NST Part II Physics | Michaelmas Term 2021

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ADVANCED QUANTUM PHYSICS

Examples Sheet Solutions - Revision

1. **Operator methods and measurement**

(a) We are told that $\hat{H}|\psi_1\rangle = E_1|\psi_1\rangle$ and $\hat{H}|\psi_2\rangle = E_2|\psi_2\rangle$, where $E_1 \neq E_2$. Therefore

$$\langle\psi_1|\hat{H}|\psi_2\rangle = \int \psi_1^* \hat{H}\psi_2 \,\mathrm{d}x = \int \psi_1^* E_2 \psi_2 \,\mathrm{d}x = E_2\langle\psi_1|\psi_2\rangle\,.$$

Since $\hat{H}$ is Hermitian, the eigenvalues E_1 and E_2 are real, and we can write

$$\langle\psi_1|\hat{H}|\psi_2\rangle = \int (\hat{H}\psi_1)^*\psi_2 \,\mathrm{d}x = \int (E_1\psi_1)^*\psi_2 \,\mathrm{d}x = E_1^*\langle\psi_1|\psi_2\rangle = E_1\langle\psi_1|\psi_2\rangle\,.$$

Therefore $(E_1 - E_2)\langle\psi_1|\psi_2\rangle = 0$ and, if $E_1 \neq E_2$ we must have $\langle\psi_1|\psi_2\rangle = 0$.

(b) Adding and subtracting the relations $\hat{A}|\psi_1\rangle = |\psi_2\rangle$ and $\hat{A}|\psi_2\rangle = |\psi_1\rangle$ gives

$$\hat{A}(|\psi_1\rangle + |\psi_2\rangle) = |\psi_1\rangle + |\psi_2\rangle\,, \qquad \hat{A}(|\psi_1\rangle - |\psi_2\rangle) = -(|\psi_1\rangle - |\psi_2\rangle)\,.$$

Hence $\hat{A}$ has an eigenvalue $a = +1$ corresponding to a normalized eigenvector $(|\psi_1\rangle + |\psi_2\rangle)/\sqrt{2}$ and an eigenvalue $a = -1$ corresponding to eigenvector $(|\psi_1\rangle - |\psi_2\rangle)/\sqrt{2}$.

(c) The initial measurement of $\hat{A}$, giving the result $a = -1$, puts the system into the corresponding eigenstate of $\hat{A}$:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\big[|\psi_1\rangle - |\psi_2\rangle\big]\,.$$

The time-dependent Schrödinger equation is $\hat{H}\psi = E\psi = i\hbar(\partial\psi/\partial t)$; hence the eigenstates of $\hat{H}$ evolve with time dependence $e^{-iEt/\hbar}$. Thus the system evolves as

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[|\psi_1\rangle e^{-iE_1 t/\hbar} - |\psi_2\rangle e^{-iE_2 t/\hbar}\right]\,.$$

The probability that a measurement of $\hat{A}$ again gives the result $a = -1$ is then

$$\begin{aligned} P(t) = |\langle\psi(0)|\psi(t)\rangle|^2 &= \frac{1}{4}\Big|\big[\langle\psi_1| - \langle\psi_2|\big]\big[|\psi_1\rangle e^{-iE_1 t/\hbar} - |\psi_2\rangle e^{-iE_2 t/\hbar}\big]\Big|^2 \\ &= \frac{1}{2}\big[1 + \cos((E_1 - E_2)t/\hbar)\big] = \cos^2((E_1 - E_2)t/2\hbar)\,. \end{aligned}$$

2. **Probability flux**

$$\psi = Ae^{ikx} + Be^{-ikx}$$

$$\begin{aligned}
j &= \frac{\hbar}{2mi}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right) \\
&= \frac{\hbar}{2mi}[\left(A^*e^{-ikx} + B^*e^{ikx}\right) ik \left(Ae^{ikx} - Be^{-ikx}\right) \\
&\qquad\qquad - \left(Ae^{ikx} + Be^{-ikx}\right)(-ik)\left(A^*e^{-ikx} - B^*e^{ikx}\right)] \\
&= \frac{\hbar k}{2m}[\left(|A|^2 - |B|^2 - A^*Be^{-2ikx} + B^*Ae^{2ikx}\right) \\
&\qquad\qquad + \left(|A|^2 - |B|^2 - AB^*e^{2ikx} + BA^*e^{-2ikx}\right)] \\
&= \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right)
\end{aligned}$$

3. **Ladder operators**

(a) From the definitions of $\hat{a}$ and $\hat{a}^\dagger$, we have

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

Using $\langle n|\hat{a}|n\rangle = \sqrt{n}\langle n|n-1\rangle = 0$ and $\langle n|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\langle n|n+1\rangle = 0$ then gives

$$\boxed{\langle n|\hat{x}|n\rangle = \langle n|\hat{p}|n\rangle = 0}\,.$$

(b) The expectation value of the potential $V(x) = (1/2)m\omega^2x^2$ requires $\langle \hat{x}^2\rangle$:

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

$$\begin{aligned}
\langle n|\hat{x}^2|n\rangle &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{\hbar}{2m\omega}\left[\sqrt{n}\sqrt{n-1}\langle n|n-2\rangle + \sqrt{n+1}\sqrt{n+2}\langle n|n+2\rangle + (n+1)\langle n|n\rangle + n\langle n|n\rangle\right] \\
&= \frac{\hbar}{2m\omega}(2n+1)\ .
\end{aligned}$$

Hence

$$\langle n|V(\hat{x})|n\rangle = \frac{1}{2}m\omega^2\,\frac{\hbar}{2m\omega}(2n+1) = \frac{1}{2}(n+1/2)\hbar\omega\ .$$

(c) The uncertainties Δx and Δp are given by

$$(\Delta x)^2 \equiv \langle \hat{x}^2\rangle - \langle \hat{x}\rangle^2 = \frac{\hbar}{2m\omega}(2n+1) - 0 = \frac{\hbar}{2m\omega}(2n+1)$$

$$(\Delta p)^2 \equiv \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2 = \frac{m\hbar\omega}{2}(2n+1) - 0 = \frac{m\hbar\omega}{2}(2n+1)$$

Hence

$$\boxed{\Delta x \Delta p = \hbar(n+1/2)}\ .$$

4. **Matrix methods**

The basis states $|\phi_1\rangle = |Y_{11}\rangle$, $|\phi_0\rangle = |Y_{10}\rangle$, $|\phi_{-1}\rangle = |Y_{1,-1}\rangle$ are eigenstates of $\hat{L}_z$, with eigenvalues $+\hbar$, 0, $-\hbar$. Therefore the matrix representation of $\hat{L}_z$ is diagonal:

$$\hat{L}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \ .$$

The ladder operators $\hat{L}_\pm$ act on the basis states as

$$\hat{L}_\pm |\ell m\rangle = \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}|\ell, m\pm 1\rangle\ ,$$

from which we can straightforwardly obtain the matrix representations

$$\hat{L}_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \ ; \qquad \hat{L}_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \ .$$

From these we can infer

$$\hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-) = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} ; \qquad \hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-) = i\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} .$$

Using these results, the operator

$$\hat{H} = \frac{\hat{L}_x^2}{2I_x} + \frac{\hat{L}_y^2}{2I_y} + \frac{\hat{L}_z^2}{2I_z}$$

can then be written in matrix form as

$$\hat{H} = \frac{\hbar^2}{4} \begin{pmatrix} I_x^{-1} + I_y^{-1} + 2I_z^{-1} & 0 & I_x^{-1} - I_y^{-1} \\ 0 & 2I_x^{-1} + 2I_y^{-1} & 0 \\ I_x^{-1} - I_y^{-1} & 0 & I_x^{-1} + I_y^{-1} + 2I_z^{-1} \end{pmatrix} \ .$$

The eigenvalues can be found by subtracting E from the diagonal of this matrix, and setting the determinant to zero, yielding

$$\left(\frac{\hbar^2}{4I_x} + \frac{\hbar^2}{4I_y} + \frac{\hbar^2}{2I_z} - E\right)^2 \left(\frac{\hbar^2}{2I_x} + \frac{\hbar^2}{2I_y} - E\right) = \left(\frac{\hbar^2}{4I_x} - \frac{\hbar^2}{4I_y}\right)^2 \left(\frac{\hbar^2}{2I_x} + \frac{\hbar^2}{2I_y} - E\right),$$

from which we readily obtain the energy eigenvalues and eigenstates:

$$\frac{\hbar^2}{2}\left(\frac{1}{I_x} + \frac{1}{I_y}\right) \qquad \frac{\hbar^2}{2}\left(\frac{1}{I_x} + \frac{1}{I_z}\right) \qquad \frac{\hbar^2}{2}\left(\frac{1}{I_y} + \frac{1}{I_z}\right)$$

$$\begin{pmatrix}0\\1\\0\end{pmatrix} \qquad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix} \qquad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}$$

5. **Spin**

The spin operator in the (θ, ϕ) direction, $\hat{\boldsymbol{S}}_{\theta\phi}$, can be found by forming the scalar product $\hat{\boldsymbol{S}} \cdot \boldsymbol{n}$ of the spin operator $\hat{\boldsymbol{S}}$ with a unit vector $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ in the (θ, ϕ) direction. In the basis of states $|\uparrow\rangle_z$, $|\downarrow\rangle_z$, the operator $\hat{\boldsymbol{S}}$ has matrix representation $\hat{\boldsymbol{S}} = (\hbar/2)\boldsymbol{\sigma}$, where the σ_i are the Pauli matrices. Therefore

$$\hat{\boldsymbol{S}}_{\theta\phi} = \frac{\hbar}{2}\begin{pmatrix}\cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta\end{pmatrix}.$$

We need the eigenvalues of the matrix, i.e.

$$\frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta\end{pmatrix}\begin{pmatrix}u\\v\end{pmatrix} = \lambda\begin{pmatrix}u\\v\end{pmatrix}.$$

Eliminating u and v, we find $\lambda^2 = 1$ and hence the eigenvalues of $\hat{\boldsymbol{S}}_{\theta\phi}$ are $\pm\hbar/2$, as expected. Substituting the values $\lambda = \pm 1$ back into the equations relating u and v, we can infer the ratios, $u/v = e^{-i\phi}\cot(\theta/2)$ and $-e^{-i\phi}\tan(\theta/2)$. So, in matrix notation, the eigenstates are

$$|\uparrow\rangle_{\theta\phi} = \begin{pmatrix}\cos(\theta/2)\\ e^{i\phi}\sin(\theta/2)\end{pmatrix}, \qquad |\downarrow\rangle_{\theta\phi} = \begin{pmatrix}\sin(\theta/2)\\ -e^{i\phi}\cos(\theta/2)\end{pmatrix},$$

(up to multiplication by arbitrary overall phases) for eigenvalues $+\hbar/2$ and $-\hbar/2$ respectively.

The spin states in the x-direction are obtained by setting $\theta = \pi/2$, $\phi = 0$:

$$|\uparrow\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_z + |\downarrow\rangle_z\big), \qquad |\downarrow\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_z - |\downarrow\rangle_z\big).$$

The spin states in the y-direction are obtained by setting $\theta = \pi/2$, $\phi = \pi/2$:

$$|\uparrow\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_z + i|\downarrow\rangle_z\big), \qquad |\downarrow\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_z - i|\downarrow\rangle_z\big).$$

6. **Identical particles**

A single particle in the potential well has the (unnormalized) wavefunction $\psi_n(x) = \sin(n\pi x/L)$, and energy $E = (\hbar^2\pi^2/2mL^2)n^2 \equiv \epsilon n^2$. The wavefunction for a system of two indistinguishable particles must be either symmetric or antisymmetric under particle interchange $1 \leftrightarrow 2$, i.e.

$$\psi(x_1, x_2) = \sin(n_1\pi x_1/L)\sin(n_2\pi x_2/L) \pm \sin(n_2\pi x_1/L)\sin(n_1\pi x_2/L),$$

with energy $(n_1^2 + n_2^2)\epsilon$. If $E = 5\epsilon$, we must have $n_1 = 1$, and $n_2 = 2$ (or *vice versa*).

(a) Spin-zero particles are bosons and must have a symmetric wavefunction,

$$\begin{aligned}\psi(x_1, x_2) &= \sin(\pi x_1/L)\sin(2\pi x_2/L) + \sin(2\pi x_1/L)\sin(\pi x_2/L)\\ &= 2\sin(\pi x_1/L)\sin(\pi x_2/L)\left[\cos(\pi x_1/L) + \cos(\pi x_2/L)\right] .\end{aligned}$$

This has zeros for $x_1 = 0$, $x_1 = L$, $x_2 = 0$, $x_2 = L$, and $x_1 + x_2 = L$.

(b) Spin 1/2 particles are fermions and must have an antisymmetric wavefunction. In the singlet case, the spin wavefunction is antisymmetric, and hence the spatial wavefunction is symmetric, just as in (a).

(c) In the triplet case, the spin wavefunction is symmetric, and hence the spatial wavefunction must be antisymmetric, i.e.

$$\begin{aligned}\psi(x_1, x_2) &= \sin(\pi x_1/L)\sin(2\pi x_2/L) - \sin(2\pi x_1/L)\sin(\pi x_2/L)\\ &= 2\sin(\pi x_1/L)\sin(\pi x_2/L)\left[\cos(\pi x_1/L) - \cos(\pi x_2/L)\right] .\end{aligned}$$

This has zeros for $x_1 = 0$, $x_1 = L$, $x_2 = 0$, $x_2 = L$, and $x_1 = x_2$.

If the particles were charged, they would repel each other through the Coulomb interaction. Therefore, in the spin 1/2 case, the triplet state would have the lower energy, because the particles tend to be further apart. This is an example of the exchange interaction, and is a simplified model of what happens in the Helium atom.

7. **Heisenberg picture**

The time derivative of a Heisenberg picture operator $\hat{A}(t) \equiv e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}$ is

$$\frac{\mathrm{d}\hat{A}(t)}{\mathrm{d}t} = \frac{i\hat{H}}{\hbar}e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar} - e^{i\hat{H}t/\hbar}\hat{A}\frac{i\hat{H}}{\hbar}e^{-i\hat{H}t/\hbar} = \frac{i}{\hbar}e^{i\hat{H}t/\hbar}[H, A]e^{-i\hat{H}t/\hbar} ,$$

giving the equation of motion

$$\frac{\mathrm{d}\hat{A}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[H, \hat{A}(t)] .$$

For the one-dimensional harmonic oscillator, the Hamiltonian is

$$\hat{H} = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega ,$$

where the ladder operators $\hat{a}$ and $\hat{a}^\dagger$ satisfy the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$. Therefore $[\hat{a}^\dagger\hat{a}, \hat{a}] = -\hat{a}$, and the commutator of the Hamiltonian with $\hat{a}$ is given by

$$[\hat{H}, \hat{a}] = -\hbar\omega\hat{a} .$$

Thus also

$$[\hat{H}, \hat{a}(t)] = -\hbar\omega\hat{a}(t) ,$$

and the Heisenberg equation of motion for $\hat{a}(t)$ is therefore

$$\frac{\mathrm{d}\hat{a}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{a}(t)] = -i\omega\hat{a}(t) .$$

We can integrate this to find that

$$\boxed{\hat{a}(t) = e^{-i\omega t}\hat{a}(0)\ , \qquad \hat{a}^\dagger(t) = e^{i\omega t}\hat{a}^\dagger(0)}\,.$$

From the definition of the ladder operators, the position operator is

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

This relation holds also for the operators in the Heisenberg picture. We have

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = \sqrt{\frac{\hbar}{2m\omega}}\left(-i\omega\hat{a} + i\omega\hat{a}^\dagger\right) = \sqrt{\frac{\hbar\omega}{2m}}(-i)\left(\hat{a} - \hat{a}^\dagger\right) = \frac{\hat{p}}{m}\ .$$

For a more general Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})\ ,$$

the Heisenberg equation of motion gives

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)] = \frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m}, \hat{x}(t)\right]\ .$$

Repeatedly using $[\hat{x}, \hat{p}] = i\hbar$, the commutator $[\hat{p}^2, \hat{x}]$ is

$$[\hat{p}^2, \hat{x}] = \hat{p}\hat{p}\hat{x} - \hat{x}\hat{p}\hat{p} = \hat{p}(\hat{x}\hat{p} - i\hbar) - (i\hbar + \hat{p}\hat{x})\hat{p} = -2i\hbar\hat{p}\ .$$

Hence we again obtain

$$\boxed{\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{\hat{p}(t)}{m}}\ .$$