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Examination, course FY8104 Symmetry in physics
Friday December 7, 2007
Time: 09.00–13.00

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Allowed to use: Calculator, mathematical tables.

All subproblems are given the same weight in the grading.

Problem 1:

A general three dimensional rotation matrix $\mathbf{R}$, with $\det \mathbf{R} = 1$, may be written as

$$\mathbf{R} = \exp(\alpha \vec{n} \cdot \vec{\boldsymbol{\lambda}}) = \exp(\alpha(n_1 \boldsymbol{\lambda}_1 + n_2 \boldsymbol{\lambda}_2 + n_3 \boldsymbol{\lambda}_3)) \,,$$

where α is the rotation angle, the unit vector $\vec{n}$ is the rotation axis, and

$$\boldsymbol{\lambda}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

A general three dimensional reflection matrix $\mathbf{S}$, with $\det \mathbf{S} = -1$, may be written as $\mathbf{S} = -\mathbf{R}$, where $\mathbf{R}$ is a rotation matrix. Then

$$\begin{aligned} \mathbf{R} \exp(\beta \vec{m} \cdot \vec{\boldsymbol{\lambda}}) \mathbf{R}^{-1} &= \exp(\beta \mathbf{R}(\vec{m} \cdot \vec{\boldsymbol{\lambda}}) \mathbf{R}^{-1}) = \exp(\beta (\mathbf{R}\vec{m}) \cdot \vec{\boldsymbol{\lambda}}) \,, \\ \mathbf{S} \exp(\beta \vec{m} \cdot \vec{\boldsymbol{\lambda}}) \mathbf{S}^{-1} &= \exp(\beta \, \mathbf{S} \, (\vec{m} \cdot \vec{\boldsymbol{\lambda}}) \, \mathbf{S}^{-1}) = \exp(\beta (\mathbf{R}\vec{m}) \cdot \vec{\boldsymbol{\lambda}}) \,. \end{aligned}$$

To the SO(3) matrix $\mathbf{R}$ corresponds the SU(2) matrix

$$\mathbf{U} = \exp\left(-\mathrm{i} \frac{\alpha}{2} \vec{n} \cdot \vec{\boldsymbol{\sigma}}\right) = \cos\left(\frac{\alpha}{2}\right) \mathbf{I} - \mathrm{i} \sin\left(\frac{\alpha}{2}\right) \vec{n} \cdot \vec{\boldsymbol{\sigma}} \,,$$

where $\mathbf{I}$ is the identity matrix and the components of $\vec{\boldsymbol{\sigma}}$ are the Hermitean Pauli matrices

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Then

$$\mathbf{U} \exp\left(-\mathrm{i} \frac{\beta}{2} \vec{m} \cdot \vec{\boldsymbol{\sigma}}\right) \mathbf{U}^{-1} = \exp\left(-\mathrm{i} \frac{\beta}{2} \mathbf{U}(\vec{m} \cdot \vec{\boldsymbol{\sigma}}) \mathbf{U}^{-1}\right) = \exp\left(-\mathrm{i} \frac{\beta}{2} (\mathbf{R}\vec{m}) \cdot \vec{\boldsymbol{\sigma}}\right).$$

a) Describe the conjugation classes of the groups SO(3), O(3), and SU(2).

b) What is the centre of SU(2) (the subset of group elements commuting with all group elements)?

What is the centre of SU(3)?

Hint: You may use Schur's lemma, since both SU(2) and SU(3) are irreducible representations of themselves.

c) Define, for every $\mathbf{U} \in \mathrm{SU}(2)$,

$$\begin{aligned} \rho_1(\mathbf{U}) &= \mathbf{U} \,, \\ \rho_2(\mathbf{U}) &= \mathbf{U}^* = \text{the complex conjugate of } \mathbf{U} \,. \end{aligned}$$

Both ρ_1 and ρ_2 are representations of SU(2) (since $\rho_1(\mathbf{UV}) = \rho_1(\mathbf{U})\rho_1(\mathbf{V})$ and $\rho_2(\mathbf{UV}) = \rho_2(\mathbf{U})\rho_2(\mathbf{V})$).

Show that they are equivalent representations.

What can this result tell us about the characters $\chi_1(\mathbf{U}) = \mathrm{Tr}\,\rho_1(\mathbf{U}) = \mathrm{Tr}\,\mathbf{U}$?

Hint: The direct proof of equivalence is to find a complex 2×2 matrix $\mathbf{V}$, for example $\mathbf{V} \in \mathrm{SU}(2)$, such that $\mathbf{U}^* = \mathbf{VUV}^{-1}$ for every $\mathbf{U} \in \mathrm{SU}(2)$.

d) Define, for every $\mathbf{U} \in \mathrm{SU}(3)$,

$$\begin{aligned} \rho_1(\mathbf{U}) &= \mathbf{U} \,, \\ \rho_2(\mathbf{U}) &= \mathbf{U}^* \,. \end{aligned}$$

Show that ρ_1 and ρ_2 are inequivalent representations of SU(3).

e) The quaternion group has eight elements ± 1, $\pm \mathrm{i}$, $\pm \mathrm{j}$, and $\pm \mathrm{k}$, with the multiplication rules

$$\mathrm{i}^2 = \mathrm{j}^2 = \mathrm{k}^2 = -1 \,, \quad \mathrm{ij} = -\mathrm{ji} = \mathrm{k} \,, \quad \mathrm{jk} = -\mathrm{kj} = \mathrm{i} \,, \quad \mathrm{ki} = -\mathrm{ik} = \mathrm{j} \,.$$

It is a subgroup of SU(2), for example with the identifications

$$1 \leftrightarrow \mathbf{I} \,, \quad \mathrm{i} \leftrightarrow -\mathrm{i}\sigma_1 \,, \quad \mathrm{j} \leftrightarrow -\mathrm{i}\sigma_2 \,, \quad \mathrm{k} \leftrightarrow -\mathrm{i}\sigma_3 \,.$$

Find the character table of the quaternion group.

The following orthogonality relations hold for a finite group of order N.

Let $\chi_i^{(\mu)}$ be the character of the conjugation class i, with N_i elements, in the irreducible representation μ. Then

$$\begin{aligned} \sum_i N_i (\chi_i^{(\mu)})^* \chi_i^{(\nu)} &= N \, \delta_{\mu\nu} \,, \\ \sum_\mu (\chi_i^{(\mu)})^* \chi_j^{(\mu)} &= \frac{N}{N_i} \, \delta_{ij} \,. \end{aligned}$$

Problem 2:

Figure 1 shows a planar hexagonal lattice, describing for example the arrangement of carbon atoms in a monatomic layer of graphene. The basic translation vectors $\vec{a}_1$ and $\vec{a}_2$ are shown. The translational symmetry group of the lattice consists of all translations $\vec{a} = m\vec{a}_1 + n\vec{a}_2$ with m and n integer.

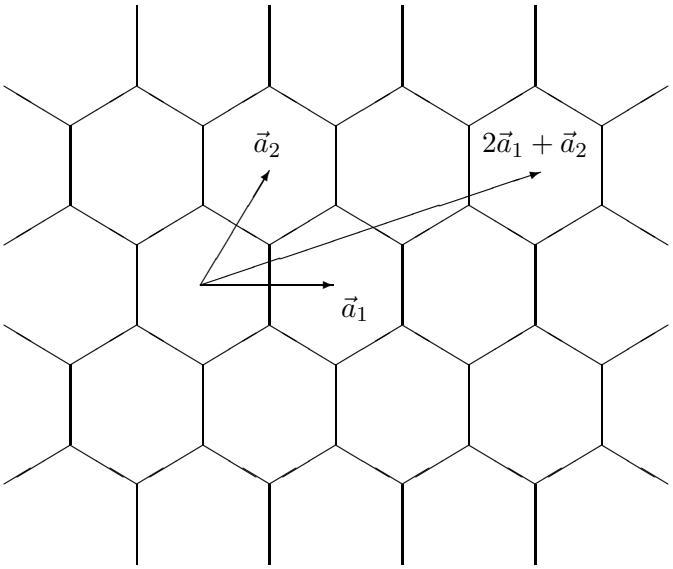

Figure 1: A planar hexagonal lattice (graphene).

a) Describe the full three dimensional point group of the hexagonal lattice.

What is the order (number of elements) of this group?

For simplicity, in what follows we will regard the hexagonal lattice as a two dimensional structure. Then the point group is C_{6v}, having a six-fold rotation axis and six vertical reflection planes.

The two dimensional reciprocal lattice is spanned by the reciprocal basis vectors $\vec{b}_1$ and $\vec{b}_2$, defined by the duality conditions

$$\vec{b}_1 \cdot \vec{a}_1 = \vec{b}_2 \cdot \vec{a}_2 = 1 \,, \qquad \vec{b}_1 \cdot \vec{a}_2 = \vec{b}_2 \cdot \vec{a}_1 = 0 \,.$$

A wave vektor $\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2$ defines an irreducible unitary representation of the translation group such that

$$\vec{a} = m\vec{a}_1 + n\vec{a}_2 \rightarrow \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{a}} = \mathrm{e}^{-\mathrm{i}(k_1 m + k_2 n)} \,. \tag{1}$$

Figure 2 shows the so called first Brillouin zone of wave vectors defining irreducible representations of the translation group of the hexagonal lattice.

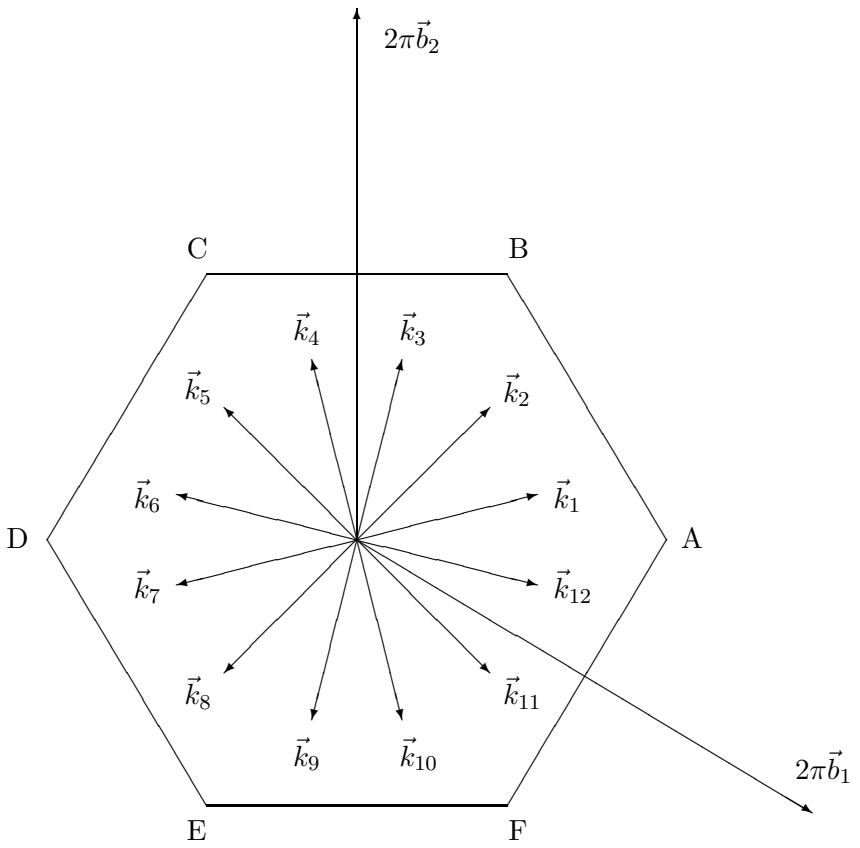

Figure 2: The first Brillouin zone.

The Brillouin zone includes all irreducible representations of the discrete translation group, since two wave vectors $\vec{k}$ and $\vec{k} + 2\pi(m'\vec{b}_1 + n'\vec{b}_2)$ with m' and n' integer define the same irreducible representation. For a wave vector on the edge of the Brillouin zone there is at least one other wave vector on the edge defining the same irreducible representation. Thus, the edge AB, in direction from A to B, is identified with the edge ED, in direction from E to D. The edges BC and FE are identified, as are the edges CD and AF. The corners A, B, C, D, E, F are special cases, since the three corners A, C, E define the same representation, and B, D, F define the same representation.

b) An irreducible unitary representation of the translation group must be one dimensional, as in Equation (1). Why?

c) We consider one electron moving in a potential with the symmetry of the planar hexagonal lattice. For simplicity, we disregard the intrinsic spin of the electron and take the physical state of the electron to be described by a scalar wave function $\psi = \psi(\vec{r})$.

A symmetry transformation $\vec{r} \to \vec{r}\,' = f(\vec{r})$ transforms the wave function ψ into ψ', such that $\psi'(\vec{r}\,') = \psi(\vec{r})$. That is,

$$\psi'(\vec{r}) = \psi(f^{-1}(\vec{r})) \; .$$

We write $\psi' = U(f)\psi$, where $U(f)$ is the unitary operator representing the transformation f. In particular, $U(\vec{a})$ and $U(R)$ are the unitary operators representing the translation $\vec{a} = m\vec{a}_1 + n\vec{a}_2$ and the rotation or reflection R.

Show that if $U(\vec{a})\psi = \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{a}}\psi$, and $\psi' = U(R)\psi$, then $U(\vec{a})\psi' = \mathrm{e}^{-\mathrm{i}\vec{k}'\cdot\vec{a}}\psi'$ with $\vec{k}' = R\vec{k}$.

With the same notation, show that ψ and ψ' are orthogonal if $\mathrm{e}^{-\mathrm{i}\vec{k}'\cdot\vec{a}} \neq \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{a}}$.

Hint: You may show more generally that eigenstates of a unitary operator with different eigenvalues are orthogonal.

d) Given a typical wave vector $\vec{k}_1$ inside the Brillouin zone, and a wave function ψ_1 with $U(\vec{a})\psi_1 = \mathrm{e}^{-\mathrm{i}\vec{k}_1\cdot\vec{a}}\psi_1$.

The wave vector $\vec{k}_1$ is transformed by the point group C_{6v} into a star of 12 wave vectors $\vec{k}_1$ to $\vec{k}_{12}$, as shown in Figure 2. Similarly, the wave function ψ_1 is transformed into a set of 12 orthogonal wave functions ψ_1 to ψ_{12}. These 12 wave functions are orthogonal basis vectors defining a 12 dimensional unitary matrix representation of the whole space group, including translations, rotations and reflections.

Show that this is a reducible representation of the point group C_{6v}, and find the multiplicities of the irreducible representations it contains.

The character table of the group C_{6v} is given below, on page 6.

e) In the above 12 dimensional matrix representation of the space group, the translations are represented by diagonal matrices.

Show that if a 12×12 matrix commutes with all the translations, then it must be diagonal.

Show further that if a diagonal matrix commutes with all the rotations and reflections, then all its diagonal elements must be equal.

In conclusion, any 12×12 matrix which commutes with all translations, rotations and reflections must be a multiple of the identity.

Does this prove that we have an irreducible representation of the space group?
Explain why or why not.

f) A carbon nanotube is a sheet of graphene rolled up into a cylinder. The rolling up is described by two integers M and N, in such a way that a point $\vec{r}$ in the plane becomes identified with the point $\vec{r} + M\vec{a}_1 + N\vec{a}_2$.

See Figure 1 for an example with $M = 2$, $N = 1$.

The point group of the nanotube is a subgroup of C_{6v}. Which subgroup?

The answer may depend on the integers M and N.

For which values of M and N does the point group of the nanotube include reflection symmetries?

A nanotube is said to be *chiral* if it has no reflection symmetry.

g) The translation $M\vec{a}_1 + N\vec{a}_2$ is the identity transformation on the nanotube, and this fact imposes a restriction on the set of wave vectors defining representations of the translation group.

It is possible to regard the Brillouin zone of the nanotube as a subset of the Brillouin zone of the hexagonal lattice. Describe this subset.

The irreducible characters of C_{6v}

Notation:
E: unit element;
C_n: order n rotation, $(C_n)^n = E$;
σ: reflection;
A, B: one dimensional representations;
E: two dimensional representations.

	E	C_2	$2C_3$	$2C_6$	$3\sigma_d$	$3\sigma_v$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	−1	−1
B_1	1	−1	1	−1	−1	1
B_2	1	−1	1	−1	1	−1
E_1	2	−2	−1	1	0	0
E_2	2	2	−1	−1	0	0