

Handout 22

Electron Transport: The Boltzmann Equation

In this lecture you will learn:

- Non-equilibrium distribution functions
- The Liouville equation
- The Boltzmann equation
- Relaxation time approximation
- Scattering beyond the relaxation time approximation



Ludwig Eduard Boltzmann
(1844-1906)

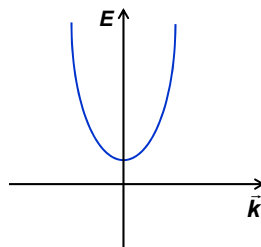
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Note on Notation

In this handout, unless states otherwise, we will assume a conduction band with a dispersion given by:

$$E(\vec{k}) = E_c + \frac{\hbar^2}{2} \vec{k}^T \cdot M^{-1} \cdot \vec{k}$$

$$\Rightarrow \vec{v}(\vec{k}) = M^{-1} \cdot \hbar \vec{k}$$



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Momentum Equation with Scattering and Problems

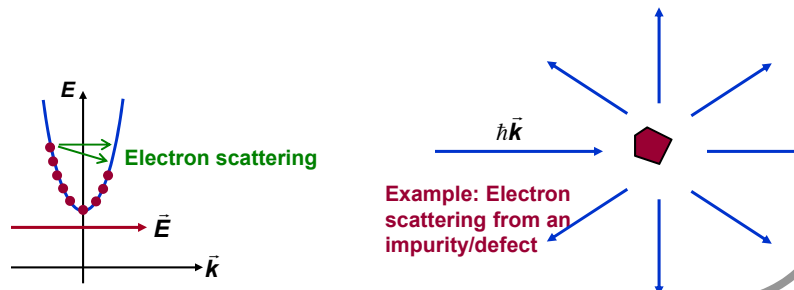
In any energy band the electrons obey the dynamical equation:

$$\frac{d \hbar \vec{k}(t)}{dt} = -e \vec{E}$$

In the presence of scattering, we wrote:

$$\frac{d \hbar \vec{k}(t)}{dt} = -e \vec{E} - \left(\frac{\hbar \vec{k}(t) - \hbar \vec{k}}{\tau} \right)$$

- We need a more general and rigorous description of electron scattering than is captured by adding damping to the momentum equation



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The Non-Equilibrium Distribution Function

In thermal equilibrium, the electron distribution (or the electron occupation probability) is given by the Fermi-Dirac distribution:

$$f_0(\vec{k}) = \frac{1}{1 + e^{(E(\vec{k}) - E_f)/kT}}$$

And the electron density can be written as:

$$n = 2 \times \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f_0(\vec{k})$$

We generalize this concept to non-equilibrium situations (which happen, for example, when electric fields are applied from outside)

The electron distribution (or occupation probability) more generally is given by a time-dependent distribution function:

$$f(\vec{k}, t)$$

that also obeys:

$$n = 2 \times \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f(\vec{k}, t)$$

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The Non-Equilibrium Distribution Function

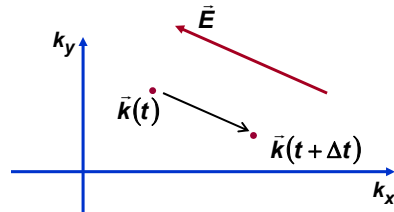
Consider a single electron state in k-space in the presence of an electric field

Assume no scattering

$$\frac{d \hbar \bar{k}(t)}{dt} = -e \bar{E}$$

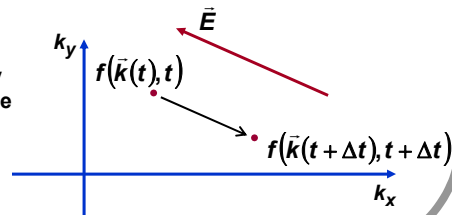
$$\Rightarrow \bar{k}(t) = \bar{k}(t=0) - \frac{e}{\hbar} \bar{E} t$$

$$\Rightarrow \bar{k}(t + \Delta t) = \bar{k}(t=0) - \frac{e}{\hbar} \bar{E} (t + \Delta t)$$



Suppose there exists a time dependent function $f(\bar{k}, t)$ that gives the probability of electron occupying any state in k-space

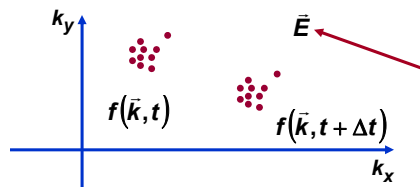
$$\Rightarrow f(\bar{k}(t + \Delta t), t + \Delta t) = f(\bar{k}(t), t)$$



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Case of No Scattering: Liouville Equation

Question: How does the non-equilibrium distribution function behave in time in the absence of scattering?



Consider an initial non-equilibrium distribution at time "t", as shown

There is also an applied electric field, as shown

In time " Δt " each electron would have moved according to the dynamical equation:

$$\frac{d \hbar \bar{k}(t)}{dt} = -e \bar{E}$$

$$\left\{ \begin{array}{l} \bar{k}(t) = \text{initial momentum value} \\ \bar{k}(t + \Delta t) = \text{final momentum value} \end{array} \right.$$

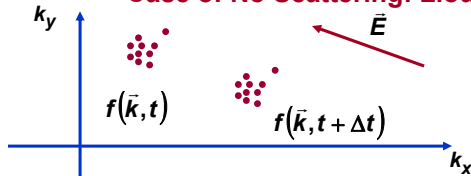
The distribution at time " $t + \Delta t$ " must obey the equation:

$$f(\bar{k}(t + \Delta t), t + \Delta t) = f(\bar{k}(t), t)$$

This is because in time " Δt " the electron with initial momentum $\bar{k}(t)$ would have gone over to the state with momentum $\bar{k}(t + \Delta t)$

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Case of No Scattering: Liouville Equation



$$\frac{d \hbar \bar{k}(t)}{dt} = -e \bar{E}$$

We have: $f(\bar{k}(t + \Delta t), t + \Delta t) = f(\bar{k}(t), t)$

$$\Rightarrow f\left(\bar{k}(t) + \frac{d\bar{k}(t)}{dt} \Delta t, t + \Delta t\right) = f(\bar{k}(t), t) \longrightarrow \left[\bar{k}(t) \text{ is arbitrary} \right]$$

$$\Rightarrow f\left(\bar{k} + \frac{d\bar{k}(t)}{dt} \Delta t, t + \Delta t\right) = f(\bar{k}, t)$$

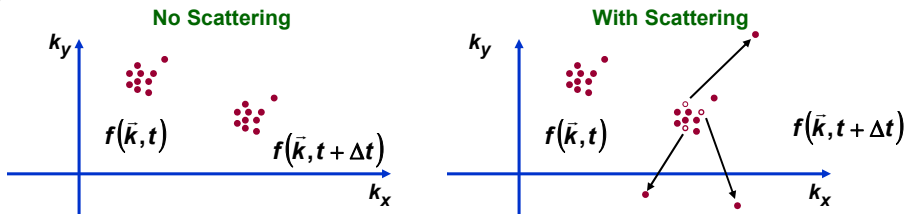
$$\Rightarrow f(\bar{k}, t) + \nabla_{\bar{k}} f(\bar{k}, t) \cdot \frac{d\bar{k}(t)}{dt} \Delta t + \frac{\partial f(\bar{k}, t)}{\partial t} \Delta t = f(\bar{k}, t)$$

The above equation implies that the underlined term must be zero:

$$\frac{\partial f(\bar{k}, t)}{\partial t} + \nabla_{\bar{k}} f(\bar{k}, t) \cdot \frac{d\bar{k}(t)}{dt} = 0 \longrightarrow \text{Liouville equation}$$

Describes the deterministic evolution of electron distribution in k-space

Boltzmann's Equation: Liouville Equation with Scattering



Now we have:

$$f(\bar{k}(t + \Delta t), t + \Delta t) = f(\bar{k}(t), t) + \{ \text{changes due to scattering} \} \Delta t$$

$$\Rightarrow f\left(\bar{k} + \frac{d\bar{k}(t)}{dt} \Delta t, t + \Delta t\right) = f(\bar{k}, t + \Delta t) + \{ \text{changes due to scattering} \} \Delta t$$

$$\Rightarrow f(\bar{k}, t) + \nabla_{\bar{k}} f(\bar{k}, t) \cdot \frac{d\bar{k}(t)}{dt} \Delta t + \frac{\partial f(\bar{k}, t)}{\partial t} \Delta t = f(\bar{k}, t) + \{ \text{changes due to scattering} \} \Delta t$$

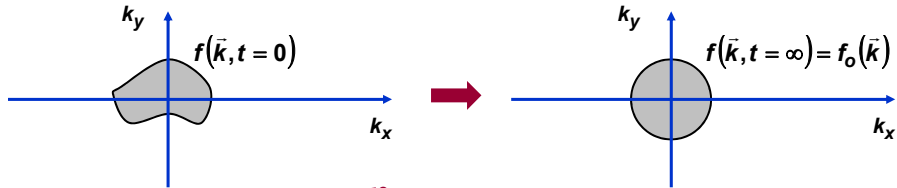
$$\Rightarrow \underbrace{\frac{\partial f(\bar{k}, t)}{\partial t} + \nabla_{\bar{k}} f(\bar{k}, t) \cdot \frac{d\bar{k}(t)}{dt}}_{\text{Deterministic evolution}} = \underbrace{\{ \text{changes due to scattering} \}}_{\text{Non-deterministic evolution}} \longrightarrow \text{Boltzmann's equation}$$

Relaxation Time Approximation

Suppose no external fields are applied: $\vec{E} = 0$

The initial non-equilibrium distribution is given: $f(\vec{k}, t = 0)$

Scattering must eventually restore the equilibrium distribution function



$$\frac{\partial f(\vec{k}, t)}{\partial t} + \nabla_{\vec{k}} f(\vec{k}, t) \cdot \frac{d\vec{k}(t)}{dt} = \{ \text{changes due to scattering} \}$$

$$\Rightarrow \frac{\partial f(\vec{k}, t)}{\partial t} = \{ \text{changes due to scattering} \}$$

Scattering must “relax” the non-equilibrium distribution to the equilibrium Fermi-Dirac distribution at time $t = \infty$

Question: What should be the form of the expression on the RHS in the Boltzmann equation so that equilibrium Fermi-Dirac distribution is indeed restored at time $t = \infty$

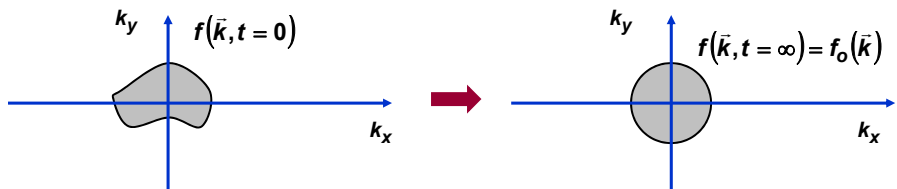
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Relaxation Time Approximation

Case I:

Suppose no external fields are applied: $\vec{E} = 0$

The initial non-equilibrium distribution is given: $f(\vec{k}, t = 0)$



In the **relaxation time approximation**, the RHS is assumed to be as follows:

$$\frac{\partial f(\vec{k}, t)}{\partial t} = \{ \text{changes due to scattering} \} = - \frac{[f(\vec{k}, t) - f_0(\vec{k})]}{\tau}$$

$$\Rightarrow \frac{\partial f(\vec{k}, t)}{\partial t} = - \frac{[f(\vec{k}, t) - f_0(\vec{k})]}{\tau}$$

Solution is: $f(\vec{k}, t) = f(\vec{k}, t = 0) e^{-t/\tau} + f_0(\vec{k}) [1 - e^{-t/\tau}]$

As $t \rightarrow \infty$, $f(\vec{k}, t) \rightarrow f_0(\vec{k})$

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DC External Electric Field

When the external field is not zero, then we get:

$$\frac{\partial f(\vec{k}, t)}{\partial t} + \nabla_{\vec{k}} f(\vec{k}, t) \cdot \frac{d\vec{k}(t)}{dt} = - \frac{[f(\vec{k}, t) - f_o(\vec{k})]}{\tau}$$

Case II:

Suppose a DC external field is applied: \vec{E}

The steady state distribution function is desired

Since: $\frac{d\vec{k}(t)}{dt} = - \frac{e\vec{E}}{\hbar}$

and since in steady state the distribution function cannot depend on time, we have:

$$\cancel{\frac{\partial f(\vec{k})}{\partial t}} - \nabla_{\vec{k}} f(\vec{k}) \cdot \frac{e\vec{E}}{\hbar} = - \frac{[f(\vec{k}) - f_o(\vec{k})]}{\tau}$$

$$\Rightarrow f(\vec{k}) = f_o(\vec{k}) + \nabla_{\vec{k}} f_o(\vec{k}) \cdot \frac{e\tau\vec{E}}{\hbar}$$

We will keep terms that are linear in the applied field (assuming the applied field is small) and so the distribution in the second term on the RHS can be approximated by the equilibrium distribution:

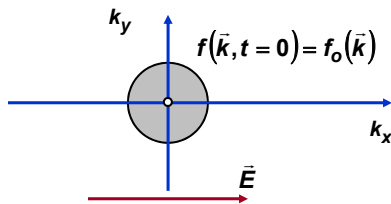
$$f(\vec{k}) \approx f_o(\vec{k}) + \nabla_{\vec{k}} f_o(\vec{k}) \cdot \frac{e\tau\vec{E}}{\hbar} \quad \longrightarrow \quad \text{Final answer}$$

DC External Electric Field

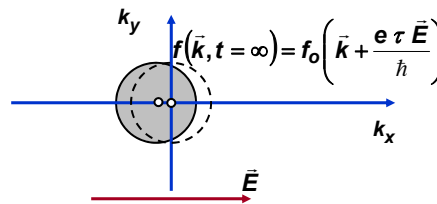
The final answer: $f(\vec{k}) \approx f_o(\vec{k}) + \nabla_{\vec{k}} f_o(\vec{k}) \cdot \frac{e\tau\vec{E}}{\hbar}$ → 1st two terms of a Taylor expansion

can also be written approx. as: $f(\vec{k}) \approx f_o\left(\vec{k} + \frac{e\tau\vec{E}}{\hbar}\right)$ → Shifted equilibrium distribution

Initial Distribution



Steady State Distribution

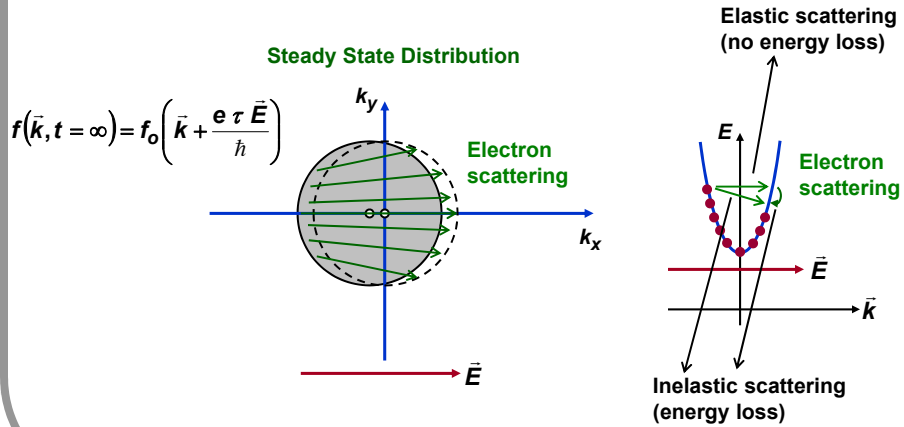


Shifted equilibrium distribution
SAME AS BEFORE!

Everything from here onwards is the same as discussed earlier.....

DC External Electric Field

Steady state distribution: $f(\vec{k}) \approx f_0\left(\vec{k} + \frac{e\tau\vec{E}}{\hbar}\right)$ \longrightarrow Shifted equilibrium distribution



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DC External Electric Field - Current Density

$$f(\vec{k}) \approx f_0(\vec{k}) + \nabla_{\vec{k}} f_0(\vec{k}) \cdot \frac{e\tau\vec{E}}{\hbar} \approx f_0\left(\vec{k} + \frac{e\tau\vec{E}}{\hbar}\right)$$

Example: Consider the conduction band of a semiconductor with the following dispersion:

$$E(\vec{k}) = E_c + \frac{\hbar^2}{2} \vec{k}^T \cdot M^{-1} \cdot \vec{k} \quad \vec{v}(\vec{k}) = M^{-1} \cdot \hbar \vec{k}$$

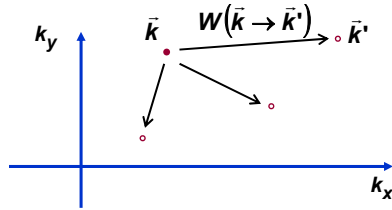
The current density becomes:

$$\begin{aligned} \vec{J} &= -2e \times \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f(\vec{k}) \vec{v}(\vec{k}) = -2e \times \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f_0\left(\vec{k} + \frac{e\tau\vec{E}}{\hbar}\right) \vec{v}(\vec{k}) \\ &= -2e \times \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f_0(\vec{k}) \vec{v}\left(\vec{k} - \frac{e\tau\vec{E}}{\hbar}\right) = -2e \times \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f_0(\vec{k}) M^{-1} \cdot \hbar \left(\vec{k} - \frac{e\tau\vec{E}}{\hbar}\right) \\ &= e^2 \tau \int_{\text{FBZ}} \frac{d^d \vec{k}}{(2\pi)^d} f_0(\vec{k}) M^{-1} \cdot \vec{E} \\ &= n e^2 \tau M^{-1} \cdot \vec{E} \\ &= \vec{\sigma} \cdot \vec{E} \end{aligned}$$

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Scattering Rates

Consider a single electron state in k-space:



The electron in the initial state \bar{k} can scatter to another state \bar{k}' with a scattering rate given by $W(\bar{k} \rightarrow \bar{k}')$ due to phonons, defects, impurities, etc.

But to get the actual transition rate one must weigh $W(\bar{k} \rightarrow \bar{k}')$ by the probabilities that the final state is empty and the initial state is occupied:

$$R(\bar{k} \rightarrow \bar{k}') = W(\bar{k} \rightarrow \bar{k}') f(\bar{k}, t) [1 - f(\bar{k}', t)]$$

Total transition rate out of the state \bar{k} :

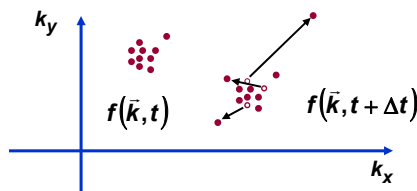
$$\sum_{\bar{k}'} R(\bar{k} \rightarrow \bar{k}') = \sum_{\bar{k}'} W(\bar{k} \rightarrow \bar{k}') f(\bar{k}, t) [1 - f(\bar{k}', t)]$$

Total transition into the state \bar{k} :

$$\sum_{\bar{k}'} R(\bar{k}' \rightarrow \bar{k}) = \sum_{\bar{k}'} W(\bar{k}' \rightarrow \bar{k}) f(\bar{k}', t) [1 - f(\bar{k}, t)]$$

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Boltzmann Equation: Beyond the Relaxation Time Approximation



$$\frac{\partial f(\bar{k}, t)}{\partial t} + \nabla_{\bar{k}} f(\bar{k}, t) \cdot \frac{d\bar{k}(t)}{dt} = \{ \text{changes due to scattering} \}$$

The term that represents the changes in the distribution due to scattering can be written as:

$$\frac{\partial f(\bar{k}, t)}{\partial t} + \nabla_{\bar{k}} f(\bar{k}, t) \cdot \frac{d\bar{k}(t)}{dt} = \sum_{\bar{k}'} W(\bar{k}' \rightarrow \bar{k}) f(\bar{k}', t) [1 - f(\bar{k}, t)] - \sum_{\bar{k}'} W(\bar{k} \rightarrow \bar{k}') f(\bar{k}, t) [1 - f(\bar{k}', t)] \approx - \frac{[f(\bar{k}, t) - f_0(\bar{k})]}{\tau}$$

$W(\bar{k} \rightarrow \bar{k}')$ is the rate of scattering of an electron from momentum state \bar{k} to \bar{k}' due to impurities, defects, phonons, etc. The RHS can be shown to reduce to the **relaxation time approximation** expression in many cases of practical interest.

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Boltzmann Equation: Beyond the Relaxation Time Approximation

$$\frac{\partial f(\vec{k}, t)}{\partial t} + \nabla_{\vec{k}} f(\vec{k}, t) \cdot \frac{d\vec{k}(t)}{dt} = \sum_{\vec{k}'} W(\vec{k}' \rightarrow \vec{k}) f(\vec{k}', t) [1 - f(\vec{k}, t)] - \sum_{\vec{k}'} W(\vec{k} \rightarrow \vec{k}') f(\vec{k}, t) [1 - f(\vec{k}', t)]$$

Assume thermal equilibrium:

$$f(\vec{k}, t) = f_0(\vec{k}) \quad \frac{d\vec{k}(t)}{dt} = 0$$

Therefore:

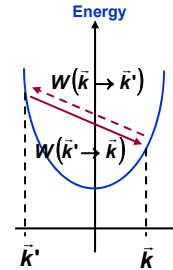
$$0 = \sum_{\vec{k}'} W(\vec{k}' \rightarrow \vec{k}) f_0(\vec{k}') [1 - f_0(\vec{k})] - \sum_{\vec{k}'} W(\vec{k} \rightarrow \vec{k}') f_0(\vec{k}) [1 - f_0(\vec{k}')]]$$

$$\Rightarrow 0 = \sum_{\vec{k}'} W(\vec{k}' \rightarrow \vec{k}) f_0(\vec{k}') [1 - f_0(\vec{k})] - W(\vec{k} \rightarrow \vec{k}') f_0(\vec{k}) [1 - f_0(\vec{k}')]]$$

$$\Rightarrow 0 = W(\vec{k}' \rightarrow \vec{k}) f_0(\vec{k}') [1 - f_0(\vec{k})] - W(\vec{k} \rightarrow \vec{k}') f_0(\vec{k}) [1 - f_0(\vec{k}')]]$$

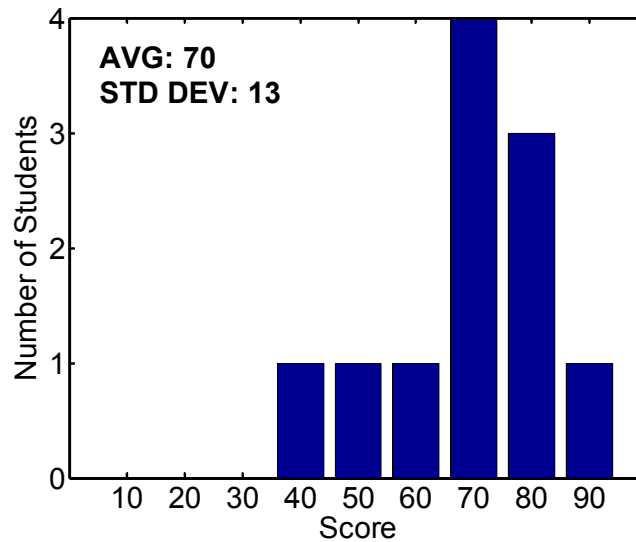
$$\Rightarrow \frac{W(\vec{k} \rightarrow \vec{k}')}{W(\vec{k}' \rightarrow \vec{k})} = \frac{f_0(\vec{k}')}{1 - f_0(\vec{k}')} \frac{1 - f_0(\vec{k})}{f_0(\vec{k})} = \frac{e^{E(\vec{k}')/KT}}{e^{E(\vec{k})/KT}}$$

Scattering rate to lower energy states is larger than scattering to higher energy states



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Exam 1: Results



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