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Group theory and symmetries in quantum mechanics
Summer semester 2017 - Exercise sheet 8
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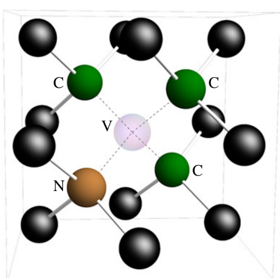
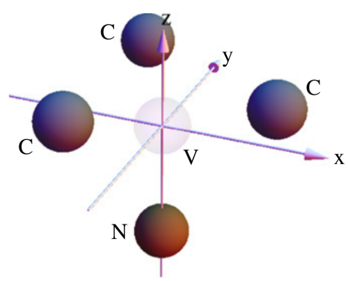
Problem 22: Interaction of the NV center in diamond with the electric field.

Consider the nitrogen-vacancy (NV) center in diamond: a point defect where two neighboring carbon atoms are replaced with a nitrogen and a vacancy. The defect has a 3-fold symmetry axis going through N and the vacancy, as well as 3 reflection planes passing through N and each of the closest to the vacancy C atoms. This corresponds to the C_{3v} symmetry group. The structure of the NV center and the C_{3v} character table are shown in the figure below.





C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

a) Let the x-axis lie in the plane containing N and one of the C neighbours of the vacancy; y-axis is set to be perpendicular to the x-axis and to the symmetry axis of the NV center, which is the z-axis then. Taking unit vectors $\bar{\mathbf{e}}_x$ and $\bar{\mathbf{e}}_y$ as basis build the IR $\mathbf{E}$ of the C_{3v} group.

b) We will say that $\phi_x^{(E)} \in \mathbf{E_x}$ and $\phi_y^{(E)} \in \mathbf{E_y}$ if they transform as the first and second rows of $\mathbf{E}$, respectively.

- Now build one more 2D representation taking the pseudovectors $\mathbf{l}_x$ and $\mathbf{l}_y$ pointing in the x and y directions, respectively, as basis.
- Check that this is an IR but it is different from $\mathbf{E}$, so $\mathbf{l}_x \notin \mathbf{E_x}$ and $\mathbf{l}_y \notin \mathbf{E_y}$.

Then the two representations must be related by a similarity transformation, which means there exists a basis change $(\mathbf{l}_1, \mathbf{l}_2) = (\mathbf{l}_x, \mathbf{l}_y)\mathbf{S}$ produced by a 2×2 matrix $\mathbf{S}$, so that $\mathbf{l}_1 \in \mathbf{E_x}$ and $\mathbf{l}_2 \in \mathbf{E_y}$. Notice that the action of rotation on $\mathbf{l}_x$ and $\mathbf{l}_y$ already agrees with $\mathbf{E}$ representation and so the transformation to a new basis should leave the rotation matrix invariant. This can only happen if the transformation matrix $\mathbf{S}$ itself corresponds to a rotation around the z-axis.

- With this in mind find the pseudovector basis of $\mathbf{E}$: $\mathbf{l}_1$ and $\mathbf{l}_2$.

c) Check that $\bar{\mathbf{e}}_z \in \mathbf{A}_1$ and $\mathbf{l}_z \in \mathbf{A}_2$.

d) Let $\phi_x^{(E)} \in \mathbf{E}_x$, $\phi_y^{(E)} \in \mathbf{E}_y$ and $\psi_x^{(E)} \in \mathbf{E}_x$, $\psi_y^{(E)} \in \mathbf{E}_y$ be two pairs of basis functions for $\mathbf{E}$, $\phi^{(A1)}$, $\psi^{(A1)}$ belong to the IR $\mathbf{A}_1$ and $\phi^{(A2)}$, $\psi^{(A2)}$ belong to the IR $\mathbf{A}_2$.

- Show that the products $\phi^{(A1)}\psi^{(A1)}$, $\phi^{(A2)}\psi^{(A2)}$ belong to $\mathbf{A}_1$ and $\phi^{(A1)}\psi^{(A2)}$, $\phi^{(A2)}\psi^{(A1)}$ belong to $\mathbf{A}_2$.

- Show that $\phi_x^{(E)}\psi^{(A2)}$, $\phi_y^{(E)}\psi^{(A2)}$ transform as $\mathbf{l}_x$, $\mathbf{l}_y$ and using the result from (b) show that $-\phi_y^{(E)}\psi^{(A2)} \in \mathbf{E}_x$, $\phi_x^{(E)}\psi^{(A2)} \in \mathbf{E}_y$ form a basis for $\mathbf{E}$.

The products $\phi_x^{(E)}\psi_x^{(E)}$, $\phi_x^{(E)}\psi_y^{(E)}$, $\phi_y^{(E)}\psi_x^{(E)}$, $\phi_y^{(E)}\psi_y^{(E)}$ transform according to $\mathbf{E}\otimes\mathbf{E} = \mathbf{E}\oplus\mathbf{A}_1\oplus\mathbf{A}_2$.

- Using the formalism of projectors, find the corresponding basis vectors for the constituting IRs in the decomposition.

e) It can be shown that the vector space corresponding to the ground state of the NV center is spanned by three eigenstates of spin-1 angular momentum operator ($|\psi_1\rangle$, $|\psi_0\rangle$, $|\psi_{-1}\rangle$). Any other operator acting in this space can be written as a function of the components of the spin angular momentum operator: $\hat{\mathbf{S}}_x, \hat{\mathbf{S}}_y, \hat{\mathbf{S}}_z$. Note that $\hat{\mathbf{S}}_x, \hat{\mathbf{S}}_y, \hat{\mathbf{S}}_z$ transform exactly as pseudovectors $\mathbf{l}_x, \mathbf{l}_y, \mathbf{l}_z$ under the group operations. There are nine functions quadratic in the spin operator components $\hat{\mathbf{S}}_x^2$, $\hat{\mathbf{S}}_y^2$, $\hat{\mathbf{S}}_z^2$, $\hat{\mathbf{S}}_x\hat{\mathbf{S}}_y$, $\hat{\mathbf{S}}_y\hat{\mathbf{S}}_x$, $\hat{\mathbf{S}}_x\hat{\mathbf{S}}_z$, $\hat{\mathbf{S}}_z\hat{\mathbf{S}}_x$, $\hat{\mathbf{S}}_y\hat{\mathbf{S}}_z$, $\hat{\mathbf{S}}_z\hat{\mathbf{S}}_y$. However, due to fundamental properties of angular momentum we have: $\hat{\mathbf{S}}_x^2 + \hat{\mathbf{S}}_y^2 + \hat{\mathbf{S}}_z^2 = 2$, $\hat{\mathbf{S}}_x\hat{\mathbf{S}}_y - \hat{\mathbf{S}}_y\hat{\mathbf{S}}_x = i\hat{\mathbf{S}}_z$, $\hat{\mathbf{S}}_y\hat{\mathbf{S}}_z - \hat{\mathbf{S}}_z\hat{\mathbf{S}}_y = i\hat{\mathbf{S}}_x$, $\hat{\mathbf{S}}_z\hat{\mathbf{S}}_x - \hat{\mathbf{S}}_x\hat{\mathbf{S}}_z = i\hat{\mathbf{S}}_y$. Then in reality we have only five independent truly quadratic combinations of operators: $\hat{\mathbf{S}}_x^2 - \hat{\mathbf{S}}_y^2$, $\hat{\mathbf{S}}_z^2$, $\{\hat{\mathbf{S}}_x, \hat{\mathbf{S}}_y\}$, $\{\hat{\mathbf{S}}_y, \hat{\mathbf{S}}_z\}$, $\{\hat{\mathbf{S}}_z, \hat{\mathbf{S}}_x\}$, where $\{\hat{\mathbf{A}}, \hat{\mathbf{B}}\} = \hat{\mathbf{A}}\hat{\mathbf{B}} + \hat{\mathbf{B}}\hat{\mathbf{A}}$ stands for the anticommutator of the two operators.

- Using the result of (d) find which of the five operators above form pairs of basis functions belonging to $\mathbf{E}_x$ and $\mathbf{E}_y$ of $\mathbf{E}$ and which form basis functions for $\mathbf{A}_1$ and $\mathbf{A}_2$.

If we apply electric field it will start to couple different spin states. This is an indirect effect due to coupling to the higher levels of the NV center.

- Apply symmetry considerations to find the most general form of the Hamiltonian linear in the electric field and quadratic in the spin operators, which acts in the vector space corresponding to the ground state of the NV center and describes its interaction with the electric field.

Note that any Hamiltonian allowed by symmetry should transform according to the identity representation when both the field and spin operators are transformed by the C_{3v} symmetry operations. You should use the result of (d) to construct it.