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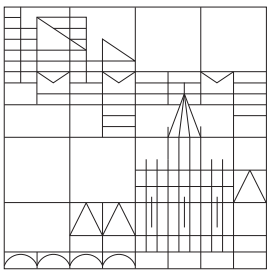

Group theory and symmetries in quantum mechanics
Summer semester 2015 - Exercise sheet 13
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Problem 35: Rotational symmetries of Bravais lattices

Let us consider a two-dimensional Bravais lattice in the $x-y$ plane and assume that a rotation by an angle ϕ around the z axis is also a symmetry of the lattice. Due to the translational invariance, the angle ϕ cannot take on arbitrary values. To show this, assume that the perpendicular rotation axis located at a lattice point and choose an in-plane coordinate system such that one of the primitive lattice vectors (say, $\mathbf{a}_1$) is along the x axis. Assuming that a rotation by $+\phi$ and $-\phi$ are symmetries of the Bravais lattice and taking into account the translational invariance, find the allowed values of ϕ ! Can the result be generalized to three-dimensional Bravais lattices?

Problem 36: 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.

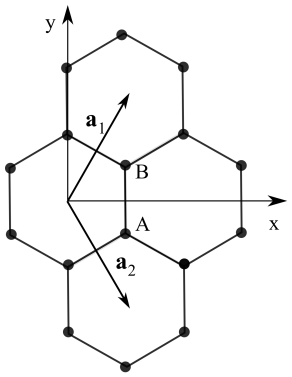

Figure 1

a) What is the point group $g_{graphene}$ 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 $g_{graphene}$? 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?