

Solutions to

Quick Questions to

2.1 Basic Band Theory

Solutions to quick questions to 2.1.1: Essentials of the Free Electron Gas

- What happens, if you do not choose $U = U_0 = 0$ but $U = U_1$?
- The Energy scale for the total energy E moves up or down by U_1 since $U_1 \cdot \psi$ can be added to $E \cdot \psi$.
- What does the [sentence](#) "...a plane wave with amplitude $(1/L)^{3/2}$ moving in the direction of the **wave vector \underline{k}** " mean? Wave vectors, after all, are defined in *reciprocal* space with a dimension **1/cm**. What, exactly, is their direction in *real* space?
- The velocity vector of a car in real space has the dimension **cm/s** - the dimension **1/cm** for wave vectors thus means nothing. The wave vector comes into being by writing the components of a plane wave as follows

$$\psi(x_i, t) = A \cdot \sin \cdot \left(\frac{2\pi x_i}{\lambda_i} - \omega \cdot t \right)$$

- With vectors we get

$$\psi(\underline{r}, t) = A \cdot \sin \cdot \left(\underline{r} \cdot \underline{k} - \omega \cdot t \right)$$

- This defines \underline{k} and by definition \underline{k} is a vector in real space, pointing in the direction of wave propagation.
- The better question is: If we know \underline{k} in reciprocal space (= Fourier transform of the real space), how can we conclude on the direction in real space? The answer is. Reciprocal lattice vectors with components $\underline{k}_{h,k,l}$ are perpendicular to the lattice plane in real space with Miller indices (hkl) - the direction in real space is thus given
- Recount what you know about the *spin* of an electron.
 - 1. Everything contained in this ["basic" module](#).
 - 2. Everything contained in [this module](#) describing the relation of spin and magnetic moment.
 - 3. The catchword "[Spintronics](#)" should also come up in this context.
- Where does the $(1/L)^{3/2}$ in the solution come from? What would one expect for a crystal with the dimension L_x, L_y, L_z ?
- From the normalizing condition. The factor should change from $(1/L)^{3/2} = (1/L^3)^{1/2}$ to $(1/V^3)^{1/2}$.
- What kind of information is contained in the wave vector \underline{k} ?
 - 1. "Number" of solution or state.
 - 2. Wave length $\lambda = 2\pi / |\underline{k}|$
 - 3. Momentum $\underline{p} = \hbar \underline{k}$
 - 4. Total energy E via dispersion relation (for free electron gas $E \propto k^2$)
 - 5. Propagation direction of plane wave with \underline{k}
- Consider a system with some given energy levels (including possibly energy continua). Distribute a number N of classical particles, of Fermions and of Bosons on these levels. Describe the basic principles.
- Fermions = Fermi-Dirac distribution
Bosons = Bose-Einstein distribution (which we don't know so far)
Classical = Boltzmann distribution and an approximation to the two fundamental ones
- Do it! Check the [link](#) for details to the Boltzmann distribution.

Fermi-Dirac distribution	Bose- Einstein distribution	Boltzmann distribution
$f(E, T) = \frac{1}{\exp\left(\frac{E - E_F}{kT}\right) + 1}$	$f(E, T) = \frac{1}{\exp\left(\frac{E - E_F}{kT}\right) - 1}$	$f(E, T) = \exp\left(-\frac{E}{kT}\right)$

How does one always derive the density of states $D(E)$?

Volume of "onion skin" in phase space.

Compare the free electron model with and without diffraction.

	Free elektron gas	Free elektron gas with diffraction
Potential $V(x, y, z)$	$V = \text{const} = 0$	$V_x = V_0 \cdot \cos(2\pi x/a_1)$ $V_y = V_0 \cdot \cos(2\pi y/a_2)$ $V_z = V_0 \cdot \cos(2\pi z/a_3)$ $V_0 \rightarrow 0$
Wavefunktion $\psi(x, y, z)$	$\psi = \left(\frac{1}{L}\right)^{3/2} \cdot e^{i\mathbf{k}\mathbf{r}}$	$\psi = \left(\frac{1}{L}\right)^{3/2} \cdot e^{i\mathbf{k}\mathbf{r}}$ <i>except</i> for wavevectors \mathbf{k}_B that are being diffracted.
Wave vectors \mathbf{k}	$k_x = \pm n_x \cdot 2\pi / L$ $k_y = \pm n_y \cdot 2\pi / L$ $k_z = \pm n_z \cdot 2\pi / L$ $n_i = 0, \pm 1, \pm 2, \dots$	$k_x = \pm n_x \cdot 2\pi / L$ $k_y = \pm n_y \cdot 2\pi / L$ $k_z = \pm n_z \cdot 2\pi / L$ $n_i = 0, \pm 1, \pm 2, \dots$
Energy E	Total energy = const = E_{kin}	Total energy = const = E_{kin} <i>except</i> for wavevectors \mathbf{k}_B that are being diffracted; then some potential energy comes into play.
Dispersion function $E(\mathbf{k})$	$E = \frac{\hbar^2 k^2}{2m}$	$E = \frac{\hbar^2 k^2}{2m}$ <i>except</i> for wavevectors \mathbf{k}_B that are being diffracted.
Density of states $D(E)$		

<p>Density of states $D(E)$</p>	$D(E) = \frac{(2m_e)^{3/2}}{2\hbar^3\pi^2} E^{1/2}$	$D(E) = \frac{(2m_e)^{3/2}}{2\hbar^3\pi^2} E^{1/2}$ <p>as a first approximation., Could be rather different, however.</p>
<p>Probability of state being occupied $f(E, T)$</p>	$f(E, T) = \frac{1}{\exp\left(\frac{E_i - E_F}{kT}\right) + 1}$	$f(E, T) = \frac{1}{\exp\left(\frac{E_i - E_F}{kT}\right) + 1}$
<p>the Fermi distributoin <i>always</i> obtains!</p>		