A Course in Mechanics by Dr. J. Tinsley Oden
Part II - Homework 4 - Solutions

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Set II.4:

1. The k-th component of the angular momentum operator is

$$L_k = \frac{\hbar}{i}\varepsilon_{nmk}\, q_n \frac{\partial}{\partial q_m},$$

with ε_{nmk} the Levi-Civita symbol. We now calculate the time derivative of its expected value

$$\begin{aligned}\frac{\mathrm{d}\langle L_k\rangle}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi^*(\mathbf{q},t), \left(\frac{\hbar}{i}\varepsilon_{nmk}\, q_n \frac{\partial}{\partial q_m}\right)\Psi(\mathbf{q},t)\rangle \\ &= \frac{\hbar}{i}\varepsilon_{nmk}\left\{\int_{\mathbb{R}^3}\frac{\partial\Psi^*}{\partial t} q_n \frac{\partial\Psi}{\partial q_m}\mathrm{d}^3\mathbf{q} + \int_{\mathbb{R}^3}\Psi^* q_n \frac{\partial}{\partial q_m}\frac{\partial\Psi}{\partial t}\mathrm{d}^3\mathbf{q}\right\}.\end{aligned}$$

Following Schrödinger's equation, we have

$$\frac{\partial\Psi}{\partial t} = \frac{1}{i\hbar}H\Psi, \qquad \frac{\partial\Psi^*}{\partial t} = -\frac{1}{i\hbar}(H\Psi)^*.$$

Then, we can write

$$\frac{\mathrm{d}\langle L_k\rangle}{\mathrm{d}t} = \frac{\hbar}{i}\varepsilon_{nmk}\left\{\int_{\mathbb{R}^3} -\frac{1}{i\hbar}(H\Psi)^* q_n \frac{\partial\Psi}{\partial q_m}\mathrm{d}^3\mathbf{q} + \int_{\mathbb{R}^3}\Psi^* q_n \frac{\partial}{\partial q_m}\frac{1}{i\hbar}(H\Psi)\mathrm{d}^3\mathbf{q}\right\}.$$

Using the Hermitian property of the Hamiltonian, assuming $q_n \frac{\partial\Psi}{\partial q_m} \in L^2(\mathbb{R}^3)$, we get

$$\begin{aligned}\frac{\mathrm{d}\langle L_k\rangle}{\mathrm{d}t} &= \varepsilon_{nmk}\left\{\int_{\mathbb{R}^3}\Psi^* H q_n \frac{\partial\Psi}{\partial q_m}\mathrm{d}^3\mathbf{q} - \int_{\mathbb{R}^3}\Psi^* q_n \frac{\partial}{\partial q_m}(H\Psi)\mathrm{d}^3\mathbf{q}\right\} \\ &= \varepsilon_{nmk}\left\{\int_{\mathbb{R}^3}\Psi^*\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{q}} + V(\mathbf{q})\right) q_n \frac{\partial\Psi}{\partial q_m}\mathrm{d}^3\mathbf{q} - \int_{\mathbb{R}^3}\Psi^* q_n \frac{\partial}{\partial q_m}\left[\left(-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{q}} + V(\mathbf{q})\right)\Psi\right]\mathrm{d}^3\mathbf{q}\right\}.\end{aligned}$$

We now observe that

$$\begin{aligned}\varepsilon_{nmk}\nabla^2_{\mathbf{q}}\left(q_n\frac{\partial\Psi}{\partial q_m}\right) &= \varepsilon_{nmk}\sum_{\ell=1}^{3}\frac{\partial^2}{\partial q_\ell^2}\left(q_n\frac{\partial\Psi}{\partial q_m}\right) = \varepsilon_{nmk}\frac{\partial}{\partial q_\ell}\left(\delta_{n\ell}\frac{\partial\Psi}{\partial q_m} + q_n\frac{\partial^2\Psi}{\partial q_m\partial q_\ell}\right) \\ &= \varepsilon_{nmk}\left(\delta_{n\ell}\frac{\partial^2\Psi}{\partial q_m\partial q_\ell} + \delta_{n\ell}\frac{\partial^2\Psi}{\partial q_m\partial q_\ell} + \sum_{\ell=1}^{3} q_n\frac{\partial^3\Psi}{\partial q_m\partial q_\ell^2}\right) \\ &= 2\varepsilon_{nmk}\frac{\partial^2\Psi}{\partial q_m\partial q_n} + \varepsilon_{nmk}\, q_n\frac{\partial}{\partial q_m}\nabla^2_{\mathbf{q}}\Psi = \varepsilon_{nmk}\, q_n\frac{\partial}{\partial q_m}\nabla^2_{\mathbf{q}}\Psi,\end{aligned}$$

where we use the antisymmetric property of ε_{nmk}. Then,

$$\begin{aligned}\frac{\mathrm{d}\langle L_k\rangle}{\mathrm{d}t} &= \varepsilon_{nmk}\Bigg\{\int_{\mathbb{R}^3}\Psi^*\left(-\frac{\hbar^2}{2m}q_n\frac{\partial}{\partial q_m}\nabla^2_{\mathbf{q}}\Psi + q_n V\frac{\partial\Psi}{\partial q_m}\right)\mathrm{d}^3\mathbf{q} \\ &\quad -\int_{\mathbb{R}^3}\Psi^*\left(-\frac{\hbar^2}{2m}q_n\frac{\partial}{\partial q_m}\nabla^2_{\mathbf{q}}\Psi + q_n V\frac{\partial\Psi}{\partial q_m} + q_n\frac{\partial V}{\partial q_m}\Psi\right)\mathrm{d}^3\mathbf{q}\Bigg\} = \int_{\mathbb{R}^3}\Psi^*\left(\varepsilon_{nmk}\,q_n\left(-\frac{\partial V}{\partial q_m}\right)\Psi\right)\mathrm{d}^3\mathbf{q} \\ &= \int_{\mathbb{R}^3}\Psi^*\left(\varepsilon_{nmk}\,q_n\,F_m\right)\Psi\mathrm{d}^3\mathbf{q} = \langle\varepsilon_{nmk}\,q_n\,F_m\rangle,\end{aligned}$$

with $F_m = -\frac{\partial V}{\partial q_m}$. Then,

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{L}\rangle = \langle\mathbf{q}\times\mathbf{F}\rangle, \quad \mathbf{F} = -\frac{\mathrm{d}V}{\mathrm{d}\mathbf{q}}}.$$

2. We find the eigenvalues of S_1: The eigenvalue problem is to find states $\mathbf{X}_i^{(1)}$, $i = 1, 2$ such that

$$S_1 \mathbf{X}_i^{(1)} = \lambda_i \mathbf{X}_i^{(1)},$$

with λ_i the eigenvalues and $\mathbf{X}_i^{(1)}$ the eigenvectors. Then,

$$S_1 \mathbf{X}_i^{(1)} = \frac{\hbar}{2} \boldsymbol{\sigma}_1 \mathbf{X}_i^{(1)} = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \mathbf{X}_i^{(1)} = \lambda_i \mathbf{X}_i^{(1)}$$

and

$$\left(\frac{\hbar}{2} \boldsymbol{\sigma}_1 - \lambda_i \mathbf{I} \right) \mathbf{X}_i^{(1)} = \begin{bmatrix} -\lambda_i & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda_i \end{bmatrix} \mathbf{X}_i^{(1)} = 0,$$

with $\mathbf{I}$ the identity matrix. To obtain the eigenvalues, we solve the characteristic equation

$$\det \left(\frac{\hbar}{2} \boldsymbol{\sigma}_1 - \lambda_i \mathbf{I} \right) = 0 = \lambda_i^2 - \left(\frac{\hbar}{2} \right)^2 \Rightarrow \lambda_i = \pm \frac{\hbar}{2}.$$

Then, the eigenvalues are

$$\boxed{\lambda_1 = \frac{\hbar}{2}, \qquad \lambda_2 = -\frac{\hbar}{2}}.$$

We now find the eigenvectors:
$\underline{\lambda_1 = \frac{\hbar}{2}}$: let $\mathbf{X}_1^{(1)} = \begin{bmatrix} a_1 \\ b_1 \end{bmatrix}$, then

$$\left(\frac{\hbar}{2} \boldsymbol{\sigma}_1 - \lambda_i \mathbf{I} \right) \mathbf{X}_1^{(1)} = \frac{\hbar}{2} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} a_1 \\ b_1 \end{bmatrix} = 0.$$

We get $-a_1 + b_1 = 0$, thus $b_1 = a_1$. The normalized eigenvector is then

$$\mathbf{X}_1^{(1)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

$\underline{\lambda_2 = -\frac{\hbar}{2}}$: similarly, we obtain

$$\mathbf{X}_2^{(1)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

3. To answer this question, we use the general spin state of an $s = 1/2$ particle

$$\mathbf{X} = a\mathbf{X}_+ + b\mathbf{X}_-, \qquad \mathbf{X}_+ = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \mathbf{X}_- = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Notice that $\langle \mathbf{X}_+, \mathbf{X}_+ \rangle = \langle \mathbf{X}_-, \mathbf{X}_- \rangle = 1$, $\langle \mathbf{X}_+, \mathbf{X}_- \rangle = \langle \mathbf{X}_-, \mathbf{X}_+ \rangle = 0$.
The spin operators have the following properties:

$$\begin{aligned}
S^2\mathbf{X}_+ &= \tfrac{3\hbar^2}{4}\mathbf{X}_+, & S^2\mathbf{X}_- &= \tfrac{3\hbar^2}{4}\mathbf{X}_-, \\
S_3\mathbf{X}_+ &= \tfrac{\hbar}{2}\mathbf{X}_+, & S_3\mathbf{X}_- &= -\tfrac{\hbar}{2}\mathbf{X}_-, \\
S_1\mathbf{X}_+ &= \tfrac{\hbar}{2}\mathbf{X}_-, & S_1\mathbf{X}_- &= \tfrac{\hbar}{2}\mathbf{X}_+, \\
S_2\mathbf{X}_+ &= i\tfrac{\hbar}{2}\mathbf{X}_-, & S_2\mathbf{X}_- &= -i\tfrac{\hbar}{2}\mathbf{X}_+.
\end{aligned}$$

We now check whether these operators are Hermitian:

- S^2:

$$\begin{aligned}
\langle \mathbf{X}, S^2\mathbf{X} \rangle &= \langle a\mathbf{X}_+ + b\mathbf{X}_-, S^2(a\mathbf{X}_+ + b\mathbf{X}_-) \rangle = \langle a\mathbf{X}_+ + b\mathbf{X}_-, \frac{3\hbar^2}{4}(a\mathbf{X}_+ + b\mathbf{X}_-) \rangle \\
&= \langle \frac{3\hbar^2}{4}(a\mathbf{X}_+ + b\mathbf{X}_-), a\mathbf{X}_+ + b\mathbf{X}_- \rangle = \langle S^2\mathbf{X}, \mathbf{X} \rangle.
\end{aligned}$$

  Then, S^2 is an observable.

- S_3:

$$\begin{aligned}
\langle \mathbf{X}, S_3\mathbf{X} \rangle &= \langle a\mathbf{X}_+ + b\mathbf{X}_-, S_3(a\mathbf{X}_+ + b\mathbf{X}_-) \rangle = \langle a\mathbf{X}_+ + b\mathbf{X}_-, \frac{\hbar}{2}(a\mathbf{X}_+ - b\mathbf{X}_-) \rangle \\
&= \frac{\hbar}{2}(a^*a - b^*b) = \langle \frac{\hbar}{2}(a\mathbf{X}_+ - b\mathbf{X}_-), a\mathbf{X}_+ + b\mathbf{X}_- \rangle \\
&= \langle S_3(a\mathbf{X}_+ + b\mathbf{X}_-), a\mathbf{X}_+ + b\mathbf{X}_- \rangle = \langle S_3\mathbf{X}, \mathbf{X} \rangle.
\end{aligned}$$

  Then, S_3 is an observable.

- S_1:

$$\begin{aligned}
\langle \mathbf{X}, S_1\mathbf{X} \rangle &= \langle a\mathbf{X}_+ + b\mathbf{X}_-, S_1(a\mathbf{X}_+ + b\mathbf{X}_-) \rangle = \langle a\mathbf{X}_+ + b\mathbf{X}_-, \frac{\hbar}{2}(a\mathbf{X}_- + b\mathbf{X}_+) \rangle = \hbar\frac{a^*b + b^*a}{2}. \\
\langle S_1\mathbf{X}, \mathbf{X} \rangle &= \langle S_1(a\mathbf{X}_+ + b\mathbf{X}_-), a\mathbf{X}_+ + b\mathbf{X}_- \rangle = \langle \frac{\hbar}{2}(a\mathbf{X}_- + b\mathbf{X}_+), a\mathbf{X}_+ + b\mathbf{X}_- \rangle = \hbar\frac{a^*b + b^*a}{2}.
\end{aligned}$$

  Then, $\langle \mathbf{X}, S_1\mathbf{X} \rangle = \langle S_1\mathbf{X}, \mathbf{X} \rangle$ and thus S_1 is an observable.

- S_2:

$$\begin{aligned}
\langle \mathbf{X}, S_2\mathbf{X} \rangle &= \langle a\mathbf{X}_+ + b\mathbf{X}_-, S_2(a\mathbf{X}_+ + b\mathbf{X}_-) \rangle = \langle a\mathbf{X}_+ + b\mathbf{X}_-, i\frac{\hbar}{2}(a\mathbf{X}_- - b\mathbf{X}_+) \rangle = \hbar\frac{a^*b - b^*a}{2i}. \\
\langle S_2\mathbf{X}, \mathbf{X} \rangle &= \langle S_2(a\mathbf{X}_+ + b\mathbf{X}_-), a\mathbf{X}_+ + b\mathbf{X}_- \rangle = \langle i\frac{\hbar}{2}(a\mathbf{X}_- - b\mathbf{X}_+), a\mathbf{X}_+ + b\mathbf{X}_- \rangle = \hbar\frac{a^*b - b^*a}{2i}.
\end{aligned}$$

  Then, $\langle \mathbf{X}, S_2\mathbf{X} \rangle = \langle S_2\mathbf{X}, \mathbf{X} \rangle$ and thus S_2 is an observable. In addition, for any complex number z, $(z+z^*)/2 \in \mathbb{R}$ and $(z-z^*)/(2i) \in \mathbb{R}$. Then, $\langle \mathbf{X}, S_1\mathbf{X} \rangle \in \mathbb{R}$ and $\langle \mathbf{X}, S_2\mathbf{X} \rangle \in \mathbb{R}$.

We now check $S_\pm$:

$$\langle \mathbf{X}, S_\pm \mathbf{X}\rangle = \langle \mathbf{X}, (S_1 \pm i S_2)\mathbf{X}\rangle = \langle \mathbf{X}, S_1\mathbf{X}\rangle \pm i\langle \mathbf{X}, S_2\mathbf{X}\rangle$$
$$\langle S_\pm \mathbf{X}, \mathbf{X}\rangle = \langle (S_1 \pm i S_2)\mathbf{X}, \mathbf{X}\rangle = \langle S_1\mathbf{X}, \mathbf{X}\rangle \mp i\langle S_2\mathbf{X}, \mathbf{X}\rangle = \langle \mathbf{X}, S_1\mathbf{X}\rangle \mp i\langle \mathbf{X}, S_2\mathbf{X}\rangle.$$

Then, $\langle \mathbf{X}, S_\pm \mathbf{X}\rangle \neq \langle S_\pm \mathbf{X}, \mathbf{X}\rangle$, and S_+, S_- are not observable. In particular, because $\langle \mathbf{X}, S_1\mathbf{X}\rangle$ and $\langle \mathbf{X}, S_2\mathbf{X}\rangle$ are real, then $\langle \mathbf{X}, S_\pm \mathbf{X}\rangle$ is not a real number and thus S_+, S_- cannot be observables.

4. For fermions, the wave function should be antisymmetric applying Pauli's principle to the combined orbitals and spins.

   (a) Let
   $$\Psi(1,2) = \varphi_{1s}(1)\,\varphi_{2s}(2)\begin{vmatrix}\alpha_1 & \beta_1\\ \alpha_2 & \beta_2\end{vmatrix} = \varphi_{1s}(1)\,\varphi_{2s}(2)\Big(\alpha_1\beta_2 - \alpha_2\beta_1\Big).$$
   Then,
   $$\Psi(2,1) = \varphi_{1s}(2)\,\varphi_{2s}(1)\Big(\alpha_2\beta_1 - \alpha_1\beta_2\Big) = -\varphi_{1s}(2)\,\varphi_{2s}(1)\Big(\alpha_1\beta_2 - \alpha_2\beta_1\Big) \neq -\Psi(1,2).$$
   Therefore, this function in not valid for the Helium atom.

   (b) Let
   $$\Psi(1,2) = \Big(\varphi_{1s}(1)\,\varphi_{2s}(2) - \varphi_{2s}(1)\,\varphi_{1s}(2)\Big)\begin{vmatrix}\alpha_1 & \beta_1\\ \alpha_2 & \beta_2\end{vmatrix} = \Big(\varphi_{1s}(1)\,\varphi_{2s}(2) - \varphi_{2s}(1)\,\varphi_{1s}(2)\Big)\Big(\alpha_1\beta_2 - \alpha_2\beta_1\Big).$$
   Then,
   $$\begin{aligned}\Psi(2,1) &= \Big(\varphi_{1s}(2)\,\varphi_{2s}(1) - \varphi_{2s}(2)\,\varphi_{1s}(1)\Big)\Big(\alpha_2\beta_1 - \alpha_1\beta_2\Big)\\ &= -\Big(\varphi_{1s}(2)\,\varphi_{2s}(1) - \varphi_{2s}(2)\,\varphi_{1s}(1)\Big)\Big(\alpha_1\beta_2 - \alpha_2\beta_1\Big)\\ &= \Big(\varphi_{1s}(1)\,\varphi_{2s}(2) - \varphi_{2s}(1)\,\varphi_{1s}(2)\Big)\Big(\alpha_1\beta_2 - \alpha_2\beta_1\Big) = \Psi(1,2).\end{aligned}$$
   Therefore, this function in not valid for the Helium atom.

   <u>Note</u>: An appropriate function for the Helium atom should be antisymmetric, i.e., it can be symmetric in its orbital part $\times$ antisymmetric in its spin part, or antisymmetric in its orbital part $\times$ symmetric in its spin part. None of the above functions satisfy this property.