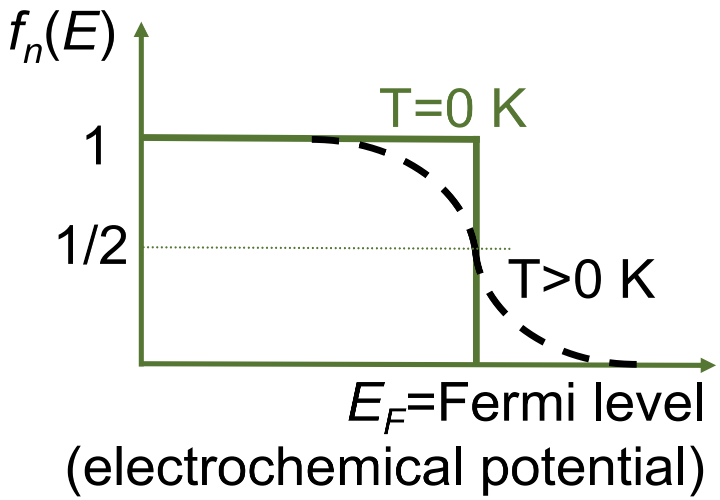
Boltzmann Transport Equation and Fermi's Golden Rule

1. Equilibrium Distribution Function

- The probability of a state with energy *E* being occupied with spin 1/2 electrons, for which the Pauli exclusion principle is valid, is given by the following function:

$$f_n(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

- Fermi-Dirac distribution function, valid in thermal equilibrium.
- In non-equilibrium conditions, one actually has to solve for the distribution function.



Approximate Non-Equilibrium Distribution Function

- **The most difficult problem in device analysis is to calculate the distribution function $f(\mathrm{r},\mathrm{k},t)$.**
- **To overcome these difficulties, reasonable guess for the distribution function is often made. Two most commonly used approaches are:**
  - Quasi-Fermi level concept.
  - Displaced Maxwellian approximation for the distribution function.

(A) Quasi-Fermi Level Concept

- Under non-equilibrium conditions, it may still be useful to represent the distribution functions for electrons and holes as

$$f_n(E) = \frac{1}{1+\exp\left(\frac{E-E_{Fn}}{k_BT}\right)} \qquad f_p(E) = 1 - f_n(E) = \frac{1}{1+\exp\left(\frac{E_{Fp}-E}{k_BT}\right)}$$

- Therefore, under non-equilibrium conditions and assuming non-degenerate statistics, we will have

$$n = N_C \exp\left(\frac{E_{Fn}-E_C}{k_BT}\right), \quad \text{and} \quad p = N_V \exp\left(\frac{E_V-E_{Fp}}{k_BT}\right)$$

- where N_C and N_V are the effective density of states of the conduction and valence band, respectively.

np-product

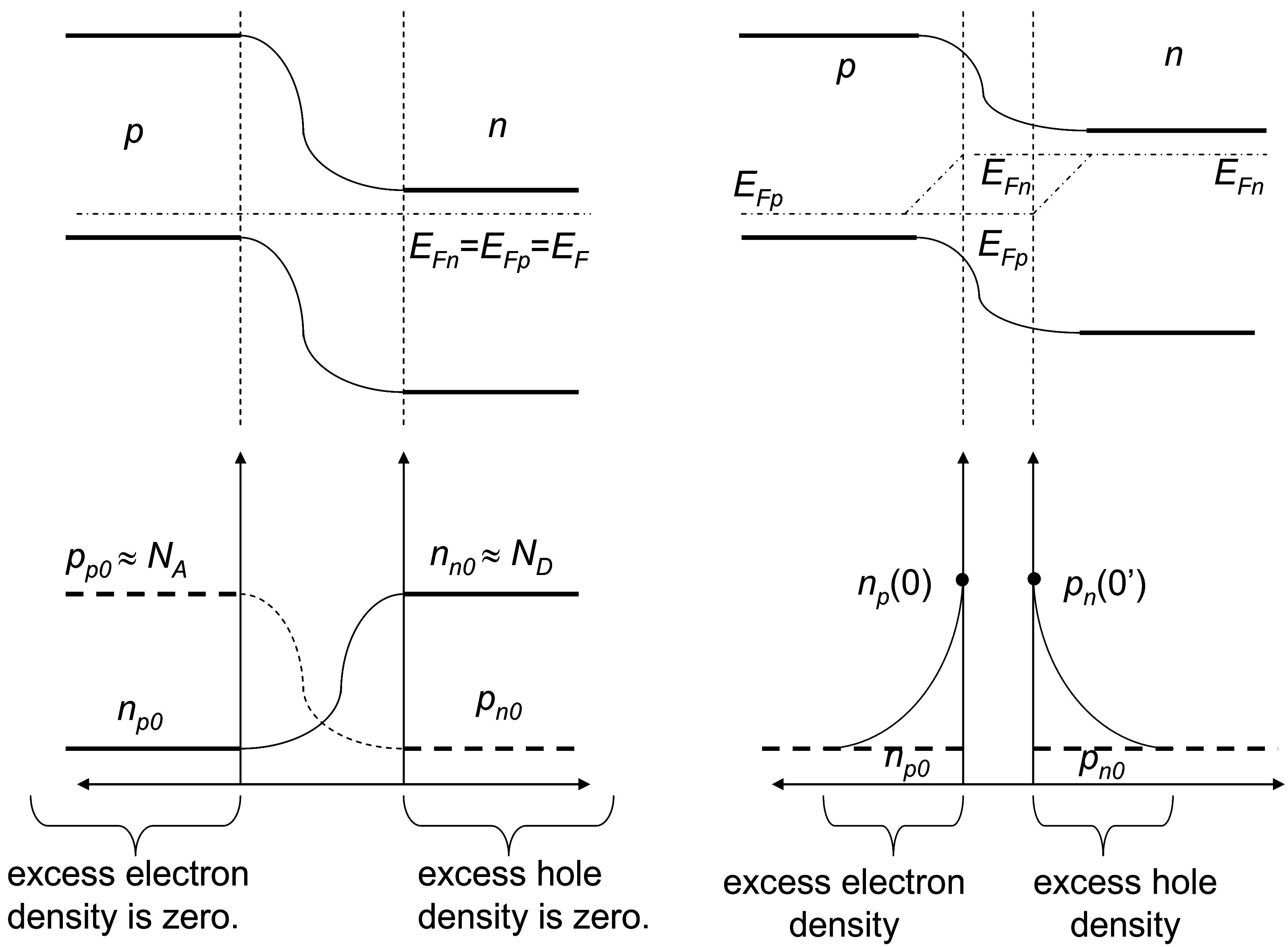
- The product

$$np = n_i^2 \exp\left(\frac{E_{Fn} - E_{Fp}}{k_B T}\right)$$

suggests that the difference E_{Fn} - E_{Fp} is a measure for the deviation from the equilibrium.

- However, this can not be correct distribution function since it is even in *k*, which means that it suggests that current can never flow in a device.
- The fact that makes it not so unreasonable is that average carrier velocities are usually much smaller than the spread in velocity

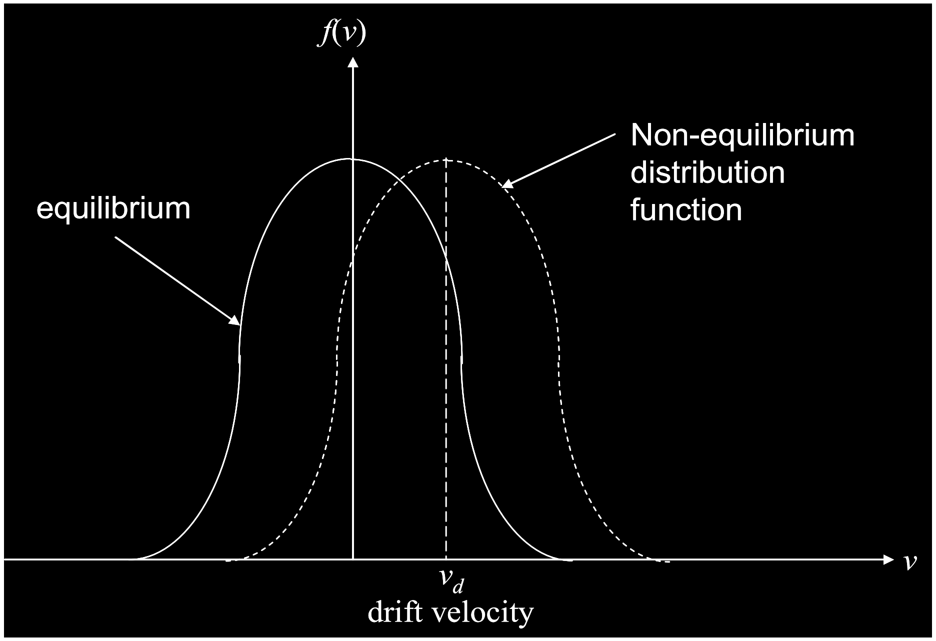
Quasi-Fermi Level Adjustment



(B) Displaced Maxwellian DF

A better guess for the distribution function $f(\mathbf{r},\mathbf{k},t)$ is to assume that the distribution function retains its shape, but that its average momentum is displaced from the origin. For example, particularly suitable form to use is

$$f(\mathbf{r},\mathbf{k},t) = \exp\left(\frac{E_{Fn} - E_{C0}}{k_B T}\right) \exp\left(-\frac{\hbar^2}{2m^* k_B T}\left|\mathbf{k} - \mathbf{k}_d\right|^2\right)$$



Displaced Maxwellian distribution function.

Drift and Thermal Energy

Using this form of the distribution function gives

$$n(\mathbf{r},t) = \frac{1}{V}\sum_{k} f(\mathbf{r},\mathbf{k},t) = N_C \exp\left(\frac{E_{Fn} - E_{C0}}{k_B T}\right)$$

In the same manner, one finds that the kinetic energy density per carrier is given by

$$u(\mathbf{r},t) = \frac{1}{2} m^* v_d^2 + \frac{3}{2} k_B T$$

The first term on the RHS represents the drift energy due to average drift velocity, and the second term is the well known thermal energy term due to collisions of carriers with phonons

2. Boltzmann Transport Equation

2.1 Derivation of the Boltzmann Transport Equation

Kinetic theory: We need to derive an equation for the single particle distribution function $f(\mathbf{v},\mathbf{r},t)$ (classical) which gives the probability of finding a particle with velocity between **v** and **v**+*d***v** and in the region **r** to **r**+*d***r**

- We assume that **v** and **r** are given simultaneously which neglects quantum mechanical nature of particles.
- $f(\mathbf{v},\mathbf{r},t)$ allows us to calculate ensemble averages over velocity and space (particle density, current density, energy density, etc.):

$$\langle A(t)\rangle = \int d\mathrm{r}\int d\mathrm{v}\, A(\mathrm{v},\mathrm{r},t) f(\mathrm{v},\mathrm{r},t)$$

- For this to give the proper average, *f* is normalized as follows:

$$\int d\mathrm{r} \int d\mathrm{v} f(\mathbf{v},\mathbf{r},t) = 1$$

- To derive an equation of motion for $f(\mathbf{v},\mathbf{r},t)$, it is somewhat easier to consider the particle density

$$n(\mathbf{v},\mathbf{r},t) = Nf(\mathbf{v},r,t)$$

where

$$N = \int d\mathrm{r} \int d\mathrm{v}\, n(\mathbf{v},\mathbf{r},t) = Total\ \#\ of\ \ particles$$

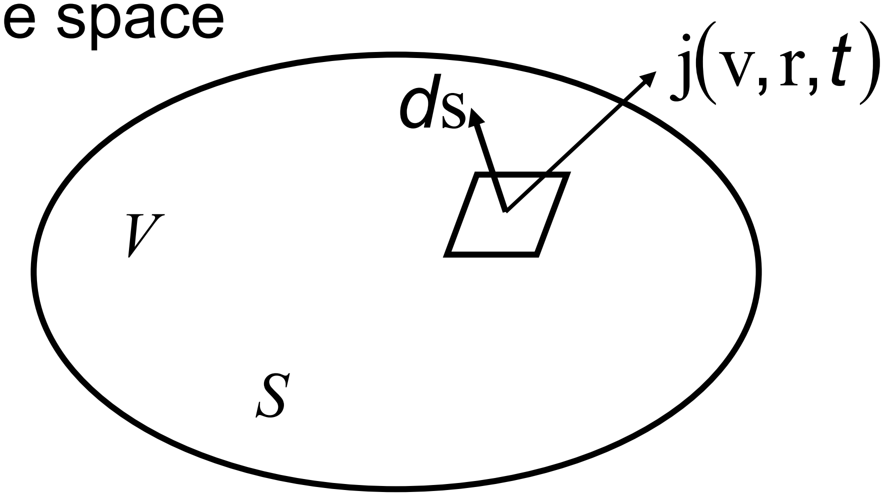
- The density $n(\mathbf{v},\mathbf{r},t)$ should satisfy a continuity equation in the 6D phase space defined by

$$x, y, z, v_x, v_y, v_z \rightarrow Independent\ variables$$

- Consider a hypervolume in phase space

j(**r**,**v**,*t*) is the flux density

j(**r**,**v**,*t*)•*d***s** is flux through hypersurface *d***s**



- Consider the particle balance through the hyper-volume *V*

$$\frac{\partial}{\partial t}\int_V d\mathrm{r}d\mathrm{v}\,n(\mathrm{v},\mathrm{r},t) = -\int_S \mathrm{j}(\mathrm{v},\mathrm{r},t)\cdot d\mathrm{s} + \int_V d\mathrm{r}d\mathrm{v}\left.\frac{\partial n}{\partial t}\right|_{Coll} +$$

Time rate of change of # particles in V

Leakage through *S*

Time rate of change due to collisions

$$+\int_V d\mathrm{r}d\mathrm{v}\{G(\mathrm{r},\mathrm{v},t) - R(\mathrm{r},\mathrm{v},t)\}$$

Time rate of change due to G-R mechanisms

- The flux density is written in terms of the time derivatives of the ‘position’ variables in 6D:

$$j\left(x,y,z,v_x,v_y,v_z\right)=v_x n(\mathrm{v},\mathrm{r},t)\hat{a}_x+v_y n\hat{a}_y+v_z n\hat{a}_z+$$

$$\frac{F_x}{m}n\hat{b}_{v_x}+\frac{F_y}{m}n\hat{b}_{v_y}+\frac{F_z}{m}n\hat{b}_{v_z}\ \textit{with}\ \dot{\mathrm{v}}=\frac{\mathrm{F}}{m}$$

- Applying the divergence theorem in 6D

$$\int_{\mathrm{S}}\mathrm{j}(\mathrm{v},\mathrm{r},t)\cdot d\mathrm{s}=\int_{V}d\mathrm{r}\,d\mathrm{v}\,\nabla\cdot\mathrm{j}(\mathrm{v},\mathrm{r},t)$$

where the divergence of **j** is

$$\nabla\cdot\mathrm{j}=v_x\frac{\partial n}{\partial x}+v_y\frac{\partial n}{\partial y}+v_z\frac{\partial n}{\partial z}+\frac{F_x}{m}\frac{\partial n}{\partial v_x}+\frac{F_y}{m}\frac{\partial n}{\partial v_y}+\frac{F_z}{m}\frac{\partial n}{\partial v_z}$$

which is written more compactly as:

$$\nabla \cdot \mathrm{j} = \mathrm{v} \cdot \nabla_r n + \frac{\mathrm{F}}{m} \nabla_v n$$

- Particle balance is therefore:

$$\int_V d\mathrm{r} d\mathrm{v} \left(\frac{\partial n}{\partial t} + \mathrm{v} \cdot \nabla_r n + \frac{\mathrm{F}}{m} \cdot \nabla_v n - \left.\frac{\partial n}{\partial t}\right|_{Coll} - \left.\frac{\partial n}{\partial t}\right|_{G-R} \right) = 0$$

Normalizing, we get the classical form of the Boltzmann transport equation:

$$\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t} = \underbrace{-\mathbf{v} \cdot \nabla_r f - \frac{\mathbf{F}}{m} \cdot \nabla_v f + \left.\frac{\partial f}{\partial t}\right|_{Coll}} + \left.\frac{\partial f}{\partial t}\right|_{G-R}$$

First two terms on the rhs are the streaming terms

- For Bloch electrons in a semiconductor, we could have considered a 6D space x, y, z, k_x, k_y, k_z where **k** is the wavevector and

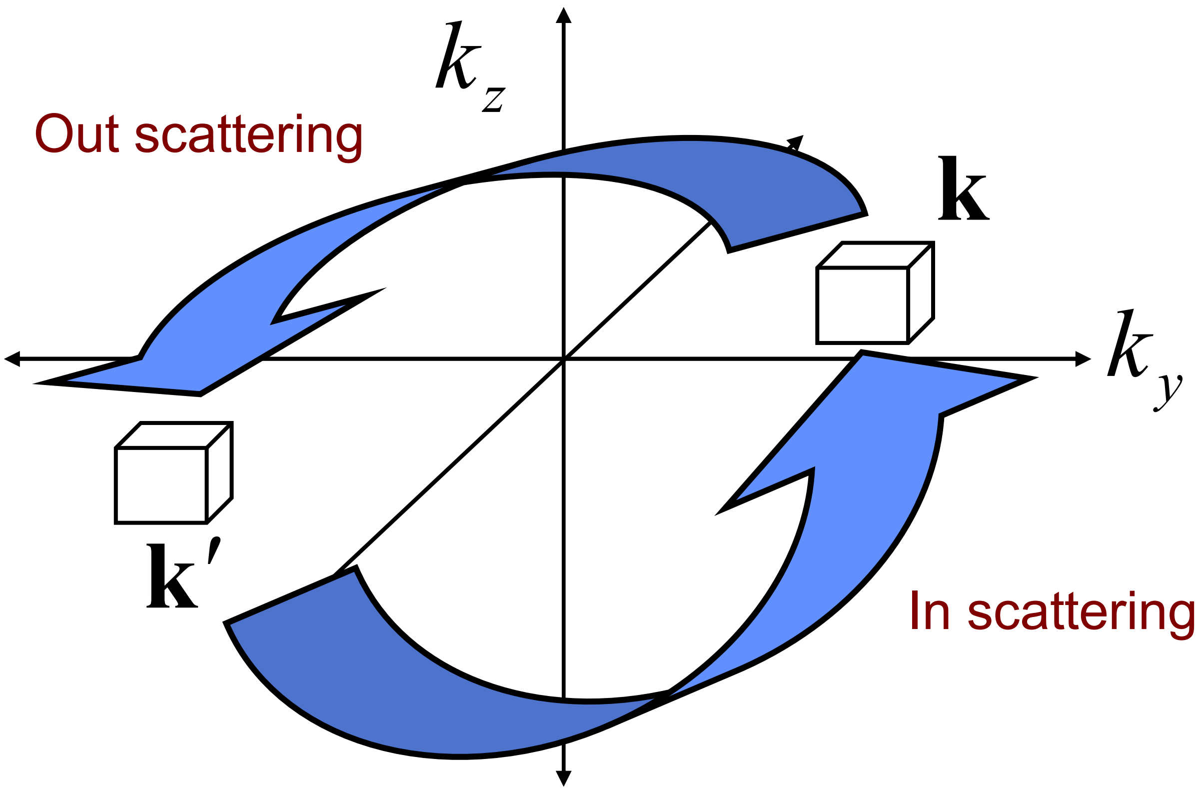
$$\mathrm{v} = \frac{1}{\hbar} \nabla_k E(\mathrm{k})$$

- The semi-classical BTE for transport of Bloch electrons is therefore

$$\frac{\partial f(\mathrm{r}, \mathrm{k}, t)}{\partial t} = -\frac{1}{\hbar} \nabla_k E(\mathrm{k}) \cdot \nabla_r f - \frac{\mathrm{F}}{\hbar} \cdot \nabla_k f + \left.\frac{\partial f}{\partial t}\right|_{Coll} + \left.\frac{\partial f}{\partial t}\right|_{G-R}$$

2.2 Collisional Integral

Assume instantaneous, single collisions which are independent of the driving force and take particles from **k** to **k**′ (out scattering) or from **k**′ to **k** (in scattering).



(A) Out Scattering

$$\Delta n(\mathrm{r},\mathrm{k},t) = -n(\mathrm{r},\mathrm{k},t)\Gamma_{\mathrm{kk}'}\Delta t$$

where $\Gamma_{\mathrm{kk}'}$ is the transition rate per particle from **k** to **k**′

Distribution function is: $f(\mathrm{r},\mathrm{k},t) = \dfrac{n(\mathrm{r},\mathrm{k},t)}{N}$

Take limit as $\Delta t \to 0$

$$\left.\frac{\partial f(\mathrm{r},\mathrm{k},t)}{\partial t}\right|_{OUT} = -f(\mathrm{r},\mathrm{k},t)\Gamma_{\mathrm{kk}'}\left[1 - f(\mathrm{r},\mathrm{k}',t)\right]$$

where the last term in brackets accounts for the Pauli exclusions principle (degeneracy of the final state after scattering).

(B) In Scattering

By an analogous argument, the rate of change of the distribution function due to in scattering is:

$$\left.\frac{\partial f(\mathrm{r},\mathrm{k},t)}{\partial t}\right|_{IN} = f(\mathrm{r},\mathrm{k}',t)\Gamma_{\mathrm{k}'\mathrm{k}}\left[1 - f(\mathrm{r},\mathrm{k},t)\right]$$

Total rate of change of *f* (**r**,**k**,*t*) around **k** is a sum over all possible initial and final states **k**′:

In scattering

$$\left.\frac{\partial f(\mathrm{r},\mathrm{k},t)}{\partial t}\right|_{Coll} = \sum_{\mathrm{k}'}\left\{f(\mathrm{r},\mathrm{k}',t)\left[1 - f(\mathrm{r},\mathrm{k},t)\right]\Gamma_{\mathrm{k}'\mathrm{k}} - \right.$$

$$\left. f(\mathrm{r},\mathrm{k},t)\left[1 - f(\mathrm{r},\mathrm{k}',t)\right]\Gamma_{\mathrm{k}\mathrm{k}'}\right\}$$

Out scattering

(C) Boltzmann Equation with Collision Integral

The sum over final states **k**′ may be converted to an integral due to the small volume of k-space associated with each state:

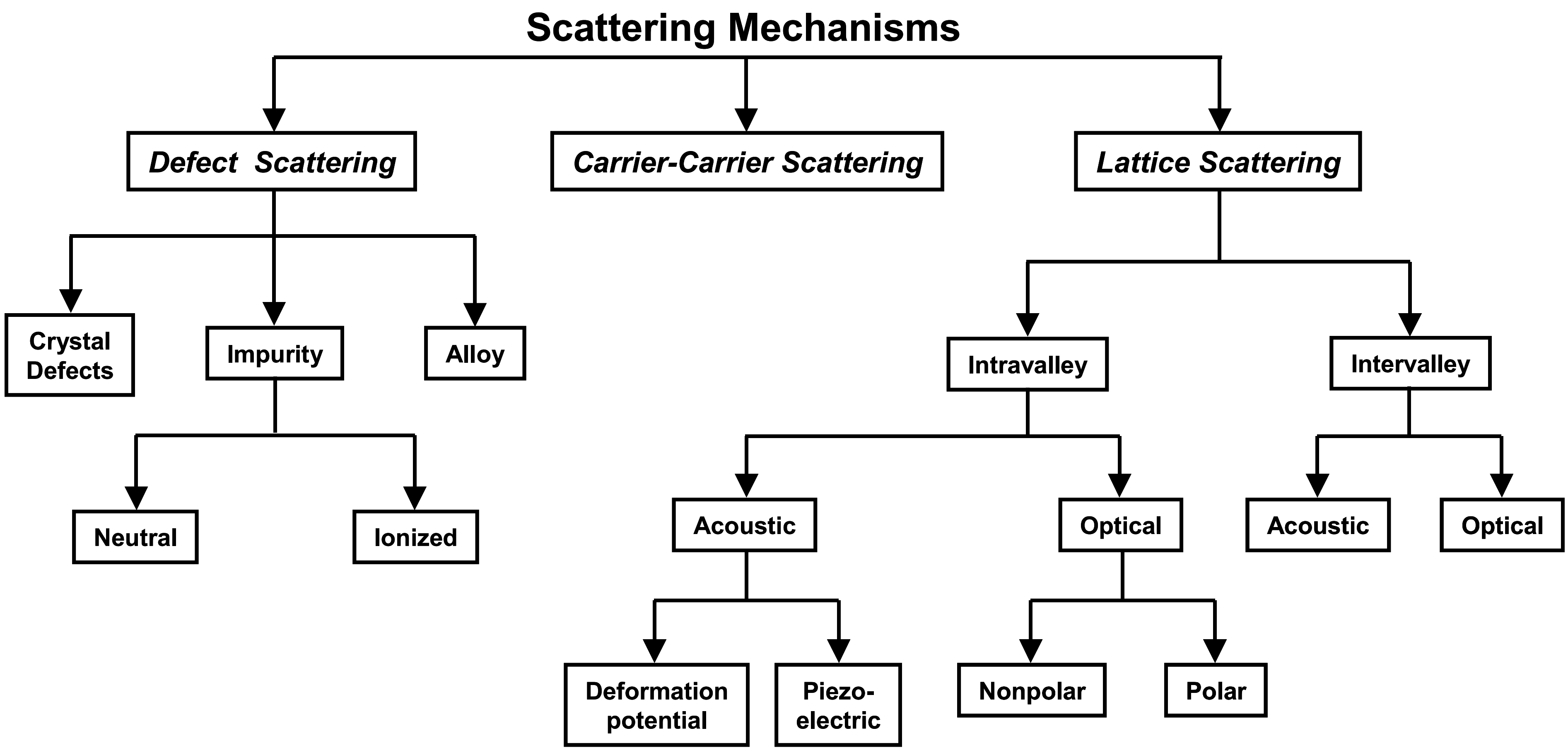
$$\sum_{k'} \rightarrow \frac{V}{8\pi^3}\int d\mathrm{k}'$$

The BTE becomes:

$$\frac{\partial f_k}{\partial t} + \frac{1}{\hbar}\nabla_k E \cdot \nabla_r f_k + \frac{\mathrm{F}}{\hbar}\nabla_k f_k =$$
$$\frac{V}{8\pi^3}\int d\mathrm{k}\left\{f_{k'}\left[1 - f_k\right]\Gamma_{\mathrm{k'k}} - f_k\left[1 - f_{k'}\right]\Gamma_{\mathrm{kk'}}\right\}$$

2.3 Scattering Theory

What contributes to $\Gamma_{kk'}$?



3. Time dependent perturbation theory

- Assume the Hamiltonian may be decomposed as $H=H_0+V_s$, where H_0 is the Hamiltonian of the perfect crystal (described by Bloch states), $V_s(\mathbf{r},t)$ is a small random potential. If $V_s \ll H_0$, then it is a good approximation to expand the solution (with random part) in terms of unperturbed eigenstates:

$$H_0\psi_k = E_k\psi_k \; ; \quad \psi_k^0(\mathrm{r},t) = \psi_k(\mathrm{r})e^{-iE_k t/\hbar}$$

- Expand actual solution in terms of these orthonormal functions:

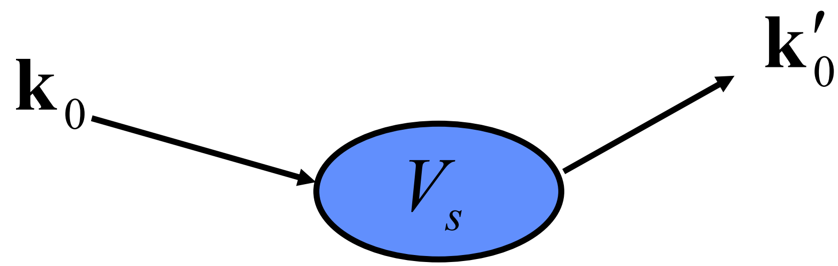
$$\psi(\mathrm{r},t) = \sum_k c_k(t)\psi_k(\mathrm{r})e^{-iE_k t/\hbar}$$

- If the initial wave packet is centered around $\mathbf{k}_o$, so that

$$c_{k_0}(t) \approx 1 \qquad c_{k \neq k_0}(t) \approx 0$$

- In the limit at $t \to \infty$, the probability of finding the particle in another state $\mathbf{k}_o'$ is

$$P_{k_0 k_0'} = \lim_{t \longrightarrow \infty} \left| c_{k_0'}(t) \right|^2$$



- Define the transition rate

$$\Gamma_{k_0 k_0'} = \lim_{t \longrightarrow \infty} \frac{\left| c_{k_0'}(t) \right|^2}{t}$$

- Solve for $c_{k_0'}$ using the S.E. and the previous expansion

$$\{H_0 + V_s\} \sum_k c_k(t) \psi_k(\mathrm{r}) e^{-iE_k t/\hbar} = i\hbar \frac{\partial}{\partial t} \sum_k c_k(t) \psi_k(\mathrm{r}) e^{-iE_k t/\hbar}$$

H_0 part cancels with phase factor on RHS

$$V_s \sum_k c_k(t) \psi_k(\mathrm{r}) e^{-iE_k t/\hbar} = i\hbar \sum_k \frac{\partial c_k(t)}{\partial t} \psi_k(\mathrm{r}) e^{-iE_k t/\hbar}$$

- Multiply both sides by $\psi_{k_0'}(\mathrm{r}) e^{-iE_{k_0'} t/\hbar}$ and integrate

$$i\hbar \frac{\partial c_{k_0'}(t)}{\partial t} = \sum_k c_k(t) \langle k_0' | V_s | k \rangle e^{-i\left(E_{k_0'} - E_k\right)t/\hbar}$$

where the *matrix element*, using Dirac notation, is defined as

$$\langle k_0' | V_s | k \rangle = \int d\mathrm{r} \psi_{k_0'}^{*} V_s(\mathrm{r}, t) \psi_{k'}$$

- Assume sufficiently weak scattering that $c_{ko} \approx 1$, and $\mathbf{c}_{k \neq ko} \approx 0$ for all time. The dominant term in the sum is:

$$i\hbar \frac{\partial c_{k_0'}(t)}{\partial t} = c_{k_0}(t) \langle k_0' | V_s | k_0 \rangle e^{-i\left(E_{k_0'} - E_{k_0}\right)t/\hbar}$$

which integrates to

$$c_{k_0'}(t) = \frac{1}{i\hbar} \int_0^t dt' \langle k_0' | V_s | k_0 \rangle e^{-i\left(E_{k_0'} - E_{k_0}\right)t'/\hbar} + c_{k_0'}(0)$$

- Suppose $V(\mathbf{r},t)$ may be Fourier decomposed, so that

$$V_s(\mathrm{r},t) = V_s(\mathrm{r}) e^{\mp i\omega t}$$

Note that this form of V(**r**,t) may correspond to interaction with lattice vibrations or with optical excitation.

- Then substituting

$$c_{k_0'}(t) = \frac{1}{i\hbar}\langle k_0' | V_s | k_0 \rangle \int_0^t dt' e^{-i\Lambda t'}; \quad \Lambda = \left(E_{k_0'} - E_{k_0} \mp \hbar\omega\right)/\hbar$$

and integrating this last expression leads to

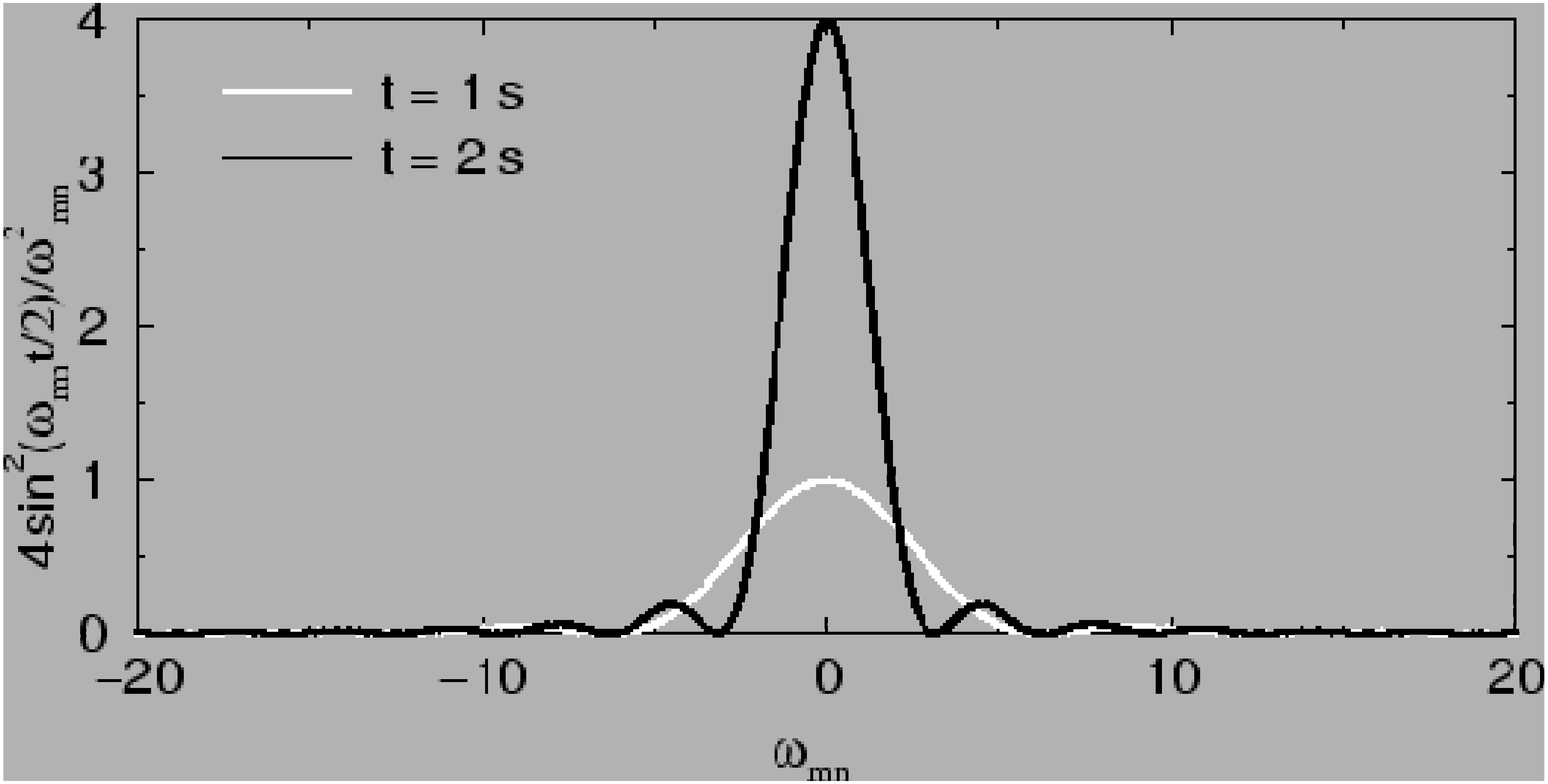
$$c_{k_0'}(t) = \frac{1}{i\hbar} V^{k_0 k_0'}{}_s \frac{e^{-i\Lambda t} - 1}{i\Lambda}$$

$$c_{k_0'}(t) = \frac{1}{i\hbar} V_s^{k_0 k_0'} e^{-i\Lambda t/2} \left(\frac{\sin(\Lambda t)}{\Lambda t}\right) t$$

- Since the probability of being in $\mathbf{k}_0'$ is given by

$$P_{k_0 k_0'} = \lim_{t \longrightarrow \infty} \left| c_{k_0'}(t) \right|^2$$

Long-Time Limit δ-Function



- Substituting for *c* and taking the magnitude squared gives

$$P_{k_0 k_0'} = \lim_{t \longrightarrow \infty} \frac{1}{\hbar^2} \left| V_s^{k_0 k_0'} \right|^2 \left(\frac{\sin(\Lambda t)}{\Lambda t} \right)^2 t^2$$

where asymptotically

$$\lim_{t \longrightarrow \infty} \left(\frac{\sin(\Lambda t)}{\Lambda t} \right)^2 = 2\pi\delta(\Lambda)/t = 2\pi\hbar\delta\left(E_{k_0'} - E_{k_0} \mp \hbar\omega\right)/t$$

This gives the famous **Fermi's Golden Rule** (droping 0s index)

$$\Gamma_{kk'} = \frac{P_{kk'}}{t} = \frac{2\pi}{\hbar} \left| V_s^{kk'} \right|^2 \delta(E_{k'} - E_k \mp \hbar\omega)$$

- Assumptions made:

(1) Long time between scattering (no multiple scattering events)
(2) Neglect contribution of other *c*'s (Collision broadening ignored)

Scattering Rate Calculations

Example: 1-D Scattering from Defect

$$U_s(z) = A_o \delta(z) \qquad (1-D)$$

$$H_{k'k} = U_{s,k-k'} = \frac{1}{L}\int_{\frac{-L}{2}}^{\frac{L}{2}} A_o \delta(z)\ \mathrm{e}^{-i(k'-k)z}\, dz$$

$$= \frac{A_o}{L}$$

$$\hbar\omega \to 0 \qquad S(k,k') = \frac{2\pi}{\hbar}\ \frac{A_o^2}{L^2}\ \delta\left(E(k') - E(k)\right)$$

- Sharply peaked potential scatters isotropically

$$indep.\ of\ \ q = k' - k$$

- Static potential scatters elastically

$$E(k') = E(k)$$