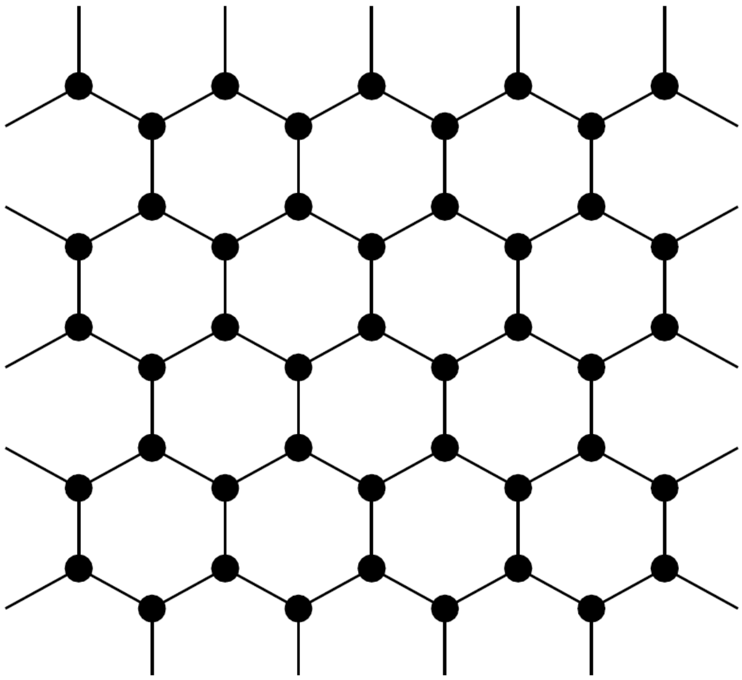
Problem 7: Point group of graphene (3 points)

Graphen is a two-dimensional sheet of carbon atoms that form a lattice with primitive vectors $\vec{a}_1 = (1,\, 0)\, a$ and $\vec{a}_2 = (-1,\, \sqrt{3})\, \frac{a}{2}$ and basis vectors $\vec{\tau}_1 = (0,\, 0)$, $\vec{\tau}_2 = \left(0,\, \frac{1}{\sqrt{3}}\right)\, a$.

a) First, consider graphene as a two-dimensional structure in a *two-dimensional* space. List all symmetry operations (according to the Schönflies notation) that let the structure invariant. Give a short description of the respective operations (e.g. C_{2z}: rotation by 180° about the z axis). Mark the respective axes and mirror planes in the figure. Which point group is formed by these operations?

b) Secondly, consider graphene as a layer of carbon atoms that exist in a three-dimensional space in the x-y plane at $z = 0$. List the additional symmetry operations that let the structure invariant. Which group is formed by *all* operations?



Problem 8: Band structure of graphen (3 points)

Graphene consists of a layer of carbon atoms that are arranged in a hexagonal structure.

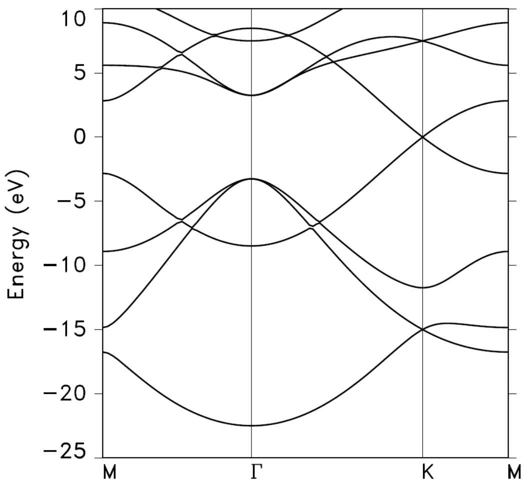
a) Give the primitive vectors $\vec{b}_1$ and $\vec{b}_2$ of the reciprocal lattice and construct the first Brillouin zone.

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.

c) Plot the band structure for $E_p = 0$ eV and $V_{pp\pi} = -2.828$ 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.



Problem 9: Time reversal (4 points)

a) The vector of the Pauli matrices is given by $\hat{\vec{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$. Proof the following relation: $\hat{\sigma}_y^{-1} \hat{\sigma} \hat{\sigma}_y = -\hat{\sigma}^*$.

b) Show that the time reversal operator $\hat{\mathcal{T}} = -i\,\hat{\sigma}_y \hat{K}$ for a particle with the spin $\frac{1}{2}$ has the following properties:

$$(1) \quad \hat{\mathcal{T}}\,\hat{\vec{r}} = \hat{\vec{r}}\,\hat{\mathcal{T}}, \qquad (2) \quad \hat{\mathcal{T}}\,\hat{\vec{p}} = -\hat{\vec{p}}\,\hat{\mathcal{T}}, \qquad (3) \quad \hat{\mathcal{T}}\,\hat{\vec{S}} = -\hat{\vec{S}}\,\hat{\mathcal{T}}.$$

$\vec{K}$ is the operator of complex conjugation. *Hint*: Apply the operators on a wave function in order to proof the relations given above.

c) Show that $\hat{\mathcal{T}}^2 \Psi = -\Psi$.

d) Give the inverse $\hat{\mathcal{T}}^{-1}$ of the time-reversal operator.

e) Consider a Hamilton operator $\hat{H}(\vec{r})$ with $\hat{\mathcal{T}}\,\hat{H}(\vec{r})\,\hat{\mathcal{T}}^{-1} = \hat{H}(\vec{r})$. Show that

$$\hat{\mathcal{T}}\,\hat{\tilde{H}}(\vec{k})\,\hat{\mathcal{T}}^{-1} = \hat{\tilde{H}}(-k) \qquad \text{for} \qquad \hat{\tilde{H}}(\vec{k}) = \mathrm{e}^{-i\,\vec{k}\cdot\vec{r}}\,\hat{H}(\vec{r})\,\mathrm{e}^{i\,\vec{k}\cdot\vec{r}}.$$

f) Give a proof of the following relations i) $\langle\Psi|\hat{\mathcal{T}}|\Phi\rangle = -\langle\Phi|\hat{\mathcal{T}}|\Psi\rangle$, ii) $\langle\hat{\mathcal{T}}\,\Psi|\hat{\mathcal{T}}\,\Phi\rangle = \langle\Phi|\Psi\rangle$. *Hint*: use

$$\Psi(\vec{r}) = \begin{pmatrix} \Psi^{(a)}(\vec{r}) \\ \Psi^{(b)}(\vec{r}) \end{pmatrix} \qquad \text{and} \qquad \Phi(\vec{r}) = \begin{pmatrix} \Phi^{(a)}(\vec{r}) \\ \Phi^{(b)}(\vec{r}) \end{pmatrix}.$$

g) Consider a hermitian operator $\hat{U}$ with $\hat{U}\,\hat{\mathcal{T}} = \hat{\mathcal{T}}\,\hat{U}$. Use the relations from c) together with $\hat{\mathcal{T}}^2 = -1$ to show that $\langle\hat{\mathcal{T}}\,\Psi|\hat{U}|\Psi\rangle = -\langle\hat{\mathcal{T}}\,\Psi|\hat{U}|\Psi\rangle$. Is it possible that $\hat{U}$ induces a transition from $|\Psi\rangle$ to $\hat{\mathcal{T}}\,|\Psi\rangle$?