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Group theory and symmetries in quantum mechanics
Summer semester 2017 - Exercise sheet 9
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Problem 23: 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.

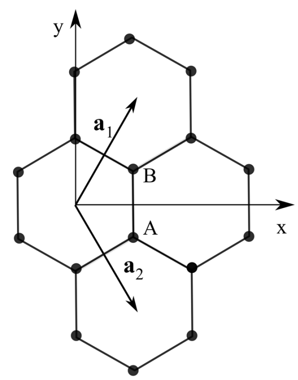

Figure 1

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?

Problem 24: Mapping SU(2) $\longrightarrow$ SO(3)**: part 1.**

In order to establish a connection between the matrix groups SU(2) and SO(3) we consider the transformation

$$\mathbf{r} \longmapsto \mathbf{r}' \equiv R\mathbf{r} \quad \text{with} \quad U\mathbf{r}\cdot\boldsymbol{\sigma}U^\dagger = \mathbf{r}'\cdot\boldsymbol{\sigma} \ ,$$

where $U \in \mathrm{SU}(2)$, $\mathbf{r} \in \mathbb{R}^3$, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^\mathrm{T}$ denotes the vector of the Pauli matrices.

a) Show that R is a linear operator and that this operator does not change angles and distances between vectors.
Hint : Consider how the scalar product of two vectors changes under this transformation and use the property $\mathrm{Sp}(\sigma_i\sigma_j) = 2\delta_{ij}$. Here and in what follows use the Einstein notation for summation.

b) Show that in the basis of cartesian coordinates the components of R can be written as

$$R_{ij} = \frac{1}{2}\mathrm{Sp}\left(\sigma_i U \sigma_j U^\dagger\right) \ .$$

c) Using a possible parametrization of U by the components of a unit vector $\mathbf{n}$ and the angle α as $U = e^{i\alpha\mathbf{n}\cdot\boldsymbol{\sigma}}$, show that

$$R_{ij} = \cos 2\alpha\,\delta_{ij} + \sin 2\alpha\,\epsilon_{ijk}n_k + (1-\cos 2\alpha)n_i n_j \ ,$$

where we use the Einstein notation for summation.
Hint : Use $e^{i\alpha\mathbf{n}\cdot\boldsymbol{\sigma}} = \mathbb{1}\cos\alpha + i\mathbf{n}\cdot\boldsymbol{\sigma}\sin\alpha$, $\sigma_j\sigma_k = \delta_{jk}\mathbb{1} + i\epsilon_{jkl}\sigma_l$ with ϵ_{jkl} being the Levi-Civita symbol, and $\epsilon_{ijk}\epsilon_{ij'k'} = \delta_{jj'}\delta_{kk'} - \delta_{jk'}\delta_{kj'}$.

d) Write R for $\mathbf{n} = \mathbf{e}_x$, $\mathbf{n} = \mathbf{e}_y$ and $\mathbf{n} = \mathbf{e}_z$. Which rotations do you get in these cases?

Problem 25: Mapping SU(2) $\longrightarrow$ SO(3)**: part 2.**

a) Using 24c show that the matrices R belong to SO(3).
Hint : In order to prove this, you should show that the components of R are real, $R^\mathrm{T}R = \mathbb{1}$, and $\det R = 1$.

b) Differentiating the result of 24c with respect to α at the following points in the parameter manifold, $\{\alpha = 0, n_x = 1, n_y = n_z = 0\}, \{\alpha = 0, n_y = 1, n_x = n_z = 0\}, \{\alpha = 0, n_x = 1, n_y = n_z = 0\}$, find a possible form of three generators of SO(3).

c) Argue why the mapping SU(2) $\longrightarrow$ SO(3) with $U \longmapsto R$ is a homomorphism. I.e. for each matrix $R \in \mathrm{SO}(3)$ there is at least one matrix $U \in \mathrm{SU}(2)$ generating the corresponding rotation, and arbitrary U_1, U_2 from SU(2) lead to $R(U_1U_2) = R(U_1)R(U_2)$.