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 bout 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 woth 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 $\lambda = 2\lambda\ /|\underline{k}|$
  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 pf 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 priciples.
- 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
$f(E, T) = \dfrac{1}{\exp\left(\dfrac{E - E_F}{kT}\right) + 1}$	$f(E, T) = \dfrac{1}{\exp\left(\dfrac{E - E_F}{kT}\right) - 1}$	$f(E, T) = \exp-\left(\dfrac{E}{kT}\right)$

- How does on always derive the density of states ***D*** **(*E*)** ?
- Volume of "onion skin" in phase space.
-
-

-
- Compare the free electron model with and withour diffraction.
-

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

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