left[E_m^{(0)}-E_n^{(0)}\right]t/\hbar}\,{}_0\langle m|V(\mathbf{r},t)|n\rangle_0 \tag{16}$$

Now let's suppose we have a simple harmonic perturbation, for which

$$V(\mathbf{r},t) = V_0(\mathbf{r})e^{\pm i\omega_0 t} \tag{17}$$

Then

$$\begin{aligned} {}_0\langle m|V(\mathbf{r},t)|n\rangle_0 &= e^{\pm i\omega_0 t}\,{}_0\langle m|V_0(\mathbf{r})|n\rangle_0 && (18)\\ &= e^{\pm i\omega_0 t}V_{mn} && (19)\end{aligned}$$

Substituting this gives

$$i\hbar\frac{\partial a_m}{\partial t} = \sum_n a_n(t)e^{i\left[E_m^{(0)}-E_n^{(0)}\pm\omega_0\hbar\right]t/\hbar}V_{mn} \tag{20}$$

What we have now is a omplete set of equations for the expansion xoefficients $a_m(t)$ and their time dependence. Matrix methods can be used to solve problems of this type, but this is generally very complicated a task.

• The approach that we will follow is as follows. We will assume that before the perturbation is turned on, the system is in a states k, i.e.,

$$\begin{aligned} \psi(r,0) &= |k\rangle_0 && (21)\\ &= \sum_n a_n(0)|n\rangle_0\delta_{n,k} && (22)\\ &= a_k(0)|k\rangle_0 && (23)\end{aligned}$$

The above expression suggests that the expansion coefficients at $t=0$ are

$$a_n(0) = \begin{cases} 1, & n=k \\ 0, & n\neq k \end{cases} \tag{24}$$

• To understand the meaning of the expansion coefficients, we consider the normalization of $\psi(r,t)$

$$\begin{aligned} 1 &= \langle\psi(r,t)|\psi(r,t)\rangle && (25)\\ &= \sum_{m,n} a_m^*(t)e^{iE_m^{(0)}t/\hbar}a_n(t)e^{-iE_n^{(0)}t/\hbar}\underbrace{{}_0\langle m|n\rangle_0}_{\delta_{m,n}} && (26)\end{aligned}$$

$$\boxed{1 = \sum_n |a_n(t)|^2} \quad \Rightarrow \quad \begin{array}{l} \text{The expansion coefficients must satisfiy} \\ \\ \text{the normalization condition} \end{array} \tag{27}$$

We now calculate the matrix element

$$\langle \psi_k^{(0)}(\mathbf{r},t)|\psi(\mathbf{r},t)\rangle = e^{iE_k^{(0)}t/\hbar} \sum_n a_n(t) e^{-iE_n^{(0)}t/\hbar} \underbrace{{}_0\langle k|n\rangle_0}_{\delta_{k,n}} \tag{28}$$

$$= a_k(t) e^{i\left[E_k^{(0)}t/\hbar - E_k^{(0)}t/\hbar\right]} \tag{29}$$

$$= a_k(t) \tag{30}$$

Hence

$$a_k(t) = \langle \psi_k^{(0)}(\mathbf{r},t)|\psi(\mathbf{r},t)\rangle \tag{31}$$

Therefore $|a_k(t)|^2$ is the probability of finding the system at time t in state $\psi_k^{(0)}(\mathbf{r},t)$ with energy $E_k^{(0)}$

• Our next task is to calcualte the amplitudes $a_m(t)$ from the coupled set of differential equations. If $V(\mathbf{r},t)$ is small perturbation, we can make the approximation that even at $t > 0$, we have

$$a_n(t) = \delta_{n,k} \tag{32}$$

i.e., that the probability that a system will stay in state $\psi_k^{(0)}(\mathbf{r},t)$ is almost unity. In this case we need to solve only

$$i\hbar \frac{\partial a_m}{\partial t} = \underbrace{a_k(t)}_{\approx 1} e^{i\left[E_m^{(0)} - E_k^{(0)} \pm \hbar\omega_0\right]t/\hbar} \tag{33}$$

Integrating the last equation from 0 to t gives

$$i\hbar\left[a_m(t) - \underbrace{\cancel{a_m(0)}}_{0 \text{ for } m \neq k}\right] = \frac{\hbar}{i\left[E_m^{(0)} - E_k^{(0)} \pm \hbar\omega_0\right]} \left[e^{i\left[E_n^{(0)} - E_k^{(0)} \pm \hbar\omega_0\right]t/\hbar} - 1\right] \tag{34}$$

Introducing the short hand notation

$$\omega_{mk} = \frac{1}{\hbar}\left[E_m^{(0)} - E_k^{(0)} \pm \hbar\omega_0\right] \tag{35}$$

gives

$$
\begin{aligned}
i\hbar a_m(t) &= \frac{V_{mk}}{i\omega_{mk}}\left(e^{i\omega_{mk}t}-1\right) && (36)\\
&= V_{mk}\frac{e^{i\omega_{mk}t/2}\left(e^{i\omega_{mk}t/2}-e^{-i\omega_{mk}t/2}\right)}{i\omega_{mn}} && (37)\\
&= e^{i\omega_{mk}t/2}V_{mk}\frac{i2\sin(\omega_{mk}t/2)}{i\omega_{ml}} && (38)\\
&= e^{i\omega_{mk}t/2}2\frac{\sin(\omega_{mk}t/2)}{\omega_{mk}}V_{mk} && (39)
\end{aligned}
$$

or

$$
a_m(t) = -i\frac{2}{\hbar}\frac{\sin(\omega_{mk}t/2)}{\omega_{mk}}e^{i\omega_{mk}t/2}V_{mk} \qquad (40)
$$

recall that we initially assumed that at $t = 0$ the system was in as state $\psi_k^{(0)}(\mathbf{r},t)$ with energy $E_k^{(0)}(\mathbf{r},t)$. Then

$|a_m(t)|^2 \longrightarrow$ probability that the system will make a transition from state $\psi_k^{(0)}(\mathbf{r},t)$ into state $\psi_m^{(0)}(\mathbf{r},t)$.
We denote this transition probability as $W_{mn}(t)$.

Therefore

$$
\begin{aligned}
W_{mk}(t) &= |a_m(t)|^2 && (41)\\
&= \frac{4|V_{mk}|^2}{\hbar^2}\frac{\sin^2\left(\frac{W_{mk}t}{2}\right)}{\left(\frac{W_{mk}t}{2}\right)^2}\frac{t^2}{4} && (42)\\
&= \frac{|V_{mk}|^2}{\hbar^2}\frac{\sin^2\left(\frac{W_{mk}t}{2}\right)}{\left(\frac{W_{mk}t}{2}\right)^2}t^2 && (43)
\end{aligned}
$$

or

$$
W_{mk}(t) = \frac{|V_{mk}|^2}{\hbar^2}tg(W_{mk}) \qquad (44)
$$

where

$$
g(W_{mk}) = t\left[\frac{\sin\left(\frac{W_{mk}t}{2}\right)}{\left(\frac{W_{mk}t}{2}\right)}\right]^2 \qquad (45)
$$

For fixes t, $g(W_{mk}t)$ is of the form shown in the figure below.

- As t gest larger, $g(\omega_{mk}t)$ becomes more and more peaked. The peak value is t, while the distance between the nearest nulls is $4\pi/t$.

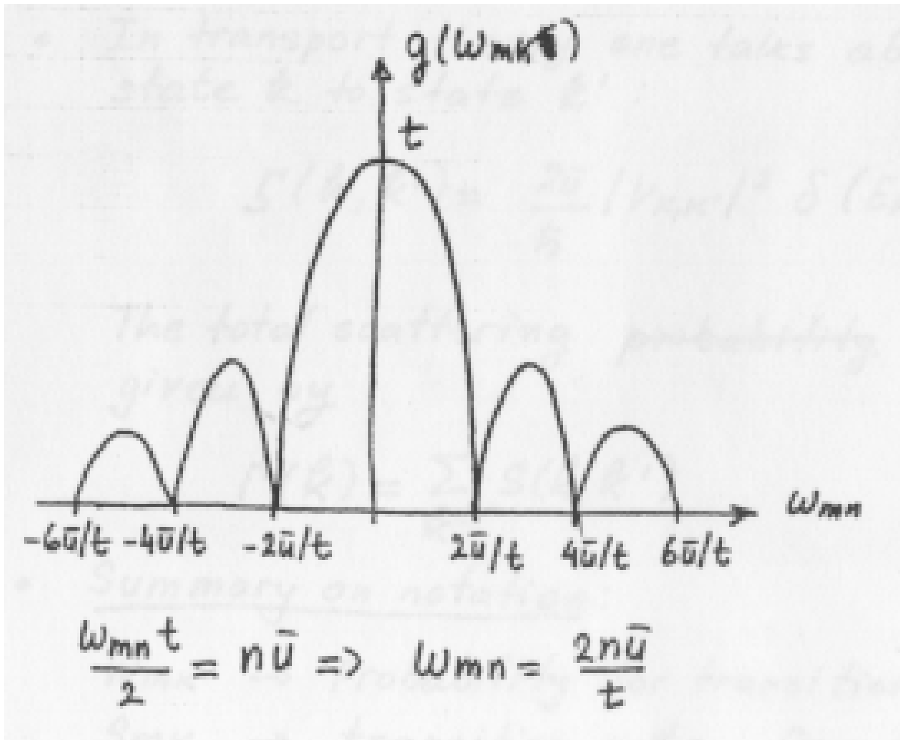

Figure 1: Figure

• It can be shown that

$$\int_{-\infty}^{\infty} g(\omega_{mk}) d\omega_{mk} = 2\pi \tag{46}$$

and is independent of t.

• For these reasons, we can view $g(\omega_{mk})$ as $t \to \infty$ as a function that is very large for $\omega_{mk} = 0$ but is non-zero around a very narrow range of ω_{mn}, so that the area is constant. Hence:

$$\lim_{t\to\infty} g(\omega_{mk}) = 2\pi\delta(\omega_{mk}) \tag{47}$$

i.e.,

$$\begin{aligned} \lim_{t\to\infty} g(\omega_{mk}) &= 2\pi\delta(\omega_{mk}) && (48) \\ &= 2\pi\delta\left(\frac{E_{mk}}{\hbar}\right) && (49) \\ &= 2\pi\hbar\delta(E_{mk}) && (50) \end{aligned}$$

• To summarize, in the limit $t \to \infty$, the probability $W_{mk}(t)$ is

$$\begin{aligned} W_{mk}(t) &= \frac{1}{\hbar^2}|V_{mk}|^2 t \cdot 2\pi\hbar\delta(E_{mk}) && (51) \\ &= t \cdot \frac{2\pi}{\hbar}|V_{mk}|^2 \delta\left(E_m^{(0)} - E_k^{(0)} \pm \hbar\omega_0\right) && (52) \\ &= tS_{mk} && (53) \end{aligned}$$

The limit $t \to \infty$ can be used only in the case when one scattering event finished before that next one starts, i.e., when the scattering in INFREQUENT.

$$\begin{aligned} S_{mk} &= \frac{W_{mk}(t)}{t} && (54) \\ &= \frac{2\pi}{\hbar}|V_{mk}|^2 \delta\left(E_m^{(0)} - E_k^{(0)} \pm \hbar\omega_0\right) && (55) \end{aligned}$$

transition rate $\to$ probability for transition in a time interval t

The formula for the transition rate S_{mk} was named by Fermi(as somw measure of importance) THE GOLDEN RULE.

• Summary of approxiamtions made in deriving Fermi's golden rule:

(a) Weak perturbation which gives no depletion of the initial state $a_k(t) = 1$ for all times.

(b) the limit $t \to \infty$ can only be used when we are in a weak (infrequent) scattering regime. It led to energy conservation in the scattering process, which is not necessarily satsified when we have heavy scattering in the system.

• In transport theory one talks about scattering (transition rate) from state k to state k' :

$$S(k,k') = \frac{2\pi}{\hbar}|V_{k,k'}|^2 \delta\left(E_{k'} - E_k \pm \hbar\omega_0\right) \tag{56}$$

The total scattering (rate) out os state k is then given by

$$\Gamma(k) = \sum_{k'} S(k,k') \tag{57}$$

• Summary on notation

$W_{mk} \to$ Probability for transition from state k to state m $[W(k,k')]$.
$S_{mk} \to$ transition rate from state k to state m $[S(k,k')]$.

$P(k) = \sum_{k'} W(k,k') \to$ total probability for scattering out of state k

$\Gamma(k) = \sum_{k'} S(k,k') \to$ total scattering rate out of state k.

(A) EXAMPLE THAT SHOWS UNDER WHAT CONDITIONS IS FERMI'S GOLDEN RULE VALID

PROBLAM STATEMENT

Consider the potentia barrier of the form

$$U_s(z) = \begin{cases} V_0, & 0 < z < d \\ 0, & z < 0; z > d \end{cases} \tag{58}$$

which we can view as a scattering potential. If one solves this problem exactly, then the probability of reflection R_B for $E > V_0$ is given by

$$R_B(E) = \frac{\sin^2(kd)}{\sin^2(kd) + 4\frac{E}{V_0}\left(\frac{E}{V_0} - 1\right)} \tag{59}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \tag{60}$$

Use Fermi's Golden Rule to calculate R_B and compare it with the exact result. Under what circumstances is the Fermi Golden Rule valid?

SOLUTION

The matrix element for transition from state k to state k' is given by

$$\begin{aligned}
V_{k,k'} &= \frac{1}{L_z}\int_0^d V_0 e^{i(k'-k_z)} dz && (61)\\
&= \frac{V_0}{L_z}\frac{1}{i(k'-k)} e^{i(k'-k)z}\Big|_0^d && (62)\\
&= \frac{V_0}{L_z}\frac{1}{i(k'-k)}\left[e^{i(k'-k)d} - 1\right] && (63)\\
&= \frac{V_0}{L_z}\frac{e^{i(k'-k)d/2}}{i(k'-k)}\underbrace{\left[e^{i(k'-k)d/2} - e^{-i(k'-k)d/2}\right]}_{i2\sin[(k'-k)d/2]} && (64)\\
&= \frac{V_0}{L_z}e^{i(k'-k)d/2}\frac{\cancel{i}2\sin[(k'-k)d/2]}{\cancel{i}(k'-k)} && (65)\\
&= \frac{V_0}{L_z}e^{i(k'-k)d/2} d\frac{\sin\left[(k'-k)\frac{d}{2}\right]}{(k'-k)\frac{d}{2}} && (66)
\end{aligned}$$

The total scattering probability out of state k is then given by

$$
\begin{aligned}
P(k) &= \frac{2\pi T}{\hbar} \sum_{k'} |V_{kk'}|^2 \delta\left(E_{k'} - E_k\right) && (67) \\
&= \frac{\cancel{2\pi} T}{\hbar} \frac{L_z}{\cancel{2\pi}} \int_{-\infty}^{\infty} dk' \delta(E_{k'} - E_k) \frac{4V_0^2}{L_z^2} \frac{\sin^2\left[(k'-k)\frac{d}{2}\right]}{(k'-k)^2} && (68)
\end{aligned}
$$

Since

$$
E_{k'} = \frac{\hbar^2 k'^2}{2m} \tag{69}
$$

(for parabolic bands); we have

$$
dE_{k'} = \frac{\hbar^2}{m} k' dk' \tag{70}
$$

From the energy conservation function we have $|k'| = |k|$, but for reflection we only need to consider $k' = -k$. Therefore

$$
\begin{aligned}
P)k) &= \frac{TL_z}{\hbar} \cdot \frac{4V_0^2}{L_z^2} \int_{-\infty}^{\infty} \frac{m^*}{\hbar^2 |k'|} \delta(E_{k'} - E_k) \frac{\sin^2\left[(k'-k)\frac{d}{2}\right]}{(k'-k)^2} dE_{k'} && (71) \\
&= \frac{4V_0^2 T}{\hbar L_z} \frac{m^*}{\hbar^2 |k|} \frac{\sin^2(k'd)}{4k^2} && (72) \\
&= \frac{TV_0^2 m^*}{\hbar^3 L_z k^3} \sin^2(kd) && (73)
\end{aligned}
$$

Now the upper limit of the integration T is equal to the time it takes for electrons to cross the length L_z, i.e.,

$$
\begin{aligned}
T &= \frac{L_z}{v} && (74) \\
&= \frac{L_z}{\hbar k} m^* && (75) \\
&\Downarrow && (76) \\
\frac{T}{L_z} &= \frac{m^*}{\hbar k} && (77)
\end{aligned}
$$

This gives

$$
\begin{aligned}
P(k) &= \frac{V_0^2 m^*}{\hbar^3 k^3} \cdot \frac{m^*}{\hbar k} \sin^2(kd) && (78) \\
&= \left(\frac{m^* V_0}{\hbar^2 k^2}\right)^2 \sin^2(kd) && (79)
\end{aligned}
$$

This is Fermi's golden rule result

• Now Consider weak scattering, i.e., $E \gg V_0$ (the electrons do not feel the presence of the barrier very much). Then the following approximations are valid

$$\begin{aligned} k^2 &= \frac{2m}{\hbar^2}(E - V_0) && (80)\\ &\approx \frac{2mE}{\hbar^2} && (81)\\ &= k^2 && (82) \end{aligned}$$

i.e.,

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad (83)$$

identical to what is
used in Fermi's golden rule

The reflection coefficient R_B is then given by

$$\begin{aligned} R_B &= \frac{\sin^2(kd)}{\sin^2(kd) + 4\frac{E}{V_0}\left(\frac{E}{V-0}01\right)} && (84)\\ &\approx \frac{\sin^2(kd)}{4\left(\frac{E}{V_0}\right)^2} && (85)\\ &= \frac{V_0^2}{4E^2}\sin^2(kd) && (86) \end{aligned}$$

$$\begin{aligned} R_B &= \frac{V_0^2}{4\left(\frac{\hbar^2 k^2}{2m}\right)^2}\sin^2(kd) && (87)\\ &= \left(\frac{mV_0}{\hbar^2 k^2}\right)^2 \sin^2(kd) && (88) \end{aligned}$$

This expression is identical to the Fermi
golden rule result, which implies that
the Fermi golden rule is valid when
the scattering is weak

(B)Elastic Scattering Of Electrons

With this example, we will demonstrate the application of Ferm's Golden Rule and simulataneously illustrate some concepts of scattering theory.

• We consider the Coulomb interaction between a charge center (Ze) and the electron as a perturbation. The perturbing potential is given by

$$V(\mathbf{r}) = \frac{Ze^2 e^{-r/L_D}}{4\pi\epsilon r} \tag{89}$$

where

$$L_D = \sqrt{\frac{\epsilon V_T}{qn}} \tag{90}$$

is the Debye screening length.

• Before we apply the result of first-order time dependent theory, we need to introduce the concept of SCATTERING CROSS SECTION (a quantity that can be measured), starting from the definition for the probability for transition from state k to state k':

$$W(k,k') = \frac{2\pi T}{\hbar}|V_{kk'}|^2 \delta(E_{k'} - E_k) \tag{91}$$

Note: Coulomb interaction is to first order time independent, which means that only $w = 0$ term will be non zero.

The total probability for scattering out os state k is then given by

$$P(k) = \sum_{k'} W(k,k') \longrightarrow \frac{\Omega}{(2\pi)^3} \int\int\int d^3k' W(k,k') \tag{92}$$

Note that the factor of 2 for spin is not included since we assume that the spin of the particle is the same before and after scattering. In spherical coordinates,

$$d^3k = k^2 dk d(\cos\theta) d\phi \tag{93}$$

which gives

$$\begin{aligned}
P(k) &= \frac{\Omega}{8\pi^3} \int_0^\infty k'^2 dk' \int_{-1}^1 d(\cos\theta) \int_0^{2\pi} d\phi W(k,k') && (94)\\
&= \frac{\Omega}{8\pi^3} \frac{2\pi T}{\hbar} \int_0^\infty k'^2 dk' \int_{-1}^1 d(\cos\theta) \int_0^{2\pi} d\phi |V_{kk'}| \delta(E_{k'} - E_k) && (95)\\
&= \int_{-1}^2 d(\cos\theta) \int_0^{2\pi} d\phi \underbrace{\frac{\Omega T}{4\pi^2\hbar} \int_0^\infty k'^2 dk' |V_{kk'}|^2 \delta(E_{k'} - E_k)}_{P(\theta,\phi)} && (96)
\end{aligned}$$

We can simplify the expression for $P(\theta, \phi)$ if we consider parabolic bands, for which

$$
\begin{aligned}
\frac{\hbar^2 k'^2}{2m^*} &= E'_k \qquad (97)\\
&\Downarrow \\
\frac{\hbar^2}{m^*} k' dk' &= dE_{k'} \qquad (98)\\
&\Downarrow \\
dk' &= \frac{m^*}{\hbar^2 |k'|} dE_{k'} \qquad (99)
\end{aligned}
$$

Therefore

$$
\begin{aligned}
P(\theta, \phi) &= \frac{\Omega T}{4\pi^2 \hbar} \int_0^\infty k'^2 |V_{kk'}|^2 \delta(E_{k'} - E_k) dk' \qquad (100)\\
&= \frac{\Omega T}{4\pi^2 \hbar} \int_0^\infty k'^{\cancel{2}} |V_{kk'}|^2 \delta(E_{k'} - E_k) \frac{m^*}{\hbar^2 \cancel{k'}} dE_{k'} \qquad (101)\\
&= \frac{m^* \Omega T}{4\pi^2 \hbar^3} \int_0^\infty k' |V_{kk'}|^2 \delta(E_{k'} - E_k) dE_{k'} \qquad (102)
\end{aligned}
$$

The δ-function in the integral requires $E_{k'} = E_k$, which means that the intital and final momenta have same magnitude, i.e., $|k'| = |k|$. This means that we can immediately perform this integration to get

$$
P(\theta, \phi) = \frac{m^* \Omega T k}{4\pi^2 \hbar^3} |V_{kk'}|^2 \bigg|_{k'=k} \qquad (103)
$$

Now, let T be the time required for the electron to traverse the box of length L_z, i.e.,

$$
T = \frac{L_z}{v} = \frac{L_z}{\hbar k} m^* = \frac{\Omega}{A} \frac{m^*}{\hbar k} \qquad (104)
$$

$A \rightarrow$ cross section of the box
$\Omega = L_z A \rightarrow$ volume of the box

With the above definitions, we have

$$
\begin{aligned}
P(\theta, \phi) &= \frac{m^* \Omega \cancel{k}}{4\pi^2 \hbar^3} \frac{\Omega m^*}{A \hbar \cancel{k}} |V_{kk'}|^2 \bigg|_{k'=k} \qquad (105)\\
&= \left(\frac{m^* \Omega}{2\pi \hbar^2} \right)^2 \frac{|V_{kk'}|^2_{k'=k}}{A} \qquad (106)
\end{aligned}
$$

$$
\begin{aligned}
&= \left(\frac{m^*}{2\pi\hbar^2}\right)^2 \frac{|\Omega V_{kk'}|^2_{k'=k}}{A} && (107) \\
&= \frac{\sigma(\theta,\phi)}{A} && (108)
\end{aligned}
$$

where

$$
\sigma(\theta,\phi) = \left(\frac{m^*}{2\pi\hbar^2}\right)^2 |\Omega V_{kk'}|^2_{k'=k} \rightarrow \text{ scattering cross section} \tag{109}
$$

To get the total scattering cross-section σ_s we need to integrate over the entire solif angle, i.e.,

$$
\sigma_s = \int_0^{2\pi} \sin\theta d\theta \int_0^{2\pi} d\phi\sigma(\theta,\phi) \tag{110}
$$

• Physical explanation of the scattering cross-section $\sigma(\theta,\phi)$

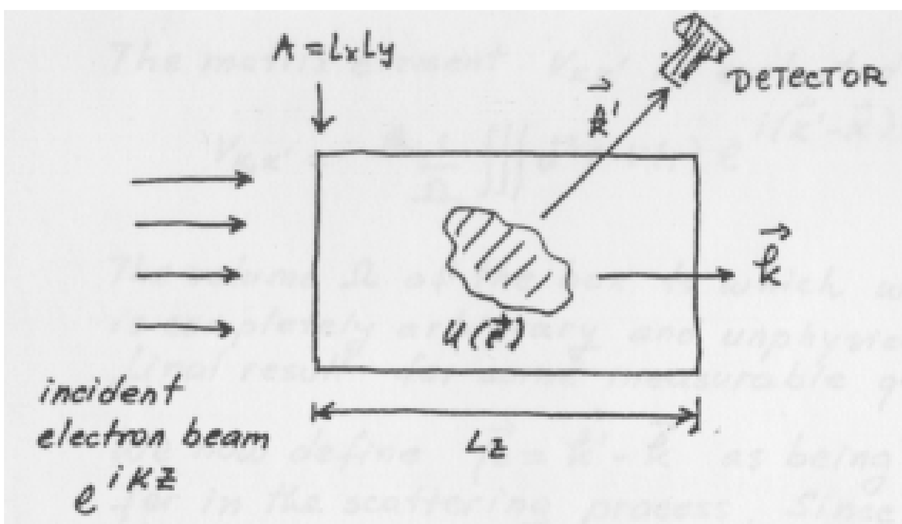

Figure 2: Figure

(1) One can view the scattere as a solid obstacle with a cross-sectional are σ_s, ehich scatters a fraction of the incident electrons equal to

$$
\frac{\sigma_s}{A} \tag{111}
$$

The analysis to be described below is only accurate when $\sigma_s \ll 1$, i.e., if the total number of scattered electrons is a small fraction of the incident electron number.

(2) Usually, we have electrons moving through a medium of certain density (N_I) of scattering centers and we want to know the probability $P_s(t)$ that an electron is scattering within a time t.

Since each scatterer scatters a fraction σ_s/A of the electrons, and the total number of scatterers encountered during time period t is

$$N_E A v t \tag{112}$$

for small t, we can write

$$\begin{aligned} P_s(t) &= \frac{\sigma_s}{\cancel{A}} N_I \cancel{A} v t & (113)\\ &= \frac{t}{\tau} & (114)\\ &= \sigma_s N_I v t & (115) \end{aligned}$$

where

$$\tau = \frac{1}{\sigma_s N_i v} \tag{116}$$

is the mean-free time, or average time between scattering events.

Therefore, to evaluate τ, we need to evaluate the total scattering cross section

$$\sigma_s = \int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\phi \sigma(\theta, \phi) \tag{117}$$

where

$$\sigma(\theta, \phi) = \left(\frac{m^*}{2\pi\hbar^2}\right)^2 |\Omega_{kk'}|^2_{k'=k} \tag{118}$$

- Calculation of the matrix element $V_{kk'}$:

The matrix element $V_{kk'}$ is evaluated from

$$V_{kk'} = \frac{1}{\Omega} \int \int \int d^3 r V(r) e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} \tag{119}$$

The volume Ω of the box to which we normalize all wavefunctions is completely arbitrary and unphysical, but it will never appear in the final result for some measurable quantity.

We now define $\boldsymbol{\beta}= \mathbf{k'} - \mathbf{k}$ as being equal to the momentum transfer in the scattering process. Since we have a freedom in choosing the coordinate system,we can choose $\boldsymbol{\beta}$ to be aligned with the $\boldsymbol{z}$-axis, i.e.,

$$\boldsymbol{\beta} \cdot \mathbf{r} = \beta \cdot r \cos\theta \tag{120}$$

With this choice of the coordinate system, we have:

$$\begin{aligned}
V_{kk'} &= \frac{1}{\Omega}\int_0^\infty \int_{-1}^1 d(\cos\theta) \int_0^{2\pi} d\phi \frac{Ze^2}{4\pi\epsilon r} e^{-r/L_D} e^{i\beta r \cos\theta} \qquad (121)\\
&= \frac{Ze^2}{4\pi\epsilon\Omega}\int_0^\infty r\,dr \int_0^{2\pi} d\phi e^{-r/L_D} \int_{-1}^1 dx e^{i\beta r x} \qquad (122)
\end{aligned}$$

$$\begin{aligned}
\int_{-1}^1 dx e^{i\beta r x} &= \frac{1}{i\beta r} e^{i\beta r x}\Big|_{-1}^{1} \qquad (123)\\
&= \frac{1}{i\beta r}\left(e^{i\beta r} - e^{-i\beta r}\right) \qquad (124)
\end{aligned}$$

or

$$\begin{aligned}
V_{kk'} &= \frac{Ze^2}{4\pi\epsilon\Omega} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \int_0^\infty \cancel{r}\, e^{-r/L_D} \frac{1}{i\beta \cancel{r}}\left(e^{i\beta r} - e^{-i\beta r}\right) dr \qquad (125)\\
&= \frac{Ze^2}{4\pi\epsilon\Omega} \cdot 2\pi \cdot \frac{1}{i\beta} \int_0^\infty \left[e^{(i\beta - 1/L_D)r} - e^{-(i\beta+1/L_D)r}\right] dr \qquad (126)\\
&= \frac{Ze^2}{2\epsilon\Omega}\frac{1}{\beta}\left[\frac{1}{i\beta - 1/L_D} e^{(i\beta-1/L_D)r}\Big|_0^\infty + \frac{1}{i\beta + 1/L_D} e^{-(i\beta+1/L_D)r}\Big|_0^\infty\right] \\
& \qquad (127)\\
&= \frac{Ze^2}{2\epsilon\Omega}\frac{1}{i\beta}\left[-\frac{1}{i\beta - 1/L_D} - \frac{1}{i\beta + 1/L_D}\right] \qquad (128)\\
&= -\frac{Ze^2}{2\epsilon\Omega}\frac{1}{i\beta}\frac{i\beta - \cancel{1/L_D} + i\beta + \cancel{1/L_D}}{-\beta^2 - 1/L_D^2} \qquad (129)\\
&= \frac{Ze^2}{2\epsilon\Omega}\frac{1}{i\beta}\frac{i2\beta}{\beta^2 + 1/L_D^2} \qquad (130)\\
&= \frac{Ze^2}{\epsilon\Omega}\frac{1}{\beta^2 + 1/L_D^2} \qquad (131)
\end{aligned}$$

Since $\boldsymbol{\beta} = \mathbf{k'} - \mathbf{k}$ and $|k'| = |k|$, we have

$$
\begin{aligned}
\beta^2 &= \boldsymbol{\beta} \cdot \boldsymbol{\beta} && (132)\\
&= (\mathbf{k}' - \mathbf{k}) \cdot (\mathbf{k}' - \mathbf{k}) && (133)\\
&= k'^2 - 2kk' \cos\theta + k^2 && (134)\\
&= 2k^2 - 2k^2 \cos\theta && (135)\\
&= 2k^2 (1 - \cos\theta) && (136)\\
&= 4k^2 \sin^2\left(\frac{\theta}{2}\right) && (137)
\end{aligned}
$$

Therefore

$$
V_{kk'} = \frac{Ze^2}{\epsilon\Omega} \frac{1}{4k^2 \sin^2\left(\frac{\theta}{2}\right) + \frac{1}{L_D^2}} \tag{138}
$$

and the scattering cross-section is given by

$$
\begin{aligned}
\sigma(\theta,\phi) &= \left(\frac{m^*}{2\pi\hbar^2}\right)^2 |\Omega V_{kk'}|^2_{k=k'} && (139)\\
&= \left(\frac{m^*}{2\pi\hbar^2}\right)^2 \left(\frac{Ze^2}{\epsilon}\right)^2 \frac{1}{\left(4k^2 \sin^2\left(\frac{\theta}{2}\right) + \frac{1}{L_D^2}\right)^2} && (140)
\end{aligned}
$$

<u>Important consideraions</u>

We define the Bohr radius

$$
a_0 = \frac{4\pi\epsilon\hbar^2}{Zm^*e^2} \tag{141}
$$

Then

$$
\begin{aligned}
\sigma(\theta,\phi) &= \left(\frac{m^* Ze^2}{2\pi\epsilon\hbar^2}\right)^2 \frac{L_D^4}{\left[1 + 4k^2 L_D^2 \sin^2\left(\frac{\theta}{2}\right)\right]^2} && (142)\\
&= \frac{4L_D^4}{a_0^2} \frac{1}{\left[1 + 4k^2 L_D^2 \sin^2\left(\frac{\theta}{2}\right)\right]^2} && (143)
\end{aligned}
$$

(a) If the Debye length is small compared to the electron De Broglie length $(= 2\pi/k)$, then

$$
\frac{L_D^2}{\left(\frac{2\pi}{k}\right)^2} = \frac{L_D^2 k^2}{4\pi^2} \ll 1 \tag{144}
$$

and the factor

$$\gamma^2 = 4k^2 L_D^2 \ll 1 \tag{145}$$

$$\Rightarrow \sigma(\theta, \phi) \approx \frac{4L_D^4}{a_0^2} = \text{const} \tag{146}$$

In this case, the scattering cross-section is nearly independent of θ and scattering is considered isotropic (low-energy electrons)

(b) If $\gamma^2 \gg 1$, i.e., k^2 is very large, then

$$\begin{aligned} \sigma(\theta, \phi) &\approx \frac{4\cancel{L_D^4}}{a_0^2} \frac{1}{16k^4 \cancel{L_D^4} \sin^4(\theta/2)} && (147) \\ &= \frac{1}{4a_0^2 k^4 \sin^4(\theta/2)} && (148) \end{aligned}$$

Scattering is anisotropic and peaked around $\theta = 0$. Therefore, high energy electrons are hardly deflected.

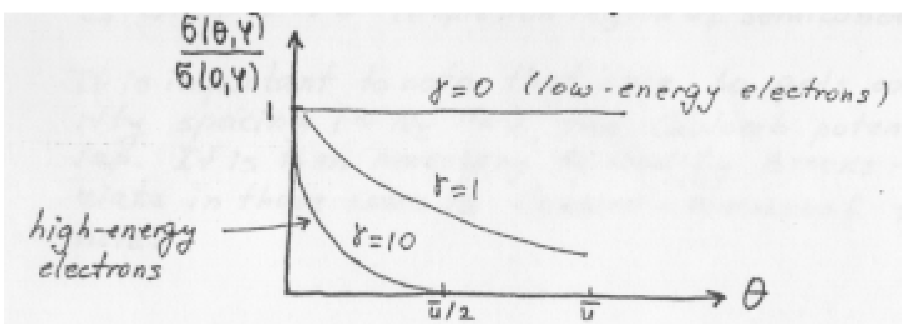

Figure 3: Figure

• To get the total cross-section, we need to integrate over the entire solid angle to get

$$\sigma_s = \int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\phi \frac{4L_D^4}{a_0^2} \frac{1}{\left[1 + \frac{\gamma^2}{2}(1 - \cos\theta)\right]^2} \tag{149}$$

Define

$$x = \cos\theta \tag{150}$$

and

$$y = 1 + \frac{\gamma^2}{2}(1 - x) \tag{151}$$

Then

$$dy = -\frac{\gamma^2}{2} dx \tag{152}$$

and the limits of integration are

$$x = \cos\theta = 1 \Rightarrow y = 1 + \frac{\gamma^2}{2}(1 - 1) = 1 \tag{153}$$

$$x = \cos\theta = -1 \Rightarrow y = 1 + \frac{\gamma^2}{2}(1 + 1) = 1 + \gamma^2 \tag{154}$$

With these substitutions we have

$$\sigma_s = \frac{4L_D^4}{a_0^2} \cdot 2\pi \cdot \int_{1+\gamma^2}^{1} \left(-\frac{2}{\gamma^2}\right) dy \frac{1}{y^2} \tag{155}$$

$$= \frac{16\pi L_D^4}{a_0^2 \gamma^2} \int_1^{1+\gamma^2} \frac{dy}{y^2} \tag{156}$$

$$= \frac{16\pi L_D^4}{a_0^2 \gamma^2} \left(-\frac{1}{y}\right) \Big|_1^{1+\gamma^2} \tag{157}$$

$$= \frac{16\pi L_D^4}{a_0^2 \gamma^2} \left[-\frac{1}{1+\gamma^2} + 1\right] \tag{158}$$

$$= \frac{16\pi L_D^4}{a_0^2 \gamma^2} \left[1 - \frac{1}{1+\gamma^2}\right] \tag{159}$$

$$\sigma_s = \frac{16\pi L_D^4}{a_0^2 \cancel{\gamma^2}} \frac{\cancel{1} + \cancel{\gamma^2} - \cancel{1}}{1+\gamma^2} \tag{160}$$

$$= \frac{16\pi L_D^4}{a_0^2} \frac{1}{1+\gamma^2} \tag{161}$$

where $\gamma^2 = 4k^2 L_D^2$
To summarize

$$\sigma_s = \frac{16\pi L_D^4}{a_0^2} \frac{1}{1 + 4k^2 L_D^2} \tag{162}$$

$$\Rightarrow \tau = \frac{1}{\sigma_s N_I v} \tag{163}$$

$$\Rightarrow \frac{1}{\tau} = \sigma_s N_I v \tag{164}$$

i.e.,

$$\frac{1}{\tau} = N_I \frac{\hbar k}{m^*} \frac{16\pi L_D^4}{a_0^2} \frac{1}{1 + 4k^2 L_D^2} \longrightarrow \text{ Brook's - Herring result} \tag{165}$$

$\longrightarrow$ low energy electrons

$$\frac{1}{\tau} \approx N_I \frac{\hbar k}{m^*} \frac{16\pi L_D^4}{a_0^2} \tag{166}$$

$\longrightarrow$ high energy electrons

$$\frac{1}{\tau} \approx N_I \frac{\hbar k}{m^*} \frac{16\pi L_D^4}{a_0^2} \frac{1}{4k^2 L_D^2} \tag{167}$$

$$\approx \frac{4\pi L_D^2 \hbar N_I}{m^* a_0^2 k} \tag{168}$$

$\longrightarrow$ when $L_D \rightarrow \infty$ (depletion region of semiconductor), σ_s and $1/\tau$ are large.

It is important to note that once L_D gets comparable to the inter-impurity spacing ($\sim N_I^{-1/3}$), the Coulomb potential of nearby impurities overlap. It is then necessary to modify Brooks-Herring theory. More appropriate in those cases is Conwell-Weisskopf theory, which is not discussed here.