Übungen zur Computational Nanoscience
– Blatt 7 –
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Aufgabe 1) Tight-Binding Model

Calculate a tight-binding energy spectrum for the 2-dimensional cubic lattice with nearest-neighbor hopping $t_1$ and next-nearest hopping $t_2$ as well as for the triangular lattice with nearest-neighbor hopping $t$. Is there is some special case where these two band structures can be similar?

Aufgabe 2) Density of States

Find the density of states (DOS) for the 1-dimensional tight-binding model with nearest-neighbor hopping $t$.

Aufgabe 3) Wannier orbitals

Proof that the Wannier orbitals are orthogonal for different bands ($n$) and different lattice sites $\vec{R}$:

$$W_n(\vec{r} - \vec{R}) = \frac{1}{N_k} \sum_k e^{-i\vec{k}\cdot\vec{R}} \psi_{kn}(\vec{r})$$

where the $\psi_{kn}(\vec{r})$ are the solution of effective Schrödinger equation in crystal.