Silicon electron density of states

Given the band structure of a solid, $\varepsilon_v(\mathbf{k})$, the electron density of states per unit volume is given by:

$$g(\varepsilon) = 2\sum_v \int \frac{d^3k}{(2\pi)^3}\delta(\varepsilon - \varepsilon_v(\mathbf{k})),$$

where the integral is over the first Brillouin zone and the factor 2 accounts for spin degeneracy. In this exercise, we calculate numerically $g(\varepsilon)$ for crystalline silicon discretizing the integral with a uniform mesh of $\mathbf{k}$ points and approximating $\delta(x)$ with a Gaussian function that depends on a parameter σ: $\tilde{\delta}(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{x^2}{2\sigma^2}}$.

1. Modify the program that calculates the band structure of crystalline silicon with empirical pseudopotentials to read in input three integer numbers N_1, N_2 and N_3 and compute all the points $\mathbf{k}$ in a uniform mesh of $N = N_1 \times N_2 \times N_3$ points:

   $$\mathbf{k}_{n_1,n_2,n_3} = \frac{(n_1-1)}{N_1}\mathbf{b}_1 + \frac{(n_2-1)}{N_2}\mathbf{b}_2 + \frac{(n_3-1)}{N_3}\mathbf{b}_3,$$

   where $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ are the primitive vectors of the reciprocal lattice, and n_i are integers with $1 \leq n_i \leq N_i$.

2. Compute the energy bands of silicon in each point $\mathbf{k}_{n_1,n_2,n_3}$ of the mesh given at point 1.

3. After computing the bands for a $\mathbf{k}$ point, accumulate in the sum

   $$\tilde{g}(\varepsilon,\sigma) = \frac{2}{N\Omega}\sum_{n_1,n_2,n_3}\sum_v \tilde{\delta}(\varepsilon - \varepsilon_v(\mathbf{k}_{n_1,n_2,n_3}))$$

   the contribution of this $\mathbf{k}$ point to the function $\tilde{g}(\varepsilon,\sigma)$. Calculate the function $\tilde{g}(\varepsilon,\sigma)$ in a uniform mesh of energy values. Consider an energy interval sufficient to include all the occupied bands an a few empty bands. The number of energy points, the minimum and the maximum energy, and the parameter σ are input parameters. Note that σ must be given in the same units used for the energy.

4. After the loop over the **k** points, write in a file the energy values and the values of the function $\tilde{g}(\varepsilon, \sigma)$. Plot the function $\tilde{g}(\varepsilon, \sigma)$ and study its dependence on σ and on the mesh size N. Consider only the case $N_1 = N_2 = N_3$.

5. Compare $\lim_{\substack{\sigma \to 0 \\ N \to \infty}} \tilde{g}(\varepsilon, \sigma)$ with the theoretical free electron density of states per unit volume that in states/(Hartree $\times$ (a.u.)^3) is equal to $g(\varepsilon) = \frac{1}{\pi^2}\sqrt{2\varepsilon}$ for $\varepsilon > 0$ (in this expression ε is in Hartree unit).