XMA344403

Coláiste na Tríonóide, Baile Átha Cliath
Trinity College Dublin
Ollscoil Átha Cliath | The University of Dublin

Faculty of Science, Technology, Engineering and Mathematics

School of Mathematics

JS Mathematics **Michaelmas Term 2021**
JS Theoretical Physics

Module MAU34403: Quantum Mechanics I

???, December 2021 **RDS ???** **14.00 — 16.00 ???**

Prof. Sergey Frolov

Instructions to candidates:

Credit will be given for the best 3 questions answered.

Each question is worth 33 marks.

Additional instructions for this examination:

Formulae and Tables are available from the invigilators, if required.

Non-programmable calculators are permitted for this examination,—please indicate the make and model of your calculator on each answer book used.

You may not start this examination until you are instructed to do so by the Invigilator.

1. The XXX Heisenberg spin-1/2 chain of length 2 is described by the Hamiltonian

$$H = \frac{3}{4}J + \frac{J}{\hbar^2}\sum_{\alpha=1}^{3} S_1^\alpha S_2^\alpha \tag{1}$$

which acts in the tensor product of 2 copies of $\mathbb{C}^2$ (spin up-down) $\mathscr{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$.

The spin-1/2 operator $S_i^\alpha = \hbar\sigma_i^\alpha/2$ acts only at the i-th site

$$S_1^\alpha = S^\alpha \otimes I\,, \quad S_2^\alpha = I \otimes S^\alpha \tag{2}$$

The Hamiltonian commutes with the total spin operator

$$\mathbb{S}^\alpha = S_1^\alpha + S_2^\alpha = S^\alpha \otimes I + I \otimes S^\alpha \tag{3}$$

The orthonormal vectors

$$|e_1\rangle \equiv\ |\uparrow\uparrow\rangle\,, \quad |e_0\rangle \equiv\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\,, \quad |e_{-1}\rangle \equiv\ |\downarrow\downarrow\rangle\,, \tag{4}$$

are eigenvectors of H with the eigenvalue $E_1 = J$ while the vector

$$|f\rangle \equiv\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \tag{5}$$

is an eigenvector of H with the eigenvalue $E_0 = 0$. These vectors are also eigenvectors of $\mathbb{S}^3$ with eigenvalues $s_1 = \hbar$, $s_0 = 0$ and $s_{-1} = -\hbar$.

Consider the state

$$]\psi\rangle = \frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle - 2|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) \tag{6}$$

(a) **10 marks.** Expand $|\psi\rangle$ over the basis $|f\rangle$ and $|e_m\rangle$, $m = 1, 0, -1$.

Find the probabilities to measure E_0 and E_1, and s_1, s_0 and s_{-1}.

Answer. We compute

$$\begin{aligned}
\langle e_1|\psi\rangle &= \langle\uparrow\uparrow|\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle - 2|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{1}{\sqrt{10}} \\
\langle e_0|\psi\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle - 2|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{1}{\sqrt{20}}(-2+1) = -\frac{1}{\sqrt{20}} \\
\langle e_{-1}|\psi\rangle &= \langle\downarrow\downarrow|\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle - 2|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{2}{\sqrt{10}} \\
\langle f|\psi\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\frac{1}{\sqrt{10}}\big(|\uparrow\uparrow\rangle - 2|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + 2|\downarrow\downarrow\rangle\big) = \frac{1}{\sqrt{20}}(-1-2) = -\frac{3}{\sqrt{20}}
\end{aligned} \tag{7}$$

Thus,

$$\begin{aligned} |\psi\rangle &= |e_1\rangle\langle e_1|\psi\rangle + |e_0\rangle\langle e_0|\psi\rangle + |e_{-1}\rangle\langle e_{-1}|\psi\rangle + |f\rangle\langle f|\psi\rangle \\ &= \frac{1}{\sqrt{10}}|e_1\rangle - \frac{1}{\sqrt{20}}|e_0\rangle + \frac{2}{\sqrt{10}}|e_{-1}\rangle - \frac{3}{\sqrt{20}}|f\rangle \end{aligned} \tag{8}$$

and

$$P(E_1) = \frac{1}{10} + \frac{1}{20} + \frac{4}{10} = \frac{11}{20}\,, \quad P(E_0) = \frac{9}{20} \tag{9}$$

$$P(s_1) = \frac{1}{10}\,, \quad P(s_0) = \frac{1}{20} + \frac{9}{20} = \frac{1}{2}\,, \quad P(s_{-1}) = \frac{4}{10} = \frac{2}{5} \tag{10}$$

(b) **6 marks.** If the result of a measurement is E_1, what is the state of the system after it?

If the result of a measurement is s_0, what is the state of the system after it?

Answer. After the measurements the system collapses into

$$\begin{aligned} |\mathcal{E}_1\rangle &= \frac{|e_1\rangle\langle e_1|\psi\rangle + |e_0\rangle\langle e_0|\psi\rangle + |e_{-1}\rangle\langle e_{-1}|\psi\rangle}{\sqrt{P(E_1)}} = \sqrt{\frac{20}{11}}\Big(\frac{1}{\sqrt{10}}|e_1\rangle - \frac{1}{\sqrt{20}}|e_0\rangle + \frac{2}{\sqrt{10}}|e_{-1}\rangle\Big) \\ &= \sqrt{\frac{2}{11}}|e_1\rangle - \frac{1}{\sqrt{11}}|e_0\rangle + \sqrt{\frac{8}{11}}|e_{-1}\rangle \end{aligned} \tag{11}$$

$$\begin{aligned} |s_0\rangle &= \frac{|e_0\rangle\langle e_0|\psi\rangle + |f\rangle\langle f|\psi\rangle}{\sqrt{P(s_0)}} = \sqrt{2}\Big(-\frac{1}{\sqrt{20}}|e_0\rangle - \frac{3}{\sqrt{20}}|f\rangle\Big) \\ &= -\sqrt{\frac{1}{10}}|e_0\rangle - \sqrt{\frac{9}{10}}|f\rangle \end{aligned} \tag{12}$$

(c) **6 marks.** What is the probability to measure first E_1 and immediately after s_0?

What is the probability to measure first s_0 and immediately after E_1?

Are these probabilities equal? Explain the result.

Answer. The probability to find s_0 by measuring $|\mathcal{E}_1\rangle$ is $|\langle e_0|\mathcal{E}_1\rangle|^2 = 1/11$. The probabilities multiply, so

$$P(E_1, s_0) = P(E_1)|\langle e_0|\mathcal{E}_1\rangle|^2 = \frac{1}{20} \tag{13}$$

Similarly,

$$P(s_0, E_1) = P(s_0)|\langle e_0|s_0\rangle|^2 = \frac{1}{20} \tag{14}$$

They are equal because H and $\mathbb{S}^3$ are compatible.

(d) **6 marks.** Find the expectation values of and the uncertainty in the Hamiltonian H and the z-component $\mathbb{S}^3$ of the total spin operator with respect to $]\psi\rangle$

Answer. We get

$$\langle H\rangle = P(E_0)E_0 + P(E_1)E_1 = \frac{9}{20}0 + \frac{11}{20}J = \frac{11}{20}J \tag{15}$$

$$\Delta H = \sqrt{P(E_0)(E_0 - \langle H\rangle)^2 + P(E_1)(E_1 - \langle H\rangle)^2} = J\sqrt{\frac{9}{20}\frac{11^2}{20^2} + \frac{11}{20}(1 - \frac{11}{20})^2} = \frac{3\sqrt{11}}{20}J \tag{16}$$

$$\langle \mathbb{S}^3\rangle = P(s_1)s_1 + P(s_0)s_0 + P(s_{-1})s_{-1} = \frac{1}{10} + \frac{1}{2}0 + \frac{2}{5}(-1) = -\frac{3\hbar}{10} \tag{17}$$

$$\Delta\mathbb{S}^3 = \sqrt{P(s_1)(s_1 - \langle\mathbb{S}^3\rangle + P(s_0)(s_0 - \langle\mathbb{S}^3\rangle)^2 + P(s_{-1})(s_{-1} - \langle\mathbb{S}^3\rangle)^2} := \frac{\hbar\sqrt{41}}{10} \tag{18}$$

(e) **5 marks.** Check that the general uncertainty relation

$$\Delta\hat{A}^2\Delta\hat{B}^2 \geq \left(\frac{1}{2}\langle[\hat{A}\,,\,\hat{B}]_+\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle\right)^2 - \frac{1}{4}\langle[\hat{A}\,,\,\hat{B}]\rangle^2 \tag{19}$$

holds for $\mathbb{S}^3$ and H

Answer. Since $\mathbb{S}^3$ and H commute the rhs of the general uncertainty relation gives

$$\left(\langle\mathbb{S}^3\,H\rangle - \langle\mathbb{S}^3\rangle\langle H\rangle\right)^2 \tag{20}$$

Then,

$$\langle\mathbb{S}^3\,H\rangle = -\frac{3\hbar J}{10} \tag{21}$$

Thus,

$$\left(\langle\mathbb{S}^3\,H\rangle - \langle\mathbb{S}^3\rangle\langle H\rangle\right)^2 = (\frac{3\hbar J}{10} - \frac{3\hbar}{10}\frac{11}{20}J)^2 \approx 0.018225\hbar^2J^2 \tag{22}$$

$$\Delta H^2 = \frac{99}{20^2}J^2\,,\quad (\Delta\mathbb{S}^3)^2 = \frac{\hbar^2 41}{100}\,,\quad \Delta H^2(\Delta\mathbb{S}^3)^2 \approx 0.101475\hbar^2J^2 \tag{23}$$

and the inequality holds.

2. Consider a particle in the following potential

$$V(x) = \begin{cases} 0 & \text{for } x < -a \\ -V_0 & \text{for } -a < x < 0 \\ +\infty & \text{for } x > 0 \end{cases} \tag{24}$$

where $a > 0\,,\,V_0 > 0$.

(a) **10 marks.** Find the wave function for a scattering state. Do not normalise it.

Solution: We need to glue the following two solutions of the time-independent Schrödinger equation

$$\begin{aligned}
&\psi_L(x) = A_L e^{\mathrm{i}\,k\,(x+a)} + B_L e^{-\mathrm{i}\,k\,(x+a)}\,, \quad k = \frac{\sqrt{2mE}}{\hbar}\,, \quad x < -a \\
&\psi_M(x) = A\sin(k_M\,x)\,, \quad k_M = \frac{\sqrt{2m(E+V_0)}}{\hbar}\,, \quad -a < x < 0
\end{aligned} \tag{25}$$

where $E > 0$, and we used that $\psi(x) = 0$ for $x > 0$.

The constants A_L and B_L are expressed in terms of A by using the continuity conditions for $\psi(x)$ and $\psi'(x)$ at $x = -a$

$$\begin{aligned}
A_L + B_L &= -A\sin(k_M\,a)\,, \\
\mathrm{i}\,k\,A_L - \mathrm{i}\,k\,B_L &= k_M A\cos(k_M\,a)
\end{aligned} \tag{26}$$

Thus,

$$\begin{aligned}
A_L &= -\frac{A}{2}\big(\sin(k_M\,a) + \mathrm{i}\,\frac{k_M}{k}\cos(k_M\,a)\big)\,, \\
B_L &= -\frac{A}{2}\big(\sin(k_M\,a) - \mathrm{i}\,\frac{k_M}{k}\cos(k_M\,a)\big)
\end{aligned} \tag{27}$$

and the wave function is given by

$$\psi(x) = \begin{cases} A\sin(k_M\,a)\cos(k(x+a)) + A\frac{k_M}{k}\cos(k_M\,a)\sin(k(x+a)) & \text{for } x < -a \\ A\sin(k_M\,x) & \text{for } -a < x < 0 \\ 0 & \text{for } x > 0 \end{cases} \tag{28}$$

(b) **10 marks.** Find the wave function for a bound state, and the quantisation condition for the bound state spectrum. Do not normalise the wave function.

Solution: We need to glue the following two solutions of the time-independent Schrödinger equation

$$\begin{aligned}
&\psi_L(x) = A_L e^{\kappa\,(x+a)}\,, \quad \kappa = \frac{\sqrt{-2mE}}{\hbar}\,, \quad x < -a \\
&\psi_M(x) = A\sin(k_M\,x)\,, \quad k_M = \frac{\sqrt{2m(E+V_0)}}{\hbar}\,, \quad -a < x < 0
\end{aligned} \tag{29}$$

where $-V_0 < E < 0$, and we used that $\psi(x) = 0$ for $x > 0$, and that $\psi_L(-\infty) = 0$.

The constant A_L is expressed in terms of A by using the continuity condition for $\psi(x)$ at $x = -a$

$$A_L = -A\sin(k_M\, a)\,. \tag{30}$$

Thus, the wave function is given by

$$\psi(x) = \begin{cases} -A\sin(k_M\, a)\, e^{\kappa\,(x+a)} & \text{for } \; x < -a \\ A\sin(k_M\, x) & \text{for } \; -a < x < 0 \\ 0 & \text{for } \; x > 0 \end{cases} \tag{31}$$

Using the continuity condition for $\psi'(x)$ at $x = -a$, we get

$$-\kappa\, A\sin(k_M\, a) = k_M A\cos(k_M\, a) \tag{32}$$

Thus, the quantisation condition is

$$-\kappa\, \sin(k_M\, a) = k_M\cos(k_M\, a) \tag{33}$$

(c) **8 marks.** Show that the energy quantisation condition can be written in the form

$$-\cot z = \sqrt{\frac{W^2}{z^2} - 1} \tag{34}$$

where z and W have to be identified.

Sketch plots of the left and right hand sides of the energy quantisation condition.

Find the values of W for which there are n bound states.

Solution: By using

$$\kappa^2 + k_M^2 = \frac{2mV_0}{\hbar^2} \tag{35}$$

and introducing

$$z \equiv k_M a\,, \quad W^2 \equiv \frac{2mV_0 a^2}{\hbar^2} \tag{36}$$

we get the equation (34).

Taking into account that $z \le W$, and that $\cot z = 0$ for $z = \pi/2 + i\pi n$, we get that the first bound state appears at $W = \pi/2$, the second at $W = 3\pi/2$, and so on, so that for $(2n-1)\pi/2 \le W < (2n+1)\pi/2$ there are n bound states.

(d) **5 marks.** Denote the energy eigenvalues by E_n, $n = 0, 1, 2, \ldots$, $E_n < E_{n+1}$. Find $E_n + V_0$ in the limit $V_0 \to \infty$. Explain the result obtained.

Solution: In this limit the energy quantisation condition becomes

$$\tan z = 0 \quad \Rightarrow \quad z_n = \pi(n+1)\,, \quad n = 0, 1, 2, \ldots \tag{37}$$

Thus,

$$E_n + V_0 = \frac{k_n^2 \hbar^2}{2m} = \frac{\pi^2 (n+1)^2 \hbar^2}{2ma^2} \tag{38}$$

These are energies of states in an infinitely deep well of width a.

3. The motion of two particles in one dimension is described by the Hamiltonian

$$H = \frac{P_1^2}{2m} + \frac{P_2^2}{2m} + \frac{k_{12}}{2} X_1 X_2 + V(X_1 - X_2) \tag{39}$$

where the potential V is given by

$$V(X) = \begin{cases} k\, X^2/2 & \text{for } \; X > 0 \\ \infty & \text{for } \; X < 0 \end{cases} \tag{40}$$

(a) **8 marks.** Introduce the centre of mass coordinate $X_{\rm cm}$, the relative coordinate X, and their conjugate momenta. Check that they satisfy the canonical commutation relations.

Express the Hamiltonian in terms of the new coordinates and momenta. In classical mechanics for which values of k_{12} and k is the energy of the system positive unless it is at rest?

Answer. We introduce the centre of mass coordinate $X_{\rm cm}$, the relative coordinate X, and their conjugate momenta

$$X_{\rm cm} = \frac{1}{2} X_1 + \frac{1}{2} X_2\,, \quad X = X_1 - X_2\,, \quad P_{\rm cm} = P_1 + P_2\,, \quad P = \frac{1}{2} P_1 - \frac{1}{2} P_2 \tag{41}$$

The new coordinates and momenta satisfy the canonical commutation relations.

The Hamiltonian takes the form

$$H = \frac{P_{\rm cm}^2}{4m} + \frac{P^2}{m} + \frac{k_{12} X_{\rm cm}^2}{2} - \frac{k_{12} X^2}{8} + V(X) = H_{\rm cm} + H_{\rm rel} \tag{42}$$

The energy is positive if

$$k - k_{12}/4 > 0 \tag{43}$$

(b) **10 marks.** Separate the variables and find the eigenvalues of the Hamiltonian for values of k_{12} and k from the previous question.

Answer. Since

$$H = H_{\rm cm} + H_{\rm rel}\,, \quad H_{\rm cm} = \frac{P_{\rm cm}^2}{4m} + \frac{k_{12}X_{\rm cm}^2}{2}\,, \quad H_{\rm rel} = \frac{P^2}{m} - \frac{k_{12}X^2}{8} + V(X) \tag{44}$$

$X_{\rm cm}$ and X can be separated, and the eigenfunctions of H factorise

$$\psi_E(x_{\rm cm}, x) = \psi_{E_{\rm cm}}(x_{\rm cm})\psi_{E_{\rm rel}}(x)\,, \quad E = E_{\rm cm} + E_{\rm rel} \tag{45}$$

where $\psi_{E_{\rm cm}}(x_{\rm cm})$ and $\psi_{E_{\rm rel}}(x)$ satisfy

$$\begin{aligned} (\frac{P_{\rm cm}^2}{4m} + \frac{k_{12}X_{\rm cm}^2}{2})\psi_{E_{\rm cm}}(x_{\rm cm}) = E_{\rm cm}\psi_{E_{\rm cm}}(x_{\rm cm}) \\ (\frac{P^2}{m} - \frac{k_{12}X^2}{8} + V(X))\psi_{E_{\rm rel}}(x) = E_{\rm rel}\psi_{E_{\rm rel}}(x) \end{aligned} \tag{46}$$

The centre-of-mass Hamiltonian is just a harmonic oscillator one with mass $2m$ and frequency $\omega^2 = k_{12}/2m$. Thus,

$$E_{\rm cm} = \hbar\,\omega\,(n_{\rm cm} + \frac{1}{2})\,, \quad n_{\rm cm} = 0, 1, \ldots \tag{47}$$

The relative-motion Hamiltonian $H_{\rm rel}$ for $x > 0$ is also a harmonic oscillator one with mass $m/2$ and frequency

$$\Omega^2 = \frac{2k - \frac{k_{12}}{2}}{m} \tag{48}$$

However, for $x < 0$ wave functions must vanish because there $V = \infty$. Therefore, only odd wave functions of the harmonic oscillator are the eigenfunctions of $H_{\rm rel}$, and, as a result

$$E_{\rm rel} = \hbar\,\Omega\,(n_{\rm rel} + \frac{1}{2})\,, \quad n_{\rm rel} = 1, 3, 5, \ldots \tag{49}$$

Thus, the total spectrum is

$$E = E_{\rm cm} + E_{\rm rel} = \hbar\,\omega\,(n_{\rm cm} + \frac{1}{2}) + \hbar\,\Omega\,(n_{\rm rel} + \frac{1}{2}) \tag{50}$$

(c) **10 marks.** Find the ground state wave function.

Answer. The ground state wave function is given by the product of

$$\psi_0(x_{\rm cm}) = \frac{1}{\sqrt{\sqrt{2\pi}\eta_{\rm cm}}} \exp\Big(-\frac{x_{\rm cm}^2}{4\eta_{\rm cm}^2}\Big)\,, \quad \eta_{\rm cm} = \sqrt{\frac{\hbar}{4m\omega}} \tag{51}$$

and

$$\begin{aligned} \psi_1(x) &= \sqrt{2}\,\frac{1}{\sqrt{2}} H_1\big(\frac{x}{\sqrt{2}\eta_{\rm rel}}\big)\,\psi_0(x) = \sqrt{2}\,\frac{x}{\eta_{\rm rel}}\,\psi_0(x)\,, \quad \text{for } \ x>0 \\ \psi_0(x) &= \frac{1}{\sqrt{\sqrt{2\pi}\eta_{\rm rel}}} \exp\Big(-\frac{x^2}{4\eta_{\rm rel}^2}\Big)\,, \quad \eta_{\rm rel} = \sqrt{\frac{\hbar}{m\Omega}} \end{aligned} \tag{52}$$

and $\psi_1(x) = 0$ for $x < 0$.

(d) **5 marks.** Under which conditions on the constants m, k and k_{12} is the spectrum degenerate?

Answer. If the spectrum is degenerate then for some energy level there are at least two sets of integers $n_{\rm cm}, n_{\rm rel}$ and $n'_{\rm cm}, n'_{\rm rel}$ such that

$$\omega\, n_{\rm cm} + \Omega\, n_{\rm rel} = \omega\, n'_{\rm cm} + \Omega\, n'_{\rm rel} \quad \Leftrightarrow \quad \omega\,(n_{\rm cm} - n'_{\rm cm}) = \Omega\,(n'_{\rm rel} - n_{\rm rel}) \tag{53}$$

Clearly, this equation has no solution if ω and Ω are incommensurable. Thus, the spectrum is degenerate if there are two integers p and q such that

$$\Omega = \frac{p}{q}\omega \quad \Rightarrow \quad 2k - \frac{k_{12}}{2} = \frac{p^2}{q^2}\frac{k_{12}}{2} \quad \Rightarrow \quad \frac{4k}{k_{12}} = \frac{p^2+q^2}{q^2} > 1 \tag{54}$$

4. (a) **11 marks.** The orbital angular momentum operator is $\vec{L} = \vec{X} \times \vec{P}$.

Use the canonical commutation relations to show that

$$[L^\alpha, X^\beta] = \sum_{\gamma=1}^{3} \mathrm{i}\,\hbar\,\epsilon^{\alpha\beta\gamma} X^\gamma\,, \quad [L^\alpha, P^\beta] = \sum_{\gamma=1}^{3} \mathrm{i}\,\hbar\,\epsilon^{\alpha\beta\gamma} P^\gamma\,, \quad [L^\alpha, L^\beta] = \sum_{\gamma=1}^{3} \mathrm{i}\,\hbar\,\epsilon^{\alpha\beta\gamma} L^\gamma\,,$$

$$[L^{\vec n}, \vec X] = \mathrm{i}\hbar\,\vec X \times \vec n\,, \quad [L^{\vec n}, \vec P] = \mathrm{i}\hbar\,\vec P \times \vec n\,, \quad [L^{\vec m}, L^{\vec n}] = \mathrm{i}\hbar\, L^{\vec m \times \vec n}\,,$$

where

$$L^{\vec n} \equiv \vec n \cdot \vec L = n^x L^x + n^y L^y + n^z L^z\,, \quad \vec n^{\,2} = 1$$

Answer. Straightforward calculation.

(b) For a particle with the Hamiltonian

$$H = \frac{\vec{P}^{\,2}}{2m} + V(\vec{X}) \tag{55}$$

i. **7 marks.** Derive the Heisenberg equation for the orbital angular momentum operator $\vec{L}$.

Answer. We get for any unit vector $\vec{n}$

$$\frac{d\vec{L}^{\vec{n}}}{dt} = \frac{\mathrm{i}}{\hbar}\big[\hat{H}\,,\,\vec{L}^{\vec{n}}\big] = \frac{\mathrm{i}}{\hbar}\big[V(\vec{X})\,,\,\vec{L}^{\vec{n}}\,\big] = \frac{\mathrm{i}}{\hbar}(-\mathrm{i}\hbar\,\vec{X}\times\vec{n})\cdot\vec{\nabla}V = (\vec{\nabla}V\times\vec{X})\cdot\vec{n} \tag{56}$$

Thus,

$$\frac{d\vec{L}}{dt} = \vec{\nabla}V \times \vec{X} \tag{57}$$

The right hand side is the torque.

ii. **4 marks.** Derive an equation for the rate of change of the expectation value of the orbital angular momentum operator $\vec{L}$.

Is it the same as the equation of motion for $\vec{L}$ in classical mechanics?

Answer. Since in the Heisenberg picture a state vector $|\psi\rangle$ is stationary, we get

$$\frac{d\langle\vec{L}\rangle}{dt} = \langle\vec{\nabla}V \times \vec{X}\rangle \tag{58}$$

It is not the same as in classical mechanics because in general

$$\langle\vec{\nabla}V \times \vec{X}\rangle \neq \frac{\partial V\big(\langle\vec{X}\rangle\big)}{\partial\langle\vec{X}\rangle} \times \langle\vec{X}\rangle \tag{59}$$

(c) **11 marks.** Show that the Hamiltonian

$$H = \frac{\vec{P}^{\,2}}{2m} - \frac{e^2}{|\vec{X}|} \tag{60}$$

of the hydrogen atom commutes with the Runge-Lenz vector

$$\vec{D} = \vec{P}\times\vec{L} - \vec{L}\times\vec{P} \;-\; 2m\,e^2\,\frac{\vec{X}}{|\vec{X}|} \tag{61}$$

Hint. Use that $[A,BC] = [A,B]C + B[A,C]$. and that $\vec{L}$ commutes with a scalar.

Answer. We first calculate

$$
\begin{aligned}
[\frac{\vec{P}^{\,2}}{2m}\,,D^\alpha] &= [\vec{P}^{\,2}\,,-e^2\,\frac{X^\alpha}{|\vec{X}|}] = -e^2\,P^\beta[P^\beta\,,\,\frac{X^\alpha}{|\vec{X}|}] - e^2\,[P^\beta\,,\,\frac{X^\alpha}{|\vec{X}|}]P^\beta \\
&= \mathrm{i}\hbar e^2\,P^\alpha\frac{1}{|\vec{X}|} - \mathrm{i}\hbar e^2\,P^\beta\,\frac{X^\alpha X^\beta}{|\vec{X}|^3} + \mathrm{i}\hbar e^2\,\frac{1}{|\vec{X}|}P^\alpha - \mathrm{i}\hbar e^2\,\frac{X^\alpha X^\beta}{|\vec{X}|^3}P^\beta
\end{aligned}
\tag{62}
$$

Then,

$$
\begin{aligned}
[\frac{1}{|\vec{X}|}\,,D^\alpha] &= [\frac{1}{|\vec{X}|}\,,\,\epsilon^{\alpha\beta\gamma}P^\beta L^\gamma - \epsilon^{\alpha\beta\gamma}L^\beta P^\gamma] \\
&= \epsilon^{\alpha\beta\gamma}[\frac{1}{|\vec{X}|}\,,\,P^\beta]L^\gamma - \epsilon^{\alpha\beta\gamma}L^\beta[\frac{1}{|\vec{X}|}\,,\,P^\gamma] \\
&= -\mathrm{i}\hbar e^{\alpha\beta\gamma}\frac{X^\beta}{|\vec{X}|^3}\,e^{\gamma\rho\sigma}X^\rho P^\sigma - \mathrm{i}\hbar e^{\gamma\rho\sigma}P^\sigma X^\rho e^{\alpha\beta\gamma}\frac{X^\beta}{|\vec{X}|^3} \\
&= -\mathrm{i}\hbar\frac{X^\beta}{|\vec{X}|^3}\,X^\alpha P^\beta + \mathrm{i}\hbar\frac{1}{|\vec{X}|}\,P^\alpha - \mathrm{i}\hbar P^\beta\frac{X^\beta}{|\vec{X}|^3}\,X^\alpha + \mathrm{i}\hbar P^\alpha\frac{1}{|\vec{X}|}
\end{aligned}
\tag{63}
$$

Thus,

$$
\begin{aligned}
[H\,,D^\alpha] &= \mathrm{i}\hbar e^2\,P^\alpha\frac{1}{|\vec{X}|} - \mathrm{i}\hbar e^2\,P^\beta\,\frac{X^\alpha X^\beta}{|\vec{X}|^3} + \mathrm{i}\hbar e^2\,\frac{1}{|\vec{X}|}P^\alpha - \mathrm{i}\hbar e^2\,\frac{X^\alpha X^\beta}{|\vec{X}|^3}P^\beta \\
&\quad - e^2\big(-\mathrm{i}\hbar\frac{X^\beta}{|\vec{X}|^3}\,X^\alpha P^\beta + \mathrm{i}\hbar\frac{1}{|\vec{X}|}\,P^\alpha - \mathrm{i}\hbar P^\beta\frac{X^\beta}{|\vec{X}|^3}\,X^\alpha + \mathrm{i}\hbar P^\alpha\frac{1}{|\vec{X}|}\big) = 0
\end{aligned}
\tag{64}
$$