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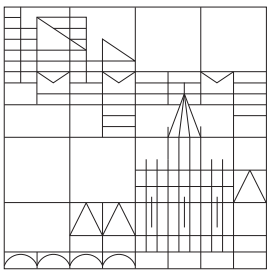

Group theory and symmetries in quantum mechanics
Summer semester 2016 - Exercise sheet 11
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Problem 30: Graphene's energy levels at the $\mathbf{k} = 0$ point in the empty-lattice approximation

Consider the lattice of the well-known one-atom thick material, graphene ! (see, e.g., `http://www.nobelprize.org/nobel_prizes/physics/laureates/2010/press.html`) There are two carbon atoms in the unit cell of graphene (denoted by A and B) and they are arranged into a honeycomb lattice, see Figure 1.

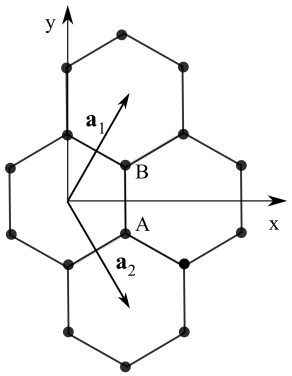

Figure 1: Schematics of the crystal structure of graphene.

a) What is the point group $\mathrm{G}_{graphene}$ of graphene's crystal lattice? Using the lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ shown in Figure 1 find the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$! Sketch the unit cell in the reciprocal space and the corresponding Brillouin zone!

b) In the so-called *empty lattice* approximation the eigenstates of the lattice-periodic Hamiltonian are given by

$$\Psi_{\mathbf{k}} = \frac{1}{\mathcal{N}} e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{G}(n_i)\cdot\mathbf{r}}$$

where $\mathcal{N}$ is a normalization factor, $\mathbf{k}$ is a wave vector in the Brillouin zone, $\mathbf{G}(n_i) = n_1\mathbf{b}_1 + n_2\mathbf{b}_2$ is a lattice vector in the reciprocal space and n_1, n_2 are integers. Note, that $u_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{G}(n_i)\cdot\mathbf{r}}$ is a lattice-periodic function. In the same approximation the eigenenergies are given by

$$E(\mathbf{k} + \mathbf{G}(n_i)) = \frac{\hbar^2}{2m}[\mathbf{k} + \mathbf{G}(n_i)][\mathbf{k} + \mathbf{G}(n_i)].$$

By choosing n_1, n_2 appropriately, find the lowest seven eigenenergies at $\mathbf{k} = 0$!

c) Some of the eigenenergies found above are degenerate. Consider now the wave functions corresponding to these degenerate eigenenergies. How do they transform under the symmetry operations of $\mathrm{G}_{graphene}$? Construct a representation of the point group operations using these degenerate

wave functions! Is this a reducible or an irreducible representation? If reducible, which irreducible representations are contained in it?

Problem 31: Time reversal and spatial symmetries

The fact that the time reversal operation $\mathcal{T}$ is anti-unitary leads to complications when one tries to consider the effects of this symmetry. Namely, consider a set of eigenfunctions $\{\Psi_\lambda\}$ of a Hamiltonian $\mathcal{H}$ which are degenerate in energy. They can be used therefore as basis functions for the point group $\mathcal{G}$ which describes the symmetries of the Hamiltonian $\mathcal{H}$. Since the time reversed wavefunctions $\mathcal{T}\Psi_\lambda$ correspond to the same energy, we find

$$\mathcal{T}G_i\Psi_\nu = \sum_\lambda D(\mathcal{T}G_i)_{\lambda\nu}\Psi_\lambda \tag{1}$$

where $G_i \in G$ and $D(\mathcal{T}G_i)$ is unitary. Consider now the operation $\mathcal{T}G_iG_j$ and show that, contrary to what one would expect, the basis $\{\Psi_\lambda\}$ cannot be used as basis functions for a representation of $\mathcal{G}$ in the degenerate subspace!