Chapter 13
Appendix D: The Ritchie Theory

The Ritchie theory describes the relationship between the dielectric function and the electron energy loss in a solid. It allows to calculate the differential inverse inelastic mean free path, the elastic mean free path, and the stopping power. The original version of the Ritchie theory can be found in Ref. [1]. Also see Refs. [2–6] for further details.

13.1 Energy Loss and Dielectric Function

The response of the ensemble of conduction electrons to the electromagnetic disturbance due to electrons passing through a solid and losing energy in it, is described by a complex dielectric function $\varepsilon(\boldsymbol{k}, \omega)$, where $\boldsymbol{k}$ is the wave vector and ω is the frequency of the electromagnetic field. If, at time t, the electron position is $\boldsymbol{r}$ and its speed is $\boldsymbol{v}$, then, indicating with e the electron charge, the electron that passes through the solid can be represented by a charge distribution given by

$$\rho(\boldsymbol{r}, t) = -e\,\delta(\boldsymbol{r} - \boldsymbol{v}t)\,. \tag{13.1}$$

The electric potential φ generated in the medium can be calculated as[1]

$$\varepsilon(\boldsymbol{k}, \omega)\,\nabla^2\varphi(\boldsymbol{r}, t) = -4\pi\,\rho(\boldsymbol{r}, t)\,. \tag{13.2}$$

In the Fourier space we have

$$\varphi(\boldsymbol{k}, \omega) = -\frac{8\pi^2 e}{\varepsilon(\boldsymbol{k}, \omega)}\frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v} + \omega)}{k^2}\,. \tag{13.3}$$

[1]The vector potential is zero due to the chosen gauge.

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In fact, on the one hand,

$$\varphi(\boldsymbol{r}, t) = \frac{1}{(2\pi)^4} \int d^3k \int_{-\infty}^{+\infty} d\omega \exp[i(\boldsymbol{k} \cdot \boldsymbol{r} + \omega\, t)]\, \varphi(\boldsymbol{k}, \omega)\,, \tag{13.4}$$

so that

$$\nabla^2 \varphi(\boldsymbol{r}, t) = -\frac{1}{(2\pi)^4} \int d^3k \int_{-\infty}^{+\infty} d\omega\, \exp[i(\boldsymbol{k} \cdot \boldsymbol{r} + \omega\, t)]\, k^2\, \varphi(\boldsymbol{k}, \omega)\,, \tag{13.5}$$

and, on the other hand,

$$\begin{aligned} \rho(\boldsymbol{k}, \omega) &= \int d^3r \int_{-\infty}^{+\infty} dt\, \exp[-i(\boldsymbol{k} \cdot \boldsymbol{r} + \omega\, t)]\, \rho(\boldsymbol{r}, t) = \\ &= \int d^3r \int_{-\infty}^{+\infty} dt\, \exp[-i(\boldsymbol{k} \cdot \boldsymbol{r} + \omega\, t)]\, [-e\, \delta(\boldsymbol{r} - \boldsymbol{v}t)] = \\ &= -2\pi e \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt\, \exp[-i(\boldsymbol{k} \cdot \boldsymbol{v} + \omega)t] = \\ &= -2\pi e\, \delta(\boldsymbol{k} \cdot \boldsymbol{v} + \omega)\,, \end{aligned} \tag{13.6}$$

so that

$$\rho(\boldsymbol{r}, t) = \frac{1}{(2\pi)^4} \int d^3k \int_{-\infty}^{+\infty} d\omega \exp[i(\boldsymbol{k} \cdot \boldsymbol{r} + \omega\, t)]\, [-\, 2\pi e\, \delta(\boldsymbol{k} \cdot \boldsymbol{v} + \omega)]\,. \tag{13.7}$$

Then, using Eqs. (13.2), (13.5), and (13.7), we obtain

$$\varepsilon(\boldsymbol{k}, \omega)\, k^2\, \varphi(\boldsymbol{k}, \omega) = -8\pi^2\, e\, \delta(\boldsymbol{k} \cdot \boldsymbol{v} + \omega))\,, \tag{13.8}$$

which is equivalent to Eq. (13.3).

We are interested in calculating the energy loss $-dE$ of an electron due to its interaction with the electric field $\boldsymbol{\mathcal{E}}$ generated by the electrons passing through the solid. Let us indicate with $\mathcal{F}_z$ the z component of the electric force, so that

$$-\, dE = \boldsymbol{\mathcal{F}} \cdot d\boldsymbol{r} = \mathcal{F}_z\, dz\,. \tag{13.9}$$

It should be noted that here and in the following equations, the electric force (and the electric field $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{F}}/e$) are considered at $\boldsymbol{r} = \boldsymbol{v}\, t$. Since

$$\mathcal{E}_z\, dz = \frac{dz}{dt}\, dt\, \mathcal{E}_z = \frac{d\boldsymbol{r}}{dt} \cdot \boldsymbol{\mathcal{E}}\, dt = \frac{\boldsymbol{v} \cdot \boldsymbol{\mathcal{E}}}{v}\, dz \tag{13.10}$$

the energy loss $-dE$ per unit path length dz, $-dE/dz$, is given by

$$-\frac{dE}{dz} = \frac{e}{v}\,\boldsymbol{v}\cdot\boldsymbol{\mathcal{E}}\,. \tag{13.11}$$

Since

$$\boldsymbol{\mathcal{E}} = -\nabla\,\varphi(\boldsymbol{r},t) \tag{13.12}$$

and $\varphi(\boldsymbol{k},\omega)$ is the Fourier transform of $\varphi(\boldsymbol{r},t)$ [see Eq. (13.4)], then

$$\begin{aligned}\boldsymbol{\mathcal{E}} &= \\ &= -\nabla\left\{\frac{1}{(2\,\pi)^4}\int d^3\,k\int_{-\infty}^{+\infty} d\omega\,\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}+\omega\,t)]\,\varphi(\boldsymbol{k},\omega)\right\}.\end{aligned} \tag{13.13}$$

As a consequence

$$\begin{aligned}-\frac{dE}{dz} &= \\ &= \mathrm{Re}\left\{-\frac{8\pi^2e^2}{(2\pi)^4 v}\,\times\right. \\ &\times\left.\int d^3k\int_{-\infty}^{+\infty} d\omega(-\nabla)\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}+\omega\,t)]\cdot\boldsymbol{v}\;\frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right|_{\boldsymbol{r}=\boldsymbol{v}\,t}\Bigg\} = \\ &= \mathrm{Re}\left\{-\frac{8\pi^2e^2}{(2\pi)^4 v}\,\times\right. \\ &\times\left.\int d^3k\int_{-\infty}^{+\infty} d\omega(-i\boldsymbol{k})\cdot\boldsymbol{v}\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}+\omega\,t)]\;\frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right|_{\boldsymbol{r}=\boldsymbol{v}\,t}\Bigg\} = \\ &= \mathrm{Re}\left\{\frac{i8\pi^2e^2}{16\pi^4 v}\,\times\right. \\ &\times\left.\int d^3k\int_{-\infty}^{+\infty} d\omega(\boldsymbol{k}\cdot\boldsymbol{v})\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}+\omega\,t)]\;\frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right|_{\boldsymbol{r}=\boldsymbol{v}\,t}\Bigg\}\,.\end{aligned} \tag{13.14}$$

Taking into account (i) that the electric field has to be calculated at $\boldsymbol{r} = \boldsymbol{v}\,t$ and (ii) of the presence in the integrand of the $\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)$ distribution, we have

$$
\begin{aligned}
&-\frac{dE}{dz} = \\
&= \mathrm{Re}\left\{\frac{i\,e^2}{2\,\pi^2\,v} \times\right. \\
&\times \left.\int d^3k \int_{-\infty}^{+\infty} d\omega\, \boldsymbol{k}\cdot\boldsymbol{v}\, \exp[i(\boldsymbol{k}\cdot\boldsymbol{v}\,t + \omega\,t)]\, \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right\} = \\
&= \mathrm{Re}\left\{\frac{i\,e^2}{2\,\pi^2\,v} \times\right. \\
&\times \left.\int d^3k \int_{-\infty}^{+\infty} d\omega\, \boldsymbol{k}\cdot\boldsymbol{v}\, \exp[i(-\omega\,t + \omega\,t)]\, \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right\} = \\
&= \mathrm{Re}\left\{\frac{i\,e^2}{2\,\pi^2\,v} \times\right. \\
&\times \left.\int d^3k \int_{-\infty}^{+\infty} d\omega\, (-\omega)\, \exp[i(-\omega\,t + \omega\,t)]\, \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right\} = \\
&= \mathrm{Re}\left\{\frac{-i\,e^2}{2\,\pi^2\,v} \int d^3k \int_{-\infty}^{+\infty} d\omega\,\omega\, \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2\,\varepsilon(\boldsymbol{k},\omega)}\right\}.
\end{aligned}
\tag{13.15}
$$

Since

$$
\begin{aligned}
&\mathrm{Re}\left\{i \int_{-\infty}^{+\infty} d\omega\,\omega\, \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{\varepsilon(\boldsymbol{k},\omega)}\right\} = \\
&= 2\,\mathrm{Re}\left\{i \int_{0}^{+\infty} d\omega\,\omega\, \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{\varepsilon(\boldsymbol{k},\omega)}\right\},
\end{aligned}
$$

we conclude that[2]

$$
-\frac{dE}{dz} = \frac{e^2}{\pi^2\,v} \int d^3k \int_0^{\infty} d\omega\,\omega\,\mathrm{Im}\left[\frac{1}{\varepsilon(\boldsymbol{k},\omega)}\right] \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2}, \tag{13.16}
$$

or

$$
-\frac{dE}{dz} = \int_0^{\infty} d\omega\,\omega\,\tau(\boldsymbol{v},\omega), \tag{13.17}
$$

where

$$
\tau(\boldsymbol{v},\omega) = \frac{e^2}{\pi^2\,v} \int d^3k\,\mathrm{Im}\left[\frac{1}{\varepsilon(\boldsymbol{k},\omega)}\right] \frac{\delta(\boldsymbol{k}\cdot\boldsymbol{v}+\omega)}{k^2} \tag{13.18}
$$

[2]Note that, for any complex number z, $\mathrm{Re}(i\,z) = -\mathrm{Im}(z)$.

is the probability of an energy loss ω per unit distance traveled by a non-relativistic electron of velocity $\boldsymbol{v}$ [1].

13.2 Homogeneous and Isotropic Solids

Let us assume now that the solid is homogeneous and isotropic, and ε is a scalar depending only on the magnitude of $\boldsymbol{k}$ and not on its direction

$$\varepsilon(\boldsymbol{k}, \omega) = \varepsilon(k, \omega) \tag{13.19}$$

so that

$$\begin{aligned}
\tau(v, \omega) &= \\
&= \frac{e^2}{\pi^2 v} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \int_{k_-}^{k_+} dk\, k^2 \sin\theta \times \\
&\times \mathrm{Im}\left[\frac{1}{\varepsilon(k, \omega)}\right] \frac{\delta(k\, v \cos\theta + \omega)}{k^2} = \\
&= \frac{2\, e^2}{\pi\, v} \int_0^{\pi} d\theta \int_{k_-}^{k_+} dk \sin\theta\, \mathrm{Im}\left[\frac{1}{\varepsilon(k, \omega)}\right] \delta(k\, v \cos\theta + \omega)
\end{aligned} \tag{13.20}$$

where

$$\hbar k_{\pm} = \sqrt{2\, m\, E} \pm \sqrt{2\, m\, (E - \hbar\omega)}\,. \tag{13.21}$$

and $E = m\, v^2 / 2$. These limits of integration come from conservation of momentum (see Sect. 5.2.3).

Let us introduce the new variable ω' defined as

$$\omega' = -k\, v \cos\theta\,, \tag{13.22}$$

so that

$$d\omega' = k\, v \sin\theta\, d\theta \tag{13.23}$$

and, hence,

$$\begin{aligned}
\tau(v, \omega) &= \frac{2\, e^2}{\pi\, v} \int_{-k\, v}^{k\, v} d\,\omega' \int_{k_-}^{k_+} \frac{dk}{k\, v}\, \mathrm{Im}\left[\frac{1}{\varepsilon(k, \omega)}\right] \delta(-\omega' + \omega) \\
&= \frac{2\, m\, e^2}{\pi\, m\, v^2} \int_{k_-}^{k_+} \frac{dk}{k}\, \mathrm{Im}\left[\frac{1}{\varepsilon(k, \omega)}\right].
\end{aligned} \tag{13.24}$$

We thus can write that

$$\tau(E,\omega) = \frac{m\,e^2}{\pi\,E}\int_{k_-}^{k_+}\frac{dk}{k}\,\mathrm{Im}\left[\frac{1}{\varepsilon(k,\omega)}\right], \tag{13.25}$$

Indicating with $W = \hbar\omega$ the energy loss and with $W_{\max}$ the maximum energy loss, the inverse electron inelastic mean free path, $\lambda_{\mathrm{inel}}^{-1}$, can be calculated as

$$\begin{aligned}\lambda_{\mathrm{inel}}^{-1} &= \\ &= \frac{m\,e^2}{\pi\,\hbar^2\,E}\int_0^{W_{\max}} d\hbar\omega \int_{k_-}^{k_+}\frac{dk}{k}\,\mathrm{Im}\left[\frac{1}{\varepsilon(k,\omega)}\right] = \\ &= \frac{1}{\pi\,a_0\,E}\int_0^{W_{\max}} d\hbar\omega \int_{k_-}^{k_+}\frac{dk}{k}\,\mathrm{Im}\left[\frac{1}{\varepsilon(k,\omega)}\right].\end{aligned} \tag{13.26}$$

13.3 Summary

The Ritchie theory [1] was described. It allows to establish the relationship between electron energy loss and dielectric function, and to calculate the differential inverse inelastic mean free path, the inelastic means free path, and the stopping power.

References

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