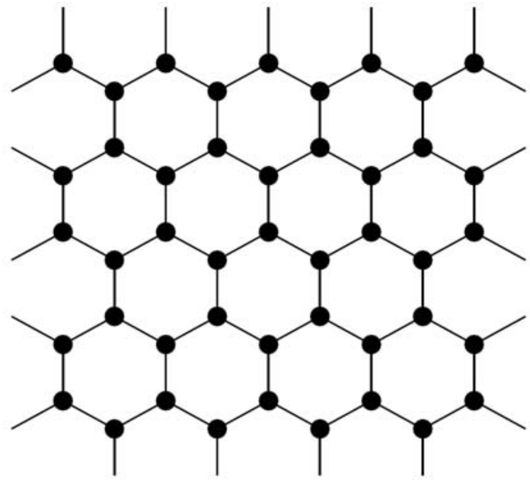
Problem 12: **Band structure of graphene** **(4 points)**

Graphene consists of a layer of carbon atoms that are arranged in a hexagonal structure. The lattice vectors are given by $\vec{a}_1 = (1, 0)\, a$ and $\vec{a}_2 = (-1, \sqrt{3})\, \frac{a}{2}$.



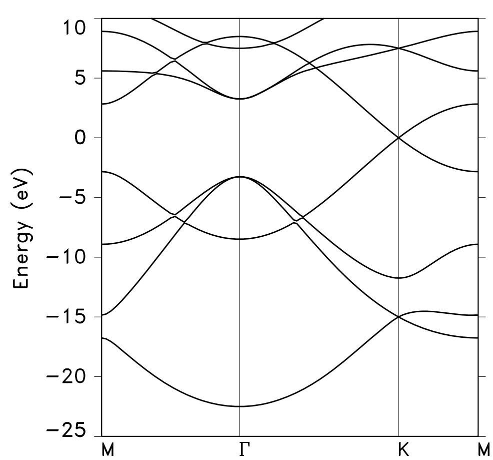
a) Give the primitive vectors $\vec{b}_1$ and $\vec{b}_2$ of the reciprocal lattice and construct the first Brillouin zone.

b) Use the empirical tight-binding method with one p_z orbital per atom to calculate the band structure $E_n\,(k_x,\, k_y)$ of graphen. The hopping term t only acts between nearest neighbours.

c) Plot the band structure for $E_0 = 0$ eV and $t = -2.828$ eV along the high-symmetry lines from Γ to K and from K to M.

$$K: \quad \left(\frac{2}{3},\, 0\right) \frac{2\,\pi}{a}, \qquad M: \quad \left(\frac{1}{2},\, \frac{-1}{2\sqrt{3}}\right) \frac{2\,\pi}{a}.$$

d) The figure shows the band structure of graphen resulting from a calculation with s, p_x, p_y and p_z orbitals. Compare your result with this band structure.



e) Show that in the vicinity of K, i. e. for $\vec{k} = K + \vec{q}$ (with small $\vec{q}$), the tight-binding method yields isotropic bands with linear dispersion $E_\pm\,(\vec{k}) \approx \pm v \cdot |\vec{q}|$ („Dirac cones of graphene“).

Problem 13: Density of states for a linear chain (2 points)

The band structure of a linear chain with one s-like orbital per atom is given within the framework of the empirical tight-binding method by $E_k = E_0 + 2t\cos(k\,a)$. Calculate the density of states $N(E) = \sum_k \delta(E - E_k)$ of the chain. *Hint*: Substitute the sum by an integral.

Problem 14: Homogeneous electron gas (6 points)

Consider N interacting electrons in a volume Ω with a neutralizing background of a constant positive density $\rho_{\mathrm{nucl}} = e\,n_{\mathrm{nucl}} = e\,\frac{N}{\Omega}$. Within the Hartree-Fock approximation, the one-particle wave functions $\Psi_{\vec{k},\sigma}(\vec{r})$ are given by the solutions of

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V_{EN}(\vec{r}) + V_{\mathrm{Coul}}(\vec{r})\right)\psi_{\vec{k},\sigma}(\vec{r})$$

$$-\sum_{\sigma'=-\frac{1}{2}}^{1/2}\sum_{\vec{k}'}\delta_{\sigma,\sigma'}\,e^2\int_\Omega \frac{\Psi^*_{\vec{k}'}(\vec{r}',\sigma')\,\Psi_{\vec{k}}(\vec{r}',\sigma)}{|\vec{r}-\vec{r}'|}\,d^3r'\,\Psi_{\vec{k}',\sigma'}(\vec{r}) = \varepsilon_{\vec{k},\sigma}\,\psi_{\vec{k}}(\vec{r},\sigma)$$

with

$$V_{EN}(\vec{r}) = -\frac{N}{\Omega}\,e^2\int_\Omega \frac{1}{|\vec{r}-\vec{r}'|}\,d^3r'$$

and

$$V_{\mathrm{Coul}}(\vec{r}) = e^2\int_\Omega \frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|}\,d^3r', \qquad n(\vec{r}) = \sum_\sigma\sum_{\vec{k}}|\Psi_{\vec{k}}(\vec{r},\sigma)|^2 .$$

The sums over $\vec{k}$ and $\vec{k}'$ include all occupied states, i. e. $|\vec{k}| \le k_F$, $|\vec{k}'| \le k_F$.

a) Show that the Hartree-Fock equations of this system are solved by plane waves

$$\Psi_{\vec{k}}(\vec{r},\sigma) = \frac{1}{\sqrt{\Omega}}\,e^{i\vec{k}\cdot\vec{r}} \qquad \text{for both spins} \qquad \left(\sigma = \pm\frac{1}{2}\right).$$

Hint: Convince yourselves that V_{EN} is compensated by V_{Coul}.

b) Calculate the eigenvalues $\varepsilon_{\vec{k},\sigma}$. To this end, convert the sum over $\vec{k}'$ into an integral.

Useful integral:

$$\int x\ln\left|\frac{x+a}{x-a}\right|dx = \frac{1}{2}(x^2 - a^2)\ln\left|\frac{x+a}{x-a}\right| + a\,x .$$

c) Plot $\varepsilon_{\vec{k},\sigma}$ and discus its behaviour at $k = k_F$.

d) The eigenvalues

$$\varepsilon_{\vec{k},\sigma} = \frac{\hbar^2}{2m}k^2 + \Sigma^{\mathrm{ex}}(\vec{k},\sigma)$$

contain the self energy $\Sigma^{\mathrm{ex}}(\vec{k},\sigma)$ (here: only exchange). Within the Hartree-Fock approximation, it contributes the exchange energy

$$E^{\mathrm{ex}} = \frac{1}{2}\sum_{\substack{\vec{k},\sigma\\ k<k_F}}\Sigma^{\mathrm{ex}}(\vec{k},\sigma)$$

to the total energy. Show that $E^{\mathrm{ex}} = -N\cdot\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\cdot n^{\frac{1}{3}}$ with $n = \frac{N}{\Omega}$.