Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 4

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The problems whose solutions you need to upload are designated with stars.

$\star$ Problem 1 $\star$ $\frac{1}{2}$-spin of electrons

Consider the following three operators:

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1}$$

There operators are $\frac{1}{2}$-spin operators.

1. Show that the above spin operators satisfying following commutation relation

$$[\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{S}_k \tag{2}$$

where ϵ_{ijk} is a Levi-Civita symbol:

$$\epsilon_{ijk} = \begin{cases} +1, & \text{if } (i,j,k) = (x,y,z), (y,z,x) \text{ and } (z,x,y) \\ -1, & \text{if } (i,j,k) = (z,y,x), (x,z,y) \text{ and } (y,x,z) \\ 0 & \text{if } i = j, \text{ or } j = k, \text{ or } i = k. \end{cases} \tag{3}$$

2. Show that eigenvalues of the spin operators are $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ and find the corresponding eigenvectors of all three spin operators. We will denote the eigenvectors of the spin operator $\hat{S}_i$ with eigenvalues $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ as $|i:\uparrow\rangle$ and $|i:\downarrow\rangle$ respectively. Finally show that the state $|x:\uparrow\rangle$ is superposition of $|z:\uparrow\rangle$ and $|z:\downarrow\rangle$ with equal probabilities.

3. Consider an operator defined as follows:

$$\hat{S}_{\hat{n}} = \vec{S}\cdot\hat{n} \tag{4}$$

where $\hat{\vec{S}} = \hat{S}_x\hat{x} + \hat{S}_y\hat{y} + \hat{S}_z\hat{z}$ and $\hat{n} = \sin\theta\cos\phi\hat{x} + \sin\theta\sin\phi\hat{y} + \cos\theta\hat{z}$. ($\hat{x}$, $\hat{y}$ and $\hat{z}$ are not operators! They are unit vectors.)

Show that eigenvalues of $S_{\hat{n}}$ are same to the $\hat{S}_i$ (i.e. $\pm\frac{\hbar}{2}$). If we denote the eigenvectors with $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ as $|\hat{n}:\uparrow\rangle$ and $|\hat{n}:\downarrow\rangle$, show that $\langle\hat{n}:\uparrow|\vec{S}|\hat{n}:\uparrow\rangle = \frac{\hbar}{2}\hat{n}$ and $\langle\hat{n}:\downarrow|\vec{S}|\hat{n}:\downarrow\rangle = -\frac{\hbar}{2}\hat{n}$.

4. Show that

$$e^{i\theta\frac{\hat{S}_{\hat{n}}}{\hbar}} = \hat{1}\cos\frac{\theta}{2} + i\frac{2}{\hbar}S_{\hat{n}}\sin\frac{\theta}{2} \tag{5}$$

where $\hat{1}$ is a 2×2 identity matrix. (Hint: see Problem 1 in Exercise Sheet 2)

5. Using the above results, show that
$$U(\theta,\phi)\hat{S}_z U^\dagger(\theta,\phi) = \hat{S}_{\hat{n}} \tag{6}$$
where $U(\theta,\phi) = e^{-i\phi\frac{\hat{S}_z}{\hbar}} e^{-i\theta\frac{\hat{S}_y}{\hbar}}$. Here $U(\theta,\phi)$ is the rotation matrix with Euler angles θ and ϕ.

Solution 1

1. Set $\sigma_i = \frac{2}{\hbar}\hat{S}_i$ then
$$\sigma_x^2 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \hat{1}, \tag{7}$$
$$\sigma_y^2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \hat{1}, \tag{8}$$
$$\sigma_z^2 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \hat{1}, \tag{9}$$
$$\sigma_x\sigma_y = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} = i\sigma_z, \tag{10}$$
$$\sigma_y\sigma_x = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix} = -i\sigma_z, \tag{11}$$
$$\sigma_y\sigma_z = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0 & i\\ i & 0\end{pmatrix} = i\sigma_x, \tag{12}$$
$$\sigma_z\sigma_y = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix} = -i\sigma_x, \tag{13}$$
$$\sigma_z\sigma_x = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = i\sigma_y, \tag{14}$$
$$\sigma_x\sigma_z = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = -i\sigma_y, \tag{15}$$
$$\tag{16}$$
From the above relations, we can easily show that
$$[\sigma_i, \sigma_y] = 2i\epsilon_{ijk}\sigma_k \tag{17}$$
which results in $[\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{S}_k$.

2. We will use σ_i. Let me start with σ_z. It is obvious that the eigenvalues of the σ_z are ± 1. Corresponding eigenvectors are given by
$$+1 : |z:\uparrow\rangle = \begin{pmatrix}1\\ 0\end{pmatrix}, \tag{18}$$
$$-1 : |z:\downarrow\rangle = \begin{pmatrix}0\\ 1\end{pmatrix} \tag{19}$$
Now let us consider σ_x. To find eigenvalues we need to solve $\det(\sigma_x - \lambda\hat{1}) = 0$
$$\det(\sigma_x - \lambda) = \det\begin{pmatrix}-\lambda & 1\\ 1 & -\lambda\end{pmatrix} = \lambda^2 - 1 = 0 \tag{20}$$
$$\Rightarrow \lambda = \pm 1 \tag{21}$$
So the eigenvalues are same to that of σ_z. The eigenvectors can be obtained as follows:
$$(\sigma_x - 1)|x:\uparrow\rangle = 0 \Rightarrow |x:\uparrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix} \tag{22}$$
$$(\sigma_x + 1)|x:\downarrow\rangle = 0 \Rightarrow |x:\downarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix} \tag{23}$$

For σ_y, we follow the same procedure then we can find that eigenvalues are ± 1 and eigenvectors are given by

$$|y:\uparrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} \tag{24}$$

$$|y:\downarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix} \tag{25}$$

Now let us express $|x:\uparrow\rangle$ using eigenvectors of $\hat{S}_z$

$$|x:\uparrow\rangle = a_\uparrow|z:\uparrow\rangle + a_\downarrow|z:\downarrow\rangle, \tag{26}$$

$$\Rightarrow \begin{cases} a_\uparrow = \langle z:\uparrow|x:\uparrow\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}, \\ a_\downarrow = \langle z:\downarrow|x:\uparrow\rangle = \begin{pmatrix}0 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}} \end{cases}. \tag{27}$$

As a result, the probability of the $|x:\uparrow\rangle$ being observed with $|z:\uparrow\rangle$ and $|z:\downarrow\rangle$ is the same

$$|a_\uparrow|^2 = |a_\downarrow|^2 = \frac{1}{2}. \tag{28}$$

3. A matrix representation of the operator $\hat{S}_{\hat{n}}$ is given by

$$\begin{aligned}\frac{2}{\hbar}\hat{S}_{\hat{n}} &= \begin{pmatrix}0 & \sin\theta\cos\phi\\ \sin\theta\cos\phi & 0\end{pmatrix} + \begin{pmatrix}0 & -i\sin\theta\sin\phi\\ i\sin\theta\sin\phi & 0\end{pmatrix} + \begin{pmatrix}\cos\theta & 0\\ 0 & -\cos\theta\end{pmatrix}\\ &= \begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}\end{aligned} \tag{29}$$

Following the same procedure in the problem 2, we can get following eigenvalues and eigenvectors:

$$\det\left(\frac{2}{\hbar}\hat{S}_{\hat{n}} - \lambda\hat{1}\right) = (\cos\theta - \lambda)(-\cos\theta - \lambda) - \sin^2\theta = \lambda^2 - 1 = 0 \tag{30}$$

$$\therefore \lambda = \pm 1 \tag{31}$$

$$\lambda = 1: \begin{pmatrix}\cos\theta - 1 & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta - 1\end{pmatrix}|\hat{n}:\uparrow\rangle = 0 \Rightarrow |\hat{n}:\uparrow\rangle = \begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix} \tag{32}$$

$$\lambda = -1: \begin{pmatrix}\cos\theta + 1 & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -\cos\theta + 1\end{pmatrix}|\hat{n}:\downarrow\rangle = 0 \Rightarrow |\hat{n}:\downarrow\rangle = \begin{pmatrix}\sin\frac{\theta}{2}\\ -\cos\frac{\theta}{2}e^{i\phi}\end{pmatrix} \tag{33}$$

Using the above results, let us calculate the $\langle\hat{n}:\uparrow|\vec{\hat{S}}|\hat{n}:\uparrow\rangle$ first.

$$\begin{aligned}\frac{2}{\hbar}\langle\hat{n}:\uparrow|\hat{S}_x|\hat{n}:\uparrow\rangle &= \begin{pmatrix}\cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{-i\phi}\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix} = \begin{pmatrix}\sin\frac{\theta}{2}e^{-i\phi} & \cos\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}\\ &= 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\cos\phi = \sin\theta\cos\phi,\end{aligned} \tag{34}$$

$$\begin{aligned}\frac{2}{\hbar}\langle\hat{n}:\uparrow|\hat{S}_y|\hat{n}:\uparrow\rangle &= \begin{pmatrix}\cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{-i\phi}\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix} = \begin{pmatrix}i\sin\frac{\theta}{2}e^{-i\phi} & -i\cos\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}\\ &= 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\sin\phi = \sin\theta\sin\phi,\end{aligned} \tag{35}$$

$$\begin{aligned}\frac{2}{\hbar}\langle\hat{n}:\uparrow|\hat{S}_z|\hat{n}:\uparrow\rangle &= \begin{pmatrix}\cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{-i\phi}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix} = \begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{-i\phi}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}\\ &= \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = \cos\theta\end{aligned} \tag{36}$$

As a result, $\langle \hat{n} :\uparrow | \vec{\hat{S}} | \hat{n} :\uparrow \rangle = \frac{\hbar}{2}\hat{n}$.

For $\langle \hat{n} :\downarrow \vec{\hat{S}} | \hat{n} :\downarrow \rangle$ following the same procedure, we can get

$$\begin{aligned}
\frac{2}{\hbar}\langle \hat{n} :\downarrow | \hat{S}_x | \hat{n} :\downarrow \rangle &= \begin{pmatrix} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{-i\phi} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} -\cos\frac{\theta}{2}e^{-i\phi} & \sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} \\
&= -2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\cos\phi = -\sin\theta\cos\phi, \qquad (37) \\
\frac{2}{\hbar}\langle \hat{n} :\downarrow | \hat{S}_y | \hat{n} :\downarrow \rangle &= \begin{pmatrix} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{-i\phi} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} -i\cos\frac{\theta}{2}e^{-i\phi} & -i\sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} \\
&= -2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\sin\phi = -\sin\theta\sin\phi, \qquad (38) \\
\frac{2}{\hbar}\langle \hat{n} :\downarrow | \hat{S}_z | \hat{n} :\downarrow \rangle &= \begin{pmatrix} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{-i\phi} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} \sin\frac{\theta}{2} & \cos\frac{\theta}{2}e^{-i\phi} \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} \\
&= -\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} = -\cos\theta \qquad (39)
\end{aligned}$$

Therefore $\langle \hat{n} :\downarrow | \vec{\hat{S}} | \hat{n} :\downarrow \rangle = -\frac{\hbar}{2}\hat{n}$.

4. Using Taylor expansion

$$e^{i\theta\frac{\hat{S}_{\hat{n}}}{\hbar}} = \sum_{k=0}^{\infty} \frac{1}{k!} i^k \left(\frac{\theta}{2}\right)^k \left(\frac{2}{\hbar}\hat{S}_{\hat{n}}\right)^k \qquad (40)$$

Using Eq. (29),

$$\begin{aligned}
&k = 1: \quad \tfrac{2}{\hbar}\hat{S}_n = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \\
&k = 2: \quad \left(\tfrac{2}{\hbar}\hat{S}_n\right)^2 = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1} \\
&\Rightarrow \begin{cases} \left(\frac{\hbar}{2}\hat{S}_{\hat{n}}\right)^k = \frac{\hbar}{2}\hat{S}_{\hat{n}}, & \text{when } k \text{ is even}(k > 0) \\ \left(\frac{\hbar}{2}\hat{S}_{\hat{n}}\right)^k = \hat{1}, & \text{when } k \text{ is odd}(k > 0) \end{cases}. \qquad (41)
\end{aligned}$$

Using the above results,

$$\begin{aligned}
e^{i\theta\frac{\hat{S}_{\hat{n}}}{\hbar}} &= \hat{1} + \sum_{k=\text{odd}(>0)} \frac{1}{k!} i^k \left(\frac{\theta}{2}\right)^k \frac{2}{\hbar}\hat{S}_{\hat{n}} + \sum_{k=\text{even}(>0)} \frac{1}{k!} i^k \left(\frac{\theta}{2}\right)^k \hat{1} \\
&= \hat{1} + \sum_{n=1}^{\infty} \frac{1}{(2n-1)!} i^{2n-1} \left(\frac{\theta}{2}\right)^{2n-1} \frac{2}{\hbar}\hat{S}_{\hat{n}} + \sum_{n=1}^{\infty} \frac{1}{(2n)!} i^{2n} \left(\frac{\theta}{2}\right)^{2n} \hat{1} \\
&= \hat{1} + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{(2n-1)!} \left(\frac{\theta}{2}\right)^{2n-1} i\frac{2}{\hbar}\hat{S}_{\hat{n}} + \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} \left(\frac{\theta}{2}\right)^{2n} \hat{1} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \left(\frac{\theta}{2}\right)^{2n} \hat{1} + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{(2n-1)!} \left(\frac{\theta}{2}\right)^{2n-1} i\frac{2}{\hbar}\hat{S}_{\hat{n}} \\
&= \cos\frac{\theta}{2}\hat{1} + \sin\frac{\theta}{2} i\frac{2}{\hbar}\hat{S}_{\hat{n}}. \qquad (42)
\end{aligned}$$

Alternatively, one can exploit the fact that we have previously diagonalized $\hat{S}_{\hat{n}}$ to find its exponential, as explained in the solutions to Exercise Sheet 2.

5. First let us find a matrix representation of $U(\theta,\phi)$.

$$
\begin{aligned}
U(\theta,\phi) = e^{-i\phi\frac{\hat{S}_z}{\hbar}} e^{-i\theta\frac{\hat{S}_y}{\hbar}} &= \Big(\cos\frac{\phi}{2}\hat{1} - i\sin\frac{\phi}{2}\frac{2}{\hbar}\hat{S}_z\Big)\Big(\cos\frac{\theta}{2}\hat{1} - i\sin\frac{\theta}{2}\frac{2}{\hbar}\hat{S}_y\Big) \\
&= \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix}
\end{aligned}
\tag{43}
$$

$$
\begin{aligned}
U(\theta,\phi)\hat{S}_z U^\dagger(\theta,\phi) &= \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} & -e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} & 2e^{-i\phi}\cos\frac{\theta}{2}\sin\frac{\theta}{2} \\ 2e^{i\phi}\cos\frac{\theta}{2}\sin\frac{\theta}{2} & -\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{-i\phi}\sin\theta & -\cos\theta \end{pmatrix} \\
&= \hat{S}_{\hat{n}}
\end{aligned}
\tag{44}
$$

⋆ Problem 2 ⋆ Projectors and spectral decomposition

Let $\hat{A}$ be a Hermitian operator with a discrete, non-degenerate spectrum (every eigenvalue has only one eigenvector)

$$
\hat{A}|n\rangle = a_n|n\rangle,\ n \in \mathrm{N}
\tag{45}
$$

where a_n is the eigenvalue of the (normalized) eigenstate $|n\rangle$. We define

$$
\hat{P}_n = |n\rangle\langle n|
\tag{46}
$$

as a projector on the eigenspace spanned by the eigenvector $|n\rangle$.

1. Show that for any state $|\psi\rangle$ a following equation holds

$$
\hat{A}\hat{P}_n|\psi\rangle = a_n\hat{P}_n|\psi\rangle
\tag{47}
$$

2. Show that this is true

$$
\hat{P}_n\hat{P}_m = \delta_{nm}\hat{P}_n
\tag{48}
$$

3. Express $\hat{A}$ using the operators $\hat{P}_n$. To do this, use the completeness of the $|n\rangle$ states (i.e. $\sum_n |n\rangle\langle n| = \hat{1}$)
4. The probability for a state $|\psi\rangle$ to be measured with eigenvalue n is given by

$$
P_{|\psi\rangle}(n) = |\langle n|\psi\rangle|^2
\tag{49}
$$

   Express $P_{|\psi\rangle}(n)$ using $\hat{P}_n$ and $|\psi\rangle$.

Now let $\hat{B}$ be a Hermitian operator with a purely continuous spectrum (such as the momentum operator $\hat{p}$):

$$
\hat{B}|b\rangle = b|b\rangle,\ b \in \mathrm{R}
\tag{50}
$$

These eigenstates satisfy following properties:

$$
\langle b|b'\rangle = \delta(b - b'),\ \int db|b\rangle\langle b| = \hat{1}
\tag{51}
$$

In analogy to Eq. (46), we now define the projector for the eigenvalues between α and β ($\alpha < \beta$)

$$
\hat{P}_{[\alpha,\beta]} = \int_\alpha^\beta db|b\rangle\langle b|.
\tag{52}
$$

5. Show that $\hat{P}_{[\alpha,\beta]}\hat{P}_{[\gamma,\delta]} = \hat{P}_{[\alpha,\beta]\cap[\gamma,\delta]}$.

6. Express the probability of measuring a value within the interval $[\alpha, \beta]$ when measuring the observable $\hat{B}$ from the state $|\psi\rangle$ using the projector $\hat{P}_{[\alpha,\beta]}$.

7. Now let $\hat{B} = \hat{p}$ be the momentum operator. Let the wave function in momentum representation be

$$\psi(p) = \langle p|\psi\rangle = \begin{cases} \frac{1}{\sqrt{2p_0}}, & \text{for} |p| < p_0 \\ 0 & \text{otherwise} \end{cases} \tag{53}$$

Using the above projectors, calculate the probability of measuring a particle with momentum $p > 0$ given a measurement of $|\psi\rangle$.

Solution 2

1. We expand the state $|\psi\rangle$ into the eigenstates of the Hermitian operator $\hat{A}$ (since its eigenstates are complete $\sum_n |n\rangle\langle n| = \hat{1}$ and orthonormal $\langle n|m\rangle = \delta_{nm}$)

$$|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle = \sum_n \psi_n|n\rangle \;\; (\langle n|\psi\rangle \equiv \psi_n) \tag{54}$$

Then

$$\hat{P}_n|\psi\rangle = |n\rangle\langle n| \sum_m \psi_m|m\rangle = |n\rangle \sum_m \psi_m\delta_{mn} = \psi_n|n\rangle \tag{55}$$

Obviously, $\hat{P}_n$ is really the projector to the $|n\rangle$ state and it holds

$$\hat{A}\hat{P}_n|\psi\rangle = \psi_n\hat{A}|n\rangle = \psi_n a_n|n\rangle = a_n\psi_n|n\rangle = a_n\hat{P}_n|\psi\rangle \tag{56}$$

2. Taking advantage of the orthogonality of the eigenstates of $\hat{A}$, it is easy to show that

$$\hat{P}_n\hat{P}_m = |n\rangle\langle n|m\rangle\langle m| = \delta_{nm}|n\rangle\langle n| = \delta_{nm}\hat{P}_n \tag{57}$$

3. We can express $\hat{A}$ using the projector as follows:

$$\hat{A} = \hat{1}\hat{A}\hat{1} = \sum_{n,m} |n\rangle\langle n|\hat{A}|m\rangle\langle m| = \sum_{n,m} a_m|n\rangle\langle n|m\rangle\langle m| = \sum_n a_n|n\rangle\langle n| = \sum_n a_n\hat{P}_n \tag{58}$$

4. We can express the probability for the state $|\psi\rangle$ to be measured with the eigenvalue a_n as follows:

$$P_{|\psi\rangle}(n) = |\langle n|\psi\rangle|^2 = \langle\psi|n\rangle\langle n|\psi\rangle = \langle\psi|\hat{P}_n|\psi\rangle = \langle\hat{P}_n\rangle \tag{59}$$

5. We consider

$$\hat{P}_{[\alpha,\beta]}\hat{P}_{[\gamma,\delta]} = \int_\alpha^\beta db \int_\gamma^\delta db'|b\rangle\langle b|b'\rangle\langle b'| \tag{60}$$

and now divide the first integral

$$\int_\alpha^\beta db = \int_\alpha^\beta \Big|_{b\in[\gamma,\delta]} db + \int_\alpha^\beta \Big|_{b\neq[\gamma,\delta]} db \tag{61}$$

so that

$$\begin{aligned} \hat{P}_{[\alpha,\beta]}\hat{P}_{[\gamma,\delta]} &= \int_\alpha^\beta \Big|_{b\in[\gamma,\delta]} db \int_\gamma^\delta db'\delta(b-b')|b\rangle\langle b'| + \int_\alpha^\beta \Big|_{b\neq[\gamma,\delta]} db \int_\gamma^\delta db'\delta(b-b')|b\rangle\langle b'| \\ &= \int_\alpha^\beta \Big|_{b\in[\gamma,\delta]} db|b\rangle\langle b| = \int_{[\alpha,\beta]\cap[\gamma,\delta]} db|b\rangle\langle b| = \hat{P}_{[\alpha,\beta]\cap[\gamma,\delta]} \end{aligned} \tag{62}$$

6. We first express $|\psi\rangle$ in terms of the $|b\rangle$ eigenstates

$$|\psi\rangle = \hat{1}|\psi\rangle = \int db|b\rangle\langle b|\psi\rangle = \int db\psi(b)|b\rangle \tag{63}$$

The probability for $|\psi\rangle$ to be in state $|b\rangle$ is then given by $|\psi(b)|^2 db$. This means that the probability of b being in $[\alpha, \beta]$ is given by

$$\begin{aligned} W([\alpha,\beta]) &= \int_\alpha^\beta |\psi(b)|^2 db = \int_\alpha^\beta db\langle b|\psi\rangle^* \langle b|\psi\rangle = \langle\psi|[\int_\alpha^\beta db|b\rangle\langle b|]|\psi\rangle \\ &= \langle\psi|\hat{P}_{[\alpha,\beta]}|\psi\rangle = \langle\hat{P}_{[\alpha,\beta]}\rangle \end{aligned} \tag{64}$$

7. With Eq. (64), probability that the state measured with $p > 0$ is given by

$$W([0,\infty]) = \int_0^\infty |\psi(p)|^2 dp = \int_0^{p_0} \frac{1}{2p_0} dp = \frac{1}{2}. \tag{65}$$

Problem 3 Free particle in a homogeneous field

A homogeneous field acting on a particle is determined by the potential

$$V(x) = -Fx \tag{66}$$

The Schrödinger equation for this system has the form of the Airy differential equation in spatial space

$$f^{''}(x) - xf(x) = 0 \tag{67}$$

However, the solution to this problem is easier to find in momentum space.

1. Give the momentum space representation for the Schrödinger equation of a particle in a homogeneous field.
2. Determine the wave function $\psi(p)$ that solves the Schrödinger equation,
3. Show that this solution, when transformed back into real space, becomes the implicit equation for the Airy function

$$A_i(\xi) = \int \frac{du}{\pi} \cos\Big(\frac{u^3}{3} + \xi\Big). \tag{68}$$

Solution 3

1. In momentum space, the Schrödinger equation is given by the first-order differential equation

$$\frac{p^2}{2m}\psi(p) - i\hbar F\frac{d\psi(p)}{dp} = E\psi(p) \tag{69}$$

2. This differential equation can be solved by separating the variables

$$-i\frac{1}{\psi}d\psi = \frac{1}{\hbar F}\Big(E - \frac{p^2}{2m}\Big)dp \tag{70}$$

and integration on both sides leads to

$$-i\log\left(\frac{\psi(p)}{\psi_0}\right) = \frac{1}{\hbar F}\left(Ep - \frac{p^3}{6m}\right) \tag{71}$$

This gives the wave function in momentum space

$$\psi(p) \propto \exp\left(i\frac{E}{\hbar F}p - i\frac{p^3}{6m\hbar F}\right) \tag{72}$$

3. Using Fourier transformation

$$\psi(x) = \int \frac{dp}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}} \psi(p) \propto \int dp \exp\left(i\left[\frac{p}{\hbar}\left(x + \frac{E}{F}\right) - \frac{p^3}{6m\hbar F}\right]\right) \tag{73}$$

In the above equation, the energy E is related to the shift in x by $x_0 = -EF$. This is precisely the classic reversal point where $E = V(x_0)$. Defining a length scale l: $l^3 = \frac{\hbar^2}{2m|F|}$ then

$$\psi(x) \propto \int \frac{dp}{\sqrt{2\pi\hbar}} \exp\left(i\left[\frac{pl}{\hbar}\frac{x - x_0}{l} - \text{sgn}(F)\frac{p^3 l^3}{3\hbar^3}\right]\right) \tag{74}$$

Let's introduce the dimensionless variables:

$$\xi = (x - x_0)/l, \quad u = \frac{pl}{\hbar}. \tag{75}$$

Since $\sin(x)$ is a odd function in x, we will get

$$\psi(\xi) \propto \int du \cos\left(\frac{u^3}{3} - \text{sgn}(F)\xi u\right) \tag{76}$$

This is just the implicit equation for the Airy function given by

$$\psi(\xi) \propto A_i(-\,\text{sgn}(F)\xi) \tag{77}$$