DENSITY OF STATES

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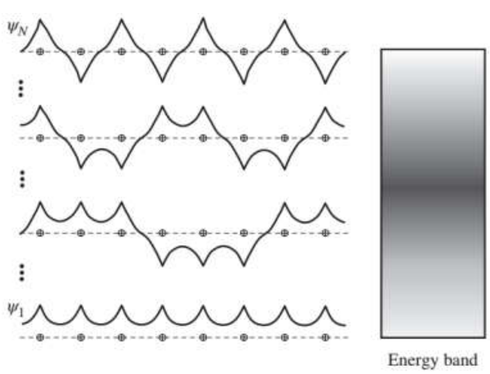
Density of States

- How many states per unit energy per unit volume?
- N atoms → N electron wavefunctions.

$$\psi_1 = \psi_A + \psi_B + \psi_C + \psi_D + \cdots$$

$$\psi_N = \psi_A - \psi_B + \psi_C - \psi_D + \cdots$$

- $g(E)$: Density of states
- $g(E)\, dE$ → number of states (*i.e.*, wavefunctions) in the energy interval E to $(E + dE)$ per unit volume of the sample.



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Density of States

- The number of states per unit volume up to some energy E'

$$S_v(E') = \int_0^{E'} g(E)\, dE$$

- The energy of an electron in a cubic *PE* well of size *L* is given by

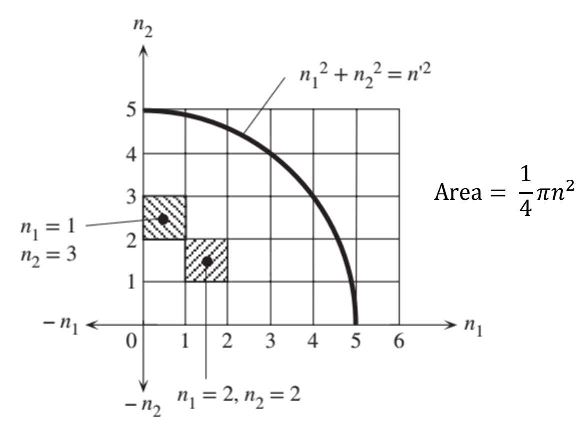
$$E = \frac{h^2}{8m_e L^2}(n_1^2 + n_2^2 + n_3^2) = n'^2$$

- The spatial dimension *L* of the well now refers to the size of the entire solid, as the electron is confined to be somewhere inside that solid. Thus, *L* is very large compared to atomic dimensions, which means that the separation between the energy levels is very small.

- Enumerate all possible choices of integers for n_1, n_2, and n_3 that satisfy $n_1^2 + n_2^2 + n_3^2 \leq n'^2$.

2D Material

- $n_1^2 + n_2^2 \leq n'^2$



3D Material

- $n_1^2 + n_2^2 + n_3^2 \leq n'^2$
- The number of orbital states $S_{\text{orb}}(n')$ within this volume is given by

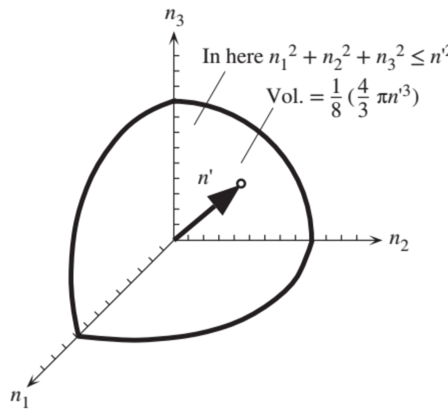
$$S_{\text{orb}}(n') = \frac{1}{8}\left(\frac{4}{3}\pi n'^3\right) = \frac{1}{6}\pi n'^3$$

- The number of states, including spin:

$$S(n') = 2S_{\text{orb}}(n') = \frac{1}{3}\pi n'^3$$

- Substitute n'^2:

$$E = \frac{h^2}{8m_e L^2} n'^2 \rightarrow n'^2 = \frac{8m_e L^2 E}{h^2}$$



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3D Material

- The number of states with $E \leq E'$:

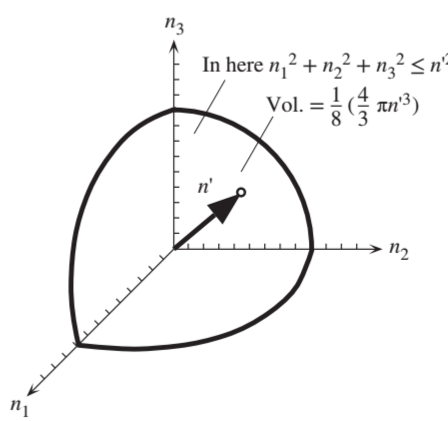
$$S(E') = \frac{\pi L^3 (8m_e E')^{3/2}}{3h^3}$$

- The number of states per unit volume:

$$S_v(E') = \frac{\pi (8m_e E')^{3/2}}{3h^3}$$

- Density of states per unit volume:

$$g(E) = \frac{S_v}{dE} = (8\sqrt{2}\pi)\left(\frac{m_e}{h^2}\right)^{3/2} E^{1/2}$$



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Carrier Statistics

- If E is the electron energy and $f(E)$ is the probability that a state with energy E is occupied, then

$$n = \int_{\text{Band}} f(E)g(E)\, dE$$

- **We need to know $f(E)$.**

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Boltzmann Probability Function

- If E is the electron energy and $f(E)$ is the probability that a state with energy E is occupied, then

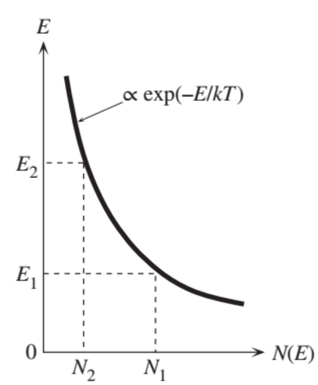
$$f(E) = A \exp\left(-\frac{E}{kT}\right)$$

- $f(E)$ decreases exponentially with energy.

- Any number of particles may have a given energy E. There is no restriction to permit only one particle per state at an energy E, as in the Pauli exclusion principle.

$$\frac{N_2}{N_1} = \exp\left(-\frac{E_2 - E_1}{kT}\right)$$

- If $E_2 \gg E_1$, then $N_2 \ll N_1$.



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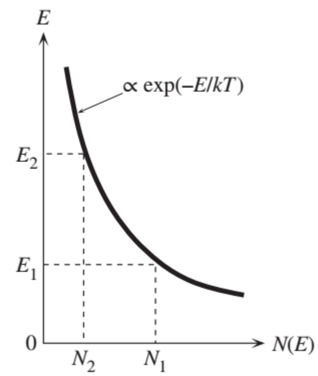
Boltzmann Probability Function

- Classical particles obey the Boltzmann statistics.
- If there are many more states than the number of particles, the likelihood of two particles having the same set of quantum numbers is negligible and we do not have to worry about the Pauli exclusion principle → We can use the Boltzmann statistics.
- **Example:** Electrons in the conduction band of a semiconductor, where usually there are many more states than electrons.



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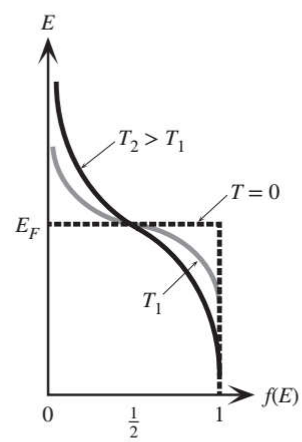
Fermi-Dirac Statistics

- If E is the electron energy and $f(E)$ is the probability that a state with energy E is occupied, then

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

- $E - E_F \gg kT$:

$$f(E) = \exp\left[-\frac{(E - E_F)}{kT}\right]$$



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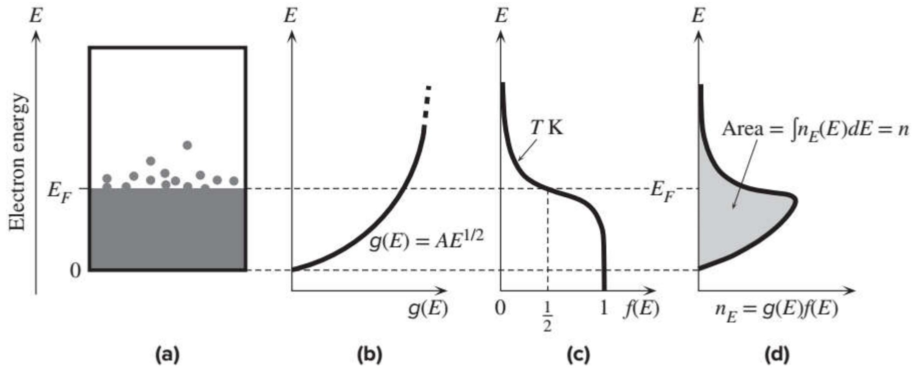
Carrier Density

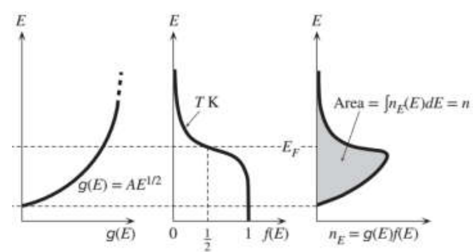
$$n_E = g(E)f(E)$$



Carrier Density

$n_E = g(E)f(E)$

- In the small energy range E to $(E + dE)$, there are $n_E\,dE$ electrons per unit volume.
- Total electrons in the band:



$$n = \int_0^{\text{Top of band}} n_E\,dE = \int_0^{\text{Top of band}} g(E)f(E)\,dE$$

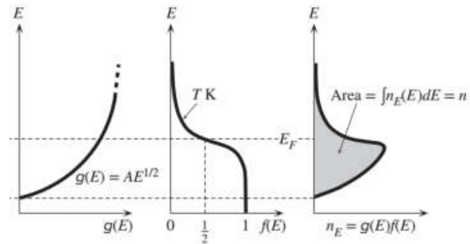
- $f \rightarrow 0$ when $E \gg E_F$

$$n = \frac{8\sqrt{2}\pi m_e^{3/2}}{h^3}\int_0^{\infty}\frac{E^{1/2}\,dE}{1+\exp\left(\frac{E-E_F}{kT}\right)}$$

Fermi Energy

- At $T = 0$ K

  $n_E = g(E)f(E)$



$$n = \frac{8\sqrt{2}\pi m_e^{3/2}}{h^3} \int_0^{E_{F0}} \frac{E^{1/2}\, dE}{1 + \exp\left(\frac{E - E_{F0}}{kT}\right)}$$

$$E_{F0} = \left(\frac{h^2}{8m_e}\right)\left(\frac{3n}{\pi}\right)^{2/3}$$

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