Problem 2: Free-electron Fermi surface

In this exercise we plot the free-electron Fermi surface. The free-electron Fermi surface of a system with N electrons per cell is a sphere with a volume equal to $N/2$ the volume of the Brillouin zone. The parts of the Fermi surface outside the Brillouin zone are refolded inside so that the shape of the Fermi surface depends on the Bravais lattice. We consider the face centered cubic lattice (fcc) and the body centered cubic lattice (bcc) with one atom per cell. The atom has from 1 up to 4 valence electrons.

In this exercise we want to plot the Fermi surface on a plane in reciprocal space as contours that represent the intersection of the Fermi surface with the plane. After the computation of the free-electron bands $\varepsilon_n(\mathbf{k})$ for a two dimensional mesh of $\mathbf{k}$ points on the plane we use a graphical program (such as `gnuplot`) to identify the contours $\varepsilon_n(\mathbf{k}) = \varepsilon_F$ (ε_F is the Fermi level).

1. Determine the value of the Fermi energy for a system with 1, 2, 3, or 4 electrons per cell with the fcc or the bcc lattice. Write it in units of $\left(\frac{2\pi}{a}\right)^2$ where a is the edge of the conventional cubic cell.

2. Modify the code that plots the free-electron bands to read three vectors $\mathbf{k}_0$, $\mathbf{v}_1$, $\mathbf{v}_2$ that define the plane $\mathbf{k} = \mathbf{k}_0 + \alpha\mathbf{v}_1 + \beta\mathbf{v}_2$ with $0 \leq \alpha \leq 1$, $0 \leq \beta \leq 1$. Moreover the input must read two integers N_1 and N_2, the number of points along $\mathbf{v}_1$ and $\mathbf{v}_2$ respectively.

3. Generate the two dimensional mesh $\mathbf{k}_{n_1,n_2} = \mathbf{k}_0 + \frac{n_1-1}{N_1-1}\mathbf{v}_1 + \frac{n_2-1}{N_2-1}\mathbf{v}_2$. Compute the bands $\varepsilon_n(\mathbf{k})$ on this grid and write them on output files: one band per file. For the fcc lattice you can consider the plane $k_z = 0$ and a size sufficient to contain the Brillouin zone, the plane $k_z = 1$ parallel to the first, and a third plane with $\mathbf{k}_0 = (0,0,0)$, $\mathbf{v}_1 = (1,1,0)$, $\mathbf{v}_2 = (0,0,1)$ in units $\frac{2\pi}{a}$. For the bcc lattice consider the plane $k_z = 0$ and a size sufficient to contain the Brillouin zone, and a plane with $\mathbf{k}_0 = (0,0,0)$, $\mathbf{v}_1 = (1/2,1/2,0)$, $\mathbf{v}_2 = (0,0,1)$ in units $\frac{2\pi}{a}$.

4. Plot the contours of the Fermi surface on these planes. For each lattice show separately the contours of the Fermi surface for 1, 2, 3, and 4 valence electrons.

5. Compare your results with the figures reported in: Phys. Rev. **118**, 1190 (1960) and Ashcroft and Mermin, Solid State Physics (Chap. 9). Describe the main features of the free-electron Fermi surfaces in the fcc and bcc lattices.

In real solids, the Fermi energy must be determined numerically. Having the bands $\varepsilon_n(\mathbf{k})$ in a uniform three dimensional mesh of $\mathbf{k}$ points, such as the one used to plot the density of states, we can use the following relationship (valid at zero temperature):

$$f(\varepsilon_F) = \frac{2}{N_{\mathbf{k}}} \sum_{\mathbf{k},n} \theta(\varepsilon_F - \varepsilon_{\mathbf{k},n}) - N = 0 \tag{1}$$

where N is the number of electrons per cell, $N_{\mathbf{k}}$ is the total number of $\mathbf{k}$ points and $\theta(x)$ is the step function: $\theta(x) = 1$ if $x > 0$, $\theta(x) = 0$ if $x < 0$. The factor two accounts for spin degeneracy. ε_F can be determined searching the zero of $f(\varepsilon_F)$. You can use the bisection method or another method of your choice to find the zero of a function. The bisection method is described in Wikipedia, or in many numerical methods books. See for instance: Press, Teukolsky, Vetterling, and Flannery, Numerical Recipes.

6. Modify the free-electron code that computes the density of states and add a routine that computes the Fermi level. Compute the Fermi level of an fcc lattice with 3 electrons per cell and compare with the analytic result.

7. Study the convergence of the calculated Fermi level as a function of the size of the $\mathbf{k}$-point mesh. Start by implementing the function $\theta(x)$ with a step function and compare with the results that you obtain by approximating $\theta(x)$ as $\tilde{\theta}(x) = \int_{-\infty}^{x} \tilde{\delta}(y)dy$ where $\tilde{\delta}(x)$ is the Gaussian introduced to calculate the density of states. Study the convergence of the Fermi energy with the value of the smearing σ and of the $\mathbf{k}$-point mesh size. (Note that the integral of a Gaussian can be computed with the help of the `erf` function provided by some `fortran` compilers — such as `gcc` — or easily found on the web.

8. Calculate the Fermi level of an fcc and of a bcc lattice with 1, 2, 3, or 4 electrons and compare with the exact result.