– Homeworks 20.07.2017 – A. AIELLO

IK-1, FAU, SS 2017

1) Consider a system of spin 1/2 (e.g., an electron) prepared in some unknown state $|\psi\rangle$. A measurement of $\hat{S}_x$ leads to the eigenvalue $+\hbar/2$. Subsequently, a measurement of $\hat{S}_\phi \equiv \hat{S}_x \cos\phi + \hat{S}_y \sin\phi$ with $\phi \in \mathbb{R}$, is carried out. What is the probability that the result is $+\hbar/2$?

– Solution –

After the first measurement of $\hat{S}_x$, the system must be in the eigenstate of $\hat{S}_x$ with eigenvalue $+\hbar/2$, denoted $|x,+\rangle$. This means that:

$$\hat{S}_x |x,+\rangle = +\frac{\hbar}{2} |x,+\rangle$$

In the basis where $\hat{S}_z$ is diagonal, we have:

$$\hat{S}_z \doteq \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z \quad \text{and} \quad \hat{S}_x \doteq \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x$$

and $\quad \hat{S}_z |\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle$

So, if we write:

$$|x,+\rangle = u|+\rangle + v|-\rangle \doteq \begin{pmatrix} u \\ v \end{pmatrix}$$

then to find $|x,+\rangle$ we have to solve the

H 20-2)

eigenvalue equation:

$$\frac{\hbar}{2}\sigma_x \begin{pmatrix} u \\ v \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} u \\ v \end{pmatrix} \Leftrightarrow \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}}_{=\begin{pmatrix} v \\ u \end{pmatrix}} = \begin{pmatrix} u \\ v \end{pmatrix}$$

Then $\begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} \Rightarrow u = v$

Since $|u|^2 + |v|^2 = 1$, we choose u real:

$$\begin{pmatrix} u \\ v \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

and

$$|x,+\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)$$

Now, to calculate the probability $P_+(\phi)$ that a measurement of $\hat{S}_\phi$ gives $+\hbar/2$, we must expand $|x,+\rangle$ in the basis of the eigenvectors of $\hat{S}_\phi$, denoted

$$\{|\phi,+\rangle, |\phi,-\rangle\}$$

and defined as:

$$\hat{S}_\phi |\phi,\pm\rangle = \pm\frac{\hbar}{2}|\phi,\pm\rangle$$

Once these states are known, it will be easy to calculate

$$|x,+\rangle = |\phi,+\rangle\langle\phi,+|x,+\rangle + |\phi,-\rangle\langle\phi,-|x,+\rangle$$

where the completeness relation

$$\hat{I} = |\phi,+\rangle\langle\phi,+| + |\phi,-\rangle\langle\phi,-|$$

has been used.

Then, the sought probability is simply:

$$P_+(\phi) = |\langle\phi,+|x,+\rangle|^2$$

So, we want to solve the eigenvalue equation that determine $|\phi,s\rangle$, with s to be found:

this is here for dimensional reasons!

$$(\hat{S}_x \cos\phi + \hat{S}_y \sin\phi)|\phi,s\rangle = s\frac{\hbar}{2}|\phi,s\rangle$$

$$\Leftrightarrow \quad \boxed{(\sigma_x \cos\phi + \sigma_y \sin\phi)\begin{pmatrix} a \\ b \end{pmatrix} = s\begin{pmatrix} a \\ b \end{pmatrix}} \qquad (1.3)$$

where we have defined:

$$|\phi,s\rangle \doteq \begin{pmatrix} a \\ b \end{pmatrix} \qquad \text{in the basis } |\pm\rangle$$

Equation (1.3) is rewritten as:

$$\begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = s\begin{pmatrix} a \\ b \end{pmatrix}$$

$$\Rightarrow \quad \begin{cases} b e^{-i\phi} = s a \\ a e^{i\phi} = s b \end{cases}$$

Multiplying side-by-side these two equations we get:

$$ab = s^2 ab \quad \Rightarrow \quad s^2 = 1$$

Therefore $\boxed{s = \pm 1}$

The eigenvector corresponding to $s = 1$ satisfies

$$a e^{i\phi} = b \quad \Leftrightarrow \quad a e^{i\phi/2} = b e^{-i\phi/2}$$

$$\Rightarrow \begin{pmatrix} a \\ b \end{pmatrix} \propto \begin{pmatrix} e^{-i\phi/2} \\ e^{i\phi/2} \end{pmatrix} \xrightarrow{\text{normalize}} \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\phi/2} \\ e^{i\phi/2} \end{pmatrix}$$

Therefore:

$$|\phi, +\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\phi/2}|+\rangle + e^{-i\phi/2}|-\rangle\right)$$

Finally, we can calculate:

$$\langle \phi,+|x,+\rangle = \frac{1}{2}\left(e^{i\phi/2}\langle +| + e^{-i\phi/2}\langle -|\right)\left(|+\rangle + |-\rangle\right)$$

$$= \frac{1}{2}\left(e^{i\phi/2} + e^{-i\phi/2}\right)$$

$$= \cos\left(\frac{\phi}{2}\right)$$

This implies that:

$$P_+(\phi) = |\langle \phi,+|x,+\rangle|^2 = \cos^2\left(\frac{\phi}{2}\right)$$

2) Consider a charged particle in a simple harmonic oscillator, for which

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2,$$

subject to a constant electric field so that

$$\lambda \hat{V} = q \mathcal{E} \hat{x} . \quad (\lambda \equiv q\mathcal{E})$$

Calculate the energy shift for the nth level to first and second order in $\lambda = q\mathcal{E}$.

— Solution —

a) Let us remind that:

$$\hat{H}_0 |n\rangle = E_n^0 |n\rangle \qquad n = 0, 1, 2, \ldots$$

where
$$E_n^0 = \hbar\omega \left(n + \frac{1}{2}\right)$$

At first order, we need to calculate:

$$\lambda E_n^1 = \langle n | \lambda \hat{V} | n \rangle$$
$$= q\mathcal{E} \langle n | \hat{x} | n \rangle$$

Remembering that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \, (\hat{a} + \hat{a}^\dagger)$$

and that

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle, \quad \hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

we easily calculate:

$$\langle n|\hat{x}|n\rangle \propto \langle n|\hat{a}+\hat{a}^+|n\rangle$$

$$= \langle n|\left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)$$

$$= \sqrt{n}\,\underbrace{\langle n|n-1\rangle}_{=0} + \sqrt{n+1}\,\underbrace{\langle n|n+1\rangle}_{=0}$$

Therefore the first-order corrections are zero:

$$\lambda E_n^1 = 0$$

b) At second-order, we have to calculate:

$$\lambda^2 E_n^2 = \sum_{k\neq n} \frac{|\langle n|\lambda\hat{V}|k\rangle|^2}{E_n^0 - E_k^0}$$

$$= q^2 \mathcal{E}^2 \sum_{k\neq n} \frac{|\langle n|\hat{x}|k\rangle|^2}{\hbar\omega(n-k)}$$

$$= \frac{q^2\mathcal{E}^2}{\cancel{\hbar}\omega} \frac{\cancel{\hbar}}{2m\omega} \sum_{k\neq n} \frac{|\langle n|\hat{a}+\hat{a}^+|k\rangle|^2}{n-k}$$

In the term

$$\langle n|\hat{a}+\hat{a}^{+}|k\rangle =$$

$$= \sqrt{k}\underbrace{\langle n|k-1\rangle}_{=\delta_{k,n+1}} + \sqrt{k+1}\underbrace{\langle n|k+1\rangle}_{=\delta_{k,n-1}}$$

$$\Rightarrow \sum_{k\neq n} \frac{|\langle n|\hat{a}+\hat{a}^{+}|k\rangle|^2}{n-k} = \frac{|\sqrt{k}|^2}{n-k}\bigg|_{k=n+1} + \frac{|\sqrt{k+1}|^2}{n-k}\bigg|_{k=n-1}$$

$$= \frac{n+1}{\cancel{n}-\cancel{n}-1} + \frac{n}{\cancel{n}-\cancel{n}+1}$$

$$= -\cancel{n}-1+\cancel{n} = -1$$

Therefore, the final result is:

$$\lambda^2 E_n^2 = -\frac{q^2\mathcal{E}^2}{2m\omega^2}$$

Notice that this number is indep of n. This is consistent with the fact that the Total potential is:

$$\frac{1}{2}m\omega^2\hat{x}^2 + q\mathcal{E}\hat{x} = \frac{1}{2}m\omega^2\left(\hat{x}^2 + \frac{2q\mathcal{E}}{m\omega^2}\hat{x}\right) = \frac{1}{2}m\omega^2\left(x+\frac{q\mathcal{E}}{m\omega^2}\right)^2 + - \frac{q^2\mathcal{E}^2}{2m\omega^2}$$

Thus, the perturbation shifts the center of the potential by $-q\mathcal{E}/(m\omega^2)$ and lowers the energy by $q^2\mathcal{E}^2/(2\omega^2 m)$, which is in agreement with our second-order results

3) Perturbation Theory with two-parameters - (H20-9)

Instead of considering the problem with

$$\hat{H} = \hat{H}_0 + \lambda \hat{V},$$

which depends on the <u>single</u> parameter λ, consider the more general perturbation

$$\hat{H} = \hat{H}_0 + x\hat{A} + y\hat{B}$$

where x, y are two "small" numerical parameters.

In this case we expect that if:

$$\hat{H}_0 |\phi_n\rangle = E_n^0 |\phi_n\rangle$$

Then

$$\hat{H} |\psi_n(x,y)\rangle = E_n(x,y) |\psi_n(x,y)\rangle$$

with

$$E_n(x,y) = E_n^0 + x E_n^x + y E_n^y + \frac{x^2}{2} E_n^{xx} + xy E_n^{xy} + \frac{y^2}{2} E^{yy} + \dots$$

and

$$|\psi_n(x,y)\rangle = |\phi_n\rangle + x|\psi_n^x\rangle + y|\psi_n^y\rangle + \dots$$

* Example 1 *

Consider a two-dimensional system with

$$\hat{H}_0 \doteq \begin{pmatrix} E_1^0 & 0 \\ 0 & E_2^0 \end{pmatrix} \quad \text{in the basis } \{|\phi_1\rangle, |\phi_2\rangle\}$$

and $\hat{A}, \hat{B}$ are two Hermitian operators represented (H20-10) by:

$$\hat{A} \doteq \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{pmatrix} \quad \text{with } A_{11}, A_{22} \in \mathbb{R}$$

$$\hat{B} \doteq \begin{pmatrix} B_{11} & B_{12} \\ B_{21}^* & B_{22} \end{pmatrix} \quad \text{with } B_{11}, B_{22} \in \mathbb{R}.$$

The matrix H: $\hat{H} \doteq H$, with

$$H = \begin{pmatrix} E_1^0 + x A_{11} + y B_{11} & x A_{12} + y B_{12} \\ x A_{12}^* + y B_{12}^* & E_2^0 + x A_{22} + y B_{22} \end{pmatrix}$$

can be diagonalized exactly, to find $E_1(x,y)$ and $E_2(x,y)$
It is not instructive doing this calculation explicitly
(Mathematica can do it in a few seconds).
So, suppose to have calculate exactly $E_1(x,y)$ and $E_2(x,y)$
If $x, y \ll 1$, we can make a Taylor expansion up to and including second-order terms:

$$E_1(x,y) \simeq E_1^0 + x A_{11} + y B_{11} + x^2 \frac{|A_{12}|^2}{E_1^0 - E_2^0} + y^2 \frac{|B_{12}|^2}{E_1^0 - E_2^0} +$$

$$+ 2xy \, \mathrm{Re} \frac{A_{12} B_{21}}{E_1^0 - E_2^0} + \cdots$$

From this expresion we can see that troubles may arise in presence of degeneracy when $E_1^0 - E_2^0 = 0$. The usual techique to diagonalize the perturbation here does not work because if we diagonalize $\hat{A}$ so that $A_{12} = 0$, we still have $B_{12} \neq 0$ and vice verse.

The only way to overcome this problem is to reduce it to the single-variable case by defining:

$$\lambda \hat{V} \equiv x \hat{A} + y \hat{B}$$

Then it is not difficult to show that:

$$E_1(x,y) \simeq E_1^0 + \lambda V_{11}(x,y) + \lambda^2 \frac{|V_{12}|^2}{E_1^0 - E_2^0} + \dots$$

and now one can diagonalize $\lambda \hat{V}$ in the degenerate case.

* Example *

Consider the 2x2 matrices:

$$H = H_0 + xA + yB$$

where

$$H_0 = \begin{pmatrix} E^0 & 0 \\ 0 & E^0 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & a \\ a^* & 0 \end{pmatrix}; \quad B = \begin{pmatrix} 0 & b \\ b^* & 0 \end{pmatrix}$$

$$a, b \in \mathbb{C}, \quad E^0 \in \mathbb{R}$$

We can easily diagonalize H.

$$H|u_\pm\rangle = E_\pm |u_\pm\rangle$$

where $$E_\pm = E^0 \pm \Delta$$

where $$\Delta = |ax + by|$$
$$= \sqrt{x^2|a|^2 + xy(ab^* + a^*b) + y|b|^2}$$

The function $\Delta(x,y)$ has a BRANCH POINT at $x=y=0$. This implies that a Taylor expansion of the form

$$\Delta(x,y) = \Delta(0,0) + x\,\Delta_x(0,0) + y\,\Delta_y(0,0) + \cdots$$

does not exist!

For example, let us calculate.

$$\Delta_x(x,y) = \frac{\partial}{\partial x}\Delta(x,y)$$
$$= \frac{2x|a|^2 + y(ab^* + a^*b)}{2|ax+by|}$$

It is easy to see that the limit
$$\lim_{\substack{x\to 0\\ y\to 0}} \Delta_x(x,y) = \text{indeterminate}$$

In fact, if we parametrize x and y as

$$x = r\cos\theta \;,\; y = r\sin\theta \quad \text{with } r \geq 0,\ \theta \in \mathbb{R}$$

Then:

$$\Delta_x(x,y) = \underbrace{\frac{2\cos\theta\,|a|^2 + \sin\theta\,(ab^* + a^*b)}{2|a\cos\theta + b\sin\theta|}}_{\text{independent of } r!}$$

for example:

$$\Delta_x(x,y)\Big|_{\theta=0} = |a| \;, \qquad \Delta_x(x,y)\Big|_{\theta=\pi/2} = \frac{ab^* + a^*b}{2|b|}$$

So, the value of $\Delta_x(0,0)$ depends on the direction in the x,y plane approaching $x=y=0$.