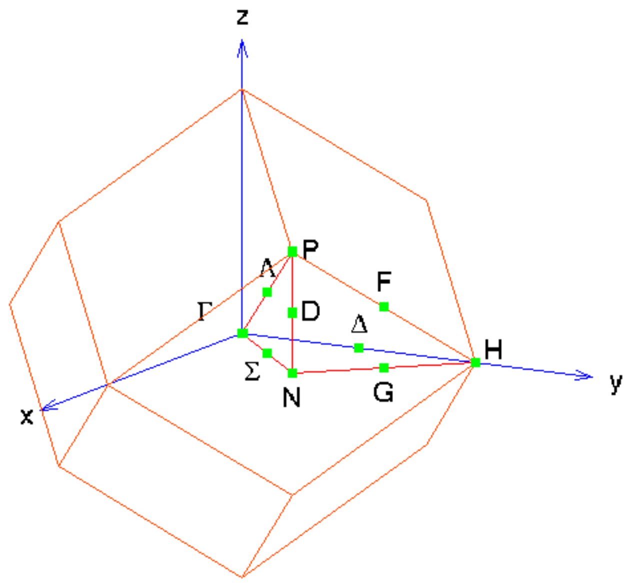
Problem 4: Band structure of Na **(5 points)**

Sodium crystallizes in a bcc structure with a lattice constant of $a = 4{,}23$ Å. The effective potential in the solid is given by a sum of atomic potentials that are represented by Gaussian functions:

$$V(\vec{r}) = V_0 \left(\left(\frac{\pi}{\gamma}\right)^{\frac{3}{2}} \frac{1}{\Omega_0} - \sum_l e^{-\gamma (\vec{r} - \vec{R}_l)^2} \right) .$$

Ω_0 is the volume of the unit cell. The sum of the lattice vectors runs over the whole space.

Use an expansion of the wave function into plane waves in order to calculate the band structure of the crystal along the high symmetry lines Λ, Σ and D (see figure) from $P(\vec{k} = \frac{\pi}{a}(1, 1, 1))$ over $\Gamma(\vec{k} = (0, 0, 0))$ to $N(\vec{k} = \frac{\pi}{a}(0, 1, 1))$ and back to P.



a) Give the reciprocal lattice vectors $\vec{b}_j$ of the bcc crystal.

b) Use two plane waves with $\vec{G}_1 = (0, 0, 0)$ and $\vec{G}_2 = \frac{2\pi}{a}(0, -1, -1)$ to calculate the band structure. Write down the resulting Hamilton matrix. First, plot the bands for $V_0 = 0$. Secondly, plot the band for $V_0 = 30$ eV and $\gamma = 0{,}2 \frac{1}{Å^2}$. How large is the splitting ΔE of the bands at the N point?

c) *Optional*: If you are interested in a more accurate calculation of the band structure, you should use all vectors with $|G_j| \le \frac{2\pi}{a}\sqrt{2}$ for the representation of the wave function. Diagonalize the corresponding Hamilton matrix and plot the respective band structure.

Hints:

$$\int_{\mathbb{R}^3} e^{-\gamma r^2} e^{i \vec{G} \vec{r}} d^3 r = \left(\frac{\hbar}{\gamma}\right)^{\frac{3}{2}} e^{-\frac{|\vec{G}|^2}{4\gamma}}$$

$$\frac{\hbar^2}{2m} = 3{,}80998 \text{ eV} \cdot Å^2$$

Problem 5: **ETBM band structure of sodium** **(2 points)**

Calculate the band structure of sodium within the framework of the empirical tight-binding method employing one s-like orbital per atom. Consider only the interactions between nearest neighbors. Determine the parameters E_s and V_{ss} in such way that the energies of the lowest band are

$$E\,(\Gamma) \,=\, 0 \text{ eV} \qquad \text{and} \qquad E\,(P) \,=\, 5.7 \text{ eV} \;.$$

(These values result from the calculation with 13 plane waves in problem 4.) Plot $E_{\vec{k}}$ along the high-symmetry lines Λ, Σ and D (see problem 4). Compare this band structure with the results of problem 4.

Problem 6: **Momentum of a Bloch electron** **(3 points)**

The solutions of the Schrödinger equation

$$\hat{H}\,\psi_{n,\vec{k}}\,(\vec{r}\,) \,=\, E_{n,\vec{k}}\,\psi_{n,\vec{k}}\,(\vec{r}\,)$$

with

$$\hat{H} \,=\, \frac{\hat{\vec{p}}^{\,2}}{2\,m} \,+\, V\,(\vec{r}\,) \qquad \text{and} \qquad V\,(\vec{r}\,) \,=\, V\,(\vec{r} \,+\, \vec{R})$$

can be represented by

$$\psi_{n,\vec{k}}\,(\vec{r}\,) \,=\, \mathrm{e}^{i\,\vec{k}\,\vec{r}}\,u_{n,\vec{k}}\,(\vec{r}\,)$$

with the lattice-periodic function $u_{n,\vec{k}}\,(\vec{r}\,)$.

a) Show that

$$\hat{\vec{p}}\,\psi_{n,\vec{k}}\,(\vec{r}\,) \,=\, \mathrm{e}^{i\,\vec{k}\,\vec{r}}\,\left(\hbar\,\vec{k} \,+\, \hat{\vec{p}}\right)\,u_{n,\vec{k}}\,(\vec{r}\,)$$

and that $u_{n,\vec{k}}\,(\vec{r}\,)$ solves the eigenvalue problem

$$\hat{\tilde{H}}\,(\vec{k})\,u_{n,\vec{k}}\,(\vec{r}\,) \,=\, E_{n,\vec{k}}\,u_{n,\vec{k}}\,(\vec{r}\,)$$

with

$$\hat{\tilde{H}}\,(\vec{k}) \,=\, \frac{1}{2\,m}\,\left(\hbar\,\vec{k} \,+\, \hat{\vec{p}}\right)^2 \,+\, V\,(\vec{r}\,) \;.$$

b) Show that $\hat{\tilde{H}}\,(\vec{k})$ can be written as

$$\hat{\tilde{H}}\,(\vec{k}) \,=\, \mathrm{e}^{-i\,\vec{k}\,\vec{r}}\,\hat{H}\,(\vec{r}\,)\,\mathrm{e}^{i\,\vec{k}\,\vec{r}} \;.$$

Hint: consider the action of $\hat{\tilde{H}}\,(\vec{k})$ on a function $f\,(\vec{r}\,)$.

c) Represent the expectation value of the momentum operator

$$\langle\hat{\vec{p}}\rangle \,=\, \int\limits_{\Omega} \psi^{*}_{n,\vec{k}}\,(\vec{r}\,)\,\hat{\vec{p}}\,\psi_{n,\vec{k}}\,(\vec{r}\,)\,d^3\,r$$

by an integral over $u^{*}_{n,\vec{k}}\,(\vec{r}\,)$ and $u_{n,\vec{k}}\,(\vec{r}\,)$.