IV. ANGULAR MOMENTUM

(Klimeš, Augustovičová)

A. Introduction

Orbital momentum of electrons and spin of particles are some of the basic examples of quantization of properties of systems at the atomic level. The aparatus used to deal with states of angular momenta is somewhat different to that usually employed in previous sections. In this section we will deal more with matrix representations or operators with defined commutation relations than with continuous wave functions. This is something to get used to and we try to help it by, *e.g.*, solving the exercises in different ways whenever possible. The exercises in this section are divided into two parts: The first one concerns properties of a single angular momentum, in the second group of examples we discuss combinations of different angular momenta.

In the first group of exercises, Ex. IV B to Ex. IV F, we refresh the basic relations for operators of angular momentum and get used to matrix representations of different operators of angular momenta. Fortunately, these matrices are small so that finding their eigenvalues is simple. Such procedures are performed in Ex. IV C and Ex. IV D for measurement of projections of spin and orbital momentum on a general axis.

The interactions between different angular momenta are important in atomic and molecular physics, chemistry, or solid state physics. An example is spin-orbit interaction, in which electron spin interacts with the movement of the electron. It allows electron transitions in which the spin changes (phosphorescence) and it also splits energy levels of electrons in solids for spin up and spin down states. A simple example of this splitting is discussed in Ex. IV G. The spin-orbital interaction causes so-called coupling of spin and orbital momentum eigenstates, they can be no longer written as products of the respective eigenstates but as combinations of products. (The first case is called “direct product basis”, the latter “coupled basis”.) In Ex. IV H and Ex. IV I we discuss how this transition is done and how different operators can be used in either bases.

In the last three exercises we study systems with two interacting spins, two electron spins in Ex. IV J and Ex. IV K, and then nuclear and electron spin of hydrogen atom in external magnetic field in Ex. IV L. The Ex. IV J and Ex. IV K solve actually the same problem, but in two different ways. The first approach in Ex. IV J rewrites the Hamiltonian using the operator of the total spin. While this solution is elegant, it can’t be used in a case of a general spin-spin interaction. Therefore, in Ex. IV K we discuss how to set-up a matrix representation of the Hamiltonian and find the new eigenstates by diagonalization of the Hamiltonian. Both approaches are used in the last exercise to deal with the more complicated interactions there.

Note that spins occur in many fields of science and there is a variety of nomenclature used to describe the different states. Here we usually use the notation $|\uparrow\rangle$ for spin-up states and $|\downarrow\rangle$ for spin-down states. In chemistry, these states can be denoted α and β, they can be also marked $|+\rangle$ and $|-\rangle$. In case of projection on a different axis, such as in Ex. IV C, we usually write the quantization axis explicitly.

B. Expectation values of $\hat{\mathsf{L}}_x$ and $\hat{\mathsf{L}}_x^2$ operators

A particle is moving in a spherically symmetric field. Calculate the expectation values of operators $\hat{\mathsf{L}}_x$ and $\hat{\mathsf{L}}_x^2$ for a state with orbital quantum number l and a projection of the angular momentum onto the z axis equal to $m\hbar$.

Solution:

The expectation value of $\hat{\mathsf{L}}_x$ can be obtained using the commutation relations for components of angular momentum: $i\hbar\hat{\mathsf{L}}_x = [\hat{\mathsf{L}}_y, \hat{\mathsf{L}}_z]$. We obtain

$$\langle\hat{\mathsf{L}}_x\rangle = \langle l,m|\,\frac{1}{i\hbar}[\hat{\mathsf{L}}_y,\hat{\mathsf{L}}_z]\,|l,m\rangle = \frac{1}{i\hbar}\,\langle l,m|\,\hat{\mathsf{L}}_y\hat{\mathsf{L}}_z - \hat{\mathsf{L}}_z\hat{\mathsf{L}}_y\,|l,m\rangle\ .$$

We now use $\hat{\mathsf{L}}_z\,|l,m\rangle = \hbar m\,|l,m\rangle$ (and its conjugate) and find

$$\langle\hat{\mathsf{L}}_x\rangle = \frac{1}{i\hbar}\,\langle l,m|\,m\hbar\hat{\mathsf{L}}_y\,|l,m\rangle - \frac{1}{i\hbar}\,\langle l,m|\,m\hbar\hat{\mathsf{L}}_y\,|l,m\rangle = 0\,.$$

The expectation value of the square of the $\hat{\mathsf{L}}_x$ operator can be obtained using the operator of the square of the magnitude of the momentum $\hat{\mathbf{L}}^2$ and of the projection onto the z axis $\hat{\mathsf{L}}_z$. As $\hat{\mathbf{L}}^2 = \hat{\mathsf{L}}_x^2 + \hat{\mathsf{L}}_y^2 + \hat{\mathsf{L}}_z^2$ and $\langle\hat{\mathsf{L}}_x^2\rangle = \langle\hat{\mathsf{L}}_y^2\rangle$ due to the symmetry of the problem, the expectation value can be expressed as

$$\langle\hat{\mathsf{L}}_x^2\rangle = \frac{1}{2}\langle\hat{\mathbf{L}}^2 - \hat{\mathsf{L}}_z^2\rangle\,.$$

Using $\hat{\mathbf{L}}^2\,|l,m\rangle = l(l+1)\hbar^2\,|l,m\rangle$ and $\hat{\mathsf{L}}_z\,|l,m\rangle = \hbar m\,|l,m\rangle$ we obtain

$$\langle\hat{\mathsf{L}}_x^2\rangle = \frac{1}{2}\hbar^2\left[l(l+1) - m^2\right]\ .$$

Alternatively, we can make use of the raising and lowering operators for angular momentum, $\hat{\mathsf{L}}_\pm = \hat{\mathsf{L}}_x \pm i\hat{\mathsf{L}}_y$, which leads to the following relation

$$\hat{\mathsf{L}}_x = \frac{1}{2}\left(\hat{\mathsf{L}}_+ + \hat{\mathsf{L}}_-\right)\ .$$

Using $\hat{\mathsf{L}}_\pm\,|l,m\rangle = \hbar\sqrt{l(l+1) - m(m\pm1)}\,|l,m\pm1\rangle$, we obtain

$$\langle\hat{\mathsf{L}}_x\rangle = \frac{1}{2}\hbar\sqrt{l(l+1)-m(m+1)}\,\langle l,m|l,m+1\rangle + \frac{1}{2}\hbar\sqrt{l(l+1)-m(m-1)}\,\langle l,m|l,m-1\rangle = 0\,,$$

as the basis of the $|l,m\rangle$ states is orthonormal.

For the expectation value of the square of the $\hat{\mathsf{L}}_x$ operator we obtain

$$\hat{\mathsf{L}}_x^2 = \frac{1}{4}\left(\hat{\mathsf{L}}_+ + \hat{\mathsf{L}}_-\right)\left(\hat{\mathsf{L}}_+ + \hat{\mathsf{L}}_-\right) = \frac{1}{4}\left(\hat{\mathsf{L}}_+\hat{\mathsf{L}}_+ + \hat{\mathsf{L}}_-\hat{\mathsf{L}}_- + \hat{\mathsf{L}}_-\hat{\mathsf{L}}_+ + \hat{\mathsf{L}}_+\hat{\mathsf{L}}_-\right)\ .$$

The expectation value of the squares of the raising or lowering operators is zero (as $\langle l,m|\,\hat{\mathsf{L}}_{\pm}^2\,|l,m\rangle = c\,\langle l,m|l,m\pm 2\rangle = 0$) and only the mixed terms remain. They can be evaluated as

$$
\begin{aligned}
\langle \hat{\mathsf{L}}_x^2\rangle &= \frac{1}{4}\langle l,m|\,\hat{\mathsf{L}}_-\hat{\mathsf{L}}_+ + \hat{\mathsf{L}}_+\hat{\mathsf{L}}_-\,|l,m\rangle \\
&= \frac{1}{4}\hbar\,\langle l,m|\,\hat{\mathsf{L}}_-\sqrt{l(l+1)-m(m+1)}\,|l,m+1\rangle \\
&\quad + \frac{1}{4}\hbar\,\langle l,m|\,\hat{\mathsf{L}}_+\sqrt{l(l+1)-m(m-1)}\,|l,m-1\rangle \\
&= \frac{1}{4}\hbar^2\,\langle l,m|\,\sqrt{l(l+1)-(m+1)(m+1-1)}\sqrt{l(l+1)-m(m+1)}\,|l,m\rangle \\
&\quad + \frac{1}{4}\hbar^2\,\langle l,m|\,\sqrt{l(l+1)-(m-1)(m-1+1)}\sqrt{l(l+1)-m(m-1)}\,|l,m\rangle \\
&= \frac{1}{2}\hbar^2\left[l(l+1)-m^2\right] .
\end{aligned}
$$

This agrees with the result obtained previously.

C. Measurement of spin along a rotated axis

An electron is prepared in a state such that the expectation value of measuring its spin along the z axis is $\frac{1}{2}\hbar$.

a) What are the possible results of measurement of spin along the x axis?

b) What is the probability of finding these states?

c) What are the possible results of measurement of spin and their probabilities if we measure the spin along axis lying in the xz plane and rotated by an angle θ from the z axis (see Fig. 21)? Assume $\theta < \pi$ and the x component of the axis vector is positive.

d) What is the expectation value for measurement of spin along the rotated axis?

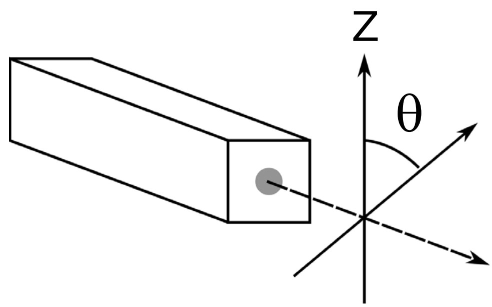

FIG. 21. Measurement of electron spin along axis rotated by an angle θ.

Solution:

a) The measurement of electron spin will give result $\pm\frac{1}{2}\hbar$ independent of the direction of measurement. For the measurement along the x axis, this can be shown explicitly by finding the eigenvalues of the $\hat{\mathsf{S}}_x$ operator that describes the act of measuring the spin along the x axis. Its eigenvalues are then the only possible results of measuring the spin (given that the system is isolated). We find the eigenvalues by diagonalizing the matrix representation of the $\hat{\mathsf{S}}_x$ operator in the basis of the states corresponding to measurement along the z axis.

The $\hat{\mathsf{S}}_x$ operator is

$$\hat{\mathsf{S}}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} .$$

The eigenvalues are found by setting the determinant of $\hat{\mathsf{S}}_x - \lambda\hat{1}$ equal to zero

$$\det\begin{pmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{pmatrix} = \lambda^2 - \frac{\hbar^2}{4} = 0\,,$$

therefore the eigenvalues are indeed $\lambda = \pm\frac{1}{2}\hbar$. The eigenvector corresponding to $\lambda = \frac{1}{2}\hbar$ is $|x_+\rangle = \frac{1}{\sqrt{2}}\binom{1}{1}$ and the eigenvector corresponding to $\lambda = -\frac{1}{2}\hbar$ is $|x_-\rangle = \frac{1}{\sqrt{2}}\binom{1}{-1}$. Note that here we use a shorthand notation where the first letter is the quantization axis and the $+$ or $-$ signs at the second position denote the sign of the spin orientation along this axis.