

Transport Theory #7

Quick Review of Classical Scattering Theory

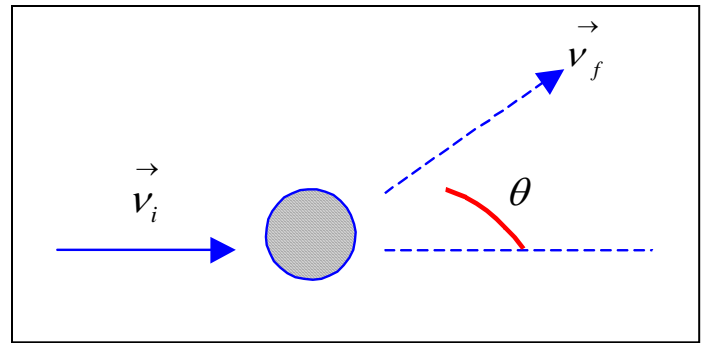
Classical mechanics teaches us of two types of particle scattering, elastic, and inelastic. In elastic scattering, momentum and energy are conserved and the scattering process between a particle and a scatterer can be understood in terms of the total geometric scatterercross section, σ_C , the density of scatterers n , and the particle velocity, which together yield a collision rate

$$f_C = n\sigma_C v \equiv \frac{1}{\tau_C} \quad (7)$$

where τ_C is the collision time. In general, the total collision cross section can be related to a differential cross section $\sigma(\theta, \phi)$ that is almost always independent of the azimuthal angle ϕ , so that

$$\sigma_C = \iint \sigma(\theta) d\Omega = 2\pi \int_0^\pi \sigma(\theta) \sin\theta d\theta \quad (8)$$

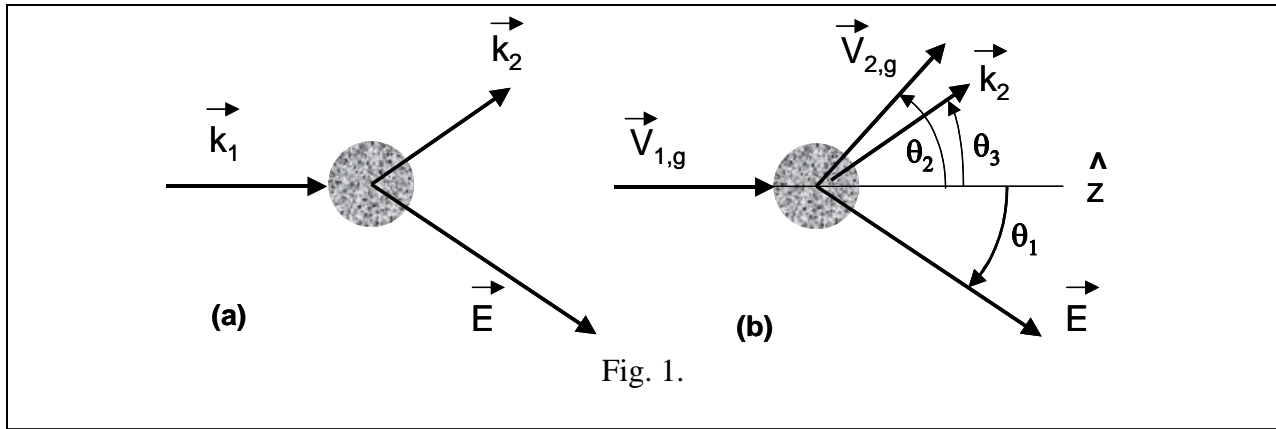
In transport we are always concerned about the flux of particles, which also constitutes a flux of momentum, even for massless “particles” like phonons. So another cross section, the momentum scattering cross section σ_m , is used to weight $\sigma(\theta)$ in the integrand of (1) by the degree to which the incident particle has its incident momentum deflected. As seen in the sketch to the right with incident velocity \vec{v}_i and final (after collision) velocity \vec{v}_f , the deflection factor should go to zero at $\theta = 0$ zero, and to a maximum at $\theta = \pi$. Clearly a deflection factor of $(1 - \cos\theta)$ makes sense in all ways, leading to the expression,



$$\sigma_m = \iint \sigma(\theta)(1 - \cos\theta) d\Omega = 2\pi \int_0^\pi \sigma(\theta)(1 - \cos\theta) \sin\theta d\theta \quad (9)$$

Although originally classical, (9) applies to quantum mechanical scattering as well, and when combined with (7) yields the useful expression.

$$1/\tau_m = n\sigma_m v = nv \cdot \iint \sigma(\theta)(1 - \cos\theta) d\Omega = 2\pi nv \cdot \int_0^\pi \sigma(\theta)(1 - \cos\theta) \sin\theta d\theta \quad (10)$$



Quantum Mechanical Scattering Theory: The Basics

Scattering theory gets particularly elegant when the particles can be represented by plane waves having wave vector \vec{k} . This occurs, of course, when the particles are “free” and have the associated energy eigenfunction

$$\psi(\vec{r}) = V^{-1/2} \exp[j(\vec{k} \cdot \vec{r})] \quad (11)$$

where the normalization is satisfied over a reference volume V . In crystals, we have the corresponding Bloch energy eigenfunction

$$\psi_{n,\vec{k}}(\vec{r}) = V^{-1/2} u_{n,\vec{k}}(\vec{r}) \exp[j(\vec{k} \cdot \vec{r})] \quad (12)$$

where V is now the volume of the primitive unit cell.

Now we assume that the particle of interest is in the form of a wavepacket made from states (12) centered (in k space) about some $\vec{k} = \vec{k}_1$. This is an inherently distributed form in which the interaction with the atomic lattice is already accounted for. We assume a defect or perturbation exists such that the perfect translational symmetry of the lattice is broken. Intuitively, we expect such a defect or perturbation, if small enough, will scatter the incident particle wavepacket to a second wave packet still formed from the states (12). A schematic diagram of the process is shown in Fig. 1. Fortunately, there is a large class of defects and perturbations in which the wavepacket after scattering is centered (in k space) about a different $\vec{k} = \vec{k}_2$ than the incident $\vec{k} = \vec{k}_1$, but the cell-periodic function $u_{n,\vec{k}}$ is nearly unchanged. Such scattering events are generally called *elastic*, since the change of \vec{k} is primarily in vector direction, not vector amplitude.

The problem of calculating the transition of a free-particle quantum-mechanical state from $\vec{k} = \vec{k}_1$ to $\vec{k} = \vec{k}_2$ is one of the oldest and most important in modern physics. It reduces to finding the probability rate $R_{1,2}$ with two key assumptions:

- (1) that there are so many possible \vec{k}_2 states and so much coupling between them that after the transition from \vec{k}_1 to \vec{k}_2 , there is negligible likelihood of the same particle making the transition from \vec{k}_2 back to \vec{k}_1 .¹
- (2) the particle energies before and after the transition are exactly equal (consistent with elastic scattering).

In this case, the transition rate can be written,²

$$R_{1,2} = \frac{2\pi}{\hbar} |H_{\vec{k}_2, \vec{k}_1}|^2 \{\delta[U(k_2) - U(k_1)]\} \equiv \frac{1}{\tau(\vec{k}_1)} \quad (13)$$

Historically, (13) was first derived by Fermi and is so useful in solid state and other branches of physics that is called the “Golden Rule.” The last step in (13) defines rigorously the scattering time added earlier to the semiclassical equations of motion as part of the single-particle relaxation time approximation. The perturbation Hamiltonian is defined by the usual quantum-mechanical expectation value

$$H_{\vec{k}_2, \vec{k}_1} = \langle \psi_{n, \vec{k}_2} | H'(\vec{k}_2, \vec{k}_1) | \psi_{n, \vec{k}_1} \rangle \quad (14)$$

Semiclassical Scattering Theorem

As in the classical analysis, τ is inherently a function of \vec{k}_1 , sometimes a strong function. So the best approach is to incorporate (13) into the semiclassical Boltzmann formalism through two collision terms:

¹ This is distinctly different than the analogous problem in isolated-atom (i.e., “atomic”) physics whereby an external perturbation acts on an atomic wave function ψ_1 , causing a transition to ψ_2 . In this case, after some time, called the Rabi “flopping” time, the atomic wave function can recycle back to ψ_1 . This assumes, of course, that no significant scattering or “dephasing” of the wave function occurs during the process.

² See any good book on Quantum Mechanics, e.g., (1) H. Kroemer, “Quantum Mechanics” (Prentice Hall, New York, 1994, or (2) C. Cohen-Tannoudji, et al. “Quantum Mechanics,” [Wiley Interscience, New York, 1977].

$$(i) \left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\substack{\text{collision} \\ 1 \rightarrow 2}} = -\frac{V}{(2\pi)^3} \int d^3k_2 R_{1,2}(\vec{k}_1, \vec{k}_2) f(\vec{k}_1) [1 - f(\vec{k}_2)] \quad (15)$$

and

$$(ii) \left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\substack{\text{collision} \\ 2 \rightarrow 1}} = +\frac{V}{(2\pi)^3} \int d^3k_2 R_{2,1}(\vec{k}_1, \vec{k}_2) f(\vec{k}_2) [1 - f(\vec{k}_1)] \quad (16)$$

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\text{collision total}} = \left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\substack{\text{collision} \\ 1 \rightarrow 2}} + \left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\substack{\text{collision} \\ 2 \rightarrow 1}} \quad (17)$$

The factor V is the volume of the sample, and $V/(2\pi)^3$ is the volume per state in k space. Both (15) and (16) display the “occupancy-to-de-occupancy” principle addressed earlier. Note that (15) and (16) do not violate the irreversible-transition assumption behind (13) since a particle that contributes to (15) and one that contributes to (16) will always be *two different particles*.

In general (15) and (16) are very difficult to solve. But just as in the case of Boltzmann classical and semiclassical transport, life gets relatively simple in the special case of low particle concentrations. Then we can approximate

$$1 - f(\vec{k}_1) \approx 1 \quad \text{and} \quad 1 - f(\vec{k}_2) \approx 1$$

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\text{collision total}} = +\frac{V}{(2\pi)^3} \int d^3k_2 [R_{2,1}(\vec{k}_1, \vec{k}_2) f(\vec{k}_2) - R_{1,2}(\vec{k}_1, \vec{k}_2) f(\vec{k}_1)] \quad (18)$$

for the nonequilibrium distribution function f . The second simplifying step is to invoke the principle of detailed balance, one of the most profound principles in all of transport theory and quantum physics for that matter. It states that in the equilibrium state, any microscopic processes involving the same two states must balance each other “in detail.” In other words, the total number of particles transferring into a quantum state must equal the number of particles transferring out. Mathematically, this can be stated in the present context as

$$R_{2,1}(\vec{k}_1, \vec{k}_2) f_0(\vec{k}_2) = R_{1,2}(\vec{k}_1, \vec{k}_2) f_0(\vec{k}_1) \quad (19)$$

where f_0 is the Fermi-Dirac function. Substitution of (19) back into (18) leads to

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\text{collision total}} = + \frac{V}{(2\pi)^3} \int d^3k_2 R_{1,2}(\vec{k}_1, \vec{k}_2) [f(\vec{k}_2) \frac{f_0(\vec{k}_1)}{f_0(\vec{k}_2)} - f(\vec{k}_1)] \quad (20)$$

where we assume $\frac{f_0(\vec{k}_1)}{f_0(\vec{k}_2)} \approx 1$ (elastic approximation)

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{\text{collision total}} \approx \frac{V}{(2\pi)^3} \int d^3k_2 R_{1,2}(\vec{k}_1, \vec{k}_2) [f(\vec{k}_2) - f(\vec{k}_1)] \quad (21)$$

where the last step follows from the assumption of elastic or near-elastic scattering

To go further, we need to apply our solution derived previously for the semiclassical Boltzmann equation (Eqn. 20 in previous section):

$$f = f_0 + \frac{\tau f_0 (1 - f_0) \vec{v}_g \cdot q \vec{E}}{k_B T} \approx f_0 + \frac{q \tau f_0 \vec{v}_g \cdot \vec{E}}{k_B T} \quad (22)$$

We can apply (22) to simplify (21) through the use of trigonometry applied to the scattering diagram in Fig. 1(b),³ with $\vec{v}_{g,1}$ defining the polar axis in spherical coordinates, $\vec{v}_{g,2}$ having polar angle θ_2 and azimuthal ϕ_2 , \vec{E} having polar angle θ_1 and azimuthal ϕ_1 , \vec{k}_2 having polar angle θ_3 and azimuthal ϕ_3 , and a relative azimuthal angle between \vec{E} and $\vec{v}_{g,2}$ of $\phi = \phi_1 - \phi_2$.

In this same coordinate system, the volume differential is

$$d^3k_2 = (k_2)^2 \sin \theta_3 d\theta_3 d\phi_3. \quad (23)$$

Given these definitions we can re-write (22) as

$$f(\vec{k}_1) \approx f_0(\vec{k}_1) + \frac{q \tau f_0 \vec{v}_{g,1} \cdot \vec{E}}{k_B T} = f_0(\vec{k}_1) + \frac{q \tau f_0 v_{g,1} E \cos \theta_1}{k_B T} \quad (24)$$

³ Note that this diagram is written in terms of group velocities rather than wave vectors, and that the group velocity, being proportional $\vec{\nabla}U(\vec{k})$ is not necessarily parallel to \vec{k} except in the special case of a spherical band.

$$f(\vec{k}_2) \approx f_0(\vec{k}_2) + \frac{q\tau f_0 v_{g,2} E}{k_B T} (\cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos \phi) \quad (25)$$

Now utilizing the elastic condition once again, $f_0(k_2) \approx f_0(k_1)$, $k_2 \approx k_1$, and $v_{g1} \approx v_{g2}$. Hence, substitution of (23), (24) and (25) into (22) yields:

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{total}^{coll} \approx \frac{V}{(2\pi)^3} \int d^3 k_2 R_{1,2} \frac{q\tau f_0 v_{g,1} E}{k_B T} [\cos \theta_1 (\cos \theta_2 - 1) + \sin \theta_1 \sin \theta_2 \cos \phi] \sin \theta_3 d\theta_3 d\phi_3 \quad (26)$$

where the last step uses an elegant theorem from spherical trigonometry for the dot product between two vectors (spherical law of cosines), each oriented away from the polar axis.⁴

Depending on the geometry, ϕ and ϕ_3 will be different by just a constant, so that the last term in the integrand of (26) that depends on $\cos \phi$ will be zero in the $d\phi_3$ integral from 0 to 2π . Thus, carrying out the $d\phi_3$ integral over the first term and substitution of (24) back into (26) yields,

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{total}^{collision} \approx \frac{V[f(\vec{k}_1) - f_0(\vec{k}_1)]}{(2\pi)^2} \int k_2^2 dk_2 \int R_{1,2} (\cos \theta_2 - 1) \sin \theta_3 d\theta_3 \quad (27)$$

which can be re-written in the elegant form

$$\left. \frac{\partial f(\vec{k})}{\partial t} \right|_{total}^{collision} \approx -\frac{[f(\vec{k}_1) - f_0(\vec{k}_1)]}{\tau_m(\vec{k}_1)} \quad (28)$$

$$\frac{1}{\tau_m(\vec{k}_1)} \approx \frac{V}{(2\pi)^2} \int k_2^2 dk_2 \int R_{1,2} (1 - \cos \theta_2) \sin \theta_3 d\theta_3 \quad (29)$$

The development culminating in (28) is sometimes called the *semiclassical scattering theorem*, but also constitutes a proof of the relaxation-time approximation we adopted previously for the semiclassical Boltzmann transport equation. But now we have a rigorous expression for calculating the relaxation time ! And because we assumed that the scattering was elastic (or quasi-elastic), τ_m is the time required to change the *crystal momentum*. Hence it is usually called the *momentum relaxation time*, and hence the subscript “m”. This is the most useful form of relaxation time in solid-state transport theory. The energy relaxation time – the other one commonly used – is generally much greater than the momentum relaxation time, but becomes

⁴ See, for example, CRC Standard Mathematical Tables 25th Ed. (CRC Press, W. Palm Beach, FL., 1978), p. 176.

more and more important as external field(s) get larger and drive the distribution function f further away from equilibrium.

Calculation of Momentum Relaxation Time with Quantum Mechanics

The most common application of (29) occurs when the carriers lie in a band that is spherical, or at least “spherical enough” that \vec{v}_g is approximately parallel to \vec{k} at all points of the constant energy surface. In that case, $\theta_3 \approx \theta_2$, and

$$\frac{1}{\tau_m(\vec{k}_1)} \approx \frac{V}{(2\pi)^2} \int k_2^2 dk_2 \int R_{1,2} (1 - \cos \theta_2) \sin \theta_2 d\theta_2 \quad (30)$$

As we shall see shortly, (30) is very handy in direct band gap semiconductors, such as GaAs as InP, in both the conduction band (exactly spherical or spheroidal), and valence band (warped sphere).

The factor in the integrand $\sin\theta (1-\cos\theta)$ is reminiscent of the same factor in the classical scattering theory (9) and (10). To make the correspondence, we switch the order of the integration in (30) to get

$$\frac{1}{\tau_m(\vec{k}_1)} \approx \frac{V}{(2\pi)^2} \int \left(\int R_{1,2} k_2^2 dk_2 \right) (1 - \cos \theta_2) \sin \theta_2 d\theta_2 \quad (31)$$

This is the momentum relaxation time for one particle and one scatterer. But the expression (10) was for one particle and a large number $N = nV$ of scatterers. For one scatterer we can re-write (10) as

$$\frac{1}{\tau_m} = 2\pi \frac{v}{V} \cdot \int_0^\pi \sigma(\theta) (1 - \cos \theta) \sin \theta d\theta \quad (32)$$

where, again, V is the volume of the entire sample and v is the incident particle velocity – now necessarily a group velocity. Direct comparison of (31) and (32) yields,

$$\sigma(\theta) \approx \frac{V^2}{(2\pi)^3 v} \int R_{1,2} k_2^2 dk_2 \quad (33)$$

an elegant expression that is a bit confusing until we remember that k_2 is the radial variable in the spherical-coordinate basis of k space with k_1 defining the polar axis, and θ is the polar angle in

this same basis. Eqn (33) is also a good exercise in dimensional analysis to show that $\sigma(\theta)$ has units of *area*.

The most common application of (33) in solids occurs when $R_{1,2}$ can be approximated from time-dependent perturbation theory by Fermi's Golden rule

$$R_{1,2} = \frac{2\pi}{\hbar} |H_{\bar{k}_2, \bar{k}_1}|^2 \{\delta[U(k_2) - U(k_1)]\} \quad (34)$$

$$\sigma(\theta) \approx \frac{V^2}{(2\pi)^2 \hbar v_1} \int |H_{\bar{k}_2, \bar{k}_1}|^2 \{\delta[U(k_2) - U(k_1)]\} k_2^2 dk_2 \quad (35)$$

To use (35) properly, we must remember that the Dirac delta function $\delta(x)$ has dimensions $[x]^{-1}$, in order that it be normalized over the domain of x . So we need to rewrite the differential taking advantage of our assumption of spherical (or near-spherical) bands,

$$dk_2 = m^* dU_2 / (\hbar^2 k_2) \quad (36)$$

and
$$v_1 = \hbar k_1 / m^* \quad (37)$$

$$\sigma(\theta) \approx \frac{V^2 m^*}{(2\pi)^2 \hbar^3 v_1} \int |H_{\bar{k}_2, \bar{k}_1}|^2 \{\delta[U(k_2) - U(k_1)]\} k_2 dU_2 \quad (38)$$

$$\sigma(\theta) \approx \frac{V^2 (m^*)^2}{(2\pi)^2 \hbar^4 k_1} |H_{\bar{k}_2, \bar{k}_1}(k_1 = k_2)|^2 \cdot k_1 = \frac{V^2 (m^*)^2}{(2\pi)^2 \hbar^4} |H_{\bar{k}_2, \bar{k}_1}(k_1 = k_2)|^2 \quad (39)$$

where the last equation follows from the *sifting* property of the Dirac delta function. Eqns (39) and (32) comprise a very useful pair in the theory of semiconductors, (39) based on the quantum mechanics of scattering and (32) based on transport principles. We will next apply this pair to a variety of important scattering problems in a number of practical materials, ranging from silicon to GaN.