## Transport Theory \#8



Fig. 1.

## Canonical Examples of Semiclassical Scattering Theory

## 1. Ionized Impurity Scattering

Ionized point-like defects, such as donor and acceptors in semiconductors, are fundamentally important and common in solids. And because they are not charge-neutral, they create an electrostatic potential that can scatter "free" carriers such as electrons or holes. But when the solid is a metal, semi-metal or semiconductor, there is generally a high enough concentration of such carriers that the electrostatic potential is not the simple Coulomb potential from electrostatics. There is a collective effect of the charge carriers as a whole to "screen" the impurity potential such that the normal $1 / r$ variation of the Coulomb potential is multiplied by another term - a decaying exponential - that causes the potential to decay away much faster at great distance from the impurity. This is the screened Coulomb electrostatic potential (for impurity charge $\mathrm{q}_{\mathrm{s}}$, ionization number Z )

$$
\begin{equation*}
V(r)=\left(q_{S} / 4 \pi \varepsilon_{r} \varepsilon_{0} r\right) \exp \left(-r / L_{D}\right) \tag{1}
\end{equation*}
$$

At low carrier densities, $\mathrm{L}_{\mathrm{D}}$ is the Debye length,

$$
\begin{equation*}
\mathrm{L}_{\mathrm{D}}=\left[\left(\mathrm{k}_{\mathrm{B}} \mathrm{~T} \varepsilon_{\mathrm{r}} \varepsilon_{0} /\left(\mathrm{ne}^{2}\right)\right]^{1 / 2}\right. \tag{2}
\end{equation*}
$$

and at higher densities it becomes the Thomas-Fermi screening length.
To calculate the scattering effects with (1) and (2), we first need the perturbation Hamiltonian from a Bloch state $\mathrm{k}_{1}$ to a Bloch state $\mathrm{k}_{2}$. In the spatial representation this is given by

$$
\begin{equation*}
H_{k_{2}, k_{1}}=\frac{q_{p}}{V} \int V[r] \exp \left[j\left(\overrightarrow{\boldsymbol{k}}_{1}-\overrightarrow{\boldsymbol{k}}_{2}\right) \cdot \overrightarrow{\boldsymbol{r}}\right] d^{3} r \tag{3}
\end{equation*}
$$

where $\mathrm{q}_{\mathrm{P}}$ is the charge of the incident particle.

$$
\begin{array}{r}
=\frac{q_{P} q_{S}}{4 \pi \varepsilon_{r} \varepsilon_{0} V} \int \frac{\exp \left(-r / L_{D}\right)}{r} \exp \left[j\left(\overrightarrow{\boldsymbol{k}}_{1}-\overrightarrow{\boldsymbol{k}}_{2}\right) \cdot \overrightarrow{\boldsymbol{r}}\right] d^{3} r \\
=\frac{q_{P} q_{S}}{4 \pi \varepsilon_{r} \varepsilon_{0} V} \iiint \frac{\exp \left(-r / L_{D)}\right.}{r} \exp \left[j\left(\overrightarrow{\boldsymbol{k}}_{1}-\overrightarrow{\boldsymbol{k}}_{2}\right) \cdot \overrightarrow{\boldsymbol{r}}\right] r^{2} \sin \theta d r d \theta d \phi \tag{5}
\end{array}
$$

where the last step is just re-expression in spherical coordinates. This is a classic integral of science and can be solved simply by first defining the direction of the vector $\overrightarrow{\boldsymbol{k}}_{1}-\overrightarrow{\boldsymbol{k}}_{2}$ (which is fixed during the integration) arbitrarily along the z axis of a same spherical coordinate system. Hence, $\left(\overrightarrow{\boldsymbol{k}}_{1}-\overrightarrow{\boldsymbol{k}}_{2}\right) \cdot \overrightarrow{\boldsymbol{r}}=\left|\overrightarrow{\boldsymbol{k}}_{1}-\overrightarrow{\boldsymbol{k}}_{2} \| \overrightarrow{\boldsymbol{r}}\right| \cos \theta \equiv \Delta k \cdot r \cdot \cos \theta$, and there is no dependence on azimuthal angle, so that (5) becomes,

$$
\begin{equation*}
H_{k_{2}, k_{1}}=\frac{q_{P} q_{S}}{2 \varepsilon_{r} \varepsilon_{0} V} \iint \frac{\exp \left(-r / L_{D)}\right.}{r} \exp [j(\Delta k \cdot r) \cos \theta] r^{2} \sin \theta d r d \theta \tag{6}
\end{equation*}
$$

The $\theta$ integral is straightforward and yields

$$
\begin{gathered}
H_{k_{2}, k_{1}}=\frac{q_{P} q_{S}}{2 \varepsilon_{r} \varepsilon_{0} V} \int \frac{\exp \left(-r / L_{D)}\right.}{r} r^{2} d r \cdot\left(\left.\frac{-\exp [j(\Delta k \cdot r) \cos \theta]}{j(\Delta k \cdot r)}\right|_{0} ^{\pi}\right) \\
=\frac{q_{P} q_{S}}{\varepsilon_{r} \varepsilon_{0} V} \int_{0}^{\infty} \exp \left(-r / L_{D}\right) \frac{\sin (\Delta k \cdot r)}{\Delta k} d r
\end{gathered}
$$

From standard integral tables or a good symbolic integration tool, this can be evaluated as

$$
\begin{gather*}
=\left.\frac{q_{P} q_{S}}{\varepsilon_{r} \varepsilon_{0} V \Delta k}\left\{\exp \left(-r / L_{D}\right) \frac{\left[\left(-1 / L_{D}\right) \sin \Delta k r-\Delta k \cos (\Delta k r)\right]}{\left[\left(1 / L_{D}\right)^{2}+(\Delta k)^{2}\right]}\right\}\right|_{0} ^{\infty} \\
H_{k_{2}, k_{1}}=\frac{q_{P} q_{S}}{\varepsilon_{r} \varepsilon_{0} V\left[\left(1 / L_{D}\right)^{2}+(\Delta k)^{2}\right]} \tag{7}
\end{gather*}
$$

a remarkably simple result. To turn this into a differential scattering cross section for use in transport calculations, we note from the trigonometry of Fig. 1 that $\Delta \mathrm{k}=2 \mathrm{k}_{1} \sin (\theta / 2)$, so that $(\Delta \mathrm{k})^{2}=\left(2 \mathrm{k}_{1}\right)^{2} \sin ^{2}(\theta / 2)=2\left(\mathrm{k}_{1}\right)^{2}(1-\cos \theta)$, where the last step uses a trigonometric identity. Hence, from the central result of the quantum mechanical scattering theory,

$$
\begin{equation*}
\sigma(\theta) \approx \frac{V^{2}\left(m^{*}\right)^{2}}{(2 \pi)^{2} \hbar^{4}}\left|H_{\vec{k}_{2}, \vec{k}_{1}}\left(k_{1}=k_{2}\right)\right|^{2}=\frac{\left(m^{*}\right)^{2}}{\left(2 \pi \varepsilon_{r} \varepsilon_{0}\right)^{2} \hbar^{4}}\left(\frac{q_{P} q_{S}}{\left(1 / L_{D}\right)^{2}+2 k_{1}^{2}-2 k_{1}^{2} \cos \theta}\right)^{2} \tag{8}
\end{equation*}
$$

One remarkable effect is already evident in (8) - the cross section does not depend on the relative signs between incident particle and scatterer !

To turn (8) into a momentum relaxation time, we need to carry out the transport
integral

$$
\begin{equation*}
1 / \tau_{m}=2 \pi n_{I} \mathrm{v} \cdot \int_{0}^{\pi} \sigma(\theta)(1-\cos \theta) \sin \theta d \theta \tag{9}
\end{equation*}
$$

where $n_{I}$ is the concentration of ionized impurities. The first term in the integrand on the RHS of (9), that goes as $\sin \theta$, is an odd function with respect to the center of the integration domain, $\theta=\pi / 2$, whereas the $\theta$-dependence of ( 8 ) is even. So the first term of ( 9 ) vanishes. The second term, through a good integral table or symbolic match tool yields,

$$
1 / \tau_{m}=\frac{n m^{*}}{(8 \pi) \hbar^{3} k_{1}^{3}}\left(\frac{q_{P} q_{S}}{\varepsilon_{r} \varepsilon_{0}}\right)^{2}\left[\ln \left(1+\beta^{2}\right)-\beta^{2} /\left(1+\beta^{2}\right)\right]
$$

where $\beta \equiv 2 \mathrm{k}_{1} \mathrm{~L}_{\mathrm{D}}$. Using the spherical-band relation $\left(\hbar k_{1}^{2}\right) /\left(2 m^{*}\right)=U_{1}$, we get

$$
\begin{equation*}
\tau_{m}=\frac{\left(2 m^{*}\right)^{1 / 2}(16 \pi) U_{1}^{3 / 2}}{n_{I}}\left(\frac{\varepsilon_{r} \varepsilon_{0}}{q_{P} q_{S}}\right)^{2}\left[\ln \left(1+\beta^{2}\right)-\beta^{2} /\left(1+\beta^{2}\right)\right]^{-1} \tag{10}
\end{equation*}
$$

To do transport evaluation, (1) should be averaged over the particle distribution function to get $\left\langle\tau_{\mathrm{m}}\right\rangle$. This can be done just over the Maxwell-Boltzmann function since the particle concentration has been assumed low from the beginning. But the expression in square brackets clearly depends on energy through the definition of $\beta$. But its dependence is much weaker than the dominant term $\left(\mathrm{U}_{1}\right)^{3 / 2}$ since in the spherical-valley approximation $U=(\hbar k)^{2} / 2 m *$ or $k=\sqrt{2 m U} / \hbar$. So we treat this expression as a constant C during the integration

$$
\ln \left[\left(1+\beta^{2}\right)-\beta^{2} /\left(1+\beta^{2}\right)\right] \equiv C \quad, \quad \tau(U) \approx \frac{16 \pi \sqrt{2 m}}{C N_{I}}\left[\frac{\varepsilon_{r} \varepsilon_{0}}{q_{p} q_{s}}\right]^{2} U^{3 / 2}
$$

This allows us to integrate (10) using a previous result for the generic form $\tau(\mathrm{U})=\mathrm{AU}^{-\mathrm{s}}$,

$$
<\tau_{m}>=\frac{4 A \cdot \Gamma(5 / 2-S)}{3 \sqrt{\pi}\left(k_{B} T\right)^{S}} \quad \text { where } \quad A=\frac{16 \pi \sqrt{2 m^{*}}}{C N_{I}}\left(\frac{\varepsilon_{r} \varepsilon_{0}}{q_{p} q_{s}}\right)^{2}
$$

Since $S=-3 / 2, \Gamma(5 / 2-S)=\Gamma(4)=3!=6$, and we get

$$
\begin{equation*}
<\tau_{m}>=\frac{128 \sqrt{2 \pi m^{*}}}{C N_{I}}\left(\frac{\varepsilon_{r} \varepsilon_{0}}{q_{p} q_{s}}\right)^{2}\left(k_{B} T\right)^{3 / 2} \tag{11}
\end{equation*}
$$

This expression is credited to H. Brooks and C. Herring and was not published until 1951 because of the rather tricky calculus needed at the end.

The most common way to handle the constant C is to evaluate it at the point $\mathrm{U}=3 \mathrm{k}_{\mathrm{B}} \mathrm{T}$ since that is where the integrand behind $<\tau_{\mathrm{m}}>$ reaches its maximum (the so-called "Brooks-

Herring" approximation). So since $k=\sqrt{2 m^{*} U} / \hbar$, we can write $k_{B H} \equiv \sqrt{6 m^{*} k_{B} T} / \hbar$

$$
\begin{equation*}
<\tau_{m}>=\frac{128 \sqrt{2 \pi m^{*}}}{N_{I} \ln \left[\left(1+\beta_{B H}^{2}\right)-\beta_{B H}^{2} /\left(1+\beta_{B H}^{2}\right)\right]}\left(\frac{\varepsilon_{r} \varepsilon_{0}}{q_{p} q_{s}}\right)^{2}\left(k_{B} T\right)^{3 / 2} \tag{12}
\end{equation*}
$$

where

$$
\beta_{\mathrm{BH}} \equiv 2 \mathrm{k}_{\mathrm{BH}} \mathrm{~L}_{\mathrm{D}}=\left(\sqrt{6 m^{*} k_{B} T} / \hbar\right)\left[\left(\mathrm{k}_{\mathrm{B}} \mathrm{~T} \varepsilon_{\mathrm{r}} \varepsilon_{0} /\left(\mathrm{ne}^{2}\right)\right]^{1 / 2}\right.
$$

And of course,

$$
<\mu>=\mathrm{e}<\tau_{\mathrm{m}}>/ \mathrm{m}^{*}
$$

which is a very handy equation to put into a spreadsheet computation.
Before applying these expressions, we note the following physically-intuitive but non-obvious aspects of (12): (1) as the temperature increases $\left.<\tau_{\mathrm{m}}\right\rangle$ and $\langle\mu>$ both increase consistent with the fact that the increasing temperature increases the mean kinetic energy of the particles, and the fact that increasing kinetic energy makes the charged scattering centers look progressively more "transparent", ${ }^{1}$ (2) as m* decreases, $\langle\mu\rangle$ increases slowly consistent with the fact that lower m* means higher mean velocity for a given temperature and, therefore, greater "transparency" of the scatterers, (3) as $\varepsilon_{\mathrm{r}}$ increases $<\tau_{\mathrm{m}}>$ and $<\mu>$ both increase rapidly consistent with the fact that higher $\varepsilon_{\mathrm{r}}$ reduces the electric field and electrostatic potential in the solid per unit ionized charge. Note that all three of these effects are favorable to the use of semiconductor devices at room temperature, particularly since semiconductors tend to have low $\mathrm{m}^{*}$ and high $\varepsilon_{\mathrm{r}}$, as we found out in our studies of band structure and electric (atomic) polarizability, respectively.

## Specific example of GaAs at 300 and 77 K

$m=m^{*}=0.067 m_{e}, \varepsilon_{r}=13.0, n_{I}=1 \times 10^{16} / \mathrm{cm}^{3}, n=1 \times 10^{16} / \mathrm{cm}^{3}$

[^0]$\Rightarrow \mathrm{L}_{\mathrm{D}}=428$ Ang $\mathrm{k}_{\mathrm{BH}}=3.7 \times 10^{8} \mathrm{~m}^{-1}, \beta_{\mathrm{BH}}=32$, and $\mathrm{C}=5.9$ at 300 K
so that $\left\langle\tau_{\mathrm{m}}\right\rangle=7.0 \mathrm{ps}$ and $\mu=18.3 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=1.8 \times 10^{5} \mathrm{~cm}^{2} / \mathrm{V}$-s which is much higher than the experimental value of $6000 \mathrm{~cm}^{2} / \mathrm{V}$-s in this grade of GaAs

But at 77 K , we get $\mathrm{L}_{\mathrm{D}}=217$ Ang $\mathrm{k}_{\mathrm{BH}}=1.9 \times 10^{8} \mathrm{~m}^{-1}, \beta_{\mathrm{BH}}=8.1$, and $\mathrm{C}=3.2$ so that $<\tau_{\mathrm{m}}>=1.7 \mathrm{ps}$ and $\mu=4.4 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=4.4 \times 10^{4} \mathrm{~cm}^{2} / \mathrm{V}$-s which is quite close to the $77-\mathrm{K}$ experimental value.

## Specific example of Si at 300 and 77 K

$m=m_{c}^{*}=0.26 m_{e}, \varepsilon_{r}=11.9, n_{I}=1 \times 10^{16} / \mathrm{cm}^{3}, n=1 \times 10^{16} / \mathrm{cm}^{3}$
At $300 \mathrm{~K}, \Rightarrow \mathrm{~L}_{\mathrm{D}}=412$ Ang $\mathrm{k}_{\mathrm{BH}}=7.3 \times 10^{8} \mathrm{~m}^{-1}, \beta_{\mathrm{BH}}=60$, and $\mathrm{C}=7.2$ at 300 K so that $\left\langle\tau_{\mathrm{m}}\right\rangle=9.7 \mathrm{ps}$ and $\mu=6.6 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=6.6 \times 10^{4} \mathrm{~cm}^{2} / \mathrm{V}$-s which is much higher than the experimental value of $\sim 1300 \mathrm{~cm}^{2} / \mathrm{V}$-s in this grade of Si
But at 77 K , we get $\mathrm{L}_{\mathrm{D}}=209 \mathrm{Ang}, \mathrm{k}_{\mathrm{BH}}=3.7 \times 10^{8} \mathrm{~m}^{-1}, \beta_{\mathrm{BH}}=15.4$, and $\mathrm{C}=4.5$ so that $<\tau_{\mathrm{m}}>=2.0 \mathrm{ps}$ and $\mu=1.4 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=1.4 \times 10^{4} \mathrm{~cm}^{2} / \mathrm{V}-\mathrm{s}$ which is close to the $77-\mathrm{K}$ experimental value.

Important practical points:
(1) The mobility is usually stated in "practical" units of $\mathrm{cm}^{2} / \mathrm{V}-\mathrm{s}$, obviously not MKSA.
(2) The great discrepancy between the $300-\mathrm{K}<\tau_{\mathrm{m}}>$ and $<\mu>$ values for GaAs and Si is caused by the fact that around room temperature and higher, ionized impurities play relatively little role in the scattering compared to phonons, which we now start to address.

## 2. Acoustic Phonon Scattering

The mobility calculated above for the ionized impurity scattering is generally very optimistic in semiconductors around room temperature because it ignores the effect of the effect of lattice vibrations. Until about 1950, this effect remained rather mysterious. Then in a very elegant theorem by Bardeen and Shockley, it was shown how the lattice waves create a uniform perturbation on the electrons because of their effect on the lattice constant and, therefore, the potential energy. By this time it was known that the carriers in semiconductors generally lie (in k space) near band edges, and that the band-edge energy represented the potential energy $U_{P}$ of the electrons relative to the conventional zero of infinity.

The simplest form of the Bardeen-Shockley proof utilizes elasticity theory to relate the band-edge energy to the strain $\eta$ through the relation:

$$
\begin{equation*}
\delta \mathrm{U}_{\mathrm{P}}=\Xi \eta \tag{13}
\end{equation*}
$$

where $\Xi$ is the deformation-potential constant - generally a known parameter for most semiconductors and usually a surprisingly big number, $\sim 10 \mathrm{eV}$. The large size of $\Xi$ can be traced back to the large change of cohesive energy with small change of interatomic separation away from the equilibrium point, or similarly, the very small thermodynamic compressibility of most semiconductors (and solids, in general).

To relate (13) to the temperature and statistical-mechanics of phonons, we recall that each phonon represents the quantized amplitude of a specific lattice wave (in phasor form),

$$
\begin{equation*}
\left.\vec{u}=A \cos \left(\vec{k}_{p} \cdot \vec{r}\right)\right] \hat{k}_{p}=A \cdot \operatorname{Re}\left\{\exp \left[ \pm j\left(\vec{k}_{p} \cdot \vec{r}\right)\right]\right\} \hat{k}_{p} \tag{14}
\end{equation*}
$$

where u is the deformation at each lattice away from the equilibrium position, A is the amplitude, $\mathrm{k}_{\mathrm{p}}$ is the phonon wave vector (to not confuse with k for the carriers), and $\omega_{\mathrm{p}}$ is the circular frequency associated with the dispersion curve $\omega$ vs kp. Elasticity theory taught us that the strain can and should be defined in terms of the divergence of the deformation, so that from (14),

$$
\eta \equiv \vec{\nabla} \cdot \vec{u}= \pm j\left(\vec{k}_{p} \cdot \vec{u}\right)
$$

clearly a phasor representation. So if we restrict the analysis temporarily to longitudinal modes, so that $u$ and $k_{p}$ are parallel, $\eta= \pm j k_{p} u$, and (13) becomes

$$
\begin{equation*}
\delta \mathrm{U}_{\mathrm{P}}=\mathrm{j} \Xi \mathrm{k}_{\mathrm{p}} \mathrm{u}=\mathrm{j} \Xi \mathrm{k}_{\mathrm{p}} \operatorname{Aexp}\left[\mathrm{j}\left(\mathbf{k}_{\mathrm{p}} \cdot \mathbf{r}\right)\right] \tag{15}
\end{equation*}
$$

The reason (15) is so elegant is that it can be put directly into Fermi's Golden rule with the understanding that $\mathrm{H}_{\mathrm{k} 1, \mathrm{k} 2}=\delta \mathrm{U}_{\mathrm{P}}$ ! This leads to the perturbation Hamiltonian

$$
\left|H_{k_{2}, k_{1}}\right|=\left|\frac{j \Xi k_{p} A}{V} \int \exp \left[j\left(\vec{k}_{1}-\vec{k}_{2} \pm \vec{k}_{p}\right) \cdot \vec{r}\right] d^{3} r\right|
$$

where V is the sample volume, needed for normalization of the wave functions. Since there are no external forces at work, whatever happens between the electrons and phonons should conserve total crystal-momentum conservation, (assuming of course that the electrons stay within the same band and that no photons are generated). Hence we can write:

$$
\begin{gather*}
\vec{k}_{1}-\vec{k}_{2} \pm \vec{k}_{p}=0 \\
\left|H_{k_{2}, k_{1}}\right|=\left|\frac{j \Xi k_{p} A}{V} \int d^{3} r\right|=\Xi \cdot k_{p} A \tag{16}
\end{gather*}
$$

The final preparation step for the transport calculations is to relate A to the phonon statistical mechanics. We made this correspondence in the coverage of lattice waves and phonons where we showed that the amplitude of lattice waves could be related to the mean number of phonons corresponding to that wave (see also Kittel Chap. 4, Eqn 29)

$$
\begin{equation*}
B^{2}=\frac{4\left(<n_{k}>+1 / 2\right) \hbar}{\omega_{p} \rho V} \tag{17}
\end{equation*}
$$

where $<\mathrm{n}_{\mathrm{k}}>$ is the occupancy for the phonons (Planck function), $\omega_{\mathrm{p}}$ is the phonon dispersion relation, $\rho$ is the density, and V is the volume of the sample. However in that derivation, the lattice wave was a standing wave composed of two equal-amplitude but oppositely-going
traveling waves, $\mathrm{u}=\mathrm{B} \cos (\mathrm{kx}) \cos (\omega \mathrm{t})=(\mathrm{B} / 2) \cos (\mathrm{kx}+\omega \mathrm{t})+(\mathrm{B} / 2) \cos (-\mathrm{kx}+\omega \mathrm{t})$ where the last step follows by trigonometric identity. So by comparing (14) and (17), we deduce that $\mathrm{A}=$ $B / 2$, or

$$
\begin{equation*}
A^{2}=\frac{\left(<n_{k}>+1 / 2\right) \hbar}{\omega_{p} \rho V} \tag{18}
\end{equation*}
$$

In our acoustical (long-wavelength) approximation and at room temperature, we have in
most solids $\quad<n_{k}>=\frac{1}{\exp \left(\hbar \omega / k_{B} T\right)-1} \approx \frac{k_{B} T}{\hbar \omega} \gg 1$
And $\omega \approx\left(\mathrm{C}_{\mathrm{mm}} / \rho\right)^{1 / 2} \mathrm{k}$ where $\mathrm{C}_{\mathrm{mm}}$ is the longitudinal stiffness coefficient (along the same direction as the phonon propagation). Hence, we get

$$
\begin{equation*}
\left|H_{k_{2}, k_{1}}\right|=\Xi \cdot\left[k_{B} T /\left(V C_{m m}\right)\right]^{1 / 2} \tag{19}
\end{equation*}
$$

Now we are ready to apply Fermi's golden rule to get the transport parameters. We just need to be careful to account for phonon absorption and phonon emission as separate processes, since both are tantamount to scattering of an electron. Emission of a phonon at wave vector $\vec{k}_{p}$ results in carrier energy after scattering of $U\left(\vec{k}_{1}-\vec{k}_{p}\right)$, and absorption of such a phonon results in an energy $U\left(\vec{k}_{1}+\vec{k}_{p}\right) \quad$ In most solids at room temperature, we can assume that the energy of the carrier is much greater than the energy of the acoustic phonons ( $\hbar \omega_{L}$ ) so that $U\left(\vec{k}_{1}-\vec{k}_{p}\right) \approx U\left(\vec{k}_{1}+\vec{k}_{p}\right) \approx U\left(\vec{k}_{2}\right)$ Inserting this relation and (19) into Fermi's Golden rule then yields,

$$
\begin{equation*}
R_{1,2}=\frac{k_{B} T}{V C_{m m}} \Xi^{2} \frac{2 \pi}{\hbar}\left\{\delta\left[U\left(\vec{k}_{2}\right)-U\left(\vec{k}_{1}\right)\right]\right\} \tag{20}
\end{equation*}
$$

Given this and the fact that (20) does not depend on angle or even on $\mathrm{k}_{1}$, the absorption and emission rates are practically equivalent, and the easiest route to the momentum relaxation time is just the integral

$$
\begin{align*}
& \frac{1}{\tau_{m}} \approx \frac{V}{(2 \pi)^{2}} \int\left(\int R_{1,2} k_{2}^{2} d k_{2}\right)\left(1-\cos \theta_{2}\right) \sin \theta_{2} d \theta_{2}  \tag{21}\\
& \frac{1}{\tau_{m}} \approx \frac{k_{B} T}{\pi \hbar C_{m m}} \Xi^{2} \int k_{2}^{2}\left[\delta\left[U\left(\vec{k}_{2}\right)-U\left(\vec{k}_{1}\right)\right]\right] d k_{2}
\end{align*}
$$

where the $\theta$ integral was carried out using the fact that the term in the integrand $\cos \theta \sin \theta \mathrm{d} \theta$ vanishes in the integral over the range from 0 to $\pi$, but the first term $\sin \theta \mathrm{d} \theta$ yields a factor of 2 . As before, we must be careful using the Dirac delta function, and convert from $\mathrm{dk}_{1}$ in terms of $\mathrm{dU}_{1}$ taking advantage of the spherical-band approximation that pervades scattering theory:

$$
\begin{gathered}
\frac{1}{\tau_{m}} \approx \frac{k_{B} T}{\pi \hbar C_{m m}} \Xi^{2} \int k_{2}^{2} \delta\left[U\left(\vec{k}_{2}\right)-U\left(\vec{k}_{1}\right)\right] \frac{m^{*}}{\hbar^{2} k_{2}} d U_{2} \\
\frac{1}{\tau_{m}} \approx \frac{m^{*} k_{B} T}{\pi \hbar^{3} C_{m m}} \Xi^{2} k_{1}
\end{gathered}
$$

from the sifting property of the Dirac delta function. Finally using the spherical band approximation yet again, so that $k_{1}=(2 m * U)^{1 / 2} / \hbar$ and we get

$$
\begin{gather*}
\frac{1}{\tau_{m}} \approx \frac{m^{*} k_{B} T}{\pi \hbar^{3} C_{m m}} \Xi^{2}(2 m * U)^{1 / 2} / \hbar=\frac{(2)^{1 / 2}\left(m^{*}\right)^{3 / 2} k_{B} T}{\pi \hbar^{4} C_{m m}} \Xi^{2} U^{1 / 2} \\
\tau_{m}=\frac{\pi \hbar^{4} C_{m m}}{(2)^{1 / 2}\left(m^{*}\right)^{3 / 2} k_{B} T \Xi^{2}} U^{-1 / 2} \equiv A U^{-S} \tag{22}
\end{gather*}
$$

where the last step defines the energy-dependent exponent $S=1 / 2$. Now applying our Maxwell-Boltzmann energy averaging expression once again, we get

$$
<\tau_{m}>=\frac{4 A \cdot \Gamma(5 / 2-S)}{3 \sqrt{\pi}\left(k_{B} T\right)^{S}}=\frac{\frac{4 \pi \hbar^{4} C_{m m}}{(2)^{1 / 2}\left(m^{*}\right)^{3 / 2} k_{B} T \cdot \Xi^{2}} \cdot \Gamma(5 / 2-1 / 2)}{3 \sqrt{\pi}\left(k_{B} T\right)^{S}}=\frac{(2 / 3) \sqrt{2 \pi} \hbar^{4} C_{m m}}{\left(m^{*}\right)^{3 / 2} \Xi^{2}\left(k_{B} T\right)^{3 / 2}}
$$

using the fact that $\Gamma(2)=1!=1$. Finally, we get a trivial step for the mobility:

$$
\begin{equation*}
<\mu>=\frac{e<\tau_{m}>}{m^{*}}=\frac{e(2 / 3) \sqrt{2 \pi} \hbar^{4} C_{m m} T^{-3 / 2}}{\left(m^{*}\right)^{5 / 2} \Xi^{2}\left(k_{B}\right)^{3 / 2}} \tag{23}
\end{equation*}
$$

This is the famous Bardeen-Shockley $\mathrm{T}^{-3 / 2}$ law for the mobility of electrons (or holes) by acoustic phonons. It is the most basic of a long list of phonon-scattering formulae for semiconductors, so deserves attention. Specifically, it has some physical properties that deserve mentioning: (1) $<\mu>$ and $<\tau_{\mathrm{m}}>$ both go down with increasing temperature, consistent with the fact that the amplitude of all lattice waves (and therefore population of the corresponding phonon modes) increases with temperature, so there is more deformation of the lattice to scatter the electrons, (2) $<\mu>$ and $<\tau_{\mathrm{m}}>$ both increase with crystal stiffness, consistent with the fact that a stiffer crystal suffers less deformation of the lattice for a unit amount of lattice-wave energy, (3) $<\mu>$ and $<\tau_{m}>$ both decrease rapidly with increasing deformation potential consistent with the fact that this potential is the perturbative coupling coefficient in the problem, and (4) $<\mu>$ and $<\tau_{\mathrm{m}}>$ increase even more rapidly with decreasing m * consistent with the fact that smaller m * means higher acceleration and, therefore, a greater distance traversed by the carrier before a deformation can disturb it.

To use (23) it is important to have the values of $\mathrm{C}_{\mathrm{mm}}, \mathrm{m}^{*}$, and $\Xi$ at hand. These values are tabulated below for two important compound semiconductors: a narrow-band-gap (InSb) and a "normal" band gap (GaAs), as well as Si.

| Material | $\varepsilon_{\mathrm{r}}$ | $\mathrm{m} * / \mathrm{m}_{\mathrm{e}}$ | $\mathrm{C}_{11}[\mathrm{Nt} / \mathrm{m} 2]$ | $\Xi[\mathrm{eV}]$ <br> (longitudinal) |
| :---: | :---: | :---: | :---: | :---: |
| GaAs | 13.0 | 0.067 | $119 \times 10^{9}$ | 9.3 |
| InP | 12.4 | 0.077 | $?$ | 6.4 |
| InSb | 17.5 | 0.014 | $67 \times 10^{9}$ | 7.7 |
| Si | 11.8 | 0.26 | $166 \times 10^{9}$ | 9.2 |

Specific example of GaAs at 300 and 77 K
$m=m_{c}^{*}=0.067 m_{e}, \varepsilon_{r}=12.9, C_{11}=119 \times 10^{9} \mathrm{~N} / \mathrm{m}^{2}, \Xi=9.3 \mathrm{eV}$
So at $300 \mathrm{~K},\left\langle\tau_{\mathrm{m}}\right\rangle=2.8 \mathrm{ps}$ and $\mu=7.2 \mathrm{~m}^{2} / \mathrm{V}$-s $=7.2 \times 10^{4} \mathrm{~cm}^{2} / \mathrm{V}$-s which is much higher than the experimental value of $6000 \mathrm{~cm}^{2} / \mathrm{V}$-s in this grade of GaAs

At 77 K , we get $<\tau_{\mathrm{m}}>=21 \mathrm{ps}$ and $\mu=56 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=5.6 \times 10^{5} \mathrm{~cm}^{2} / \mathrm{V}$-s which is way above the experimental value.

## Specific example of Si at 300 and 77 K

$m=m_{c}^{*}=0.26 m_{e}, \varepsilon_{r}=11.9, C_{11}=166 \times 10^{9} \mathrm{~N} / \mathrm{m}^{2}, \Xi=9.2 \mathrm{eV}$
At $300 \mathrm{~K}<\tau_{\mathrm{m}}>=0.5 \mathrm{ps}$ and $\mu=0.36 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=3.6 \times 10^{3} \mathrm{~cm}^{2} / \mathrm{V}$-s which is about a factor of 2.5 higher than the experimental value of $\sim 1300 \mathrm{~cm}^{2} / \mathrm{V}$-s in this grade of Si

At 77 K , we get $\left\langle\tau_{\mathrm{m}}\right\rangle=4.0 \mathrm{ps}$ and $\mu=2.7 \mathrm{~m}^{2} / \mathrm{V}-\mathrm{s}=2.7 \times 10^{4} \mathrm{~cm}^{2} / \mathrm{V}$-s which is higher than the $77-\mathrm{K}$ experimental value.

## Clearly, the Bardeen-Shockley model for scattering by acoustic phonons

 overestimates $\langle\tau\rangle$ and $\langle\mu\rangle$ in both GaAs and in Si. As we shall see shortly, the reason for this is that it ignores inelastic scattering, which is not so important with acoustical phonons, but becomes very important with optical phonons. This is particularly true at room temperature where the optical phonon modes are beginning to become significantly populated, and where the thermal kinetic energy of the carriers $\sim \mathrm{k}_{\mathrm{B}} \mathrm{T}$, becomes great enough to start emitting optical phonons- a mechanism that is profoundly important in most modern electronic devices because it is ultimately the "braking" mechanism that causes carriers to saturate their drift velocity in moderate to high bias electric fields.
## 3. Combined Ionized Impurity and Acoustic Phonon Scattering: <br> A Lucid Demonstration of Mathiessen's Rule

Notwithstanding the above limitations on the Bardeen Shockley model, it is instructive to combine the ionized-impurity expression (12) with the acoustical phonon expression (23) to form a total mobility. This is done simply by Mathiessen's summation rule for scattering rates, which means that the net mobility for two scattering mechanisms will go as,

$$
\begin{equation*}
\mu_{t o t a l}=\frac{\mu_{1} \mu_{2}}{\mu_{1}+\mu_{2}} \tag{24}
\end{equation*}
$$

Fig. 2 shows the plot of the mobility of silicon for each separate mechansim along with the combination according to (24). We assume the same materials parameters for the Si as before: $m=m_{c}^{*}=0.26 m_{e}, \varepsilon_{r}=11.9, n_{I}=1 \times 10^{16} / \mathrm{cm}^{3}, n=1 \times 10^{16} / \mathrm{cm}^{3}$, and $C_{11}=166 \times 10^{9} \mathrm{~N} / \mathrm{m}^{2}, \Xi=9.2 \mathrm{eV}$. The combination curve displays a distinct maximum around 90 K that is close to the temperature of a maximum observed experimentally. This peak makes it advantageous to cool devices to 77 K - liquid nitrogen temperature - if it is a device type in which the mobility increase improves performance. As we shall see shortly, the inclusion of inelastic scattering reduces the mobility value at the peak.



[^0]:    ${ }^{1}$ First observed by E. Rutherford and his group in the early part of the $20^{\text {th }}$ century on the experimental studies of scattering of charged particle beams from charged stationary target

