FYS3410 - Module III

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2. Born-von Karman boundary conditions

Introduce periodic (Born-von Karman) boundary conditions and derive the density of states (DOS) for FEFG in a finite 3D sample. Calculate values of ε_F, k_F, v_F and T_F, i.e. Fermi energy, wavevector, velocity and temperature, respectively, for alkali metals. Explain the trend.

A FEFG in 3D can at first approximation be described by the free particle Schrödinger equation in three dimensions

$$-\frac{\hbar^2}{2m}\nabla^2\boldsymbol{\psi}_{\boldsymbol{k}}(r) = \boldsymbol{\epsilon}_{\boldsymbol{k}}\boldsymbol{\psi}_{\boldsymbol{k}}(\boldsymbol{r}) \tag{1}$$

Confining the electrons to a cube whose sides have length L we get the following solution for the wavefunctions

$$\boldsymbol{\psi}_n(\boldsymbol{r}) = A\sin(\pi n_x x/L)\sin(\pi n_y y/L)\sin(\pi n_z z/L), \quad n_x, n_y, n_z \in \mathbb{Z} \tag{2}$$

Next we want to apply Born-von Karman boundary conditions. The Born-von Karman boundary condition can be represented mathematically as certain restrictions on the wavefunction in a crystal under the assumption that the wavefunction is periodic. The condition can be stated as

$$\boldsymbol{\psi}(x+L, y, z) = \boldsymbol{\psi}(x, y, z) \tag{3}$$

For the x-direction and similarly for y and z.

This is a classical particle in box problem that we know from quantum mechanics. The boundary conditions gives us the familiar solution of

$$\boldsymbol{\psi}_{\boldsymbol{k}}(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tag{4}$$

With the special requirement that the wavevectors are on the form

$$\boldsymbol{k}_x = \frac{2n_x\pi}{L}$$

It is easily shown that this satisfies equation (3)

$$\begin{aligned}
\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) &= \exp(i\boldsymbol{k}\cdot(\boldsymbol{r}+L\boldsymbol{e}_x)) \\
\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) &= \exp(i\boldsymbol{k}\cdot\boldsymbol{r})\cdot\exp(iL\boldsymbol{k}_x) \\
\exp(iL\boldsymbol{k}_x) &= 1 \implies Lk_x = 2n_x\pi
\end{aligned}$$

Substituting equation (4) into (1) we get an expression for the energies related to each wavevector

$$2 \tag{5}$$

3. Temperature dependence of energy and chemical potential for the Fermi-Dirac distribution

4. DOS in 1D & 2D FEFG

6. k-space considerations of some cubic lattices