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Advanced Quantum mechanics

All Exercises

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Contents

1 Recap of quantum mechanics

1.1 Harmonic oscillator spectrum

Compute the energy spectrum of the harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \tag{1.1}$$

using the ladder operators $a, a^\dagger$ with

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \mathrm{i}\frac{p}{m\omega}\right) \tag{1.2}$$

Solution: At first the Hamiltonian H is expressed as a function of the ladder operators. Therefore the product $a^\dagger a$ is computed:

$$\begin{aligned} a^\dagger a &= \frac{m\omega}{2\hbar}\left[\left(x - \mathrm{i}\frac{p}{m\omega}\right)\cdot\left(x + \mathrm{i}\frac{p}{m\omega}\right)\right] \\ &= \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2} + \mathrm{i}\frac{xp - px}{m\omega}\right) \\ &= \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2} - \frac{\hbar}{m\omega}\right) \\ &= \frac{1}{\omega\hbar}\Big(\underbrace{\frac{m\omega^2 x^2}{2} + \frac{p^2}{2m}}_{=H} - \frac{\hbar\omega}{2}\Big) \\ &= \frac{H}{\omega\hbar} - \frac{1}{2}. \end{aligned} \tag{1.3}$$

In the third step the relation for the commutator $[x, p_x] = \mathrm{i}\hbar$. Therefore the Hamiltonian can be written as

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right). \tag{1.4}$$

Another important relation is the commutator $[a, a^\dagger]$ which can be derived by using (1.3)

$$[a, a^\dagger] = a\,a^\dagger - a^\dagger a = \left(\frac{H}{\omega\hbar} + \frac{1}{2}\right) - \left(\frac{H}{\omega\hbar} - \frac{1}{2}\right) = \mathbb{1}. \tag{1.5}$$

The operator $N := a^\dagger a$ is a Hermitian operator (because the Hamiltonian is hermitian) and it therefore has only real eigenvalues. It can be easily checked, that N and H commute because $H \propto N +$ const. This implies that N and H are compatible operators with the same eigenvectors. Consider an eigenstate $|\lambda\rangle$ of N with eigenvalue λ

$$N|\lambda\rangle = \lambda|\lambda\rangle \quad \Rightarrow \quad H|\lambda\rangle = \left(\lambda + \frac{1}{2}\right)|\lambda\rangle. \tag{1.6}$$

It can also be shown that λ is positive by calculating

$$\langle\lambda|N|\lambda\rangle = \langle\lambda|\lambda|\lambda\rangle = \lambda\,\langle\lambda|\lambda\rangle = \lambda \tag{1.7}$$

and comparing it with the definition of $N = a^\dagger a$

$$\left\langle \lambda|a^\dagger a|\lambda \right\rangle = (a\,|\lambda\rangle)^\dagger (a\,|\lambda\rangle) = ||a\,|\lambda\rangle\,||^2 \geq 0. \tag{1.8}$$

Furthermore the commutaror $[N,a]$ can be calculated as

$$[N,a] = [a^\dagger a, a] = a^\dagger \underbrace{[a,a]}_{=0} + \underbrace{[a^\dagger,a]}_{\overset{(1.5)}{=}-1} a = -a. \tag{1.9}$$

If the operator $N\,a$ is applied to the state $|\lambda\rangle$ it follows

$$N\,a\,|\lambda\rangle = (a\,N + [N,a])\,|\lambda\rangle = (a\,N - a)\,|\lambda\rangle = (\lambda - 1)\,a\,|\lambda\rangle\,. \tag{1.10}$$

It can be shown recursively that

$$N\,a^k\,|\lambda\rangle = (\lambda - k)\,a^k\,|\lambda\rangle\,, \quad k \in \mathbb{N}. \tag{1.11}$$

For values $k > \lambda$ the eigenvalues of N would become negative which is in conflict with equation (1.8). Therefore there must be a $k \in \mathbb{N}$ for which the eigenvalue is zero in order to stop the following eigenvalues to become negative. This implies that λ must be a positive integer

$$N\,|\lambda\rangle = \lambda\,|\lambda\rangle \quad \Rightarrow \quad \lambda = n \in \mathbb{N}. \tag{1.12}$$

The same calculation of (1.11) can be done with $a^\dagger$ which leads to

$$N\,a^{\dagger k}\,|n\rangle = (n + k)\,a^{\dagger k}\,|n\rangle\,, \quad k \in \mathbb{N}. \tag{1.13}$$

Therefore all positive integers $n + k \in \mathbb{N}$ are eigenvalues of N. Therefore the energy spectrum of the harmonic oscillator can be written as (1.4)

$$H\,|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle\,, \quad n \in \mathbb{N}. \tag{1.14}$$

1.2 Angular momentum spectrum

Compute the eigenvalues of the orbital angular momentum $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$

- *Show $[L_i, L_j] = \mathrm{i}\hbar\epsilon_{ijk}L_k$ and $[L^2, L_j] = 0$.*
- *Use the operators $L_\pm = L_x \pm \mathrm{i}L_y$ to derive the spectrum (Hint: compute the commutators with L_i and L^2 and express L^2 in terms of $L_\pm$ and L_z).*

Solution: The cross product of $\boldsymbol{r}$ and $\boldsymbol{p}$ can be written using EINSTEINS sum convention as follows:

$$L_i = \epsilon_{ijk} x_j \, p_k. \tag{1.15}$$

By using $[AB, C] = A[B, C] + [A, C]B$ the commutator $[L_i, L_j]$ can be expressed as

$$\begin{aligned}
[L_i, L_j] &= \epsilon_{iab}\epsilon_{jcd}[x_a p_b, x_c p_d] \\
&= \epsilon_{iab}\epsilon_{jcd}(x_a[p_b, x_c p_d] + [x_a, x_c p_d]p_b) \\
&= \epsilon_{iab}\epsilon_{jcd}(x_a x_c \underbrace{[p_b, p_d]}_{=0} + x_a \underbrace{[p_b, x_c]}_{=-\mathrm{i}\hbar\delta_{bc}} p_d + x_c \underbrace{[x_a, p_d]}_{=\mathrm{i}\hbar\delta_{ad}} p_b + \underbrace{[x_a, x_c]}_{=0} p_d p_b) \\
&= \mathrm{i}\hbar\epsilon_{iab}\epsilon_{jcd}(-x_a p_d \delta_{bc} + x_c p_b \delta_{ad}) \\
&= \mathrm{i}\hbar\big(-\epsilon_{iab}\epsilon_{jbd}x_a p_d + \epsilon_{iab}\epsilon_{jca}x_c p_b \delta_{ad}\big) \\
&= \mathrm{i}\hbar\big(\epsilon_{iab}\epsilon_{jdb}x_a p_d + \epsilon_{bia}\epsilon_{jca}x_c p_b \delta_{ad}\big) \\
&= \mathrm{i}\hbar\big((\delta_{ij}\delta_{ad} - \delta_{id}\delta_{ja})x_a p_d + (\delta_{jb}\delta_{ic} - \delta_{bc}\delta_{ij})x_c p_b\big) \\
&= \mathrm{i}\hbar\big(\cancel{x_a p_a} - x_j p_j + x_i p_j - \cancel{x_c p_c}\big) \\
&= \mathrm{i}\hbar\big(x_i p_j - x_j p_i\big) = \mathrm{i}\hbar\epsilon_{ijk}L_k.
\end{aligned} \tag{1.16}$$

The expression $[L^2, L_j] = 0$ can be shown explicitly for one component L_z. It follows

$$\begin{aligned}
[L^2, L_z] &= [L_x^2 + L_y^2 + L_z^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z] + \underbrace{[L_z^2, L_z]}_{=0} \\
&= L_x \underbrace{[L_x, L_z]}_{=-\mathrm{i}\hbar L_y} + \underbrace{[L_x, L_z]}_{=-\mathrm{i}\hbar L_y} L_x + L_y \underbrace{[L_y, L_z]}_{=\mathrm{i}\hbar L_x} + \underbrace{[L_y, L_z]}_{=\mathrm{i}\hbar L_x} L_y \\
&= \mathrm{i}\hbar(-L_x L_y - L_y L_x + L_y L_x + L_x L_y) = 0.
\end{aligned} \tag{1.17}$$

This can be shown analogously for L_x and L_y as well.

Next the commutator of the z-component of the angular momentum operator and the ladder operators is computed

$$\begin{aligned}
[L_z, L_\pm] &= L_z(L_x \pm \mathrm{i}L_y) - (L_x \pm \mathrm{i}L_y)L_z \\
&= L_z L_x \pm \mathrm{i}L_z L_y - L_x L_z \mp \mathrm{i}L_y L_z \\
&= \underbrace{[L_z, L_x]}_{=\mathrm{i}\hbar L_y} \pm \mathrm{i}\underbrace{[L_z, L_y]}_{=-\mathrm{i}\hbar L_x} \\
&= \hbar(\mathrm{i}L_y \pm L_x) = \pm\hbar(\pm\mathrm{i}L_y + L_x) \\
&= \pm\hbar L_\pm.
\end{aligned} \tag{1.18}$$

Because of the fact that L^2 and L_z commute they have the same eigenvectors $|\Psi\rangle$. The eigenvalue of L_z can be written as

$$L_z|m\rangle = \hbar m|m\rangle. \tag{1.19}$$

Now consider the product $L_z L_\pm$ applied to an eigenstate $|m\rangle$. Using equation (1.18) this can be expressed as

$$\begin{aligned} L_z L_\pm |m\rangle &= ([L_z, L_\pm] + L_\pm L_z)|m\rangle \\ &\overset{(1.18)}{=} (\pm\hbar L_\pm + L_\pm L_z)|m\rangle \\ &\overset{(1.19)}{=} \hbar(m\pm 1)L_\pm|m\rangle. \end{aligned} \tag{1.20}$$

This result is compared to $L_z|m+1\rangle = \hbar(m+1)|m+1\rangle$ which leads to the conclusion that L_+ raises the state $|m\rangle$ to $|m+1\rangle$

$$L_+|m\rangle = \alpha|m+1\rangle. \tag{1.21}$$

However, since $L^2|m\rangle = (L_x^2 + L_y^2)|m\rangle + m^2\hbar^2|m\rangle$ there must exist a maximum $m = m_{\max}$ because $m^2\hbar^2 \leq L^2$ which implies

$$L_+|m_{\max}\rangle = 0. \tag{1.22}$$

The operator L^2 can be expressed as a combination of $L_\pm$ and L_z. Lets first look at the product $L_- L_+$:

$$\begin{aligned} L_- L_+ &= (L_x - \mathrm{i}L_y)(L_x + \mathrm{i}L_y) = L_x^2 + L_y^2 + \mathrm{i}\underbrace{[L_x, L_y]}_{=\mathrm{i}\hbar L_z} = L_x^2 + L_y^2 - \hbar L_z \\ \Rightarrow L_x^2 + L_y^2 &= L_- L_+ + \hbar L_z \\ \Rightarrow L^2 &= L_- L_+ + L_z^2 + \hbar L_z. \end{aligned} \tag{1.23}$$

The operator L^2 is now applied to the eigenstate of maximum value $m_{\max}$

$$\begin{aligned} L^2|m_{\max}\rangle &= L_-\underbrace{L_+|m_{\max}\rangle}_{=0} + (L_z^2 + \hbar L_z)|m_{\max}\rangle \\ &= (L_z^2 + \hbar L_z)|m_{\max}\rangle = (m_{\max}^2\hbar^2 + m_{\max}\hbar^2)|m_{\max}\rangle \\ &= \hbar^2 m_{\max}(m_{\max}+1)|m_{\max}\rangle. \end{aligned} \tag{1.24}$$

The same procedure (equation (1.21) to (1.24)) can be performed analogously for L_- which leads to a minimum value $m_{\min}$ with $L_-|m_{\min}\rangle = 0$ and

$$L^2|m_{\min}\rangle = \hbar^2 m_{\min}(m_{\min}-1)|m_{\min}\rangle. \tag{1.25}$$

Because L^2 and L_z commute, the state $|Psi\rangle$ is an eigenfunction of L^2 and its eigenvalue is independent of m. Therefore

$$\begin{aligned} \hbar^2 m_{\max}(m_{\max}+1) &= \hbar^2 m_{\min}(m_{\min}-1) \\ \Rightarrow m_{\max} &= -m_{\min}. \end{aligned} \tag{1.26}$$

The number $m_{\max}$ can be denoted as l. The energy spectrum of the operator of angular momentum can therefore be written as

$$L_z|lm\rangle = m\hbar|lm\rangle \quad m = -l, -l+1, \ldots, l-1, l \tag{1.27}$$

$$L^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle. \tag{1.28}$$

1.3 Hydrogen atom spectrum

Solve the SCHRÖDINGER *equation for the H-atom's stationary states. Assume the Hamiltonian*

$$H = \frac{p^2}{2\mu} + \frac{Ze^2}{r} = -\frac{\hbar^2}{2\mu}\Delta + \frac{Ze^2}{r}, \tag{1.29}$$

express the result in terms of the BOHR *radius and discuss the degeneracy. Discuss the symmetry of the wavefunction in the ground state.*

Solution: The stationary SCHRÖDINGER equation can be written in the following way:

$$\left(-\frac{\hbar^2}{2\mu}\Delta + \frac{Ze^2}{r}\right)\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}), \tag{1.30}$$

whereas the Laplacian operator can be written in spherical coordinates as follows

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}. \tag{1.31}$$

It is assumed that the the solution $\Psi(\boldsymbol{r})$ can be separated in the following way:

$$\Psi(r,\vartheta,\varphi) = R(r)\Theta(\vartheta)\Phi(\varphi). \tag{1.32}$$

Therefore the SCHRÖDINGER equation can be expressed as

$$\begin{aligned}
\Delta\Psi &= -\frac{2\mu}{\hbar^2}\left(E + \frac{Ze^2}{r}\right)\Psi \\
\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)\Psi &= -\frac{2\mu}{\hbar^2}\left(E + \frac{Ze^2}{r}\right)\Psi \\
\frac{\Theta\Phi}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{R\Phi}{r^2\sin\vartheta}\frac{\mathrm{d}}{\mathrm{d}\vartheta}\left(\sin\vartheta\frac{\mathrm{d}\Theta}{\mathrm{d}\vartheta}\right) + \frac{R\Theta}{r^2\sin^2\vartheta}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2} &= -\frac{2\mu}{\hbar^2}\left(E + \frac{Ze^2}{r}\right)R\Theta\Phi.
\end{aligned} \tag{1.33}$$

Both sides can be multiplied by $r^2\sin^2\vartheta/\Psi(r,\vartheta,\varphi)$:

$$\begin{aligned}
\frac{\sin^2\vartheta}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{\sin\vartheta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\vartheta}\left(\sin\vartheta\frac{\mathrm{d}\Theta}{\mathrm{d}\vartheta}\right) + \frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2} &= -\frac{2\mu}{\hbar^2}r^2\sin^2\vartheta\left(E + \frac{Ze^2}{r}\right) \\
\underbrace{\frac{\sin^2\vartheta}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{\sin\vartheta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\vartheta}\left(\sin\vartheta\frac{\mathrm{d}\Theta}{\mathrm{d}\vartheta}\right) + \frac{2\mu}{\hbar^2}r^2\sin^2\vartheta\left(E + \frac{Ze^2}{r}\right)}_{\text{Function of } r,\vartheta} &= \underbrace{-\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}}_{\text{Function of } \varphi}.
\end{aligned} \tag{1.34}$$

Since the left hand side is only dependent on r,ϑ and the right side is only dependent on φ, both sides must be equal to a constant, which is denoted as m^2, because the equation must be valid for every (r,ϑ,φ). This leads to

$$-m^2 = \frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2} \quad\Rightarrow\quad \Phi(\varphi) = A\cdot\exp\left(\mathrm{i}m\varphi\right). \tag{1.35}$$

Because $\Phi(\varphi) = \Phi(\varphi + 2\pi)$ is periodic

$$\exp\big(\mathrm{i}m\varphi\big) = \exp\big(\mathrm{i}m(\varphi+2\pi)\big) = \exp\big(\mathrm{i}m\varphi\big)\underbrace{\exp(\mathrm{i}m2\pi)}_{=1} \quad \Rightarrow m \in \mathbb{Z}. \tag{1.36}$$

The function $\Phi(\varphi)$ can be normalized in the following way

$$\int_0^{2\pi} \Phi(\varphi)\Phi^*(\varphi)\,\mathrm{d}\varphi = A^2 \cdot 2\pi \stackrel{!}{=} 1, \tag{1.37}$$

which leads to the solution

$$\boxed{\Phi(\varphi) = \frac{1}{\sqrt{2\pi}}\exp\big(\mathrm{i}m\varphi\big).} \tag{1.38}$$

The left hand side of (1.34) can be separated again into two parts, which are only dependent on r or ϑ by dividing by $\sin^2\vartheta$

$$\underbrace{\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{2\mu}{\hbar^2}r^2\left(E + \frac{Ze^2}{r}\right)}_{\text{Function of } r} = \underbrace{-\frac{1}{\Theta\sin\vartheta}\frac{\mathrm{d}}{\mathrm{d}\vartheta}\left(\sin\vartheta\frac{\mathrm{d}\Theta}{\mathrm{d}\vartheta}\right) + \frac{m^2}{\sin^2\vartheta}}_{\text{Function of } \vartheta}. \tag{1.39}$$

Both sides of the equation are set to a second constant denoted as λ. The solution of the right hand side of equation (1.39) leads in combination with (1.38) to the spherical harmonics:

$$\boxed{Y_{lm}(\vartheta,\varphi) = \sqrt{\frac{1}{4\pi}}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\vartheta)\exp\big(\mathrm{i}m\varphi\big)} \tag{1.40}$$

with $\lambda = l(l+1)$ and $P_l^m(x)$ an associated legendre polynomial

$$P_l^m(x) = \frac{(-1)^m}{2^l\,l!}(1-x^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}\big(x^2-1\big)^l. \tag{1.41}$$

The left hand side of equation (1.39) can be written as

$$\begin{aligned} \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{2\mu}{\hbar^2}\left(E + \frac{Ze^2}{r}\right)R &= l(l+1)\frac{R}{r^2} \\ \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{2\mu}{\hbar^2}\left(E + \frac{Ze^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right)R &= 0 \end{aligned} \tag{1.42}$$

2 Postulates

2.1 Basic operator properties

Show that:

- *given two complete orthonormal bases $A = \{|\alpha\rangle\}$ and $B = \{|\beta\rangle\}$, the operator U associated to the change of basis from A to B is unitary, and is expressed as*

$$U = \sum_k \left|\beta^k\right\rangle \left\langle\alpha^k\right| ; \tag{2.1}$$

- *the trace (operator) $Tr(X) = \sum_\alpha \langle\alpha|X|\alpha\rangle$ is invariant under change of basis.*

Solution: Lets first show that the operator U performs the change of basis:

$$\begin{aligned} U|\alpha\rangle &= \sum_k \left|\beta^k\right\rangle \left\langle\alpha^k|\alpha\right\rangle \\ &= \sum_k \sum_j \left|\beta^k\right\rangle \left\langle\alpha^k|c_j|\alpha^j\right\rangle \\ &= \sum_k \sum_j c_j \left|\beta^k\right\rangle \underbrace{\left\langle\alpha^k|\alpha^j\right\rangle}_{=\delta_{jk}} \\ &= \sum_k c_k \left|\beta^k\right\rangle = |\beta\rangle . \end{aligned} \tag{2.2}$$

In order to show that U is a unitary operator we compute the product $UU^\dagger$ by using the orthonormality and completeness of $A = \{|\alpha\rangle\}$ and $B = \{|\beta\rangle\}$:

$$\begin{aligned} UU^\dagger &= \sum_k \left|\beta^k\right\rangle \left\langle\alpha^k\right| \sum_j \left(\left|\beta^j\right\rangle \left\langle\alpha^j\right|\right)^\dagger = \sum_k \left|\beta^k\right\rangle \left\langle\alpha^k\right| \sum_j \left|\alpha^j\right\rangle \left\langle\beta^j\right| \\ &= \sum_k \sum_j \left|\beta^k\right\rangle \underbrace{\left\langle\alpha^k|\alpha^j\right\rangle}_{=\delta_{jk}} \left\langle\beta^j\right| \\ &= \sum_k \left|\beta^k\right\rangle \left\langle\beta^k\right| = \mathbb{1}. \end{aligned} \tag{2.3}$$

The invariance of the trace operator can be shown by using the completeness of $A = \{|\alpha\rangle\}$ and $B = \{|\beta\rangle\}$, where we can write the trace in the following way:

$$\begin{aligned} Tr(X) &= \sum_k \left\langle\alpha^k|X|\alpha^k\right\rangle = \sum_{kj} \left\langle\alpha^k|\beta^j\right\rangle \left\langle\beta^j|X|\alpha^k\right\rangle \\ &= \sum_{kj} \left\langle\beta^j|X|\alpha^k\right\rangle \left\langle\alpha^k|\beta^j\right\rangle = \sum_j \left\langle\beta^j|X\mathbb{1}|\beta^j\right\rangle = Tr(X) \end{aligned} \tag{2.4}$$

2.2 Schwarz inequality

1. *Prove the Schwarz inequality*

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2. \tag{2.5}$$

Hint: First, observe that $(\langle\alpha| + \lambda^*\langle\beta|) \cdot (|\alpha\rangle + \lambda|\beta\rangle) \geq 0$ *holds for any complex number* λ*; then choose* λ *in such a way that the above inequality reduces to the Schwarz inequality.*

2. *Show that the equality sign in the generalized uncertainty relation* $\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ *holds if the state in question satisfies*

$$\Delta A|\alpha\rangle = \lambda\Delta B|\alpha\rangle \tag{2.6}$$

with λ *purely imaginary.*

3. *Explicit calculations using the usual rules of wave mechanics show that the wave function for a Gaussian wave packet given by*

$$\langle x'|\alpha\rangle = (2\pi d^2)^{-1/4}\exp\left[\frac{i\langle p\rangle x'}{\hbar} - \frac{(x'-\langle x\rangle)^2}{4d^2}\right] \tag{2.7}$$

satisfies the minimum uncertainty relation

$$\sqrt{\langle(\Delta x)^2\rangle}\sqrt{\langle(\Delta p)^2\rangle} = \frac{\hbar}{2}. \tag{2.8}$$

Prove that the requirement $\langle x'|\Delta x|\alpha\rangle = \lambda\langle x'|\Delta p|\alpha\rangle$*, where* λ *is an imaginary number, is indeed satisfied for such a Gaussian wave packet, in agreement with Part 2.*

1. Solution: First we rewrite the relation given in the hint:

$$\begin{aligned} 0 &\leq (\langle\alpha| + \lambda^*\langle\beta|) \cdot (|\alpha\rangle + \lambda|\beta\rangle) \\ &= \langle\alpha|\alpha\rangle + |\lambda|^2\langle\beta|\beta\rangle + \lambda^*\langle\beta|\alpha\rangle + \lambda\langle\alpha|\beta\rangle. \end{aligned} \tag{2.9}$$

In order to arrive at the Schwarz inequality we need the product $|\langle\alpha|\beta\rangle|^2$. Therefore we aim for a λ which delivers this term when squared. Since the inequality to prove consists of only two terms we need to ensure that some terms cancel out. This can be achived by choosing

$$\lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}. \tag{2.10}$$

This leads to the following result when λ is substituted into (2.9)

$$\begin{aligned} 0 &\leq \langle\alpha|\alpha\rangle + \frac{|\langle\beta|\alpha\rangle|^2}{|\langle\beta|\beta\rangle|^2}\langle\beta|\beta\rangle - \frac{\langle\beta|\alpha\rangle^*}{\langle\beta|\beta\rangle}\langle\beta|\alpha\rangle - \frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}\langle\alpha|\beta\rangle \\ &= \langle\alpha|\alpha\rangle + \frac{\cancel{|\langle\beta|\alpha\rangle|^2}}{\cancel{\langle\beta|\beta\rangle}} - \frac{\cancel{|\langle\beta|\alpha\rangle|^2}}{\cancel{\langle\beta|\beta\rangle}} - \frac{|\langle\beta|\alpha\rangle|^2}{\langle\beta|\beta\rangle} \\ \Rightarrow \frac{|\langle\beta|\alpha\rangle|^2}{\langle\beta|\beta\rangle} &\leq \langle\alpha|\alpha\rangle \quad \Rightarrow \quad \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\beta|\alpha\rangle|^2 \end{aligned} \tag{2.11}$$

2. Solution: The assumption that λ is purely imaginary means that $\lambda = -\lambda^*$. The deviation ΔA ist given by

$$\Delta A = A - \underbrace{\langle A \rangle}_{\langle\alpha|A|\alpha\rangle}, \qquad \Delta B = B - \underbrace{\langle B \rangle}_{\langle\alpha|B|\alpha\rangle}. \tag{2.12}$$

Then we first evaluate the right hand side of the equation. The commutator $[\Delta A, \Delta B]$ can be written as

$$\begin{aligned}[\Delta A, \Delta B] &= [A - \langle A\rangle, B - \langle B\rangle] = [A, B - \langle B\rangle] - \underbrace{[\langle A\rangle, B - \langle B\rangle]}_{=0} \\ &= [A, B] - \underbrace{[A, \langle B\rangle]}_{=0}. \end{aligned} \tag{2.13}$$

We used the fact, that the commutator with a scalar ($\langle A\rangle, \langle B\rangle$) is zero. Now we can write the right hand side in the following way:

$$\begin{aligned}\langle [A, B]\rangle &= \langle\alpha|[A, B]|\alpha\rangle = \langle\alpha|\Delta A\Delta B - \Delta B\Delta A|\alpha\rangle \\ &= \left\langle \alpha|\lambda^*(\Delta B)^2 - \lambda(\Delta B)^2|\alpha\right\rangle \\ &= -2\lambda\left\langle(\Delta B)^2\right\rangle \end{aligned} \tag{2.14}$$

$$\Rightarrow \frac{1}{4}|\langle [A, B]\rangle|^2 = \lambda\lambda^*|\left\langle(\Delta B)^2\right\rangle|^2 = -\lambda^2|\left\langle(\Delta B)^2\right\rangle|^2 \tag{2.15}$$

The left hand side can be evaluated as

$$\left\langle(\Delta A)^2\right\rangle\left\langle(\Delta B)^2\right\rangle = -\lambda^2|\left\langle(\Delta B)^2\right\rangle|^2, \tag{2.16}$$

which is indeed equal to the left hand side.

3. Solution: In order to prove the requirement we calculate both sides of the equation and find an imaginary λ. We start the left hand side

$$\begin{aligned}\left\langle x'|\Delta X|\alpha\right\rangle &= \left\langle x'|X - \langle X\rangle|\alpha\right\rangle = x'\left\langle x'|\alpha\right\rangle - \langle x\rangle\left\langle x'|\alpha\right\rangle \\ &= (x' - \langle x\rangle)\left\langle x'|\alpha\right\rangle. \end{aligned} \tag{2.17}$$

For the calculation of the right side we use the momentum operator in position space can be expressed as $p = -\mathrm{i}\hbar\partial x'$

$$\begin{aligned}\left\langle x'|\Delta P|\alpha\right\rangle &= \underbrace{-\mathrm{i}\hbar\frac{\partial}{\partial x'}\left\langle x'|\alpha\right\rangle}_{} - \left\langle p\right\rangle\left\langle x'|\alpha\right\rangle \\ &\quad -\mathrm{i}\hbar\left(\frac{\mathrm{i}\left\langle p\right\rangle}{\hbar} - \frac{(x' - \langle x\rangle)}{2d^2}\right)\left\langle x'|\alpha\right\rangle = \left[\left\langle p\right\rangle + \frac{\mathrm{i}\hbar}{2d^2}(x' - \langle x\rangle)\right]\left\langle x'|\alpha\right\rangle \\ \left\langle x'|\Delta P|\alpha\right\rangle &= \frac{\mathrm{i}\hbar}{2d^2}(x' - \langle x\rangle)\left\langle x'|\alpha\right\rangle. \end{aligned} \tag{2.18}$$

This leads to the following result:

$$\left\langle x'|\Delta P|\alpha\right\rangle \frac{\mathrm{i}\hbar}{2d^2}\left\langle x'|\Delta X|\alpha\right\rangle, \qquad \text{with } \lambda = \frac{\mathrm{i}\hbar}{2d^2}. \tag{2.19}$$

2.3 Spin 1/2 operators and commutators

1. *Write down the* 2×2 *matrix representation of* S_i *in the basis that diagonalizes* S_z.
2. *Verify all the commutators between each pair of* S_i, S^2
3. *Defining the ladder operator as* $S_\pm = S_x \pm \mathrm{i}S_y$, *show that they are not hermitian, write down their representation in the* S_z *basis and determine their action upon the eigenvectors of* S_z.

Solution: The matrix representation of S_z can be determined using the following formula:

$$A = \sum_{a'} a' \left|a'\right\rangle \left\langle a'\right| \Rightarrow S_z = \frac{\hbar}{2}(|+\rangle\langle +| - |-\rangle\langle -|) = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{2.20}$$

The basis vectors $|S_x;\pm\rangle$ and $\left|S_y;\pm\right\rangle$ can be written in the following way:[1]

$$|S_x;\pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle) \tag{2.21}$$

$$\left|S_y;\pm\right\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm \mathrm{i}|-\rangle). \tag{2.22}$$

Using equation (2.20) we can write S_x and S_y as

$$S_x = \frac{\hbar}{2}(|S_x;+\rangle\langle S_x;+| - |S_x;-\rangle\langle S_x;-|) \overset{(2.21)}{=} \frac{\hbar}{2}(|-\rangle\langle +| + |+\rangle\langle -|) \tag{2.23}$$

$$S_y = \frac{\hbar}{2}(\left|S_y;+\right\rangle\left\langle S_y;+\right| - \left|S_y;-\right\rangle\left\langle S_y;-\right|) \overset{(2.22)}{=} \frac{\mathrm{i}\hbar}{2}(|-\rangle\langle +| - |+\rangle\langle -|). \tag{2.24}$$

Therefore the matrix representation of both operators are as follows:

$$S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad S_y = \frac{\hbar}{2}\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}. \tag{2.25}$$

The commutators between the S_i and S^2 can be verified by noting that $[S_i, S_j] = \mathrm{i}\hbar\varepsilon_{ijk}S_k$. Then the commutation relations can be shown analogously to (1.17)

$$\begin{aligned}[S^2, S_z] &= [S_x^2 + S_y^2 + S_z^2, S_z] = [S_x^2, S_z] + [S_y^2, S_z] + \underbrace{[S_z^2, S_z]}_{=0}\\ &= S_x\underbrace{[S_x, S_z]}_{=-\mathrm{i}\hbar S_y} + \underbrace{[S_x, S_z]}_{=-\mathrm{i}\hbar S_y}S_x + S_y\underbrace{[S_y, S_z]}_{=\mathrm{i}\hbar S_x} + \underbrace{[S_y, S_z]}_{=\mathrm{i}\hbar S_x}S_y\\ &= \mathrm{i}\hbar(-S_xS_y - S_yS_x + S_yS_x + S_xS_y) = 0.\end{aligned} \tag{2.26}$$

Alternatively you can compute S^2

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3\hbar^2}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{2.27}$$

[1] Sakurai: Modern Quantum mechanics, p.26

It can be seen, that S^2 is proportional to the identity matrix, which commutes with every matrix. Therefore the commutators must be zero.

In order to show that the ladder operators are not hermitian, we first show, that S_x and S_y are hermitian, which can be immediately seen by computing the hermitian conjugate of (2.25)

$$S_x^\dagger = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad S_y^\dagger = \frac{\hbar}{2}\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}. \tag{2.28}$$

Then we can write the hermitian conjugate of $S_\pm$ as

$$S_\pm^\dagger = (S_x \pm \mathrm{i}S_y)^\dagger = S_x^\dagger + (\mathrm{i}S_y)^\dagger = S_x \mp \mathrm{i}S_y \neq S_\pm. \tag{2.29}$$

The representation of the ladder operators in the S_z basis can be derived by using (2.23) and (2.24)

$$S_x \pm \mathrm{i}S_y = \frac{\hbar}{2}[(|-\rangle\langle+| + |+\rangle\langle-|) \pm \mathrm{i}^2(|-\rangle\langle+| - |+\rangle\langle-|)]. \tag{2.30}$$

Therefore the ladder operators result in

$$S_+ = \hbar|+\rangle\langle-|, \qquad S_- = \hbar|-\rangle\langle+|. \tag{2.31}$$

Their action on the eigenvectors $|+\rangle$ and $|-\rangle$ of the z-component of the spin are therefore

$$S_+|-\rangle = \hbar|+\rangle\langle-|-\rangle = \hbar|+\rangle, \qquad S_+|+\rangle = \hbar|+\rangle\langle-|+\rangle = \hbar|0\rangle \tag{2.32}$$

$$S_-|+\rangle = \hbar|-\rangle\langle+|+\rangle = \hbar|-\rangle, \qquad S_-|-\rangle = \hbar|-\rangle\langle+|-\rangle = \hbar|0\rangle. \tag{2.33}$$

The S_+ operator raises the $|-\rangle$ state to $|+\rangle$, whereas the S_- operator does the opposite. Lowering the $|-\rangle$ state and rising the $|+\rangle$ state leads to a nullket.

2.4 Beam of Spin 1/2 atoms

A beam of spin $\frac{1}{2}$ atoms goes through a series of Stern-Gerlach-type measurements as follows

1. *The first measurement accepts $s_z = \hbar/2$ atoms and rejects $s_z = -\hbar/2$ atoms.*
2. *The second measurement accepts $s_n = \hbar/2$ atoms and rejects $s_n = -\hbar/2$ atoms, where s_n is the eigenvalue of the operator $\boldsymbol{S}\cdot\hat{\boldsymbol{n}}$, with $\hat{\boldsymbol{n}}$ making an angle β in the xz-plane with respect to the z-axis.*
3. *The third measurement accepts $s_z = -\hbar/2$ atoms and rejects $s_z = \hbar/2$ atoms.*

What is the intensity of the final $s_z = -\hbar/2$ beam when the $s_z = \hbar/2$ beam surviving the first measurement is normalized to unity? How must we orient the second measuring apparaturs if we are to maximize the intensity of the final $s_z = -\hbar/2$ beam?

Solution: The rotation of the S_z apparatus can be interpreted as a rotation matrix S_n given as

$$S_n = \frac{\hbar}{2}\begin{pmatrix}\cos\beta & \sin\beta \\ \sin\beta & -\cos\beta\end{pmatrix} \quad \text{and } \boldsymbol{s}\cdot\hat{\boldsymbol{n}} = \begin{pmatrix}S_x\\S_y\\S_z\end{pmatrix}\cdot\begin{pmatrix}\sin\beta\\0\\\cos\beta\end{pmatrix}. \tag{2.34}$$

The eigenvectors of S_n can be computed as

$$|n+\rangle = \frac{1}{2}\begin{pmatrix}\cos\beta+1\\ \sin\beta\end{pmatrix}, \qquad |n-\rangle = \frac{1}{2}\begin{pmatrix}1-\cos\beta\\ -\sin\beta\end{pmatrix}. \tag{2.35}$$

Therefore the representation of the outcoming $|n+\rangle$ state in the S_z basis is

$$|n+\rangle = \frac{1}{2}(1+\cos\beta\,|+\rangle + \sin\beta\,|-\rangle). \tag{2.36}$$

The resulting intensity of the beam for a normalized $|n+\rangle$ state after the last measurement with the S_z apparatus can be written as

$$\langle -|n+\rangle = \frac{1}{4}\sin^2\beta. \tag{2.37}$$

It can be seen that the maximum intensity occurs at $\beta = \pi/2$ which is an apparatus in x-direction.
The solution can be also obtained by combining all three measurements into a single apparatus. The initial state is

$$|S_0\rangle = a\,|+\rangle + b\,|-\rangle\,. \tag{2.38}$$

The final state can then be written in the following way:

$$\begin{aligned} |S_{\text{final}}\rangle &= |-\rangle\,\langle -|n+\rangle\,\langle n+|+\rangle\,\langle +|S_0\rangle \\ \Rightarrow P = |\,|S_{\text{final}}\rangle\,| &= \underbrace{|\,\langle -|n+\rangle\,|^2}_{\sin^2(\beta/2)}\underbrace{|\,\langle n+|+\rangle\,|^2}_{\sin^2(\beta/2)}|\,\langle +|S_0\rangle\,|^2 \\ &= \sin^2\left(\frac{\beta}{2}\right)\cos^2\left(\frac{\beta}{2}\right)a^2 = \frac{a^2}{4}\sin^2\beta. \end{aligned} \tag{2.39}$$

Since the state after the first measurement ist normalized, the factor a must be equal to one. Then (2.39) and (2.37) coincide.

3 Dynamics

3.1 Free particle evolution

Consider a particle in a generic potential $V(x)$.

a) *Prove the commutator relations*

$$\big[x_i, F(\boldsymbol{p})\big] = \mathrm{i}\hbar\frac{\partial}{\partial p_i}F(\boldsymbol{p}), \qquad \big[p_i, G(\boldsymbol{x})\big] = -\mathrm{i}\hbar\frac{\partial}{\partial x_i}G(\boldsymbol{x}), \tag{3.1}$$

where F, G are generic functions of the operators $\boldsymbol{p}$ and $\boldsymbol{x}$ respectively.

b) *Show that for the Hamiltonian $H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})$ one obtains the equation*

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\boldsymbol{x}\rangle = -\left\langle\vec{\boldsymbol{\nabla}}V(\boldsymbol{x})\right\rangle \tag{3.2}$$

i.e. expectation values follow the classical equation of motion with no $\hbar$ appearing (Ehrenfest theorem).

c) *Specify the previous point to the free particle ($V = 0$) and prove the uncertainty relation*

$$\left\langle(\Delta x_i)^2\right\rangle_t \left\langle(\Delta x_i)^2\right\rangle_{t=0} \geq \frac{\hbar^2 t^2}{4m^2}. \tag{3.3}$$

d) *Calculate the diffusion of the Gaussian wave packet using the propagator*

$$K(x, t, x_0, t_0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar(t-t_0)}}\exp\left(\frac{\mathrm{i}}{\hbar}\frac{m}{2}\frac{(x-x_0)^2}{t-t_0}\right) \tag{3.4}$$

and the wave function representation.

a.) Solution: The commutation relations can be proven by applying the commutator to a generic state $|\Psi\rangle$ and multiplying with $\langle\boldsymbol{x}|$ to work in position space:

$$\begin{aligned}
\big\langle\boldsymbol{x}|[p_i, G(\boldsymbol{x})]|\Psi\big\rangle &= \big\langle\boldsymbol{x}|p_i G(\boldsymbol{x})|\Psi\big\rangle - \big\langle\boldsymbol{x}|G(\boldsymbol{x})p_i|\Psi\big\rangle \\
&= \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_i}(G(\boldsymbol{x})\Psi(\boldsymbol{x})) - G(\boldsymbol{x})\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_i}\Psi(\boldsymbol{x}) \\
&= \frac{\hbar}{\mathrm{i}}\Psi(\boldsymbol{x})\frac{\partial}{\partial x_i}G(\boldsymbol{x}) + \cancel{G(\boldsymbol{x})\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_i}\Psi(\boldsymbol{x})} - \cancel{G(\boldsymbol{x})\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_i}\Psi(\boldsymbol{x})} \\
&= -\mathrm{i}\hbar\frac{\partial}{\partial x_i}G(\boldsymbol{x})\Psi(\boldsymbol{x}) = \left\langle\boldsymbol{x}|-\mathrm{i}\hbar\frac{\partial}{\partial x_i}G(\boldsymbol{x})|\Psi\right\rangle.
\end{aligned} \tag{3.5}$$

The same procedure can be performed for the other commutator, but we evaluate it in momentum space by using that $x_i = \mathrm{i}\hbar\partial p_i$

$$\begin{aligned}
\big\langle\boldsymbol{p}|[x_i, F(\boldsymbol{p})]|\Psi\big\rangle &= \big\langle\boldsymbol{p}|x_i F(\boldsymbol{p})|\Psi\big\rangle - \big\langle\boldsymbol{p}|F(\boldsymbol{p})x_i|\Psi\big\rangle \\
&= \mathrm{i}\hbar\frac{\partial}{\partial p_i}\big(F(\boldsymbol{p})\Psi(\boldsymbol{p})\big) - F(\boldsymbol{p})\mathrm{i}\hbar\frac{\partial}{\partial p_i}\Psi(\boldsymbol{p}) \\
&= \mathrm{i}\hbar\frac{\partial}{\partial p_i}F(\boldsymbol{p})\Psi(\boldsymbol{p}) = \left\langle\boldsymbol{p}|\mathrm{i}\hbar\frac{\partial}{\partial p_i}F(\boldsymbol{p})|\Psi\right\rangle.
\end{aligned} \tag{3.6}$$

b.) Solution: We can solve this task using the Heisenberg Picture of time evolution. For a time dependent operator (which is not explicitly time dependent) we can write

$$\frac{\mathrm{d}A_H}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[A_H, H]. \tag{3.7}$$

In order to derive the Ehrenfest theorem we need to evaluate the second time derivative of the position $\boldsymbol{x}$. For the first derivative we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x} = \frac{1}{\mathrm{i}\hbar}[\boldsymbol{x}, H] &= \frac{1}{\mathrm{i}\hbar}\left[\boldsymbol{x}, \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})\right] \\ &= \frac{1}{\mathrm{i}\hbar}\left[\boldsymbol{x}, \frac{\boldsymbol{p}^2}{2m}\right] = \frac{1}{\mathrm{i}\hbar}\frac{1}{2m}[\boldsymbol{x}, \boldsymbol{p}^2] \\ &\overset{(3.1)}{=} \frac{1}{2m}\vec{\boldsymbol{\nabla}}\left(\boldsymbol{p}^2\right) = \frac{\boldsymbol{p}}{m}.\end{aligned} \tag{3.8}$$

Then we can write the second derivative as

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\boldsymbol{x} = \frac{1}{m}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p} &= \frac{1}{\mathrm{i}\hbar m}[\boldsymbol{p}, H] \\ &= \frac{1}{\mathrm{i}\hbar m}[\boldsymbol{p}, V(\boldsymbol{x})] \overset{(3.1)}{=} \frac{1}{\mathrm{i}\hbar m}(-\mathrm{i}\hbar\vec{\boldsymbol{\nabla}}V(\boldsymbol{x})) \\ \Rightarrow m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\boldsymbol{x} &= -\vec{\boldsymbol{\nabla}}V(\boldsymbol{x}).\end{aligned} \tag{3.9}$$

The Ehrenfest theorem follows directly by applying the expectation value of a generic state to both sides of the equation

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\boldsymbol{x}\rangle = -\left\langle\vec{\boldsymbol{\nabla}}V(\boldsymbol{x})\right\rangle. \tag{3.10}$$

c.) Solution: We can write the uncertainty relation in the following way:

$$\left\langle(\Delta x_i)^2\right\rangle_t\left\langle(\Delta x_i)^2\right\rangle_{t=0} \geq \frac{1}{4}|\langle[x_i(t), x_i(0)]\rangle|^2. \tag{3.11}$$

We can use (3.8) to find a relation between $x_i(t)$ and $x_i(0)$:

$$x_i(t) = x_i(0) + \frac{p_i(0)}{m}\cdot t. \tag{3.12}$$

Then we can write the commutator $[x_i(t), x_i(0)]$ as

$$[x_i(t), x_i(0)] = \left[x_i(0) + \frac{p_i(0)}{m}t, x_i(0)\right] = \left[\frac{p_i(0)}{m}t, x_i(0)\right] = -\mathrm{i}\hbar\frac{t}{m}. \tag{3.13}$$

Now we can substitute (3.13) into (3.11)

$$\left\langle(\Delta x_i)^2\right\rangle_t\left\langle(\Delta x_i)^2\right\rangle_{t=0} \geq \frac{1}{4}\left|-\mathrm{i}\hbar\frac{t}{m}\right|^2 = \frac{\hbar^2 t^2}{4m^2}. \tag{3.14}$$

d.) Solution: The initial Gaussian wave packet can be expressed as

$$\Psi(x,t_0) = \frac{1}{\sqrt[4]{\pi d^2}} \exp\left(\mathrm{i}\frac{p_0 x}{\hbar}\right) \exp\left(-\frac{x^2}{2d^2}\right). \tag{3.15}$$

Now we can use the equation given in the lecture, to use the propagator in order to compute the state $\Psi(x,t)$

$$\begin{aligned}
\Psi(x,t) &= \int_{-\infty}^{\infty} \mathrm{d}x'\, K(x,t,x',0)\Psi(x',0) \\
&= \frac{1}{\sqrt[4]{\pi d^2}} \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left(\frac{\mathrm{i}}{\hbar}\frac{m}{2}\frac{(x-x')^2}{t}\right) \exp\left(\mathrm{i}\frac{p_0 x'}{\hbar}\right) \exp\left(-\frac{x'^2}{2d^2}\right) \\
&= \sqrt{\frac{m}{2\pi\sqrt{\pi} d \mathrm{i}\hbar t}} \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left[-\underbrace{\left(\frac{1}{2d^2} - \frac{\mathrm{i}m}{2\hbar t}\right)}_{=a} x'^2 + \underbrace{\left(\frac{\mathrm{i}p_0}{\hbar} - \frac{\mathrm{i}m}{t\hbar}x\right)}_{=b} x' + \underbrace{\frac{\mathrm{i}m}{2\hbar t}x^2}_{=c} \right].
\end{aligned} \tag{3.16}$$

Now we can compute this Gaussian integral by using the following relation

$$\int_{-\infty}^{\infty} \mathrm{d}x \exp\left(-ax^2+bx+c\right) = \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(-a\left(x-\frac{b}{2a}\right)^2 + \frac{b^2}{4a} + c\right) = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a}+c\right).$$

$$\begin{aligned}
\Psi(x,t) &= \sqrt{\frac{m}{2\pi\sqrt{\pi} d \mathrm{i}\hbar t}} \sqrt{\frac{\pi}{\frac{1}{2d^2} - \frac{\mathrm{i}m}{2\hbar t}}} \exp\left[\left(\frac{\mathrm{i}m}{\hbar t}\right)^2 \left(\frac{p_0 t}{m} - x\right)^2 \left(\frac{1}{d^2} - \frac{\mathrm{i}m}{\hbar t}\right)^{-1} + \frac{\mathrm{i}m}{2\hbar t}x^2\right] \\
&\stackrel{?}{=} \sqrt{\sqrt{\pi}\left(\frac{\mathrm{i}\hbar t}{dm} + d\right)}^{-1} \exp\left[\frac{-(x-p_0 t/m)^2}{2d^2(1+\mathrm{i}\hbar t/md^2)}\right] \exp\left[\frac{\mathrm{i}p_0}{\hbar}\left(x - \frac{p_0 t}{2m}\right)\right]
\end{aligned} \tag{3.17}$$

3.2 SHO evolution

- *Sketch the time evolution of the Simple Harmonic Oscillator in the Schrödinger formulation*
- *Do the same as above, but now in the Heisenberg formulation.*
- *Hence verify Ehrenfest's theorem and the equivalence of the Schrödinger and Heisenberg pictures.*
- *Finally calculate the propagator*

$$K(x_2,T,x_1,0) = \int_{x_1,0}^{x_2,T} [\mathscr{D}x] \exp\left(\frac{\mathrm{i}S[x(t)]}{\hbar}\right) \tag{3.18}$$

for a SHO oscillating with frequency ω.

Solution: The Hamiltonian of the 1D Harmonic Oscillator can be written as

$$H = \frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2 \quad \text{or} \quad H = \hbar\omega\left(N + \frac{1}{2}\right). \tag{3.19}$$

We can write a generic state $|\Psi\rangle$ as $|\Psi\rangle = \sum_n c_n(0)\,|n\rangle$ as a superposition of eigenstates $|n\rangle$ with eigenvalue n. In the Schrödinger picture the time evoluted state can be written as

$$\begin{aligned} |\Psi, t\rangle = U\,|\Psi\rangle &= \exp\left(-\mathrm{i}\frac{Ht}{\hbar}\right)\sum_n c_n(0)\,|n\rangle \\ &= \underbrace{\sum_n c_n(0)\exp\left(-\mathrm{i}\omega\left(n+\frac{1}{2}\right)t\right)}_{c_n(t)}|n\rangle\,. \end{aligned} \tag{3.20}$$

We can use the Heisenberg picture to analyze the time evolution of the position and momentum operator. We can aquire the equation of motion via relation (3.7)

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[x, H] = \frac{1}{\mathrm{i}\hbar}\frac{1}{2m}[x, p^2] = \frac{p}{m}. \tag{3.21}$$

We can then write the second derivative as

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = \frac{1}{m}\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar m}[p, H] = \frac{\omega^2}{2\mathrm{i}\hbar}[p, x^2] = \frac{\omega^2}{2\mathrm{i}\hbar}\left(-\mathrm{i}\hbar\frac{\partial x^2}{\partial x}\right) = -\omega^2 x. \tag{3.22}$$

The general solution of this differential equation are the sine and cosine function

$$x(t) = C_1\cos(\omega t) + C_2\sin(\omega t). \tag{3.23}$$

We can determine the integration constants by demanding

$$x(t=0) = x(0) \quad p(t=0) = 0, \tag{3.24}$$

which leads to $C_1 = x(0)$ and

$$p(t) = -\omega m\sin(\omega t)x(0) + m\omega C_2\cos(\omega t) \quad \overset{t=0}{\Rightarrow} C_2 = \frac{p(0)}{m\omega}, \tag{3.25}$$

which results in

$$x(t) = x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t). \tag{3.26}$$

We can now easily verify the Ehrenfest theorem, because we already have the second derivative in equation (3.22)

$$\begin{aligned} m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle &= -\left\langle\vec{\nabla}V(x)\right\rangle \\ m\frac{\mathrm{d}^2}{\mathrm{d}t^2}x = -m\omega^2, &\quad -\vec{\nabla}V(x) = -\frac{\partial}{\partial x}\frac{m}{2}\omega^2x^2 = -m\omega^2x, \end{aligned} \tag{3.27}$$

which shows that lhs and rhs are indeed equal.

Remark: We can show that both pictures of time evolution are the same by computing the expectation value of the operators. First we confirm that the operators are the same at $t = 0$

$$x_H(0) = x_S(0) = x_0 \quad \text{and} \quad p_H(0) = p_S(0) = p_0. \tag{3.28}$$

The time evoluted operator $x_H(t)$ can be expressed as

$$x_H(t) = \exp\left(\mathrm{i}\frac{Ht}{\hbar}\right) x_0 \exp\left(-\mathrm{i}\frac{Ht}{\hbar}\right). \tag{3.29}$$

The expectation value is as follows

$$\langle x_H(t)\rangle = \left\langle \Psi | U^\dagger x_s U | \Psi \right\rangle = \langle \Psi, t | x_s | \Psi, t\rangle = \langle x_s\rangle_t . \tag{3.30}$$

3.3 Coherent states (BONUS)

A coherent state of a one-dimensional simple harmonic oscillator is defined to be an eigenstate of the non-Hermitian (i.e. $a \neq a^\dagger$) annihilation operator a:

$$a|\lambda\rangle = \lambda|\lambda\rangle, \tag{3.31}$$

where λ, because of the non Hermiticity of a, is a complex number. Coherent states are specific linear combinations of harmonic oscillator eigenfunctions that produce Gaussian wave packets that do not spread in time. Moreover, if the uncertainties in position and time are equal, then the resulting wave packet would be as close a representation of a classical particle as could be obtained within the bounds of the uncertainty principle.

a) *Prove that the following state is normalised:*

$$|\lambda\rangle = \exp\left(-\frac{|\lambda|^2}{2}\right) \exp\left(\lambda a^\dagger\right)|0\rangle . \tag{3.32}$$

b) *Show that such a state satisfies the minimum uncertainty relation*

$$\Delta x \Delta p = \frac{\hbar}{2}. \tag{3.33}$$

c) *Write $|\lambda\rangle$ as*

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle . \tag{3.34}$$

Show that the distribution of $|f(n)|^2$ with respect to n if of the Poisson form $P_n(\mu) = \mathrm{e}^{-\mu}\mu^n/n!$. Find the most probable value of n, and hence of E.

d) *Show that a coherent state can also be obtained by applying the translation (finite displacement) operator $\exp\left(-\mathrm{i}pl/\hbar\right)$ (where p is the momentum operator and l is the displacement distance) to the ground state $|0\rangle$.*

a.) Solution: We can show the normalization by multiplying the bra $\langle\lambda|$ and use the Taylor series expansion of the exponential function and $(a^\dagger)^n|0\rangle = \sqrt{n!}|n\rangle$ to prove that the coherent state can be expressed as a superposition of the eigenvectors of the harmonic oscillator

$$\begin{aligned}
\langle\lambda|\lambda\rangle &= \exp\left(-|\lambda|^2\right)\left\langle 0|\exp\left(\lambda^* a\right)\exp\left(\lambda a^\dagger\right)|0\right\rangle \\
&= \exp\left(-|\lambda|^2\right)\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\left\langle 0|\frac{(\lambda^*)^m}{m!}a^m\frac{\lambda^n}{n!}(a^\dagger)^n|0\right\rangle \\
&= \exp\left(-|\lambda|^2\right)\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\frac{(\lambda^*)^m}{m!}\left\langle 0|a^m\sqrt{n!}|n\right\rangle \\
&= \exp\left(-|\lambda|^2\right)\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\frac{(\lambda^*)^m}{m!}\left\langle 0|\frac{\sqrt{n!}}{\sqrt{(n-m)!}}\sqrt{n!}|n-m\right\rangle \\
&= \exp\left(-|\lambda|^2\right)\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\lambda^n}{\cancel{n!}}\frac{(\lambda^*)^m}{m!}\frac{\cancel{n!}}{\sqrt{(n-m)!}}\underbrace{\langle 0|n-m\rangle}_{\delta_{mn}} \\
&= \exp\left(-|\lambda|^2\right)\sum_{n=0}^{\infty}\frac{(\lambda^*\lambda)^n}{n!} = \exp\left(-|\lambda|^2\right)\exp\left(|\lambda|^2\right) = 1.
\end{aligned} \tag{3.35}$$

b.) Solution: To find an expression for the uncertainty relation we write the position and momentum operators in terms of a and $a^\dagger$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \qquad p = -\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger). \tag{3.36}$$

At first we compute some helpful relations

$$\begin{aligned}
\left\langle\lambda|a \pm a^\dagger|\lambda\right\rangle &= \mathrm{e}^{-|\lambda|^2}\left[\left\langle 0|\mathrm{e}^{\lambda^* a}a\mathrm{e}^{\lambda a^\dagger}|0\right\rangle \pm \left\langle 0|\mathrm{e}^{\lambda^* a}a^\dagger\mathrm{e}^{\lambda a^\dagger}|0\right\rangle\right] \\
&= \mathrm{e}^{-|\lambda|^2}\sum_{n,m}\frac{(\lambda^*)^m}{m!}\frac{(\lambda)^n}{n!}\left[\left\langle 0|a^{m+1}(a^\dagger)^n|0\right\rangle \pm \left\langle 0|a^m(a^\dagger)^{n+1}|0\right\rangle\right] \\
&= \mathrm{e}^{-|\lambda|^2}\sum_{n,m}\frac{(\lambda^*)^m}{m!}\frac{(\lambda)^n}{n!}\left[\left\langle 0|a^{m+1}\sqrt{n!}|n\right\rangle \pm \left\langle 0|a^m\sqrt{(n+1)!}|n+1\right\rangle\right] \\
&= \mathrm{e}^{-|\lambda|^2}\sum_{n,m}\frac{(\lambda^*)^m}{m!}\frac{(\lambda)^n}{n!}\left[\left\langle 0|\frac{n!}{\sqrt{(n-m-1)!}}|n-(m+1)\right\rangle\right. \\
&\qquad\qquad \left.\pm\left\langle 0|\frac{(n+1)!}{\sqrt{(n+1-m)!}}|n+1-m\right\rangle\right] \\
&= \mathrm{e}^{-|\lambda|^2}\left(\sum_m\frac{(\lambda^*)^m\lambda^{m+1}}{m!} \pm \sum_n\frac{(\lambda^*)^{n+1}\lambda^n}{n!}\right) \\
&= \lambda \pm \lambda^*.
\end{aligned} \tag{3.37}$$

Similarly we can show that

$$\langle\lambda|(a)^2|\lambda\rangle = \lambda^2 \qquad \left\langle\lambda|(a^\dagger)^2|\lambda\right\rangle = (\lambda^*)^2 \tag{3.38}$$

$$\left\langle\lambda|a^\dagger a|\lambda\right\rangle = \lambda^*\lambda \qquad \left\langle\lambda|aa^\dagger|\lambda\right\rangle = \left\langle\lambda|1 + a^\dagger a|\lambda\right\rangle = 1 + \lambda^*\lambda. \tag{3.39}$$

Now we can compute $\langle \Delta x \rangle$ and $\langle \Delta p \rangle$ via

$$\langle \Delta A \rangle = \langle A^2 \rangle - \langle A \rangle^2 . \tag{3.40}$$

We can use (3.38) and (3.39) for that

$$\begin{aligned} \langle x \rangle &= \langle \lambda | x | \lambda \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\lambda + \lambda^*) \\ \langle x^2 \rangle &= \frac{\hbar}{2m\omega} \left\langle \lambda | a^2 + (a^\dagger)^2 + a^\dagger a + a a^\dagger | \lambda \right\rangle = \frac{\hbar}{2m\omega} [\lambda^2 + (\lambda^*)^2 + \lambda^* \lambda + (1 + \lambda^* \lambda)]. \end{aligned} \tag{3.41}$$

This leads to the following result

$$\langle \Delta x \rangle^2 = \frac{\hbar}{2m\omega} [\lambda^2 + (\lambda^*)^2 + 2\lambda^* \lambda + 1 - (\lambda^* + \lambda)^2] = \frac{\hbar}{2m\omega}. \tag{3.42}$$

For the momentum we get similar results

$$\begin{aligned} \langle p \rangle &= \langle \lambda | p | \lambda \rangle = -\mathrm{i} \sqrt{\frac{\hbar m \omega}{2}} (\lambda - \lambda^*) \\ \langle p^2 \rangle &= -\frac{\hbar m \omega}{2} \left\langle \lambda | a^2 + (a^\dagger)^2 - a^\dagger a - a a^\dagger | \lambda \right\rangle = \frac{\hbar}{2m\omega} [\lambda^2 + (\lambda^*)^2 - \lambda^* \lambda - (1 + \lambda^* \lambda)]. \end{aligned} \tag{3.43}$$

This leads to

$$\langle \Delta p \rangle^2 = -\frac{\hbar m \omega}{2} [\lambda^2 + (\lambda^*)^2 - \lambda^* \lambda - (1 + \lambda^* \lambda) - (\lambda^* - \lambda)^2] = \frac{\hbar m \omega}{2}. \tag{3.44}$$

From (3.42) and (3.44) we immediately get the correct result

$$\langle \Delta x \rangle^2 \langle \Delta p \rangle^2 = \frac{\hbar}{2m\omega} \frac{\hbar m \omega}{2} \quad \Rightarrow \langle \Delta x \rangle \langle \Delta p \rangle = \frac{\hbar}{2}. \tag{3.45}$$

c.) Solution: First we compute $|\lambda\rangle$ by performing the Taylor series expansion

$$\begin{aligned} |\lambda\rangle &= \mathrm{e}^{-|\lambda|^2/2} \exp\left(\lambda a^\dagger\right) |0\rangle \\ &= \mathrm{e}^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (a^\dagger)^n |0\rangle = \mathrm{e}^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \sqrt{n!} |n\rangle . \end{aligned} \tag{3.46}$$

This leads to the coefficients $f(n)$

$$f(n) = \mathrm{e}^{-|\lambda|^2/2} \frac{\lambda^n}{\sqrt{n!}}. \tag{3.47}$$

Now we compute the distribution $|f(n)|^2$ with respect to n

$$P_n = |f(n)|^2 = \mathrm{e}^{-|\lambda|^2} \frac{|\lambda|^{2n}}{n!} = \mathrm{e}^{-\mu} \frac{\mu^n}{n!}, \tag{3.48}$$

with $\mu = |\lambda^2|$. The most probable value of n can be found by maximising P_n with respect to n. For that we look for the case when $P_n > P_{n-1}$

$$\frac{P_n}{P_{n-1}} = \frac{\mathrm{e}^{-\mu} \mu^n}{n!} \frac{(n-1)!}{\mathrm{e}^{-\mu} \mu^{n-1}} = \frac{\mu}{n} \overset{!}{>} 1. \tag{3.49}$$

This leads to the relation $|\lambda|^2 > n$. Therefore the most probable value of n is the largest integer $n_{\max}$ less than $|\lambda|^2$ with the energy $(n_{\max} + 1/2)\hbar\omega$.

d.) Solution: We can use equation (3.36) to express the momentum operators with the ladder operators which leads to

$$\exp\left(-\mathrm{i}\frac{p\cdot l}{\hbar}\right)|0\rangle = \exp\left(\underbrace{\sqrt{\frac{m\omega}{\hbar}}l}_{:=\xi}(a^\dagger - a)\right)|0\rangle\,. \tag{3.50}$$

Now we use the *Baker-Campbell-Hausdorff* formula to rewrite the exponential

$$\boxed{\exp(A+B) = \exp(A)\exp(B)\exp\left(-\frac{[A,B]}{2}\right)}\,. \tag{3.51}$$

This leads to

$$\begin{aligned}\exp\left(-\mathrm{i}\frac{p\cdot l}{\hbar}\right)|0\rangle &= \mathrm{e}^{\xi a^\dagger}\mathrm{e}^{-\xi a}\exp\big(\xi\underbrace{\frac{[a^\dagger,a]}{2}}_{=-1/2}\big)|0\rangle \\ &= \mathrm{e}^{-\xi/2}\mathrm{e}^{\xi a^\dagger}\sum_{n=0}^{\infty}\frac{(-\xi)^n}{n!}\underbrace{a^n|0\rangle}_{=0,n\neq 0} \\ &= \mathrm{e}^{-\xi/2}\mathrm{e}^{\xi a^\dagger}|0\rangle\,. \end{aligned} \tag{3.52}$$

We can see that because ξ is a real number, that this result is equivalent to the coherent state (3.32) given in a.) by choosing $\lambda = \xi$.

4 Electromagnetic fields and Gauge transformations

4.1 Gauge Transformation

Consider a particle in an EM field $\boldsymbol{E}, \boldsymbol{B}$.

- *Write down how the vector potentials $\boldsymbol{A}, \phi$ change under a gauge transformation.*
- *Using the above transformations, show what happens to the Lagrangian $L(\dot{x}, x)$. Comment therefore, on the effect this has on the classical equations of motion.*
- *Examine now, what happens to QM expectation values $\langle x \rangle, \langle p \rangle$, where p is the canonical momentum. Is $\langle p \rangle$ gauge independent? What about $\langle \Pi \rangle = \langle p - \frac{e}{c}\boldsymbol{A} \rangle$?*
- *Show that the probability density $\rho(t,x)$ and the probability current density j are gauge invariant, but the phase factor S in the wave function is not.*

Solution: For a general gauge transformation the potentials $\boldsymbol{A}$ and ϕ change like

$$\boldsymbol{A} \to \boldsymbol{A} + \vec{\nabla}\Lambda \tag{4.1}$$

$$\phi \to \phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda. \tag{4.2}$$

These transformations leave the electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ field invariant

$$\begin{aligned} \boldsymbol{E} &= -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{A} = -\vec{\nabla}(\phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda) - \frac{1}{c}\frac{\partial}{\partial t}\left(\boldsymbol{A} + \vec{\nabla}\Lambda\right) \\ \boldsymbol{B} &= \vec{\nabla} \times \boldsymbol{A} = \vec{\nabla} \times \boldsymbol{A} + \underbrace{\vec{\nabla} \times \vec{\nabla}\lambda}_{=0}. \end{aligned} \tag{4.3}$$

The Lagrangian of the electromagnetic field can be written as

$$\begin{aligned} \mathscr{L}(\dot{\boldsymbol{x}}, \boldsymbol{x}) &= \frac{1}{2}m\dot{\boldsymbol{x}}^2 + \frac{e}{c}\boldsymbol{A}\cdot\dot{\boldsymbol{x}} - e\phi \\ &= \frac{1}{2}m\dot{\boldsymbol{x}}^2 + \frac{e}{c}(\boldsymbol{A} + \vec{\nabla}\Lambda)\cdot\dot{\boldsymbol{x}} - e\left(\phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda\right) \\ &= \frac{1}{2}m\dot{\boldsymbol{x}}^2 + \frac{e}{c}\boldsymbol{A}\cdot\dot{\boldsymbol{x}} - e\phi + \underbrace{\frac{e}{c}\vec{\nabla}\Lambda\cdot\dot{\boldsymbol{x}} + \frac{e}{c}\frac{\partial}{\partial t}\Lambda}_{\frac{e}{c}\frac{\mathrm{d}\Lambda}{\mathrm{d}t}}. \end{aligned} \tag{4.4}$$

We can retrieve the classical equations of motion by applying the Euler-Lagrange equations

$$\frac{\partial \mathscr{L}}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{x}_i} = 0. \tag{4.5}$$

The two parts lead to

$$\begin{aligned} \frac{\partial \mathscr{L}}{\partial x_i} &= -e\frac{\partial}{\partial x_i}\phi + \frac{e}{c}\frac{\partial}{\partial x_i}(\dot{\boldsymbol{x}}\cdot\boldsymbol{A}) + \frac{e}{c}\frac{\partial}{\partial x_i}\frac{\mathrm{d}\Lambda}{\mathrm{d}t} \\ \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathscr{L}}{\partial \dot{x}_i} &= \frac{e}{c}\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t} + m\ddot{\boldsymbol{x}} + \frac{e}{c}\frac{\partial}{\partial x_i}\frac{\mathrm{d}\Lambda}{\mathrm{d}t}. \end{aligned} \tag{4.6}$$

We can see that both red terms that were caused by the gauge will cancel out in the equation of motion. In the vector representation the equations of motion are

$$\begin{aligned} m\ddot{\boldsymbol{x}} &= -e\vec{\boldsymbol{\nabla}}\phi + \frac{e}{c}\vec{\boldsymbol{\nabla}}(\boldsymbol{A}\dot{\boldsymbol{x}}) - \frac{e}{c}\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}t} \\ &= -e\vec{\boldsymbol{\nabla}}\phi + \frac{e}{c}\vec{\boldsymbol{\nabla}}(\boldsymbol{A}\dot{\boldsymbol{x}}) - \frac{e}{c}\frac{\partial \boldsymbol{A}}{\partial t} - \frac{e}{c}(\vec{\boldsymbol{\nabla}}\cdot\boldsymbol{A})\dot{\boldsymbol{x}} \\ &= e\left(-\vec{\boldsymbol{\nabla}}\phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}\right) + \frac{e}{c}\left(\vec{\boldsymbol{\nabla}}(\boldsymbol{A}\dot{\boldsymbol{x}}) - (\vec{\boldsymbol{\nabla}}\cdot\boldsymbol{A})\dot{\boldsymbol{x}}\right) \\ &= e\boldsymbol{E} + \frac{e}{c}(\dot{\boldsymbol{x}}\times\boldsymbol{B}). \end{aligned} \tag{4.7}$$

We can verify the last step by showing

$$\dot{\boldsymbol{x}}\times\boldsymbol{B} = \dot{\boldsymbol{x}}\times\vec{\boldsymbol{\nabla}}\times\boldsymbol{A} = \vec{\boldsymbol{\nabla}}(\dot{\boldsymbol{x}}\cdot\boldsymbol{A}) - (\dot{\boldsymbol{x}}\cdot\boldsymbol{\nabla})\boldsymbol{A}. \tag{4.8}$$

We can conclude, that the equations of motion do not change, because the gauge does not change the relevant quantities $\boldsymbol{E}$ and $\boldsymbol{B}$.

Now we want to examine, what happens to the QM expectation values. For that we use the relation shown in the lecture, that the operators transform in the following way:

$$x \to U^\dagger x U, \qquad \text{with } U = \exp\left(\mathrm{i}\frac{e}{\hbar c}\Lambda(x,t)\right) \quad \text{unitary.} \tag{4.9}$$

We can now compute the expectation value of the transformed x operator by using the commutator $[x,U]=0$, because U is only dependent on space and time

$$\langle\alpha|x|\alpha\rangle \to \langle\alpha|U^\dagger x U|\alpha\rangle = \langle\alpha|U^\dagger U x|\alpha\rangle = \langle\alpha|x|\alpha\rangle. \tag{4.10}$$

This shows, that x is actually gauge invariant. For the momentum p we use the commutator relation (3.1) and the gradient of the unitary operator $\vec{\boldsymbol{\nabla}}U = \mathrm{i}e/(\hbar c)\vec{\boldsymbol{\nabla}}\Lambda$ which results in

$$\begin{aligned} \langle\alpha|p|\alpha\rangle \to \langle\alpha|U^\dagger p U|\alpha\rangle &= \langle\alpha|U^\dagger(-\mathrm{i}\hbar\vec{\boldsymbol{\nabla}}U + Up)|\alpha\rangle = \langle\alpha|-\mathrm{i}\hbar U^\dagger\vec{\boldsymbol{\nabla}}U + p|\alpha\rangle \\ &= \langle p\rangle - \mathrm{i}\hbar\frac{\mathrm{i}e}{\hbar c}\left\langle\vec{\boldsymbol{\nabla}}\Lambda\right\rangle = \langle\alpha|p|\alpha\rangle + \frac{e}{c}\langle\alpha|\vec{\boldsymbol{\nabla}}\Lambda|\alpha\rangle. \end{aligned} \tag{4.11}$$

We can see that the momentum p is not gauge invariant. However, the kinematical momentum $\Pi = p - \frac{e}{c}\boldsymbol{A}$ is gauge invariant:

$$\langle\alpha|\Pi|\alpha\rangle \to \langle\alpha|U^\dagger\left(p - \frac{e}{c}(\boldsymbol{A}+\vec{\boldsymbol{\nabla}}\Lambda)\right)U|\alpha\rangle = \langle\alpha|U^\dagger p U|\alpha\rangle - \frac{e}{c}\langle\alpha|U^\dagger(\boldsymbol{A}+\vec{\boldsymbol{\nabla}}\Lambda)U|\alpha\rangle. \tag{4.12}$$

Now we use the property that $\boldsymbol{A}(x,t)$ and $\Lambda(x,t)$ commute with $U(x,t)$. Then we get

$$\begin{aligned} \langle\alpha|U^\dagger\Pi U|\alpha\rangle &= \langle p\rangle + \frac{e}{c}\cancel{\left\langle\vec{\boldsymbol{\nabla}}\Lambda\right\rangle} - \frac{e}{c}(\langle A\rangle + \cancel{\left\langle\vec{\boldsymbol{\nabla}}\Lambda\right\rangle}) \\ &= \langle\alpha|p - \frac{e}{c}\boldsymbol{A}|\alpha\rangle. \end{aligned} \tag{4.13}$$

Under the gauge transformations the function ψ undergoes some changes too. For that we consider the time dependent Schrödinger equation

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial\Psi}{\partial t} &= \frac{1}{2m}\left(-\mathrm{i}\hbar\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\right)^2\psi + e\phi\psi \\ \Rightarrow \mathrm{i}\hbar\frac{\partial\Psi}{\partial t} &= \frac{1}{2m}\left(-\mathrm{i}\hbar\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A} - \frac{e}{c}\vec{\boldsymbol{\nabla}}\Lambda\right)^2\psi + q\phi\psi - q\frac{\partial\Lambda}{\partial t}\psi. \end{aligned} \tag{4.14}$$

We can see that for the choice

$$\psi' = \exp(\mathrm{i}\lambda(x,t))\psi, \quad \lambda = \frac{e}{\hbar}\Lambda, \tag{4.15}$$

the Schrödinger equation (4.14) remains unchanged. We can use this finding to test the behaviour of the probability density ρ and probability current j. The invariance of ρ can be found by using $\rho = \psi\psi^* \rightarrow \exp(\mathrm{i}\lambda(x,t))\psi\exp(-\mathrm{i}\lambda(x,t))\psi^* = \psi\psi^* = \rho$.

We can investigate the probability current j by considering the continuity equation for a free spin-0 particle in an electromagnetic field:

$$j = \frac{1}{2m}\left[(\psi^* p\psi - \psi p\psi^*) - 2q\boldsymbol{A}|\psi|^2\right]. \tag{4.16}$$

When the gauge transformation is applied, this leads to

$$\begin{aligned}
j &= \frac{1}{2m}\left[(\mathrm{e}^{-\mathrm{i}\lambda}\psi^* p\mathrm{e}^{\mathrm{i}\lambda}\psi - \mathrm{e}^{\mathrm{i}\lambda}\psi p\mathrm{e}^{-\mathrm{i}\lambda}\psi^*) - 2q(\boldsymbol{A}+\vec{\boldsymbol{\nabla}}\Lambda)|\psi|^2\right] \\
&= \frac{1}{2m}\left[\psi^* p\psi + \mathrm{e}^{\mathrm{i}\lambda}\psi^*\psi\frac{\hbar}{\mathrm{i}}\vec{\boldsymbol{\nabla}}\left(\mathrm{e}^{\mathrm{i}\lambda}\right) - \psi p\psi^* - \mathrm{e}^{-\mathrm{i}\lambda}\psi\psi^*\frac{\hbar}{\mathrm{i}}\vec{\boldsymbol{\nabla}}\left(\mathrm{e}^{-\mathrm{i}\lambda}\right) - 2e(\boldsymbol{A}+\vec{\boldsymbol{\nabla}}\Lambda)|\psi|^2\right] \\
&= \frac{1}{2m}\left[\psi^* p\psi + \mathrm{e}^{\mathrm{i}\lambda}|\psi|^2\frac{\hbar}{\mathrm{i}}\frac{e\mathrm{i}}{\hbar}\vec{\boldsymbol{\nabla}}\Lambda - \psi p\psi^* - \mathrm{e}^{-\mathrm{i}\lambda}|\psi|^2\frac{\hbar}{\mathrm{i}}\frac{-e\mathrm{i}}{\hbar}\vec{\boldsymbol{\nabla}}\Lambda - 2e(\boldsymbol{A}+\vec{\boldsymbol{\nabla}}\Lambda)|\psi|^2\right] \\
&= \frac{1}{2m}\left[\psi^* p\psi - \psi p\psi^* + 2|\psi|^2 e\vec{\boldsymbol{\nabla}}\Lambda - 2e(\boldsymbol{A}+\vec{\boldsymbol{\nabla}}\Lambda)|\psi|^2\right] \\
&= \frac{1}{2m}\left[\psi^* p\psi - \psi p\psi^* - 2e\boldsymbol{A}|\psi|^2\right].
\end{aligned} \tag{4.17}$$

4.2 Landau levels

- *Solve the Landau level problem in Landau gauge, find the energies and eigenfunctions.*
- *Is the wavefunction gauge independent? Is there degeneracy? Discuss.*

Solution: We are starting from the expression of $L(\dot{x}, x)$ from the previous question and derive the expression of the Hamiltonian $H(p, x)$

$$H(\boldsymbol{p}, \boldsymbol{x}) = \frac{\partial \mathscr{L}}{\partial \dot{\boldsymbol{x}}} \dot{\boldsymbol{x}} - \mathscr{L}(\dot{\boldsymbol{x}}, \boldsymbol{x}). \tag{4.18}$$

The canonical momentum can be computed as

$$p = \frac{\partial \mathscr{L}}{\partial \dot{\boldsymbol{x}}} = m\dot{\boldsymbol{x}} + \frac{e}{c}\boldsymbol{A}, \tag{4.19}$$

which leads to the Hamiltonian

$$\begin{aligned} H(\boldsymbol{p}, \boldsymbol{x}) &= m\dot{\boldsymbol{x}}^2 + \frac{e}{c}\boldsymbol{A}\dot{\boldsymbol{x}} - \frac{m}{2}\dot{\boldsymbol{x}}^2 - \frac{e}{c}\boldsymbol{A}\dot{\boldsymbol{x}} + e\phi \\ &= \frac{m}{2}\dot{\boldsymbol{x}}^2 + e\phi \\ &= \frac{1}{2m}(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})^2 + e\phi. \end{aligned} \tag{4.20}$$

Now we show that $H(\boldsymbol{p}, \boldsymbol{x})$ respond to the gauge transformation by

$$H'(\boldsymbol{p}, \boldsymbol{x}) = H(\boldsymbol{p}, \boldsymbol{x}) - \frac{1}{c}\frac{\partial \Lambda}{\partial t}, \tag{4.21}$$

where $\Lambda = \Lambda(q, t)$ is the gauge transformation function. For that we use (4.4) and computed the new canonical momentum

$$\boldsymbol{p} = \frac{\partial \mathscr{L}}{\partial \dot{\boldsymbol{x}}} = m\dot{\boldsymbol{x}} + \frac{e}{c}\boldsymbol{A} + \frac{e}{c}\vec{\boldsymbol{\nabla}}\Lambda, \tag{4.22}$$

which leads to the Hamiltonian

$$\begin{aligned} H'(\boldsymbol{p}, \boldsymbol{x}) &= \boldsymbol{p}\dot{\boldsymbol{x}} - \mathscr{L}(\dot{\boldsymbol{x}}, \boldsymbol{x}) \\ &= m\dot{\boldsymbol{x}}^2 + \cancel{\frac{e}{c}\boldsymbol{A}\dot{\boldsymbol{x}}} + \cancel{\frac{e}{c}\vec{\boldsymbol{\nabla}}\Lambda\dot{\boldsymbol{x}}} - \left(\frac{1}{2}m\dot{\boldsymbol{x}}^2 + \cancel{\frac{e}{c}\boldsymbol{A}\cdot\dot{\boldsymbol{x}}} - e\phi + \cancel{\frac{e}{c}\vec{\boldsymbol{\nabla}}\Lambda\cdot\dot{\boldsymbol{x}}} + \frac{e}{c}\frac{\partial}{\partial t}\Lambda\right) \\ &= \frac{1}{2}m\dot{\boldsymbol{x}}^2 + e\phi - \frac{e}{c}\frac{\partial \Lambda}{\partial t} = H(\boldsymbol{p}, \boldsymbol{x}) - \frac{e}{c}\frac{\partial \Lambda}{\partial t}. \end{aligned} \tag{4.23}$$

For a purely magnetic field the equations of motion will be

$$m\ddot{\boldsymbol{x}} = e\dot{\boldsymbol{x}} \times B. \tag{4.24}$$

We can see that the acceleration is perpendicular to the velocity which leads to a circular motion. We can work out the commutation relation of the kinematical momentum Π as

$$\begin{aligned}[\Pi_a, \Pi_b] &= [p_a - \frac{e}{c}A_a, p_b - \frac{e}{c}A_b] \\ &= -\frac{e}{c}([p_a, A_b] - [A_a, p_b]) = -\frac{e}{c}(-\mathrm{i}\hbar\partial_a A_b + \mathrm{i}\hbar\partial_b A_a) \\ &= \mathrm{i}\hbar\frac{e}{c}\varepsilon_{abc}B_c. \end{aligned} \tag{4.25}$$

Now we specialise to a geometry $\boldsymbol{B} = Bz$. Therefore the Hamiltonian will be $H = \frac{1}{2m}(\Pi_x^2 + \Pi_y^2)$. Now we try to express the Hamiltonian in terms of

$$\Pi_\pm = \sqrt{\frac{c}{2e\hbar B}}(\Pi_x \pm \mathrm{i}\Pi_y). \tag{4.26}$$

Analagously to the SHO we find the Hamiltonian by identifying $a^\dagger = H_-$. Hence

$$H = \hbar\left(\frac{eB}{mc}\right)\left(\Pi_-\Pi_+ + \frac{1}{2}\right). \tag{4.27}$$

As a further specialisation we choose the *Landauian Gauge* with $\boldsymbol{A} = xB\boldsymbol{e}_y$. The Hamiltonian can the be written as

$$H = \frac{1}{2}(\Pi_x^2 + \Pi_y^2) = \frac{1}{2m}\left[p_x^2 + \left(p_y - \frac{q}{c}xB\right)^2\right]. \tag{4.28}$$

We see that the Hamiltonian is not dependent on y. Therefore y is a cyclic coordinate. This motivates a separation like

$$\psi(x, y) = \mathrm{e}^{\mathrm{i}ky} f(x). \tag{4.29}$$

So now if we want to solve for the eigenspectrum we use the time independent Schrödinger equation

$$\begin{aligned} H\psi(x, y) &= E\psi \\ \frac{1}{2m}\left[p_x^2 + \left(\hbar k - \frac{e}{c}xB\right)^2\right] f(x) &= Ef(x) \\ \left[\frac{p_x^2}{2m} + \frac{m}{2}\left(\frac{eB}{mc}\right)^2\left(x - \frac{c\hbar k}{eB}\right)^2\right] f(x) &= Ef(x). \end{aligned} \tag{4.30}$$

We now see that the last expression is a SHO with a frequency given by $\omega_B = eB/mc$ and a centre at $x = \frac{c\hbar k}{eB}$. The eigenvalues are well known and given by

$$E_n = \hbar\omega_B\left(n + \frac{1}{2}\right). \tag{4.31}$$

The eigenspectrum on the other hand looks like

$$\psi_{kn} \sim \mathrm{e}^{\mathrm{i}ky} H_n(x - kl_B^2) \exp\left[\frac{1}{2}\left(\frac{x - kl_B^2}{l_B}\right)^2\right], \quad \text{with } l_B \equiv \sqrt{\frac{\hbar}{eB}}. \tag{4.32}$$

We see that the eigenspectrum contains both k and n, whereas the eigenvalues only depend on n. Hence there is an infinite degeneracy at a particular energy level.

4.3 Landau levels in a finite box

Let us consider an experiment in which electrons on a rectangular plane with surface $S = L_x L_y$ are immersed in a magnetic field directed along the z axis $\boldsymbol{B} = Bz$. In this case translational invariance is broken and the Landau levels are resolved into a cluster of levels. However, for sufficiently intense B the cluster can be approximated by a degenerate level with a certain multiplicity $\mathcal{N}$.

a) *Apply a semi-classical argument to show that $\mathcal{N} \approx \frac{S}{h/eB}$.*

b) *Give an interpretation to the quantity h/eB.*

c) *Looking at the results above, why is a large B required to see this effect?*

a.) Solution: Since the energy levels only depend on the quantum number n and not on k, degeneracy is given by the number of states with different k for a fixed n inside the finite box. Thus, to calculate the total number of levels in S, wen need to restrictions on the wavenumbers k_x, k_y in both directions. The choice of the Landauian gauge $\boldsymbol{A} = xB\boldsymbol{e}_y$ is invariant in the y-direction but not in the x-direction. This implies that the corresponding wavefunction has the same properties of invariance.

Given the symmetry properties of the wave function (4.32) we can find k_y exactly as for a particle in a box. We find that $k_y = k = 2\pi\mathcal{N}/L_y$ with an integer $\mathcal{N}$. Thus, $\mathcal{N} = kL_y/2\pi$. We see in equation (4.32), that the wavefunction is exponentially localised around the central position $x = k\frac{\hbar}{eB}$. Now we can use the restriction $0 \leq x \leq L_x$ to find $0 \leq k \leq L_x/l_B^2$. With that we can calculate $\mathcal{N}$

$$\mathcal{N} = k\frac{L_y}{2\pi} = \frac{L_x L_y}{2\pi l_B^2} = \frac{S}{h/eB}. \tag{4.33}$$

b.) Solution: The quantity h/eB has units of area

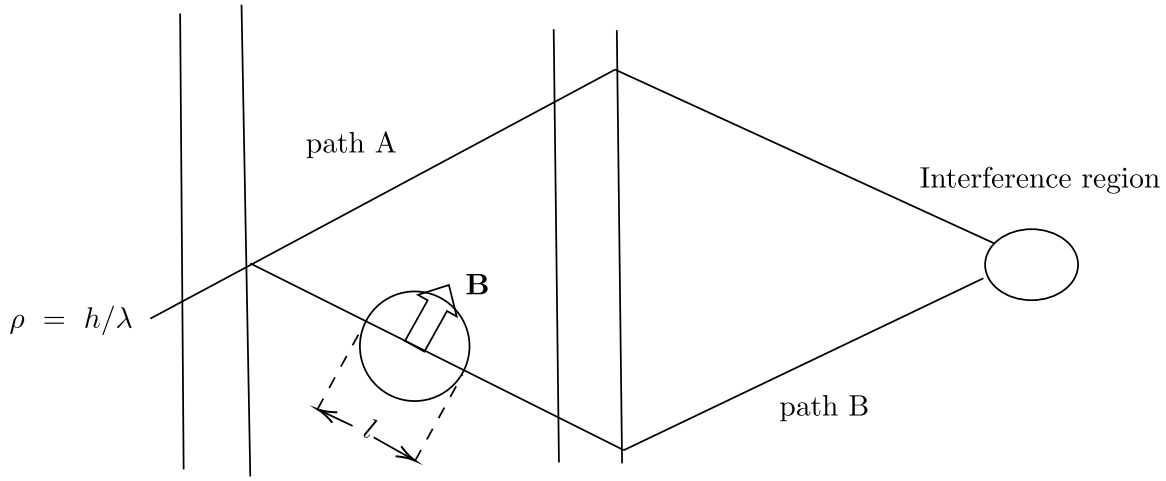
$$\frac{[h]}{[e][B]} = \frac{\mathrm{J\,s}}{\mathrm{C}\frac{\mathrm{N\,s}}{\mathrm{C\,m}}} = \mathrm{m}^2. \tag{4.34}$$

We can call the square root of this quantity the *magnetic length*. Actually the magnetic length is defined as l_B with $\hbar$ instead of h. However, this quantity characterises the length scales which govern any quantum pheonomena in a magnetic field. For an electro in a magnetic field of 1 T, we get $l_B \approx 2{,}5 \cdot 10^{-8}\,\mathrm{m}$.

c.) Solution We found that the degeneracy $\mathcal{N}$ is proportional to B. Thus, for bigger fields the degeneracy is higher and more electrons can fit into each finite Landau level.

4.4 Interference Experiment

Consider the neutron interferometer below, where a nearly monoenergetic beam of thermal neutrons with momentum $\rho = h/\lambda$ is split into two parts-path A and B (see Figure). Path A always goes through a magnetic field-free region, in contrast path B enters a small region of length l where a magnetic field B is present.



- *Write the time evolution of the initial state $|\alpha\rangle$ from the source to the interference point via the path A. Use the time evolution operator $U(t)$.*
- *Repeat the computation for the particle moving along path B. Observe that the neutrons moving along path B present a phase shift with respect to those going through A. What is the expression of this phase difference and how is it related to the time T spent by the particles in the $B \neq 0$ region?*
- *Using the properties of the Pauli matrices, prove that*

$$\exp(\pm \mathrm{i} k t \sigma_z) = \cos(kt) \pm \mathrm{i} \sin(kt) \sigma_z = \begin{pmatrix} \mathrm{e}^{\pm \mathrm{i} k t} & 0 \\ 0 & \mathrm{e}^{\mp \mathrm{i} k t} \end{pmatrix} \tag{4.35}$$

  and apply it to the phase shift computed above.
- *The finale state ket β at the interference region is given by the combination of kets which wen through the two different paths. Calculate the norm of this state and deduce the maxima in the counting rates from it.*
- *Prove that the increment in the magnetic field that separates two successive maxima in the counting rates is given by*

$$\Delta B = \frac{4\pi\hbar c}{e g_n \lambda l}. \tag{4.36}$$

4.5 Classical particle in a magnetic field (Bonus)

Consider a particle of mass m and charge e moving in a constant magnetic field $\boldsymbol{B} = Bz$. Assume that the vector potential has the form $\boldsymbol{A} = B/2(-y, x, 0)$.

a) *Prove that $P_1 = p_x - \frac{eB}{2c}y, P_2 = p_y + \frac{eB}{2c}x$ and $P_3 = p_z$ are constants of motion.*

b) *Calculate the infinitesimal generators of translation $G_{\boldsymbol{a}}(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{a} \cdot (\boldsymbol{p} - \frac{e}{c}\boldsymbol{x} \times \boldsymbol{B})$ for the* translation $(\boldsymbol{x}, \boldsymbol{p}) \rightarrow (\boldsymbol{x}+\boldsymbol{a}, \boldsymbol{p}+\frac{e}{c}\vec{\boldsymbol{\nabla}}\Lambda(\boldsymbol{x}, \boldsymbol{a}))$ *in the gauge $\boldsymbol{A}(\boldsymbol{x}+\boldsymbol{a}) - \boldsymbol{A}(\boldsymbol{x}) = \vec{\boldsymbol{\nabla}}\Lambda(\boldsymbol{x}, \boldsymbol{a})$ where both correspond to the same $\boldsymbol{B}$.*

5 Angular momentum

5.1 Rotation matrices

Consider the usual rotation matrices in $\mathbb{R}^3$, namely $\mathscr{R}(\hat{x},\alpha)$, $\mathscr{R}(\hat{y},\alpha)$, $\mathscr{R}(\hat{z},\alpha)$, where $\hat{x},\hat{y},\hat{z}$ are the rotational axes and α is the angle of rotation. Prove the equation

$$\mathscr{R}(\hat{x},\alpha)\mathscr{R}(\hat{y},\alpha)-\mathscr{R}(\hat{y},\alpha)\mathscr{R}(\hat{x},\alpha)=\mathscr{R}(\hat{z},\alpha^2)-\mathbb{1} \tag{5.1}$$

in the limit in which α is small. $\mathbb{1}$ is the identity matrix.

Solution: The Rotation matrices $\mathscr{R}(\hat{x},\alpha)\equiv\mathscr{R}_{\hat{x}}$ in $\mathbb{R}^3$ are given by

$$\mathscr{R}_{\hat{x}}=\begin{pmatrix}1&0&0\\0&\cos\alpha&-\sin\alpha\\0&\sin\alpha&\cos\alpha\end{pmatrix},\quad \mathscr{R}_{\hat{y}}=\begin{pmatrix}\cos\alpha&0&\sin\alpha\\0&1&0\\-\sin\alpha&0&\cos\alpha\end{pmatrix},\quad \mathscr{R}_{\hat{z}}=\begin{pmatrix}\cos\alpha&-\sin\alpha&0\\\sin\alpha&\cos\alpha&0\\0&0&1\end{pmatrix}.$$

For small α we can approxiamte the sine and cosine by their first two orders of the Taylor series expansion, which leads to

$$\mathscr{R}_{\hat{x}}=\begin{pmatrix}1&0&0\\0&1-\frac{\alpha^2}{2}&-\alpha\\0&\alpha&1-\frac{\alpha^2}{2}\end{pmatrix},\quad \mathscr{R}_{\hat{y}}=\begin{pmatrix}1-\frac{\alpha^2}{2}&0&\alpha\\0&1&0\\-\alpha&0&1-\frac{\alpha^2}{2}\end{pmatrix},\quad \mathscr{R}_{\hat{z}}=\begin{pmatrix}1-\frac{\alpha^2}{2}&-\alpha&0\\\alpha&1-\frac{\alpha^2}{2}&0\\0&0&1\end{pmatrix}.$$

Now we can calculate $\mathscr{R}(\hat{x},\alpha)\mathscr{R}(\hat{y},\alpha)$ and $\mathscr{R}(\hat{y},\alpha)\mathscr{R}(\hat{x},\alpha)$ by neglecting all terms of α with higher order than two

$$\mathscr{R}_{\hat{x}}\mathscr{R}_{\hat{y}}=\begin{pmatrix}1-\frac{\alpha^2}{2}&0&\alpha\\\alpha^2&1-\frac{\alpha^2}{2}&-\alpha\\-\alpha&\alpha&1-\alpha^2\end{pmatrix},\quad \mathscr{R}_{\hat{y}}\mathscr{R}_{\hat{x}}=\begin{pmatrix}1-\frac{\alpha^2}{2}&\alpha^2&\alpha\\0&1-\frac{\alpha^2}{2}&-\alpha\\-\alpha&\alpha&1-\alpha^2\end{pmatrix}. \tag{5.2}$$

Now if we subtract both results in (5.2) we get

$$\mathbb{R}_{\hat{x}}\mathbb{R}_{\hat{y}}-\mathbb{R}_{\hat{y}}\mathbb{R}_{\hat{x}}=\begin{pmatrix}0&-\alpha^2&0\\\alpha^2&0&0\\0&0&0\end{pmatrix}=\begin{pmatrix}1&-\alpha^2&0\\\alpha^2&1&0\\0&0&1\end{pmatrix}-\mathbb{1}. \tag{5.3}$$

We can now compute $\mathscr{R}_{\hat{z}}(\alpha^2)$ again by ignoring higher order terms

$$\mathscr{R}_{\hat{z}}(\alpha^2)=\begin{pmatrix}1-\frac{\alpha^4}{2}&-\alpha^2&0\\\alpha^2&1-\frac{\alpha^4}{2}&0\\0&0&1\end{pmatrix}=\begin{pmatrix}1&-\alpha^2&0\\\alpha^2&1&0\\0&0&1\end{pmatrix}. \tag{5.4}$$

We can compare that result to verify equation (5.1).

5.2 Pauli matrices

Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ are very important in Quantum Mechanics, containing the algebraic properties of spin operators $S_{x,y,z} = \hbar/2\sigma_{x,y,z}$. After writing down the expressions of Pauli matrices in the basis which diagonalizes σ_z, prove the following properties:

i.) $\sigma_k^2 = \mathbb{1}$

ii.) $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$

iii.) $[\sigma_i, \sigma_j] = 2\mathrm{i}\varepsilon_{ijk}\sigma_k$

iv.) $\sigma_k^\dagger = \sigma_k$

v.) $det\sigma_k = -1$

vi.) $Tr\sigma_k = 0$

Solution: The Pauli matrices in the basis which diagonalizes σ_z are given as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.5}$$

i.) We can verify this property by noticing that for all matrices all column vectors are orthorgonal zu each other. Therefore we can conclude that σ_i must be unitary. Because σ_i is also hermitian (see **iv**), we get immediately $\mathbb{1} = \sigma_i^\dagger \sigma_i = \sigma_i^2$.

ii.) For $i = j$ we already showed that $\sigma_i^2 = \mathbb{1}$. Then $\{\sigma_i, \sigma_i\} = 2\mathbb{1}$. So now lets compute $\{\sigma_i, \sigma_j\}$ for $i \neq j$:

$$\sigma_x\sigma_y = \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix} = \mathrm{i}\sigma_z, \qquad \sigma_y\sigma_x = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix} = -\mathrm{i}\sigma_z \tag{5.6}$$

$$\sigma_y\sigma_z = \begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} = \mathrm{i}\sigma_x, \qquad \sigma_z\sigma_y = \begin{pmatrix} & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix} = -\mathrm{i}\sigma_x \tag{5.7}$$

$$\sigma_z\sigma_x = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathrm{i}\sigma_y, \qquad \sigma_x\sigma_z = \begin{pmatrix} & -1 \\ 1 & 0 \end{pmatrix} = -\mathrm{i}\sigma_y \tag{5.8}$$

We can see that $\sigma_i\sigma_j = -\sigma_j\sigma_i$ which leads to $\{\sigma_i, \sigma_j\} = 0$.

iii.) We can see from last point already, that $\sigma_i\sigma_j = \mathrm{i}\varepsilon_{ijk}\sigma_k$. Because $\sigma_i\sigma_j = -\sigma_j\sigma_i$ we see that $[\sigma_i, \sigma_j] = 2\sigma_i\sigma_j = 2\mathrm{i}\varepsilon_{ijk}\sigma_k$.

iv.) By noting that σ_x and σ_z are real and symmetric and σ_y is imaginary and antisymmetric we can immediately verify the hermitian property.

v.) We can easily compute the determinant of a matrix $\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$, which can be used to verify $\det\sigma_i = -1$ for all three matrices.

vi.) Since σ_x, σ_y do not have entries on the diagonal, the relation is trivial. For σ_z we also see that $\mathrm{Tr}\,\sigma_z = 1 - 1 = 0$.

5.3 Clebsch-Gordan coefficients

Consider a system composed of two subsystems with angular momenta $j_1 = 1$ and $j_2 = 1$. The z-components of these angular momenta are denoted by m_1 and m_2. The states of the total system are characterized by the total angular momentum j and corresponding magnetic quantum number m. Compute the Clebsch-Gordan coefficients for the quantum numbers given in the following tables.

$m=0$		$j=2$	$j=1$	$j=0$
$m_1=1,$	$m_2=-1$			
$m_1=0,$	$m_2=0$			
$m_1=-1,$	$m_2=1$			

$m=1$		$j=2$	$j=1$
$m_1=1,$	$m_2=0$		
$m_1=0,$	$m_2=1$		

Solution: We can calculate all of the Clebsch-Gordan coefficients by using the recursion relation and the orthonormality condition. The recursion relation is defined as follows

$$\sqrt{(j\mp m)(j\pm m+1)}\left\langle m_1 m_2\middle| j\, m\pm 1\right\rangle = \sqrt{(j_1\mp m_1+1)(j_1\pm m_1)}\left\langle m_1\mp 1, m_2\middle| j\, m\right\rangle + \sqrt{(j_2\mp m_2+1)(j_2\pm m_2)}\left\langle m_1, m_2\mp 1\middle| j\, m\right\rangle. \tag{5.9}$$

Remember that the recursion relation only acts for constant j. In order to find relations between different j we need to use the orthonormality relation. We call J_+ the operation taking the upper signs of equation (5.9) and J_- the operation with the lower signs. We can find the first Clebsch-Gordan coefficient in the highest state with maximum j, m_j with

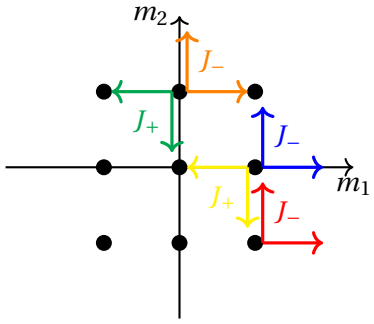
$$\left\langle m_1=1, m_2=1\middle| j=2, m=2\right\rangle = \langle 1\,1|2\,2\rangle = 1. \tag{5.10}$$

We can construct the first lower state by applying J_- to the Clebsch-Gordan coefficient $\langle 1\,0|2\,1\rangle$ which leads to

$$\begin{aligned}\sqrt{(j+m)(j-m+1)}\,\langle 1\,0|2\,1\rangle &= \sqrt{(j_1+m_1+1)(j_1-m_1)}\underbrace{\langle 2\,0|2\,2\rangle}_{=0} \\ &\quad + \sqrt{(j_2+m_2+1)(j_2-m_2)}\,\langle 1\,1|2\,2\rangle \\ 2\,\langle 1\,0|2\,1\rangle &= \sqrt{2}\underbrace{\langle 1\,1|2\,2\rangle}_{=1} \quad \Rightarrow \langle 1\,0|2\,1\rangle = \frac{1}{\sqrt{2}}.\end{aligned} \tag{5.11}$$

We can further apply J_- to the unknown coefficient $\langle 1\,-1|2\,0\rangle$ which leads to

$$\begin{aligned}\sqrt{(j+m)(j-m+1)}\,\langle 1\,-1|2\,0\rangle &= \sqrt{(j_1+m_1+1)(j_1-m_1)}\underbrace{\langle 2\,-1|2\,1\rangle}_{=0} \\ &\quad + \sqrt{(j_2+m_2+1)(j_2-m_2)}\,\langle 1\,0|2\,1\rangle \\ \sqrt{6}\,\langle 1\,0|2\,1\rangle &= \sqrt{2}\underbrace{\langle 1\,0|2\,1\rangle}_{=1/\sqrt{2}} \quad \Rightarrow \langle 1\,-1|2\,0\rangle = \frac{1}{\sqrt{6}}.\end{aligned} \tag{5.12}$$



If we now apply J_+ to the $\langle 10|21\rangle$ coefficient this will yield the $\langle 00|20\rangle$ state

$$\begin{aligned}\sqrt{(j-m)(j+m+1)}\,\langle 10|20\rangle &= \sqrt{(j_1-m_1+1)(j_1+m_1)}\,\langle 00|20\rangle \\ &\quad + \sqrt{(j_2-m_2+1)(j_2+m_2)}\,\langle 1-1|20\rangle \\ \sqrt{6}\underbrace{\langle 10|21\rangle}_{1/\sqrt{2}} &= \sqrt{2}\,\langle 00|20\rangle + \sqrt{2}\underbrace{\langle 1-1|20\rangle}_{1/\sqrt{6}} \quad \Rightarrow \langle 00|20\rangle = \sqrt{\frac{2}{3}}.\end{aligned} \tag{5.13}$$

The next coefficient can be constructed by applying J_- to $\langle 01|21\rangle$

$$\begin{aligned}\sqrt{(j+m)(j-m+1)}\,\langle 01|21\rangle &= \sqrt{(j_1+m_1+1)(j_1-m_1)}\,\langle 11|22\rangle \\ &\quad + \sqrt{(j_2+m_2+1)(j_2-m_2)}\underbrace{\langle 02|22\rangle}_{0} \\ 2\,\langle 01|21\rangle &= \sqrt{2}\underbrace{\langle 11|22\rangle}_{1} \quad \Rightarrow \langle 01|21\rangle = \frac{1}{\sqrt{2}}.\end{aligned} \tag{5.14}$$

Again the second term vanishes because $m_j > j$ is not possible. The last coefficient for $j=2$ can be constructed by applying J_+ to the same coefficient as before

$$\begin{aligned}\sqrt{(j-m)(j+m+1)}\,\langle 01|21\rangle &= \sqrt{(j_1-m_1+1)(j_1+m_1)}\,\langle -11|20\rangle \\ &\quad + \sqrt{(j_2-m_2+1)(j_2+m_2)}\,\langle 00|20\rangle \\ \sqrt{6}\underbrace{\langle 01|21\rangle}_{1/\sqrt{2}} &= \sqrt{2}\,\langle -11|20\rangle + \sqrt{2}\underbrace{\langle 00|20\rangle}_{\sqrt{2}/\sqrt{3}} \quad \Rightarrow \langle -11|20\rangle = \frac{1}{\sqrt{6}}.\end{aligned} \tag{5.15}$$

Our table now looks like

$m=0$		$j=2$	$j=1$	$j=0$
$m_1=1,$	$m_2=-1$	$1/\sqrt{6}$		
$m_1=0,$	$m_2=0$	$\sqrt{2}/\sqrt{3}$		
$m_1=-1,$	$m_2=1$	$1/\sqrt{6}$		

$m=1$		$j=2$	$j=1$
$m_1=1,$	$m_2=0$	$1/\sqrt{2}$	
$m_1=0,$	$m_2=1$	$1/\sqrt{2}$	

Now we can use the orthonormality relation

$$\boxed{\sum_j \langle m_1 m_2|jm\rangle\langle m_1 m_2|jm\rangle = 1} \tag{5.16}$$

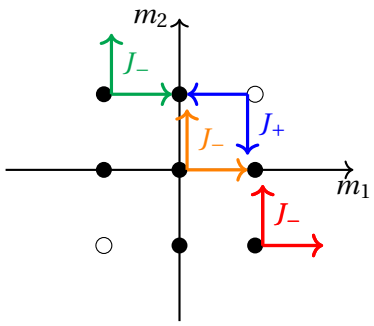
to find an expression for a Clebsch-Gordan coefficient with $j = 1$

$$\underbrace{\langle 1\,0|2\,1\rangle^2}_{=1/2} + \langle 1\,0|1\,1\rangle^2 = 1 \quad \Rightarrow \langle 1\,0|1\,1\rangle = \frac{1}{\sqrt{2}}. \tag{5.17}$$

We will choose the plus sign solution, because we use the *Condon-Shortley* phase convention which states that

$$\left\langle j_1, j_2, m_1 = j_1, m_2 \middle| j\ m \right\rangle \in \mathbb{R}, > 0. \tag{5.18}$$

Due to orthogonality of the two columns of the right table we can immediately deduce the coefficient for $\langle 0\,1|1\,1\rangle = -1/\sqrt{2}$. Alternatively we can obtain this result by applying J_+ to the zero coefficient $\langle 1\,1|1\,2\rangle$.



We can obtain the $\langle 1\,-1|1\,0\rangle$ coefficient by applying J_-

$$\begin{aligned}
\sqrt{(j+m)(j-m+1)}\,\langle 1\,-1|1\,0\rangle &= \sqrt{(j_1+m_1+1)(j_1-m_1)}\,\underbrace{\langle 2\,-1|1\,1\rangle}_{=0} \\
&\quad + \sqrt{(j_2+m_2+1)(j_2-m_2)}\,\langle 1\,0|1\,1\rangle \\
\sqrt{2}\,\langle 1\,-1|1\,0\rangle &= \sqrt{2}\,\underbrace{\langle 1\,0|1\,1\rangle}_{=1/\sqrt{2}} \quad \Rightarrow \langle 1\,-1|1\,0\rangle = \frac{1}{\sqrt{2}}.
\end{aligned} \tag{5.19}$$

Now we can apply J_- to $\langle -1\,1|1\,0\rangle$

$$\begin{aligned}
\sqrt{(j+m)(j-m+1)}\,\langle -1\,1|1\,0\rangle &= \sqrt{(j_1+m_1+1)(j_1-m_1)}\,\langle 0\,1|1\,1\rangle \\
&\quad + \sqrt{(j_2+m_2+1)(j_2-m_2)}\,\underbrace{\langle -1\,2|1\,1\rangle}_{0} \\
\sqrt{2}\,\langle -1\,1|1\,0\rangle &= \sqrt{2}\,\underbrace{\langle 0\,1|1\,1\rangle}_{-1/\sqrt{2}} \quad \Rightarrow \langle -1\,1|1\,0\rangle = -\frac{1}{\sqrt{2}}.
\end{aligned} \tag{5.20}$$

The last coefficient can be constructed by applying J_- to $\langle 0\,0|1\,0\rangle$

$$\begin{aligned}
\sqrt{(j+m)(j-m+1)}\,\langle 0\,0|1\,0\rangle &= \sqrt{(j_1+m_1+1)(j_1-m_1)}\,\langle 1\,0|1\,1\rangle \\
&\quad + \sqrt{(j_2+m_2+1)(j_2-m_2)}\,\langle 0\,1|1\,1\rangle \\
\sqrt{2}\,\langle 0\,0|1\,0\rangle &= \sqrt{2}\,\underbrace{\langle 1\,0|1\,1\rangle}_{1/\sqrt{2}} + \sqrt{2}\,\underbrace{\langle 0\,1|1\,1\rangle}_{-1/\sqrt{2}} = 0.
\end{aligned} \tag{5.21}$$

We can now easily fill in the last column of the first table by again applying the orthogonality relation for the rows. Because of *Condon-Shortley* phase convention we know that $\langle 1\,-1|1\,0\rangle$ is positive

$$\underbrace{\langle 1\,-1|20\rangle^2}_{1/6}+\underbrace{\langle 1\,-1|1\,0\rangle^2}_{1/2}+\langle 1\,-1|1\,0\rangle^2=1 \quad \Rightarrow \langle 1\,-1|1\,0\rangle=\frac{1}{\sqrt{3}}. \tag{5.22}$$

$m=0$	$j=2$	$j=1$	$j=0$
$m_1=1, m_2=-1$	$1/\sqrt{6}$	$1/\sqrt{2}$	$1/\sqrt{3}$
$m_1=0, m_2=0$	$\sqrt{2}/\sqrt{3}$	0	$-1/\sqrt{3}$
$m_1=-1, m_2=1$	$1/\sqrt{6}$	$-1/\sqrt{2}$	$1/\sqrt{3}$

$m=1$	$j=2$	$j=1$
$m_1=1, m_2=0$	$1/\sqrt{2}$	$1/\sqrt{2}$
$m_1=0, m_2=1$	$1/\sqrt{2}$	$-1/\sqrt{2}$

5.4 Rotations in Quantum mechanics

Recall that a finite rotation operator in Quantum Mechanics is given by

$$T[\boldsymbol{\theta}] = \exp\left(-\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right) \tag{5.23}$$

where $\boldsymbol{J}$ is the generalised generator of rotation. Show that if a classical observable $S(t,x)$ transforms like a scalar under rotation, the quantum operator must satisfy

$$[S, J_i] = 0. \tag{5.24}$$

Hence show also that to be a vector $\boldsymbol{V}(t,x)$ under rotation, the condition to be satisfied is

$$[V_a, J_b] = \mathrm{i}\varepsilon_{abc}V_c. \tag{5.25}$$

Deduce, therefore the transformation of $\langle \boldsymbol{V}|\boldsymbol{V}\rangle$ under a rotation. Hint: Think of transformations in the Heisenberg formulation. You can use the Baker-Campbell-Hausdorff formula for the second part.

Solution: Working in the Heisenberg formulation, we see that the action of rotation upon an operator O is given by

$$O_R(\boldsymbol{\theta}) = T^\dagger OT = \exp\left(\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right)O\exp\left(-\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right). \tag{5.26}$$

For a vector under rotation let us first see what happens under an infinitesimal rotation $\delta\boldsymbol{\theta}$. Then

$$\begin{aligned} V_a(R[\delta\boldsymbol{\theta}]) &= \left(1+\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right)V_a\left(1-\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right) = \left(1+\mathrm{i}\frac{J_k n_k\delta\theta}{\hbar}\right)V_a\left(1-\mathrm{i}\frac{J_k n_k\delta\theta}{\hbar}\right) \\ &= V_a - \frac{\mathrm{i}}{\hbar}[V_a, J_k]n_k\delta\theta. \end{aligned} \tag{5.27}$$

So if now the commutation relation $[V_a, J_k] = \mathrm{i}\hbar\varepsilon_{akl}V_l$ is satisfied[2], then

$$V_a(R[\delta\boldsymbol{\theta}]) = V_a + \varepsilon_{akl}n_k\delta\theta V_l = V_a + (\delta\boldsymbol{\theta}\times\boldsymbol{V})_a \tag{5.28}$$

which exactly corresponds to the small rotation. The factor of $\hbar$ is just to keep the formula dimensionally consistent.

Now lets attempt to prove the relation for finite rotations. Without loss of generality we can set the rotation axis to be the z-axis. Let us look at the x component of a vector $\boldsymbol{V}$

$$\begin{aligned} V_x(R[\boldsymbol{\theta}]) &= \left(1+\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right)V_a\left(1-\mathrm{i}\frac{\boldsymbol{J}\cdot\boldsymbol{\theta}}{\hbar}\right) \quad \text{BCH formula} \\ &= V_x + \mathrm{i}\theta[J_z, V_x] + \frac{(\mathrm{i}\theta)^2}{2!}[J_z,[J_z,V_x]] + \frac{(\mathrm{i}\theta)^3}{3!}[J_z,[J_z,[J_z,V_x]]] + \ldots \\ &= V_x\left(1-\frac{\theta^2}{2!}+\frac{\theta^4}{4!}+\ldots\right) - V_y\left((\theta-\frac{\theta^3}{3!}+\frac{\theta^5}{5!}+\ldots)\right) \\ \langle V_x(R[\boldsymbol{\theta}])\rangle &= \langle V_x\rangle\cos\theta - \langle V_y\rangle\cos\theta \end{aligned} \tag{5.29}$$

[2] In the task the commutation relation was given with $\hbar \equiv 1$.

In deriving the above we have made repeated use of the commutation relation. Thus we see that the rhs is exactly the rotation operator $R_z(\theta)$ applied to $\langle V_x \rangle$. In an analogous way the transformations for $\langle V_y \rangle$ can also be found

$$\langle V_y(R[\boldsymbol{\theta}]) \rangle = \langle V_x \rangle \sin\theta + \langle V_y \rangle \cos\theta \tag{5.30}$$

also as $[J_z, V_z] = 0$, so $\langle V_z(R[\boldsymbol{\theta}]) \rangle = \langle V_z \rangle$. The total rotation matrix R can now be written as

$$R = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} = R_z. \tag{5.31}$$

This can now be generalised to arbitrary axes by use of Euler angles.

5.5 Coupling of three angular momenta (BONUS)

A system consists of three spin-1/2 particles. Construct an orthonormal basis $|S, S_z\rangle$ of eigenvectors of $\boldsymbol{S}^2$ and S_z, where

$$\boldsymbol{S} = \boldsymbol{S}_1 + \boldsymbol{S}_2 + \boldsymbol{S}_3 \tag{5.32}$$

is the total spin of the system.
Hint: *Write down the $|3/2, 3/2\rangle$ state and build the other $s = 3/2$ states by repeatedly applying the $S_- = S_-^{(1)} + S_-^{(2)} + S_-^{(3)}$ operator. To obtain the $s = 1/2$ states consider one of the three possible pairs of particles in the $s = 0$ singlet state and couple it to the third particle. Are the states you obtain all linearly independent?*

Solution: At first we write down the $\left|\frac{3}{2}, \frac{3}{2}\right\rangle$ which can only be achieved if all three spins are pointing upwards. We can write this as

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle = |\uparrow\uparrow\uparrow\rangle. \tag{5.33}$$

We can now apply the ladder operator S_- to this state, which can be expressed in the $\uparrow\downarrow$ basis as

$$S_- = S_{1-} + S_{2-} + S_{3-}, \tag{5.34}$$

where S_{i-} only acts on the state of spin i. First we apply the ladder operator to the new basis

$$\begin{aligned} S_- \left|\frac{3}{2}, \frac{3}{2}\right\rangle &= \hbar\sqrt{(s+m)(s-m+1)} \left|\frac{3}{2}, \frac{1}{2}\right\rangle \\ &= \hbar\sqrt{\left(\frac{3}{2}+\frac{3}{2}\right)\left(\frac{3}{2}-\frac{3}{2}+1\right)} \left|\frac{3}{2}, \frac{1}{2}\right\rangle = \hbar\sqrt{3} \left|\frac{3}{2}, \frac{1}{2}\right\rangle. \end{aligned} \tag{5.35}$$

We can also apply the ladder operator to the old basis

$$\begin{aligned} S_{1-}|\uparrow\uparrow\uparrow\rangle &= \hbar\sqrt{(s_1+m_1)(s_1-m_1+1)}\,|\downarrow\uparrow\uparrow\rangle \\ &= \hbar\sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\,|\downarrow\uparrow\uparrow\rangle = \hbar|\downarrow\uparrow\uparrow\rangle\,. \end{aligned} \tag{5.36}$$

We can apply this for all three ladder operators separately which yields

$$S_-|\uparrow\uparrow\uparrow\rangle = \hbar(|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle). \tag{5.37}$$

We can now compare (5.35) and (5.37) resulting in

$$\left|\frac{3}{2},\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}(|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle). \tag{5.38}$$

We find the same results for the symmtetric case of three down spins

$$\left|\frac{3}{2},\frac{3}{2}\right\rangle = |\downarrow\downarrow\downarrow\rangle\,. \tag{5.39}$$

Here we can instead apply the climbing ladder operator S_+ which leads us to a similar result

$$\left|\frac{3}{2},-\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle), \tag{5.40}$$

which can be obtained by just switching the signs of all spins. Alternatively we could apply the ladder operator again to (5.38).

In order to obtain the state for $s = 1/2$ we can use a system of two spin $1/2$ particles with total spin $S = 0$ and take the tensor product with a third spin particle. The singlet state of the 2-spin system was derived in the lecture as

$$|00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \tag{5.41}$$

We can construct the $S = 1/2$ state by applying the tensor product of (**??**) with $|\uparrow\rangle$

$$\begin{aligned} \underbrace{|00\rangle \otimes |\uparrow\rangle}_{|1/2,1/2\rangle} &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \otimes |\uparrow\rangle \\ \left|\frac{1}{2},\frac{1}{2}\right\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle). \end{aligned} \tag{5.42}$$

In order to obtain the $|1/2,-1/2\rangle$ state we can take the tensor product with $|\downarrow\rangle$

$$\begin{aligned} \underbrace{|00\rangle \otimes |\downarrow\rangle}_{|1/2,-1/2\rangle} &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \otimes |\downarrow\rangle \\ \left|\frac{1}{2},-\frac{1}{2}\right\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle). \end{aligned} \tag{5.43}$$

6 Time independent perturbation theory

6.1 Perturbation of Harmonic Oscillator

Consider the quartic Oscillator

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}\mu\omega^4 x^4. \tag{6.1}$$

Treating the last term as a perturbation to the SHO problem, find the resulting new eigenvalues for an arbitrary energy state $|E_k\rangle$ up to the 2nd order. What would be the new eigenvalues for the ground state $|E_0\rangle$ at the 3rd order?
Hint: Write down the Hamiltonian as $H_0 + \lambda H_p$, where H_0 and H_p mean the unperturbed and the perturbing Hamiltonians. Similarly expand both E_n and Ψ_n in powers of λ (order of expansion). Collect the terms at a given order to derive the nature of the perturbation equation at that order.

Solution: We can write the Hamiltonian as

$$H(x,p) = H_0 + \frac{\lambda}{2}\mu\omega^4 x^4. \tag{6.2}$$

We can write the uperturbed solution as

$$H_0 \left|E_n^{(0)}\right\rangle = E_n^{(0)} \left|E_n^{(0)}\right\rangle \quad E_n^{(0)} = \hbar\omega\left(n + \frac{1}{2}\right). \tag{6.3}$$

We can additionally introduce the effects of the ladder operators on the eigenstates

$$\begin{aligned} a^\dagger \left|E_n^{(0)}\right\rangle &= \sqrt{n+1}\left|E_{n+1}^{(0)}\right\rangle \\ a\left|E_n^{(0)}\right\rangle &= n\left|E_{n-1}^{(0)}\right\rangle. \end{aligned} \tag{6.4}$$

We can now express the perturbation with the ladder operator

$$a = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \mathrm{i}\frac{P}{\mu\omega}\right) \quad \rightarrow \quad x = \sqrt{\frac{\hbar}{2\mu\omega}}(a + a^\dagger). \tag{6.5}$$

The perturbation can then be written as

$$H_p = \frac{1}{8}\frac{\hbar^2\omega^2}{\mu}(a + a^\dagger)^4. \tag{6.6}$$

In the lecture we derived a formula for the perturbed energies δ_k and perturbed states η_k

$$\delta_k = \langle E_0|H_p|\eta_{k-1}\rangle = \underbrace{\frac{1}{8}\frac{\hbar^2\omega^2}{\mu}}_{:=K}\left\langle E_0|(a + a^\dagger)^4|\eta_{k-1}\right\rangle. \tag{6.7}$$

We denote the unperturbed eigenstates $\left|E_n^{(0)}\right\rangle$ as $|n\rangle$. We first calculate

$$\begin{aligned} H_p\left|\eta_0\right\rangle &= K(a+a^\dagger)^4|0\rangle = K(a+a^\dagger)^3|1\rangle \\ &= K(a+a^\dagger)^2(|0\rangle+\sqrt{2}|2\rangle) \\ &= K(a+a^\dagger)(|1\rangle+2|1\rangle+\sqrt{6}|3\rangle) \\ &= K(3|0\rangle+6\sqrt{2}|2\rangle+2\sqrt{6}|4\rangle). \end{aligned} \tag{6.8}$$

This immediately leads to

$$\delta_1 = \left\langle E_0|H_p|E_0\right\rangle = \langle 0|K(3|0\rangle+3\sqrt{2}|2\rangle+2\sqrt{6}|4\rangle) = 3K. \tag{6.9}$$

The general formula of the corrected state is

$$\boxed{\left|\eta_k\right\rangle = R_0\sum_j^{k-1}\delta_j\left|\eta_{k-1}\right\rangle - R_0H_p\left|\eta_{k-1}\right\rangle}, \tag{6.10}$$

where R_0 is the *resolvent*

$$R_0|n\rangle = \begin{cases} \frac{1}{n}|n\rangle & n>0 \\ 0 & \text{otherwise.} \end{cases} \tag{6.11}$$

We can now calculate the state correction of the first order

$$\begin{aligned} \left|\eta_1\right\rangle &= -R_0H_p\left|\eta_0\right\rangle = -R_0K(3|0\rangle+6\sqrt{2}|2\rangle+2\sqrt{6}|4\rangle) \\ &= -K\left(3\sqrt{2}|2\rangle+\frac{\sqrt{6}}{4}|4\rangle\right). \end{aligned} \tag{6.12}$$

In order to calculate the second corrected energy state $\left|\eta_2\right\rangle$ we first calculate

$$\begin{aligned} (a+a^\dagger)^4|2\rangle &= (a+a^\dagger)^3(\sqrt{2}|1\rangle+\sqrt{3}|3\rangle) \\ &= (a+a^\dagger)^2(\sqrt{2}|0\rangle+5|2\rangle+2\sqrt{3}|4\rangle) \\ &= (a+a^\dagger)(6\sqrt{2}|1\rangle+9\sqrt{3}|3\rangle+2\sqrt{3}\sqrt{5}|5\rangle) \\ &= 6\sqrt{2}|0\rangle+39|2\rangle+28\sqrt{3}|4\rangle+6\sqrt{2}\sqrt{5}|6\rangle. \end{aligned} \tag{6.13}$$

Analogously we can calculate

$$\begin{aligned} (a+a^\dagger)^4|4\rangle &= (a+a^\dagger)^3(2|3\rangle+\sqrt{5}|5\rangle) \\ &= (a+a^\dagger)^2(2\sqrt{2}|2\rangle+9|4\rangle+\sqrt{5}\sqrt{6}|6\rangle) \\ &= (a+a^\dagger)(2\sqrt{6}|1\rangle+24|3\rangle+15\sqrt{5}|5\rangle+\sqrt{5}\sqrt{6}\sqrt{7}|7\rangle) \\ &= 2\sqrt{6}|0\rangle+28\sqrt{3}|2\rangle+123|4\rangle+22\sqrt{5}\sqrt{6}|6\rangle+\sqrt{5}\sqrt{6}\sqrt{7}\sqrt{8}|8\rangle. \end{aligned} \tag{6.14}$$

First we compute the energy correction

$$\begin{aligned} \delta_2 &= -K^2\Big(3\sqrt{2}\underbrace{\left\langle 0|(a+a^\dagger)^4|2\right\rangle}_{6\sqrt{2}}+\frac{\sqrt{6}}{2}\underbrace{\left\langle 0|(a+a^\dagger)^4|4\right\rangle}_{2\sqrt{6}}\Big) \\ &= -K^2(18\cdot 2+6) = -42K^2 = -\frac{21}{32}\frac{\hbar^4\omega^4}{\mu^2}. \end{aligned} \tag{6.15}$$

6.2 Spherical tensors

Consider a spinless particle bound to a fixed center by a central force potential.

a) *Using only the Wigner-Eckart theorem, relate (i. e. consider the ratio between) the matrix elements*

$$\left\langle n',l',m'\right| \mp\frac{1}{\sqrt{2}}(x\pm \mathrm{i}y)\left|n,l,m\right\rangle \qquad \text{and} \qquad \left\langle n',l',m'|z|n,l,m\right\rangle \tag{6.16}$$

stating under what conditions the matrix elements are nonvanishing.
Hint: You can recognize the matrix elements above as the elements of a spherical tensor of rank 1.

b) *Do the same problem again using wave functions $\psi(\boldsymbol{x}) = \mathscr{R}_{nl}Y_l^m(\vartheta,\varphi)$, i. e. ψ is factorized in a radial and angular part.*

a.) Solution: The Wigner-Eckart theorem for a generic tensor operator of rank k $R_q^{(k)}$ reads

$$\left\langle n',l',m'|R_q^{(k)}|n,l,m\right\rangle = \frac{\left\langle lk;mq|lk;l'm'\right\rangle\left\langle n'l'||R^{(1)}||nl\right\rangle}{\sqrt{2l+1}}. \tag{6.17}$$

The double bar matrix element is independent of m and m'. As was given in the hint, the matrix elements form a spherical tensor of rank $k=1$ which can be written as

$$R_\pm^{(1)} = \mp\frac{1}{\sqrt{2}}(x\pm \mathrm{i}y) \qquad \text{and} \qquad R_0^{(1)} = z. \tag{6.18}$$

From the requirement that the Clebsch-Gordan coefficient is nonvanishing we obtain the m selection rule $m' = m+q$ and also the triangular relation $|l-k| \le l' \le |l+k|$. In the special case of rank 1 tensors this translates to

$$|l-1| \le l' \le |l+1| \quad \Rightarrow l' = |l\pm 1|, 0. \tag{6.19}$$

We can further restrict this selection rule based on a parity argument. For a central potential $|nlm\rangle$ is an eigenvector of the parity operator U_p. We obtain

$$U_p|nlm\rangle = (-1)^l|nlm\rangle \qquad U_p^{-1}R^{(1)} = -R^{(1)}. \tag{6.20}$$

Hence we can write the left hand side of the Wigner-Eckart theorem as

$$-\left\langle n',l',m'|R^{(1)}|n,l,m\right\rangle = (-1)^l(-1)^{l'}\left\langle n',l',m'|R^{(1)}|n,l,m\right\rangle. \tag{6.21}$$

This implies that $l+l'$ has to be odd, therefore $l' \neq l$. We can now consider the ratio

$$\begin{aligned}\frac{\left\langle n',l',m'\right|R_\pm^{(1)}\left|n,l,m\right\rangle}{\left\langle n',l',m'\right|R_0^{(1)}\left|n,l,m\right\rangle} &= \frac{\left\langle l,1,m_1,\pm1|l,1,l',m_1'\right\rangle}{\left\langle l,1,m_2,0|l,1,l',m_2'\right\rangle}\frac{\left\langle n',l'||R^{(1)}||n,l\right\rangle\sqrt{2l+1}}{\left\langle n',l'||R^{(1)}||n,l\right\rangle\sqrt{2l+1}} \\ &= \frac{\left\langle l,1,m_1,\pm1|l,1,l',m_1'\right\rangle}{\left\langle l,1,m_2,0|l,1,l',m_2'\right\rangle},\end{aligned} \tag{6.22}$$

where $q=\pm1,0$ and l',m' satisfy the selection rules found above.

b.) Solution: Now we use the wave function $\Psi(\boldsymbol{x}) = \mathscr{R}_{nl}(r)\,Y_l^m(\theta,\phi)$. We can evaluate the matrix element using $q = \pm 1, 0$

$$\begin{aligned}\left\langle n',l',m'|R_q^{(1)}|n,l,m\right\rangle &= \int \mathscr{R}^*_{n'l'}(r)\,Y_{l'}^{m'*}(\vartheta,\varphi)[R_q^{(1)}]\mathscr{R}_{nl}(r)\,Y_l^m(\vartheta,\varphi)\,\mathrm{d}^3\boldsymbol{x}\\ &= \sqrt{\frac{4\pi}{3}}\int_0^\infty r^2\mathscr{R}^*_{n'l'}\,r\mathscr{R}_{nl}\int Y_{l'}^{m'*}\,Y_1^q\,Y_l^m\,\mathrm{d}\Omega\,. \end{aligned} \tag{6.23}$$

Here we use the fact that $R_q^{(1)}$ can be written in terms of spherical harmonics

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\vartheta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \quad\Rightarrow\quad z = r\,Y_1^0\sqrt{\frac{4\pi}{3}} \tag{6.24}$$

$$Y_1^{\pm1} = \mp\frac{x\pm\mathrm{i}y}{r\sqrt{2}}\sqrt{\frac{3}{4\pi}} \quad\Rightarrow\quad R_\pm^{(1)} = \mp\frac{x\pm\mathrm{i}y}{\sqrt{2}} = r\,Y_1^{\pm1}\sqrt{\frac{4\pi}{3}}. \tag{6.25}$$

For whatever value of q, $R_q^{(1)}$ contains the prefactor $\sqrt{\frac{4\pi}{3}}$, an r and the spherical harmonic Y_1^q.

We can now use an identity for the integral of three generic spherical harmonics[3]

$$\int \mathrm{d}\Omega\,Y_l^{m*}\,Y_{l_1}^{m_1}\,Y_{l_2}^{m_2} = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}}\,\langle l_1 l_2;00|l_1 l_2;l0\rangle\,\langle l_1 l_2;m_1 m_2|l_1 l_2;lm\rangle\,. \tag{6.26}$$

We can insert this now into (6.23) to obtain

$$\begin{aligned}\left\langle n',l',m'|R_q^{(1)}|n,l,m\right\rangle &= \sqrt{\frac{4\pi}{3}}\int_0^\infty r^2\mathscr{R}^*_{n'l'}\,r\mathscr{R}_{nl}\sqrt{\frac{(2l+1)3}{4\pi(2l'+1)}}\,\langle l_1 1;00|l1;l'0\rangle\,\langle l_1 q;mq|l1;l'm'\rangle\\ &= \int_0^\infty r^2\mathscr{R}^*_{n'l'}\,r\mathscr{R}_{nl}\sqrt{\frac{(2l+1)}{(2l'+1)}}\,\langle l_1 1;00|l1;l'0\rangle\,\langle l_1 q;mq|l1;l'm'\rangle\,. \end{aligned} \tag{6.27}$$

This value is only nonzero if $l \neq l'$. The selection rules come directly from the orthogonality of the spherical harmonics. We find the same result as in a.) when taking the ratio between the matrix elements with $l' = |l\pm1|$ and $m_1' = m_1 \pm 1, m_2' = m_2$.

[3] see Sakurai, 2nd edition, p.217

6.3 Time independent perturbations and degeneracy

p-orbital electron characterized by $|n, l = 1, m = \pm 1, 0\rangle$ (ignore spin) is subjected a potential

$$V = \lambda(x^2 - y^2) \qquad \lambda = const. \tag{6.28}$$

a) *Obtain the* correct *zeroth-order energy eigenstates that diagonalize the perturbation. You need not evaluate the energy shifts in detail, but show that the original threefold degeneracy is now completely removed.*

b) *Because V is invariant under time reversal and because there is no longer any degeneracy, we expect each of the energy eigenstates obtained in a) to go into itself (up to a phase factor or sign) under time reversal. Check this point explicitly.*

a.) Solution: We can first express the perturbation as a function of spherical harmonics Y_l^m. Then we can use the selection rules for the matrix elements in order to identify all nonzero elements. We can rewrite the potential

$$V = \lambda(x^2 - y^2) = \lambda((x + \mathrm{i}y)^2 + (x - \mathrm{i}y)^2). \tag{6.29}$$

Now we identify the spherical harmonics $Y_2^{\pm 2}$ as

$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} \frac{(x \pm \mathrm{i}y)^2}{r^2} \quad \Rightarrow V = \underbrace{2\lambda\sqrt{\frac{15}{32\pi}}}_{=\alpha}(r^2 Y_2^2 + r^2 Y_2^{-2}). \tag{6.30}$$

We can now use the selection rules for

$$\begin{aligned} \langle nlm'|V|nlm\rangle &= \alpha \langle nlm'|(r^2 Y_2^2 + r^2 Y_2^{-2})|nlm\rangle \\ &= \alpha\left[\langle nlm'|r^2 Y_2^2|nlm\rangle + \langle nlm'|r^2 Y_2^{-2}|nlm\rangle\right]. \end{aligned} \tag{6.31}$$

The first term is nonzero if $m' = m+2$ while for the second term $m' = m-2$. Since for $l = 1$, m is $\{-1, 0, 1\}$ the only non-zero components are $\langle nl1|r^2 Y_2^2|nl-1\rangle$ and $\langle nl-1|r^2 Y_2^2|nl1\rangle$. We can compute the expectation values as

$$\langle nlm'|V|nlm\rangle = \alpha \int r^2 R_{nl}^2 (Y_l^{m'})^* Y_2^q Y_l^m \,\mathrm{d}^3\boldsymbol{r}\,. \tag{6.32}$$

For the p-orbital electron we have $|n = 2, l = 1\rangle$. Therefore

$$\begin{aligned} \langle 111|\alpha r^2 Y_2^2|11-1\rangle &= \alpha \int r^2 R_{21}^2 (Y_1^1)^* Y_2^2 Y_1^{-1} \,\mathrm{d}^3\boldsymbol{r} \\ &= -\alpha\frac{3}{8\pi}\int r^2 R_{21}^2 \sin^2\vartheta \mathrm{e}^{-2\mathrm{i}\varphi} Y_2^2 \,\mathrm{d}^3\boldsymbol{r} = -\alpha\frac{3}{8\pi}\int r^2 R_{21}^2 \sin^4\vartheta\sqrt{\frac{15}{32}}\,\mathrm{d}^3\boldsymbol{r} \end{aligned} \tag{6.33}$$

$$\begin{aligned} \langle 11-1|\alpha r^2 Y_2^2|111\rangle &= \alpha \int r^2 R_{21}^2 (Y_1^{-1})^* Y_2^{-2} Y_1^1 \,\mathrm{d}^3\boldsymbol{r} \\ &= -\alpha\frac{3}{8\pi}\int r^2 R_{21}^2 \sin^2\vartheta \mathrm{e}^{+2\mathrm{i}\varphi} Y_2^{-2} \,\mathrm{d}^3\boldsymbol{r} = -\alpha\frac{3}{8\pi}\int r^2 R_{21}^2 \sin^4\vartheta\sqrt{\frac{15}{32}}\,\mathrm{d}^3\boldsymbol{r}\,. \end{aligned} \tag{6.34}$$

We see that both integrals are the same, we denote the result as ξ. In a Matrix Form we can write $\langle V \rangle$ as

$$\langle V \rangle = \begin{pmatrix} 0 & 0 & \xi \\ 0 & 0 & 0 \\ \xi & 0 & 0 \end{pmatrix}. \tag{6.35}$$

In order to find the diagonalizing energy eigenstates we solve the eigenvalue problem. We recieve the following eigenkets and corresponding eigenvalues $0, \pm\xi$

- $\psi_0 = |210\rangle$ with $\Delta E = 0$
- $\psi_1 = \frac{1}{\sqrt{2}}(|211\rangle + |21-1\rangle)$ with $\Delta E = \xi$
- $\psi_1 = \frac{1}{\sqrt{2}}(|211\rangle - |21-1\rangle)$ with $\Delta E = -\xi$.

We see that Ψ_0 with $m = 0$ has the original energy eigenvalue, the electric potential forces the other two states to occupy different energy levels. The original degeneracy has been completely removed.

6.4 Asymptotic and Convergent series

A sequence of function $\{\varphi_n\}$ with $\varphi_n : C/z_0 \to C, n = 0,1,2,\ldots$ is called an asymptotic sequence as $z \to z_0$ if for each $n = 0,1,2,\ldots$ we have that

$$\varphi_{n-1}(z) = o(\varphi_n(z)), \quad z \to z_0. \tag{6.36}$$

Let $f(z)$ be a continuous function such that $f(z) : z \in C/z_0 \to f(z) \in C$. We say that $f(z)$ allows an asymptotic series expansion for $z \to z_0$ if there exist an asymptotic sequence $\{\varphi_n\}$, such that for each $N = 1,2,\ldots$

$$|f(z) - \sum_{n=0}^{N-1} a_n \varphi_n(z)| = O(\varphi_N(z)), \quad z \to z_0 \tag{6.37}$$

or, equivalently

$$|f(z) - \sum_{n=0}^{N-1} a_n \varphi_n(z)| = o(\varphi_{N-1}(z)), \quad z \to z_0. \tag{6.38}$$

Asymptotic series often appear in many branches of physics when performing perturbatie expansions. Note that asymptotic series need not converge; in fact, in typical cases of interes, an asymptotic series will never converge. Similarly, a convergent series need not be asymptotic.

a) *Consider the (uniformly convergent) Taylor series for the exponential function $f(z) = e^z$. Prove that it does not define an asymptotic series for e^z when $|z| \to \infty$.*

b) *Consider now the function*

$$-E_i(-x) = E_1(x) = \int_x^\infty \frac{\exp(-t)}{t}\,dt \tag{6.39}$$

and prove that $E_1(x)$ does not converge in any standard sense, but admits an symptotic expansion for $x \to \infty$.

a.) Solution: In order to prove that the series is not asymptotic to e^z we need to identify the corresponding asymptotic sequence $\{\varphi_n\}$ and apply the second definition (6.38). We need to show then that the limit

$$\lim_{|z|\to\infty} \frac{e^z - \sum_{n=0}^{N} a_n \varphi_n}{\varphi_N} \neq 0. \tag{6.40}$$

We can perform this calculation by noting that $a_n = 1/n!$ and $\varphi_n = z^n$ for the exponential function

$$\begin{aligned}
\lim_{|z|\to\infty} \frac{e^z - \sum_{n=0}^{N} a_n \varphi_n}{\varphi_N} &= \lim_{|z|\to\infty} \frac{1}{z^N}\left(e^z - \sum_{n=0}^{N} \frac{z^n}{n!}\right) \\
&= \lim_{|z|\to\infty} \frac{1}{z^N}\left(\sum_{k=0}^{\infty} \frac{z^k}{k!} - \sum_{n=0}^{N} \frac{z^n}{n!}\right) \\
&= \lim_{|z|\to\infty} \frac{1}{z^N}\left(\sum_{n=N+1}^{\infty} \frac{z^n}{n!}\right) \\
&= \lim_{|z|\to\infty} \sum_{n=N+1}^{\infty} \frac{z^{n-N}}{n!} = \infty.
\end{aligned} \tag{6.41}$$

Note that, the summands are all positive because $n > N$. For $|z| \to \infty$ this tends to infinity and the Taylor series for the exponential function is not an asymptotic series.

b.) Solution: We can find the asymptotic series by repeatedly integration $E_1(x)$ by parts where we find an expression for $E_1(x) - \sum_0^N a_n \varphi_n$

$$\begin{aligned}
E_1(x) &= \int_x^\infty \frac{\exp(-t)}{t}\,\mathrm{d}t = \left(-\frac{\exp(-t)}{t}\right)\Big|_x^\infty - \int_x^\infty \frac{\exp(-t)}{t^2}\,\mathrm{d}t \\
&= \frac{e^{-x}}{x} - \left(-\frac{\exp(-t)}{t^2}\right)\Big|_x^\infty - 2\int_x^\infty \frac{\exp(-t)}{t^3}\,\mathrm{d}t \\
&= \frac{e^{-x}}{x} - \frac{e^{-x}}{x^2} + 2!\frac{e^{-x}}{x^3} + 3!\int_x^\infty \frac{\exp(-t)}{t^4}\,\mathrm{d}t \\
&= \frac{e^{-x}}{x}\left(1 - \frac{1}{x} + \frac{2!}{x^2} - \frac{3!}{x^3} + \ldots + (-1)^n \frac{n!}{x^n}\right) + (-1)^{n+1}(n+1)!\int_x^\infty \frac{\exp(-t)}{t^{n+1}}\,\mathrm{d}t.
\end{aligned}$$

We can now identify the asymptotic sequence as $\{\varphi_n\} = \{e^{-x}x^{-(n+1)}\}$ and $\{a_n\} = \{(-1)^n n!\}$. The corresponding sum

$$\sum_n^\infty \frac{e^{-x}}{x^{n+1}}(-1)^n n! \tag{6.42}$$

does not converge in any standard sense. For any fixed x the magnitude of the terms increases as n grows, which implies that this alternating sum diverges. However, it is asymptotic to $E_1(x)$. We can show this by computing (6.40) and showing, that the limit is zero

$$\lim_{|x|\to\infty} \frac{E_1(x) - \sum_n^N \frac{\mathrm{e}^{-x}}{x^{n+1}}(-1)^n n!}{\mathrm{e}^{-x}x^{-(N+1)}} = \lim_{|x|\to\infty} x^{n+2}\mathrm{e}^x(-1)^{n+1}(n+1)! \int_x^\infty \frac{\exp(-t)}{t^{n+1}}\,\mathrm{d}t > 0. \tag{6.43}$$

We can now use the fact that

$$\int_x^\infty \frac{\exp(-t)}{t^n}\,\mathrm{d}t < x^{-n}\int_x^\infty \exp(-t)\,\mathrm{d}t \tag{6.44}$$

to simplify our expression

$$\begin{aligned}\lim_{|x|\to\infty} \frac{E_1(x) - \sum_n^N \frac{\mathrm{e}^{-x}}{x^{n+1}}(-1)^n n!}{\mathrm{e}^{-x}x^{-(N+1)}} &< \lim_{|x|\to\infty} \cancel{e^x} x^{n+2}(-1)^{n+1}(n+1)! \underbrace{\int_x^\infty \exp(-t)\,\mathrm{d}t}_{\cancel{\mathrm{e}^{-x}}} \\ &= \lim_{|x|\to\infty} \frac{1}{x}(-1)^{n+1}(n+1)! = 0.\end{aligned} \tag{6.45}$$

That shows that the limit is sandwiched between zero on the lower bound (because all terms are positive) and zero for the last evaluation which proves, that the series is asymptotic.

7 Time independent perturbation theory cont.

7.1 Stark Effect

Consider a hydrogen atom in a uniform electric field $\boldsymbol{E} = E^z$ along the z-direction. The effect of the electric field on the hydrogen atom can be modelled by the inclusion of the potential $V = eEz$ as a perturbation in the Hamiltonian of the hydrogen atom. In order to compute the energy shifts caused by the presence of the electric field to the non-degenerate ground state $|100\rangle$ and the fourfold degenerate first excited states $|2lm\rangle$, one has to compute the matrix elements $\langle n'l'm'|z^2|nlm\rangle$ and $\langle n'l'm'|z|nlm\rangle$, respectively. According to the selection rules there are only three non-vanishing matrix elements: $\langle 100|z^2|100\rangle$, $\langle 200|z|210\rangle$ and $\langle 210|z|200\rangle$. Compute explicitly these matrix elements and show that the latter two are equal.
*(*Hint*: Because of spherical symmetry $\langle 100|z^2|100\rangle = \frac{1}{3}\langle 100|r^2|100\rangle$. In order to compute the matrix elements use the analytic expressions for the states $|100\rangle$, $|200\rangle$ and $|210\rangle$.)*

Solution: First we note the analytic expressions of the wave functions:

$$\begin{aligned}
\Psi_{100} &= \sqrt{\frac{4Z^3}{a_0^3}}\exp\left(-\frac{Zr}{a_0}\right)\sqrt{\frac{1}{4\pi}} \\
\Psi_{200} &= \sqrt{\frac{Z^3}{8a_0^3}}\left(-\frac{Zr}{a_0}+2\right)\exp\left(-\frac{Zr}{2a_0}\right)\sqrt{\frac{1}{4\pi}} \\
\Psi_{210} &= \sqrt{\frac{Z^3}{8a_0^3}}\left(\frac{Zr}{a_0}\right)\exp\left(-\frac{Zr}{2a_0}\right)\sqrt{\frac{1}{4\pi}}\cos\vartheta.
\end{aligned} \tag{7.1}$$

We start by calculating the first matrix element:

$$\begin{aligned}
\langle 100|z^2|100\rangle &= \int \Psi_{100}^* \underbrace{z^2}_{r^2\cos^2\vartheta} \Psi_{100}\,\mathrm{d}^3r \\
&\overset{Z=1}{=} \frac{1}{a_0^3\pi}\int \exp\left(-\frac{2r}{a_0}\right) r^2\cos^2\vartheta\, r^2\sin\vartheta\,\mathrm{d}r\,\mathrm{d}\vartheta\,\mathrm{d}\varphi \\
&= \frac{2\pi}{a_0^3\pi}\underbrace{\left[-\frac{1}{3}\cos^3\vartheta\right|_0^\pi}_{2/3}\int r^4\exp\left(-\frac{2r}{a_0}\right)\mathrm{d}r\,.
\end{aligned} \tag{7.2}$$

We can solve the radial integral by using the FEYNMANN integration rule:

$$\begin{aligned}
\int r^4\exp\left(-\frac{2r}{a_0}\right)\mathrm{d}r &= \left(\frac{a_0}{2}\right)^5\int u^4\mathrm{e}{-u}\,\mathrm{d}u = \left(\frac{a_0}{2}\right)^5\frac{\mathrm{d}^4}{\mathrm{d}\alpha^4}\underbrace{\int \mathrm{e}^{-u\alpha}\,\mathrm{d}u}_{=-1/\alpha}\Bigg|_{\alpha=1} \\
&= \frac{a_0^5}{32}\frac{\mathrm{d}^4}{\mathrm{d}\alpha^4}\left(-\frac{1}{\alpha}\right)\Bigg|_{\alpha=1} = \frac{a_0^5}{32}\frac{24}{\alpha^5}\Bigg|_{\alpha=1} = a_0^5\frac{3}{4} \\
\Rightarrow \langle 100|z^2|100\rangle &= a_0^2.
\end{aligned} \tag{7.3}$$

The two other matrix elements are matrix elements $\langle 200|z|210\rangle$ and $\langle 210|z|200\rangle$ are indeed equal, because the wavefunctions Ψ_{200} and Ψ_{210} are real:

$$\begin{aligned}
\langle 200|z|210\rangle &= \frac{1}{8a_0^3}\frac{1}{4\pi}\int\left(-\frac{r}{a_0}+2\right)\left(\frac{r}{a_0}\right)\exp\left(-\frac{r}{a_0}\right)\cos\vartheta\underbrace{z}_{r\cos\vartheta}\mathrm{d}^3r \\
&= \frac{1}{8a_0^3}\frac{1}{4\pi}\int\left(-\frac{r^2}{a_0^2}+\frac{2r}{a_0}\right)\exp\left(-\frac{r}{a_0}\right)r^3\underbrace{\cos^2\vartheta\sin\vartheta}_{\to 2/3}\mathrm{d}r\,\mathrm{d}\vartheta\,\mathrm{d}\varphi \\
&= \frac{\frac{4}{3}\pi}{8a_0^3\cdot 4\pi}\int\left(-\frac{r^5}{a_0^2}+\frac{2r^4}{a_0}\right)\exp\left(-\frac{r}{a_0}\right)\mathrm{d}r \qquad r=a_0\,u,\quad \mathrm{d}r=a_0\,\mathrm{d}u \\
&= \frac{a_0^4}{24a_0^3}\left(\int 2u^4\mathrm{e}^{-u}\,\mathrm{d}u-\int u^5\mathrm{e}^{-u}\,\mathrm{d}u\right) \\
&= \frac{a_0}{24}\Big(2\underbrace{\frac{\mathrm{d}^4}{\mathrm{d}\alpha^4}\left(-\frac{1}{\alpha}\right)\Big|_{\alpha=1}}_{=24}-\underbrace{\frac{\mathrm{d}^5}{\mathrm{d}\alpha^5}\left(-\frac{1}{\alpha}\right)\Big|_{\alpha=1}}_{=120}\Big) \\
&= -a_0\frac{72}{24}=-3a_0.
\end{aligned} \tag{7.4}$$

7.2 Spin-orbit correction for Hydrogen atom

The Hamiltonian for a hydrogen-like atom with a single electron reads

$$H_0=\frac{\boldsymbol{p}^2}{2m}-\frac{Ze^2}{r} \tag{7.5}$$

where Z is the atomic number and the potential term is the Coulomb potential. With this Hamiltonian, for any operator A the following relation holds

$$\langle nlm|\,[H_0,A]\,|nlm\rangle=0 \tag{7.6}$$

since H_0 acting to the right or left just gives $E_n^{(0)}$ (i. e. energy levels of the unperturbed Hamiltonian). Specify $A=p_r$, i. e. the radial component of the momentum operator and evaluate the commutator above, finding an expression for $\langle r^{-3}\rangle$.

Solution: In order to find an expression for $\langle r^{-3}\rangle$ we try to express the Hamiltonian for a fixed angular momentum l. For the quantum mechanical angular momentum $\hat{\boldsymbol{L}}=(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{p}})$ we find

$$\hat{\boldsymbol{L}}^2=r^2\hat{\boldsymbol{p}}^2-(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}})^2+\mathrm{i}\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}. \tag{7.7}$$

In spherical coordinates we have $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}=-\mathrm{i}\hbar\nabla=-\mathrm{i}\hbar r\partial_r$. Therefore we can find

$$\hat{\boldsymbol{p}}^2=\frac{\hat{\boldsymbol{L}}^2}{r^2}-\frac{\hbar^2}{r^2}[(r\partial_r)^2+r\partial_r]=\frac{\hat{\boldsymbol{L}}^2}{r^2}-\hbar^2\left[\partial_r^2+\frac{2}{r}\partial_r\right]. \tag{7.8}$$

We can express the last term as

$$-\hbar^2\left[\partial_r^2+\frac{2}{r}\partial_r\right]=(p_r)^2,\qquad p_r=-\mathrm{i}\hbar\frac{1}{r}\partial_r r. \tag{7.9}$$

Then we can rewrite the Hamiltonian as

$$H_0=\frac{p_r^2}{2m}+\frac{\hat{\boldsymbol{L}}^2}{2mr^2}-\frac{Ze^2}{r}=\frac{p_r^2}{2m}+\frac{\hbar^2 l(l+1)}{2mr^2}-\frac{Ze^2}{r}, \tag{7.10}$$

where we used the known eigenvalues of $\hat{\boldsymbol{L}}^2$. We can now calculate the commutator by applying it to a generic Ψ state.

$$[H_0,p_r]\Psi=\left[\frac{\hbar^2 l(l+1)}{2mr^2}-\frac{Ze^2}{r},p_r\right]\Psi=\left[\frac{\hbar^2 l(l+1)}{2mr^2},p_r\right]\Psi-\left[\frac{Ze^2}{r},p_r\right]\Psi. \tag{7.11}$$

We first compute

$$\begin{aligned}\left[\frac{\hbar^2 l(l+1)}{2mr^2},p_r\right]\Psi&=\frac{\hbar^2 l(l+1)}{2m}\left[\frac{1}{r^2},-\mathrm{i}\hbar\frac{1}{r}\partial_r r\right]\\&=\mathrm{i}\hbar\frac{\hbar^2 l(l+1)}{2m}\left(-\frac{1}{r^3}\partial_r(r\Psi)+\frac{1}{r}\partial_r\left(\frac{1}{r}\Psi\right)\right)\\&=\mathrm{i}\hbar\frac{\hbar^2 l(l+1)}{2m}\left(-\frac{1}{r^3}\Psi-\cancel{\frac{1}{r^2}\partial_r(\Psi)}-\frac{1}{r^3}\Psi+\cancel{\frac{1}{r^2}\partial_r(\Psi)}\right)\\&=-\mathrm{i}\hbar\frac{\hbar^2 l(l+1)}{mr^3}\Psi.\end{aligned} \tag{7.12}$$

Now we compute the second commutator

$$\begin{aligned}-\left[\frac{Ze^2}{r},p_r\right]\Psi&=Ze^2\mathrm{i}\hbar\left[\frac{1}{r},\frac{1}{r}\partial_r r\right]\\&=Ze^2\mathrm{i}\hbar\left(\frac{1}{r^2}\partial_r(r\Psi)-\frac{1}{r}\partial_r(\Psi)\right)\\&=Ze^2\mathrm{i}\hbar\left(\frac{1}{r^2}\Psi+\cancel{\frac{1}{r}\partial_r(\Psi)}-\cancel{\frac{1}{r}\partial_r(\Psi)}\right)\\&=\mathrm{i}\hbar\frac{Ze^2}{r^2}\Psi.\end{aligned} \tag{7.13}$$

Now we can combine the results to find the total commutator

$$[H_0,p_r]=\mathrm{i}\hbar\left(\frac{Ze^2}{r^2}-\frac{\hbar^2 l(l+1)}{mr^3}\right). \tag{7.14}$$

Now we can use (7.6) to find

$$\begin{aligned}0&=\mathrm{i}\hbar\left\langle nlm\middle|\frac{Ze^2}{r^2}-\frac{\hbar^2 l(l+1)}{mr^3}\middle|nlm\right\rangle\\\Rightarrow\left\langle\frac{Ze^2}{r^2}\right\rangle&=\left\langle\frac{\hbar^2 l(l+1)}{mr^3}\right\rangle\\\Rightarrow\left\langle r^{-3}\right\rangle&=\frac{mZe^2}{\hbar^2 l(l+1)}\left\langle r^{-2}\right\rangle=\frac{1}{a_0}\frac{1}{l(l+1)}\left\langle r^{-2}\right\rangle.\end{aligned} \tag{7.15}$$

7.3 2-state system

The Hamiltonian for a 2-state system can be written as

$$H = \begin{pmatrix} E_1^0 & \lambda\Delta \\ \lambda\Delta & E_2^0 \end{pmatrix}. \tag{7.16}$$

What are the eigenfunctions for the unperturbed problem, i e. $\lambda = 0$?

1. *Solve the $\lambda \neq 0$ problem exactly, in the eigenbasis of the unperturbed Hamiltonian, by calculating eigenvalues and eigenfunctions.*
2. *Now, in the above picture, treat the problem perturbatively, i. e. $|\lambda\Delta| \ll |E_1^0 - E_2^0|$. Calculate the energies up to second order, and compare with the exact solution.*
3. *Finally, let $E_1^0 \to E_2^0$. How should we now solve this problem? Find the first order perturbed eigenvalues. Compare once again to the exact solution.*

Solution: For the unperturbed problem, the energy eigenvalues are $E = E_1^0, E_2^0$ with the eigenfunctions $|E_1\rangle$ and $|E_2\rangle$. For the case $\lambda \neq 0$ we can calculate the eigenvalues by demanding

$$\det\begin{pmatrix} E_1^0 - E & \lambda\Delta \\ \lambda\Delta & E_2^0 - E \end{pmatrix} = (E_1^0 - E)(E_2 - E) - \lambda^2\Delta^2 \stackrel{!}{=} 0 \tag{7.17}$$

$$\Rightarrow E^2 - E(E_1^0 + E_2^0) + E_1 E_2 - \lambda^2\Delta^2 = 0. \tag{7.18}$$

We can solve this quadratic equation which yields

$$E = \frac{E_1 + E_2}{2} \pm \frac{1}{2}\sqrt{(E_1^0 - E_2^0)^2 + 4\lambda^2\Delta^2}. \tag{7.19}$$

In a perturbative approach we approximate the energy eigenvalues by using $\varepsilon = \frac{\lambda\Delta}{[E_1^0 - E_2^0]} \ll 1$. We use the expansion $\sqrt{1+x} \approx 1 + \frac{1}{2}x$ which leads to

$$\begin{aligned} E &= \frac{E_1 + E_2}{2} \pm \frac{1}{2}(E_1^0 - E_2^0)\sqrt{1 + 4\frac{\lambda^2\Delta^2}{E_1^0 - E_2^0}} \\ &= \frac{E_1 + E_2}{2} \pm \frac{1}{2}(E_1^0 - E_2^0)\sqrt{1 + 4\varepsilon^2} \\ &= \frac{E_1 + E_2}{2} \pm \frac{1}{2}(E_1^0 - E_2^0)\big(1 + 2\varepsilon^2 + \ldots\big). \end{aligned} \tag{7.20}$$

This leads to the energy modifications

$$E_+ = E_1 + (E_1 - E_2)\varepsilon^2 = E_1 + \frac{\lambda^2\Delta^2}{E_1 - E_2} \tag{7.21}$$

$$E_- = E_2 - (E_1 - E_2)\varepsilon^2 = E_1 - \frac{\lambda^2\Delta^2}{E_1 - E_2}. \tag{7.22}$$

7.4 Zeeman Effect (BONUS)

Consider a gas of excited particles immersed in a constant magnetic field. Its emission spectrum will be characterized by a multiplicity of lines such that each line, single in absence of the magnetic field, splits into more lines[4]*.When dealing with low-intensity magnetic*

fields, the lines appear to be very close to each other. This phenomenon is called Zeeman effect. Traditionally, one distinguished the Zeeman effect into two subcategories: the normal Zeeman effect, that could be interpreted even without recurring to quantum mechanics, and the "abnormal" effect, which instead required the introduction of the concept of spin.

Classically, the energy I radiated by a charged particle in motion over a unit of time can be computed from the dipole approximation as

$$I = \frac{2}{3}\frac{e^2}{c^3}\ddot{\boldsymbol{r}}^2. \tag{7.23}$$

In quantum mechanics the equation above is valid when considering mean values, hence $\ddot{\boldsymbol{r}} \to \langle\ddot{\boldsymbol{r}}\rangle$. The matric element of $\ddot{\boldsymbol{r}}$ between two generic stationary states $|nlm\rangle$ of the hydrogen state is given by

$$\left\langle n'l'm'|\ddot{\boldsymbol{r}}|nlm\right\rangle = -\omega_{n,n'}^2\left\langle n'l'm'|\boldsymbol{r}|nlm\right\rangle, \tag{7.24}$$

where $\omega_{n,n'} = \frac{E_n - E_{n'}}{\hbar}$. From the requirement $I \neq 0$ one finds that an atom can transition between two different energy levels $|nlm\rangle$ and $\left|n'l'm'\right\rangle$ only if $l' = l \pm 1$ and $m' = \pm 1$. Indeed, because of parity, transitions with $l' = l$ are not allowed. Moreover, since spin is conserved, when considering the spin quantum number m_s we find the rule $m_s' = m_s$. Now consider a hydrogen-like atom immersed in a magnetic field. Let us denote with H_0 the Hamiltonian in the absence of a magnetic field. If the atom has no spin, then the total Hamiltonian will be simply given by

$$H = H_0 + \frac{e}{2mc}\boldsymbol{B}\cdot\boldsymbol{L} = H_0 + \frac{e}{2mc}B\,L_z \tag{7.25}$$

where we assumed that the field B is directed along the z-axis.

- *Compute the energy spectrum of the atom and compare it to the energy spectrum you would obtain in absence of the field. How many distinct energy levels can you have for a fixed value of n? What is their separation?*
- *Discuss the possible transitions permitted by the rules you derived above.*

The fact, that H_0 and L_z commute, shows that both operators have the same eigenstates $|nlm\rangle$. We can calculate the new energy eigenstates by using the SCHRÖDINGER equation $H|\Psi\rangle = E|\Psi\rangle$:

$$\left(H_0 + \frac{e}{2m_e c}B\,L_z\right)|nlm\rangle = \left(H_0 + \frac{e}{2m_e c}B\,m\hbar\right)|nlm\rangle$$
$$E = E_n + \mu_B\,m\,B, \qquad \mu_B = \frac{e\hbar}{2m_e c}. \tag{7.26}$$

[4] A similar multiplication of lines is found when the gas is immersed in an external electric field. This effect is called Stark effect, c. f. Landau-Lifschitz, page 314 and following.

For a given n, we have $l = 0, \ldots, n-1$ and for each l, m varies between $-l$ and $+l$ which leads to $2l+1$ sub-states. The energy level E_n is therefore effectively divided in $2(n-1)+1 = 2n-1$ values. The energy separation Δ_m is $\Delta_m = \mu_B B m$. Instead of transmissions with $\Delta E = E_n - E_{n'}$ we now find transitions $\Delta E = (E_n + \Delta_m) - (E_{n'} + \Delta_{m'})$ with the condition $m' = m$ or $m' = m \pm 1$.

One of the critical empirical pieces of information that came from the study of the ZEEMAN *spectra is that also the levels corresponding to orbital angular momentum $l = 0$ can split. This "anomalous" level multiplication suggested that particles might have an intrinsic angular momentum, which has been interpreted as spin.*

- *To account for the contribution of spin in our Hamiltonian, write*

$$H = H_0 + \frac{e}{2m_e c} B(L_z + 2S_z) \tag{7.27}$$

  and repeat the two points above.

When we also consider spins without relativistic corrections, we can easily repeat the procedure by noting that the spin operator $\boldsymbol{S}$ acts in a different space from $\boldsymbol{L}$ and thus surely commutes with H. Then we can find eigenvalues of S_z as $\hbar m_s$ which leads to energies

$$E = E_n + \frac{e}{2m_e c} B\hbar(m + 2m_s). \tag{7.28}$$

For a fixed n, we will have as many energy levels as the values $m+2m_s$ can take on. From the addition of angular momenta we know that $-(l+2s) \leq m+2m_s \leq l+2s$ holds, meaning that we have $2l+4s+1$ different values if $l \neq 0$ and $2s+1$ values if $l = 0$. We find, that the energy separation is $\Delta = \mu_B B(m+2m_s)$. Since we have $m_s' = m_s$, there will be no difference from the emission lines obtained in the spinless case.

- *To account for relativistic effects we should also include in H_0 the spin-orbit interaction, which is proportional to a term $\boldsymbol{L}\cdot\boldsymbol{S}$. With this addition, the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is still a conserved quantity. Are the $\boldsymbol{L}$ and $\boldsymbol{S}$ vector components still conserved? And what about $\boldsymbol{L}^2$ and $\boldsymbol{S}^2$? From the considerations above, deduce that a good basis of eigenstates is given by the states $\{|l\, s\, j\, m_j\rangle\}$, where l, s, j, m_j are respectively quantum numbers of $\boldsymbol{L}^2, \boldsymbol{S}^2, \boldsymbol{J}^2, J_z$.*

We can see that the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is still conserved, as

$$\begin{aligned}
[\boldsymbol{L}\cdot\boldsymbol{S}, J_i] &= [\boldsymbol{L}\cdot\boldsymbol{S}, L_i + S_i] = [L_k S_k, L_i] + [L_k S_k, S_i] \\
&= [L_k, L_i] S_k + L_k \underbrace{[S_k, L_i]}_{=0} + L_k [S_k, S_i] + \underbrace{[L_k, S_i]}_{=0} S_k \\
&= [L_k, L_i] S_k + L_k [S_k, S_i] = \mathrm{i}\varepsilon_{kij} L_j S_k + \mathrm{i}\varepsilon_{kij} S_j L_k \\
&= \mathrm{i}\varepsilon_{kij} \underbrace{(L_j S_k + S_j L_k)}_{\text{symmetric}}.
\end{aligned} \tag{7.29}$$

With the same strategy we can show that L_i, S_i are not conserved. On the other hand, both $\boldsymbol{L}^2$ and $\boldsymbol{S}^2$ are conserved, since $[L_i, \boldsymbol{L}^2] = 0 = [S_i, \boldsymbol{S}^2]$

$$[\boldsymbol{L}\cdot\boldsymbol{S}, \boldsymbol{L}^2] = [L_k S_k, \boldsymbol{L}^2] = \underbrace{[L_k, \boldsymbol{L}^2]}_{=0} S_k + L_k \underbrace{[S_k, \boldsymbol{L}^2]}_{=0} = 0. \tag{7.30}$$

This suggests, that the good basis of eigenstates is indeed $\{|l\, s\, j\, m_j\rangle\}$.

- *prove that the first order modification induced by the presence of the magnetic field is given by*

$$\Delta E_J = B\left(\mu_B m_J + \frac{e}{2m_e c}\langle S_z\rangle\right). \tag{7.31}$$

  Hint*: Rewrite the Hamiltonian as*

$$H = H_0 + \frac{e}{2m_e c}B(J_z + S_z). \tag{7.32}$$

  This form highlights that the perturbation due to the magnetic field on the eigenstates of H_0 is given by the sum of two terms, one proportional to J_z and one to S_z. In principle, one should apply time-independent perturbation theory in the case of degenerate eigenstates. However, since the eigenstates of H_0 are also eigenstates of J_z and that J_z breaks the degeneracy, you can instead consider S_z as an ulterior perturbation of the non-degenerate states.

As already hinted in the task, we can simply use non-degenerate perturbation theory to compute the first energy correction. If we rewrite the Hamiltonian as in (7.32), we see that, because J_z commutes with H_0, it has the same eigenstates and thus eigenvalues $\hbar m_j$. If we apply non-degenerate perturbation theory we find

$$\begin{aligned}\Delta E &= \left\langle nlm|\frac{e}{2m_e c}B(J_z + S_z)|nlm\right\rangle \\ &= B\left(\mu_B m_j + \frac{e}{2m_e c}\langle S_z\rangle\right).\end{aligned} \tag{7.33}$$

Compute $\langle S_z\rangle$. From the expression $\Delta E_j = g\mu_B B m_j$ identify the Landè factor g. Proceed as follows:

- *Using that $[J_k, S_l] = \mathrm{i}\varepsilon_{klm}S_m$ prove that*

$$[J_-, S_+] = -2S_z, \qquad [J_+, S_+] = 0 \tag{7.34}$$

  with $J_\pm = J_x \pm \mathrm{i}J_y$ and $S_\pm = S_x \pm \mathrm{i}S_y$.

- *By evaluating the matrix element $\langle jls(m_j+1)|[J_+, S_+]|jls(m_j-1)\rangle$ prove that the matrix elements of J_+ and S_+ are proportional:*

$$\frac{\langle jls(m_j+1)|J_+|jlsm_j\rangle}{\langle jls(m_j+1)|S_+|jlsm_j\rangle} = \frac{\langle jlsm_j|J_+|jls(m_j-1)\rangle}{\langle jlsm_j|S_+|jls(m_j-1)\rangle} = \alpha. \tag{7.35}$$

  Use the completeness of the $|jlsm_j\rangle$ base.

- *Evaluate $\langle jlsm_j|[J_-S_+]|jlsm_j\rangle = \alpha m_j$.*

- *Evaluate the mean value of $\boldsymbol{J}\cdot\boldsymbol{S} = (\boldsymbol{J}^2 + \boldsymbol{S}^2 - \boldsymbol{L}^2)/2$ on the state $|jlsm_j\rangle$. Repeat the procedure, using $\boldsymbol{J}\cdot\boldsymbol{S} = (J_+S_- + J_-S_+)/2 + J_zS_z$. Compare the two results and find α*

At first we prove the commutation relations

$$\begin{aligned}[J_\pm, S_+] &= [J_x \pm \mathrm{i}J_y, S_x + \mathrm{i}S_y] = [L_x + S_x \pm \mathrm{i}(L_y + S_y), S_x + \mathrm{i}S_y] \\ &= [S_x, S_x + \mathrm{i}S_y] \pm \mathrm{i}[S_y, S_x + \mathrm{i}S_y] = \mathrm{i}[S_x, S_y] \mp \mathrm{i}[S_x, S_y] \\ &= \begin{cases} 0 & J_+ \\ -2S_z & J_- \end{cases}. \end{aligned} \tag{7.36}$$

Since $[J_+, S_+] = 0$ we can write

$$\begin{aligned} 0 &= \langle jls(m_j+1)|[J_+, S_+]|jls(m_j-1)\rangle \\ &= \langle jls(m_j+1)|J_+S_+|jls(m_j-1)\rangle - \langle jls(m_j+1)|S_+J_+|jls(m_j-1)\rangle \\ &= \langle jls(m_j+1)|J_+\left|jlsm_j\right\rangle\langle jlsm_j\left|S_+|jls(m_j-1)\right\rangle \\ &\quad - \langle jls(m_j+1)|S_+\left|jlsm_j\right\rangle\langle jlsm_j\left|J_+|jls(m_j-1)\right\rangle. \end{aligned} \tag{7.37}$$

This immediately yields (7.35). This implies that the matrix elements of J_+ are proportional to those of S_+, which helps us to evaluate

$$\begin{aligned} \langle jlsm_j|[J_-S_+]|jlsm_j\rangle &= \langle jlsm_j|J_-S_+|jlsm_j\rangle - \langle jlsm_j|J_+S_-|jlsm_j\rangle \\ &= \langle jlsm_j|J_-\left|jls(m_j+1)\right\rangle\langle jls(m_j+1)\left|S_+|jlsm_j\right\rangle. \end{aligned} \tag{7.38}$$

8 Time Dependent Perturbation Theory

8.1 Dirac (interaction) picture

Recall the "interaction" picture from your lectures in the context of a time dependent perturbation. Starting with a Hamiltonian given by

$$H(t) = H_0 + V(t), \quad V(0) = 0, \quad H_0 \neq H_0(t). \tag{8.1}$$

Sketch the time evolution of interaction kets $|\alpha, t\rangle_I = \exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)|\alpha, t\rangle$ *and interaction operators* $A_I(t) = \exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right) A(t) \exp\left(-\frac{\mathrm{i}H_0 t}{\hbar}\right)$.

Solution: First we try to express the time evolution of the interaction kets:

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial}{\partial t}|\alpha, t\rangle_I &= \mathrm{i}\hbar\frac{\partial}{\partial t}\left(\exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)|\alpha, t\rangle\right) \\
&= \mathrm{i}\cancel{\hbar}\exp\left(\frac{\mathrm{i}H_0 t}{\cancel{\hbar}}\right)\frac{\mathrm{i}H_0}{\hbar}|\alpha, t\rangle + \exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)\underbrace{H}_{H_0+V(t)}|\alpha, t\rangle \\
&= \exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)(-H_0 + H_0 + V(t))|\alpha, t\rangle \\
&= \underbrace{\exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)V(t)\exp\left(-\frac{\mathrm{i}H_0 t}{\hbar}\right)}_{V_I(t)}\underbrace{\exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)|\alpha, t\rangle}_{|\alpha,t\rangle_I} \\
\mathrm{i}\hbar\frac{\partial}{\partial t}|\alpha, t\rangle_I &= V_I(t)|\alpha, t\rangle_I .
\end{aligned} \tag{8.2}$$

In the second step we used the SCHRÖDINGER equation $\mathrm{i}\hbar\partial_t|\Psi\rangle = H|\Psi\rangle$. We can now also evaluate the time evolution of the operator $A_I(t)$ assuming, that $A(t)$ ist not explicitly time dependent:

$$\begin{aligned}
\frac{\mathrm{d}A}{\mathrm{d}t} &= \frac{\partial}{\partial t}\left(\exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)\right)A(t)\exp\left(-\frac{\mathrm{i}H_0 t}{\hbar}\right) + \exp\left(\frac{\mathrm{i}H_0 t}{\hbar}\right)A(t)\frac{\partial}{\partial t}\left(\exp\left(-\frac{\mathrm{i}H_0 t}{\hbar}\right)\right) \\
&= \frac{\mathrm{i}H_0}{\hbar}A_I(t) - A_I(t)\frac{\mathrm{i}H_0}{\hbar} \\
&= \frac{1}{\mathrm{i}\hbar}[A_I(t), H_0].
\end{aligned} \tag{8.3}$$

8.2 Spin-Magnetic Resonance

Consider a spin 1/2 system (e.g., a bound electron) subjected to a time independent uniform magnetic field in the z-direction and, in addition, to a time dependent magnetic field rotating in the x-y-plane:

$$\boldsymbol{B} = B_0\hat{\boldsymbol{z}} + B_1(\hat{\boldsymbol{x}}\cos(\omega t) + \hat{\boldsymbol{y}}\sin(\omega t)), \tag{8.4}$$

with B_0 and B_1 constant. Apply the solution of the two-state problem to this system. Identify the resonant frequency, and find the time separation between two different instants in which the probability of the system being entirely in the spin-up state is maximum.
Hint*: Recall that the Hamiltonian of this system is $H = \boldsymbol{\mu}\cdot\boldsymbol{B}$, with $\boldsymbol{\mu} = \frac{e}{m_e c}\boldsymbol{S}$. Write the S_i operators in their ket-bra form, i. e. as linear combinations of $\{|+\rangle\langle+|, |-\rangle\langle-|, |\pm\rangle\langle\mp|\}$.*

Solution: We start by writing down the components of the spin operator $\boldsymbol{S}$:

$$S_z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|), \qquad S_x = \frac{\hbar}{2}(|-\rangle\langle+| + |+\rangle\langle-|), \qquad S_y = \frac{\mathrm{i}\hbar}{2}(|-\rangle\langle+| - |+\rangle\langle-|).$$

We can now write the Hamiltonian as

$$\begin{aligned} H = \boldsymbol{\mu}\cdot\boldsymbol{B} &= \frac{e}{m_e c}\boldsymbol{S}\cdot\boldsymbol{B} \\ &= \frac{e}{m_e c}\big(S_z B_0 + B_1(S_x\cos(\omega t) + S_y\sin(\omega t))\big) \\ &= \frac{\hbar e}{2m_e c}\big[\underbrace{S_z B_0}_{H_0} + B_1\big((|-\rangle\langle+| + |+\rangle\langle-|)\cos(\omega t) + \mathrm{i}(|-\rangle\langle+| - |+\rangle\langle-|)\sin(\omega t)\big)\big] \\ &= \frac{\hbar e}{2m_e c}\big[H_0 + B_1\mathrm{e}^{\mathrm{i}\omega t}|-\rangle\langle+| + B_1\mathrm{e}^{-\mathrm{i}\omega t}|+\rangle\langle-|\big]. \end{aligned} \tag{8.5}$$

We can write the time dependent part of the Hamiltonian as a harmonic perturbation

$$V(t) = \hbar\gamma\big(\mathrm{e}^{\mathrm{i}\omega t}|-\rangle\langle+| + \mathrm{e}^{-\mathrm{i}\omega t}|+\rangle\langle-|\big), \qquad \text{with } \gamma = \frac{B_1 e}{2m_e c}. \tag{8.6}$$

We can identify the resonant frequency by finding the energy eigenvalues of H_0 for both states $|+\rangle$ and $|-\rangle$ which are $\pm\frac{e}{m_e c}B_0\frac{\hbar}{2}$:

$$\omega_\pm = \frac{1}{\hbar}\left(\frac{e}{m_e c}B_0\frac{\hbar}{2} + \frac{e}{m_e c}B_0\frac{\hbar}{2}\right) = \frac{eB_0}{m_e c}. \tag{8.7}$$

We can find the coefficients $c_n(t)$ for the time evoluted state by using

$$\mathrm{i}\hbar\dot{c}_n(t) = \sum_m \mathrm{e}^{\mathrm{i}\omega_{nm}t}V_{nm}c_m(t). \tag{8.8}$$

This leads to

$$\begin{aligned} \mathrm{i}\dot{c}_+ &= \mathrm{e}^{\mathrm{i}\omega_\pm t}\gamma\mathrm{e}^{-\mathrm{i}\omega t}c_- = \gamma\mathrm{e}^{\mathrm{i}(\omega_\pm-\omega)t}c_- \\ \mathrm{i}\dot{c}_- &= \gamma\mathrm{e}^{-\mathrm{i}(\omega_\pm-\omega)t}c_+. \end{aligned} \tag{8.9}$$

We can combine both differential equations into a single second order equation by differentiating:

$$-\ddot{c}_- = \gamma e^{-i(\omega_\pm-\omega)t}\underbrace{(i\dot{c}_+)}_{\gamma\exp(i(\omega_\pm-\omega)t)c_-} + \gamma(\omega_\pm-\omega)\underbrace{e^{-i(\omega_\pm-\omega)t}c_+}_{i/\gamma c_-}$$

$$\Rightarrow 0 = \ddot{c}_- + \gamma^2 c_- + i(\omega_\pm-\omega)\dot{c}_-. \tag{8.10}$$

If we choose the boundary conditions in such a way, that the system is in state $|+\rangle$ at $t=0$, so that $c_1(0)=1$ and $c_2(0)=0$ we find a solution to (8.10) as

$$c_-(t) = -i\frac{\gamma}{\Omega}e^{\frac{i}{2}(\omega-\omega_\pm)t}\sin(\Omega t), \quad \text{with } \Omega^2 = \gamma^2 + \frac{1}{4}(\omega-\omega_\pm)^2. \tag{8.11}$$

We now want to find two different instants in which the probability of the system being entirely in state $|+\rangle$ is maximum. This obviously occurs at $\omega=\omega_\pm$ because then Ω is minimized. The distance between those two instants is governed by the $\sin(\Omega t)$ term. For $\Omega=\gamma$ we find for the period of such an oscillation

$$\gamma\cdot T = 2\pi \quad \Rightarrow \quad T = \frac{2\pi}{\gamma} = \frac{4\pi m_e c}{B_1}. \tag{8.12}$$

8.3 Spin states in time

A composite system is made up of two spin $\frac{1}{2}$ objects. For $t < 0$, the Hamiltonian is independent on spin and can be considered 0 by properly adjusting the energy scale. For $t > 0$, instead, the Hamiltonian is

$$H = \left(\frac{4\Delta}{\hbar^2}\right)\boldsymbol{S}_1 \cdot \boldsymbol{S}_2. \tag{8.13}$$

The system is in $|+-\rangle$ for $t \leq 0$. Find the probability of finding the system in the states $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$ as a function of time:

1. *By solving the problem exactly.*
2. *By solving the problem using first-order time-dependent perturbation theory with H as a perturbation switched on at $t = 0$. Compare this solution with the previous point and state under which condition it is correct.*

1.) Solution: We start solving this problem by computing $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$ using the representations of S_x, S_y, S_z. We obtain the following expression

$$\begin{aligned}
\boldsymbol{S}_1\boldsymbol{S}_2 &= S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z} \\
&= \frac{\hbar^2}{4}\Big((|-\rangle\langle+| + |+\rangle\langle-|)_1(|-\rangle\langle+| + |+\rangle\langle-|)_2 + \mathrm{i}^2(|-\rangle\langle+| - |+\rangle\langle-|)_1(|-\rangle\langle+| - |+\rangle\langle-|)_2 \\
&\quad + (|+\rangle\langle+| - |-\rangle\langle-|)_1(|+\rangle\langle+| - |-\rangle\langle-|)_2\Big) \\
&= \frac{\hbar^2}{4}\Big(\cancel{|--\rangle\langle++|} + |-+\rangle\langle+-| + |+-\rangle\langle-+| + \cancel{|++\rangle\langle--|} \\
&\quad + \mathrm{i}^2(\cancel{|--\rangle\langle++|} - |-+\rangle\langle+-| - |+-\rangle\langle-+| + \cancel{|++\rangle\langle--|}) \\
&\quad + \ (|++\rangle\langle++| + |-+\rangle\langle-+| + |+-\rangle\langle+-| + |--\rangle\langle--|)\Big) \\
&= \frac{\hbar^2}{4}\Big(2|-+\rangle\langle+-| + 2|+-\rangle\langle-+| + |++\rangle\langle++| + |-+\rangle\langle-+| + |+-\rangle\langle+-| + |--\rangle\langle--|\Big).
\end{aligned}$$

We can rewrite the Hamiltonian now in matrix representation using $|1\rangle = |++\rangle, |2\rangle = |+-\rangle, |3\rangle = |-+\rangle, |4\rangle = |--\rangle$ as

$$H = \Delta\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{8.14}$$

The outer part of this matrix is already diagonalized, so we just concentrate on the inner part:

$$\det\begin{pmatrix} -1-\lambda & 2 \\ 2 & -1-\lambda \end{pmatrix} = (1+\lambda)^2 - 4 \stackrel{!}{=} 0. \tag{8.15}$$

This leads to the eigenvalues $\lambda = 1, -3$. We can calculate the corresponding eigenvectors simply by solving the eigenvalue equation

$$\lambda = 1: \qquad \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = 1 \begin{pmatrix} x \\ y \end{pmatrix}. \tag{8.16}$$

This leads to $-x + 2y = x$ which gives the solution $x = y$. We normalize the eigenvector $x^2 + y^2 = 1$ which results in $x = y = 1/\sqrt{2}$.

For $\lambda = -3$ we perform the same steps:

$$\lambda = -3: \qquad \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = -3 \begin{pmatrix} x \\ y \end{pmatrix}. \tag{8.17}$$

This results in $-x + 2y = -3x$ giving the solution $x = -y$. We choose x to be positive with the normalized value of $x = 1/\sqrt{2}$.

This result suggests a new basis with the following vectors

$$\begin{cases} |1\rangle = |{+}{+}\rangle & E = \Delta \\ |2\rangle = |{-}{-}\rangle & E = \Delta \\ |3\rangle = \dfrac{1}{\sqrt{2}}(|{+}{-}\rangle + |{-}{+}\rangle) & E = \Delta \\ |4\rangle = \dfrac{1}{\sqrt{2}}(|{+}{-}\rangle - |{-}{+}\rangle) & E = -3\Delta \end{cases} \tag{8.18}$$

We have now created a diagonalized and time independent Hamiltonian $H = \mathrm{diag}(1, 1, 1, -3)$. We time evolution is simply given by applying the time evolution operator

$$U(t, t_0 = 0) = \exp\left(-\mathrm{i}\frac{H\,t}{\hbar}\right), \quad |\alpha, t\rangle = U(t)\,|\alpha\rangle\,. \tag{8.19}$$

The probability of finding the system in the states given in the task is just $p = |\langle\beta|\alpha, t\rangle|^2$. For $|{+}{+}\rangle$ and $|{-}{-}\rangle$ we immediately obtain

$$p(|{+}{-}\rangle \to |{+}{+}\rangle) = 0 = p(|{+}{-}\rangle \to |{-}{-}\rangle), \tag{8.20}$$

because both states are orthogonal to $|{+}{-}\rangle$ and for time independent Hamiltonians, orthogonal states stay orthogonal under time evolution (intrinsic property of unitary transformations such as the time evolution operator).

In order to find the probability for the other two states we write $|{+}{-}\rangle$ in the new basis as $|{+}{-}\rangle = \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle)$. This leads to an expression for the time evoluted state $|\alpha, t\rangle$

$$\begin{aligned} |\alpha, t\rangle = U(t)\,|{+}{-}\rangle &= \frac{1}{\sqrt{2}}(|3\rangle + |4\rangle) \\ &= \frac{1}{\sqrt{2}}\left(\underbrace{\exp\left(-\mathrm{i}\frac{H\,t}{\hbar}\right)}_{H\to\Delta}|3\rangle + \underbrace{\exp\left(-\mathrm{i}\frac{H\,t}{\hbar}\right)}_{H\to-3\Delta}|4\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(\mathrm{e}^{-i\omega t}\,|3\rangle + \mathrm{e}^{\mathrm{i}\omega t}\,|4\rangle\right) \qquad (8.21) \\ &= \frac{1}{\sqrt{2}}\left[\left(\mathrm{e}^{-\mathrm{i}\omega t} + \mathrm{e}^{\mathrm{i}3\omega t}\right)|{+}{-}\rangle + (\mathrm{e}^{-\mathrm{i}\omega t} - \mathrm{e}^{\mathrm{i}3\omega t})\,|{-}{+}\rangle\right]. \qquad (8.22) \end{aligned}$$

Now we can calculate the probability

$$\begin{aligned} p = |\langle + - | \alpha, t\rangle|^2 &= \left|\frac{1}{2}(\langle 3| + \langle 4|)\left(\mathrm{e}^{-i\omega t}|3\rangle + \mathrm{e}^{\mathrm{i}\omega t}|4\rangle\right)\right|^2 \\ &= \left|\frac{1}{2}(\mathrm{e}^{-i\omega t} + \mathrm{e}^{\mathrm{i}\omega t})\right|^2 \\ &= \frac{1}{4}\left(\mathrm{e}^{-i\omega t}|3\rangle + \mathrm{e}^{\mathrm{i}\omega t}|4\rangle\right)\cdot\left(\mathrm{e}^{i\omega t}|3\rangle + \mathrm{e}^{-\mathrm{i}\omega t}|4\rangle\right) \\ &= \frac{1}{4}\left(2 + \mathrm{e}^{\mathrm{i}4\omega t} + \mathrm{e}^{-\mathrm{i}4\omega t}\right) \\ &= \frac{1}{2}[1 + \cos(4\omega t)]. \end{aligned} \tag{8.23}$$

Analogously we find

$$p = |\langle - + | \alpha, t\rangle|^2 = \frac{1}{2}[1 - \cos(4\omega t)]. \tag{8.24}$$

We can summarize this to

$$p = \begin{cases} 0 & |++\rangle, |--\rangle \\ \frac{1}{2}[1 + \cos(4\omega t)] \approx 1 - 4\omega^2 t^2 & |+-\rangle \\ \frac{1}{2}[1 - \cos(4\omega t)] \approx 4\omega^2 t^2 & |-+\rangle \end{cases} \tag{8.25}$$

2.) Solution: We now try to solve this problem perturbatively with H as a perturbation. We note that $H = H_0 + V = V$. Using the results from the lecture for zeroth and first order perturbation, we find that

$$c_n^{(0)} = \delta_{ni} \tag{8.26}$$

$$c_n^{(1)} = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}\omega_{ni}t'} V_{ni}(t'). \tag{8.27}$$

Because $H_0 = 0$ all energy the transition frequency $\omega_{ni} = 0$ is always zero. The perturbation matrix V is just (8.14) in the old basis.

The initial state is $|i\rangle = |+-\rangle \equiv |2\rangle$. We obtain the transition probability $p(i \to n)$ by

$$p(i \to n) = |c_n^{(0)}(t) + c_n^{(1)}(t)|^2. \tag{8.28}$$

Let us start with $|n\rangle = |++\rangle \equiv |1\rangle$ and $|n\rangle = |--\rangle \equiv |4\rangle$. The zeroth order is obivously zero because $i \neq n$. The first order can be calculated using (8.27). We note that $V_{12} = 0 = V_{42}$ and therefore the first order vanishes, too.

Lets move on to $|n\rangle = |+-\rangle$. We can calculate the first order as

$$c_n^{(1)} = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \underbrace{\mathrm{e}^{\mathrm{i}\omega_{ni}t'}}_{=1}\underbrace{V_{ni}(t')}_{=-\Delta} = \mathrm{i}\omega t, \quad \text{with } \omega = \frac{\Delta}{\hbar}. \tag{8.29}$$

Therefore the transition amplitude can be written as

$$p(|+-\rangle \to |+-\rangle) = |1 + \mathrm{i}\omega t|^2 = 1 - \omega^2 t^2. \tag{8.30}$$

The last calculation is for $|n\rangle = |-+\rangle$ which is in first order

$$c_n^{(1)} = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \underbrace{\mathrm{e}^{\mathrm{i}\omega_{ni}t'}}_{=1}\underbrace{V_{ni}(t')}_{=-2\Delta} = -\mathrm{i}2\omega t, \quad \text{with } \omega = \frac{\Delta}{\hbar}. \tag{8.31}$$

The transition amplitude is then

$$p(|+-\rangle \to |-+\rangle) = |-\mathrm{i}2\omega t|^2 = 4\omega^2 t^2. \tag{8.32}$$

We can summarize the results as

$$p = \begin{cases} 0 & |++\rangle, |--\rangle \\ 1-\omega^2 t^2 & |+-\rangle \\ 4\omega^2 t^2 & |-+\rangle \end{cases} \tag{8.33}$$

The reason why the solution for the $|+-\rangle$ state does not equal the approximation in (8.25), is that higher order perturbations also lead to more contributions of second order $\omega^2 t^2$.

The approximation is only valid for $\omega t \ll 1$.

9 Time Dependent Perturbation Theory cont.

9.1 Dipole Approximation

The validity of the dipole approximation

$$e^{i\frac{\omega}{c}\hat{\boldsymbol{n}}\boldsymbol{x}} = 1 + i\frac{\omega}{c}\hat{\boldsymbol{n}}\boldsymbol{x} + \dots \tag{9.1}$$

relies on the fact that the emission wavelength λ is much larger than the typical atomical dimension. Prove this by relying on scaling arguments.
Hint: *Consider an hydrogen-like atom: the radiation $\hbar\omega$ must be of the same order of magnitude of the atomic level spacing. Use that $R_{\text{atom}} \sim a_0/Z$ and the fine structure constant $\alpha = \frac{1}{137} = \frac{e^2}{c\hbar}$.*

Solution: We want to show that the wavelength of the typical radiation involved in emission and absorption processes is much larger than the typical atomic dimensions R_{atom}.

We start with the atomic level spacing in hydrogen. The energy levels are given by the following formula:

$$E_n = -\frac{1}{2}\frac{m_e e^4}{\hbar^2}\frac{1}{n^2} = -\frac{1}{2}m_e c^2\alpha^2\frac{1}{n^2}. \tag{9.2}$$

The typical atomic dimensions are of the order of the Bohr radius given as

$$R_{\text{atom}} \sim a_0 = \frac{\hbar^2}{m_e e^2} = \frac{\hbar}{m_e c\alpha}. \tag{9.3}$$

The dipole approximation is valid if $\frac{\omega}{c}\hat{\boldsymbol{n}}\boldsymbol{x} \ll 1$. If we identify $R_{\text{atom}} = \hat{\boldsymbol{n}}\boldsymbol{x}$, then we get for $n = 1$

$$\begin{aligned} \underbrace{\frac{\omega}{c}}_{E_n/(\hbar c)} R_{\text{atom}} &\ll 1 \\ \Rightarrow \frac{1}{2}m_e c^2\alpha^2\frac{1}{\hbar c}\cdot\frac{\hbar}{m_e c\alpha} &\ll 1 \\ \Rightarrow \frac{1}{2}\alpha \approx \frac{1}{274} &\ll 1 \end{aligned} \tag{9.4}$$

that the wavelength of the atomic levels is much larger than R_{atom}

$$\frac{\omega}{c}R_{\text{atom}} \ll 1 \Rightarrow 2\pi\frac{R_{\text{atom}}}{\lambda} \ll 1 \Rightarrow R_{\text{atom}} \ll \lambda. \tag{9.5}$$

9.2 Matrix elements of the position of the SHO

Derive the matrix elements $\langle n|x|n'\rangle$ of the position operator x for the simple harmonic oscillator.
Hint: *First express x in terms of the ladder operators, then use the action of the latter on the energy eigenstates $|n\rangle$ and the orthonormality of $|n\rangle$.)*

Solution: At first we identify the ladder operators that were already given in (1.2) as

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \mathrm{i}\frac{p}{m\omega}\right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \mathrm{i}\frac{p}{m\omega}\right). \tag{9.6}$$

We can easily see that the x operator can be obtained by the following combination of ladder operators:

$$x = \frac{1}{2}\sqrt{\frac{2\hbar}{m\omega}}(a + a^\dagger). \tag{9.7}$$

We also note the action of the ladder operators on the eigenstates $|n\rangle$ on the SHO

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \qquad a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{9.8}$$

We can now simply calculate the matrix element as follows

$$\begin{aligned}
\langle n|x|n'\rangle &= \frac{1}{2}\sqrt{\frac{2\hbar}{m\omega}}\left\langle n|a + a^\dagger|n'\right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\langle n|a|n'\rangle + \left\langle n|a^\dagger|n'\right\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\underbrace{\langle n|n'-1\rangle}_{\delta_{n,n'-1}} + \sqrt{n'+1}\underbrace{\langle n|n'+1\rangle}_{\delta_{n,n'+1}}\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\delta_{n,n'-1} + \sqrt{n'+1}\delta_{n,n'+1}\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta_{n,n'-1} + \sqrt{n}\delta_{n,n'+1}\right).
\end{aligned} \tag{9.9}$$

9.3 Radiation from a Harmonic Oscillator

Calculate the power emitted through spontaneous emission from a SHO. (Obviously the SHO has a mass m_e and carries an electric charge $e \neq 0$. Otherwise, the solution is trivial) Show that at the n-th level the mean power emitted is given by

$$P = \frac{2n\hbar e^2\omega^3}{3m_e c^3}. \tag{9.10}$$

Compare with the power emitted from a classical oscillator, and see the similarity, if there is any.
Hint: *You need to calculate the spontaneous transition rate from a final state f to a initial state i, w_{fi}^{spn}. You may make use of the "detailed balance principle" and the well known forms of the transition rates for absorption and stimulated emission induced by unpolarized isotropic radiation:*

$$\begin{aligned} R(i \to f)^{abs} &= \frac{4\pi^2}{3\hbar^2} d_{if}^2 \varrho(\omega_{fi}) \\ R(f \to i)^{stm} &= \frac{4\pi^2}{3\hbar^2} d_{if}^2 \varrho(\omega_{if}), \end{aligned} \tag{9.11}$$

where the matrix element of the dipole moment $\boldsymbol{d}_{if} = \langle f|\boldsymbol{d}|i\rangle$ and $\varrho(\omega_{fi})$ is the Blackbody spectrum at the emission/absorption frequency.

Solution: We start with the detailed balance principle that was given in the lecture:

$$\frac{R(i \to f)}{\varrho(\omega_{if})} = \frac{R(f \to i)}{\varrho(\omega_{fi})}. \tag{9.12}$$

This leads to $R(i \to f) = R(f \to i)$. We now assume a thermodynamical equilibrium. We note the rate of spontaneous emission as $\bar{R}(f \to i)$. We can then write

$$N_f(R(f \to i) + \bar{R}(f \to i)) = N_i R(f \to i). \tag{9.13}$$

We can now insert (9.11) and solve for the energy density $\varrho(\omega_{if})$

$$\begin{aligned} \Rightarrow R(f \to i) &= \frac{N_f}{N_i - N_f} \bar{R}(f \to i) \\ \Rightarrow \varrho(\omega_{if}) &= \frac{1}{d_{if}^2} \frac{3\hbar^2}{4\pi^2} \bar{R}(f \to i) \frac{1}{\frac{N_i}{N_f} - 1}. \end{aligned} \tag{9.14}$$

We can further assume that the population of the energy states follows a Boltzmann distribution, namely $N(E_n) = \exp\left(-\beta E_n\right)$ with $\beta = \frac{1}{k_B T}$. Then we can rewrite $\frac{N_i}{N_f} = \exp\left(-\beta(E_i - E_f)\right) = \exp\left(\beta\hbar\omega_{fi}\right)$. This leads to

$$\varrho(\omega_{fi}) = \frac{1}{d_{if}^2} \frac{3\hbar^2}{4\pi^2} \bar{R}(f \to i) \frac{1}{\exp\left(\beta\hbar\omega_{fi}\right) - 1}. \tag{9.15}$$

In the classical limit $\hbar \to 0$ we expect the energy density to correspond to the Rayleigh-Jeans law given as

$$\varrho(\omega_{fi}) = \frac{\omega_{fi}^2}{\pi^2 c^3} \frac{1}{\beta}. \tag{9.16}$$

For $\hbar \to 0$ we can approximate $\exp(\beta\hbar\omega_{fi}) = 1 + \beta\omega_{fi}$. Inserting (9.15) into (9.3) yields

$$\begin{aligned} \frac{\omega_{fi}^2}{\cancel{\pi^2} c^3} \frac{1}{\cancel{\beta}} &= \frac{1}{d_{if}^2} \frac{3\hbar^2}{4\cancel{\pi^2}} \bar{R}(f \to i) \frac{1}{\cancel{1} + \cancel{\beta}\hbar\omega_{fi} - \cancel{1}} \\ \Rightarrow \bar{R}(f \to i) &= \frac{4}{3} \frac{\omega_{fi}^3}{\hbar c^3} d_{if}^2. \end{aligned} \tag{9.17}$$

The expectation value of the dipole moment d_{fi} can be calculated using the result from Task 1. For $f = i + 1$ we can write the expectation value as

$$\begin{aligned} d_{fi} &= \langle f | ex | i \rangle = e \sqrt{\frac{\hbar}{2m\omega_{fi}}} \left(\sqrt{n+1} \underbrace{\delta_{n,n'-1}}_{=0} + \sqrt{n} \underbrace{\delta_{n,n'+1}}_{=1} \right) \\ d_{fi}^2 &= e^2 \frac{\hbar n}{2m\omega_{fi}}. \end{aligned} \tag{9.18}$$

We can insert this result into (9.17) giving

$$\bar{R}(f \to i) = \frac{4}{3} \frac{\omega_{fi}^3}{\cancel{\hbar} c^3} \cdot e^2 \frac{\cancel{\hbar} n}{2m\omega_{fi}} = \frac{2}{3} \frac{\omega_{fi}^2 e^2 n}{c^3 m_e}. \tag{9.19}$$

Now we can find the emitted power by stimulated emission as the product of the photon energy and the transition rate $\bar{R}(f \to i)$:

$$P = \hbar\omega_{fi} \bar{R}(f \to i) = \frac{2n\hbar e^2 \omega_{fi}^3}{3 m_e c^3}. \tag{9.20}$$

9.4 Time-dependent perturbed SHO

Consider a one-dimensional simple harmonic oscillator whose classical angular frequency is ω_0. For $t<0$ it is known to be in the ground state. For $t>0$ there is also a time-dependent potential

$$V(t) = F_0 x \cos(\omega t), \tag{9.21}$$

where F_0 is constant in both space and time. Obtain an expression for the expectation value $\langle x\rangle$ as a function of time using time-dependent perturbation theory to lowest nonvanishing order. Is this procedure valid for $\omega \approx \omega_0$?

$$\text{Hint: } \textit{You may use } \langle n'|x|n\rangle = \sqrt{\hbar/2m\omega_0}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}). \tag{9.22}$$

Solution: We use again the time dependent perturbation coefficients to obtain an expression for the time evoluted state $|n(t)\rangle$ by using that $|n(t=0)\rangle = |0\rangle$

$$c_n^{(0)} = \langle n|\mathbb{1}|0\rangle = \delta_{n0}. \tag{9.23}$$

The energy of a harmonic oscillator in the level n is given as $E_n = \hbar\omega_0\left(n+\frac{1}{2}\right)$.
The formula for the first order was given in the lecture as

$$\begin{aligned}
c_n^{(1)} &= -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau\, \langle n|V_I|0\rangle = -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau \left\langle n|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H_0\tau}F_0 x\cos(\omega\tau)\mathrm{e}^{\frac{-\mathrm{i}}{\hbar}H_0 t}|0\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(E_n-E_0)\tau}F_0\cos(\omega\tau)\,\langle n|x|0\rangle \overset{(9.22)}{=} -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_0 n\tau}F_0\cos(\omega\tau)\sqrt{\frac{n\hbar}{2m\omega_0}}\delta_{n,1} \\
c_1^{(1)} &= -\frac{1}{\sqrt{2m\hbar\omega_0}}F_0 \underbrace{\int_0^t \mathrm{d}\tau\, \frac{\mathrm{i}}{2}\mathrm{e}^{\mathrm{i}\omega_0\tau}\left(\mathrm{e}^{\mathrm{i}\omega\tau}+\mathrm{e}^{-\mathrm{i}\omega\tau}\right)}_{} \\
&= \frac{\mathrm{i}}{2}\int_0^t \mathrm{d}\tau\left(\mathrm{e}^{\mathrm{i}(\omega_0+\omega)\tau}+\mathrm{e}^{\mathrm{i}(\omega_0-\omega)\tau}\right) = \frac{\mathrm{i}}{2}\left[\frac{\mathrm{e}^{\mathrm{i}(\omega_0+\omega)\tau}}{\mathrm{i}(\omega_0+\omega)}+\frac{\mathrm{e}^{\mathrm{i}(\omega_0-\omega)\tau}}{\mathrm{i}(\omega_0-\omega)}\right]_0^t \\
&= \frac{1}{2}\left[\frac{\mathrm{e}^{\mathrm{i}(\omega_0+\omega)t}-1}{\mathrm{i}(\omega_0+\omega)}+\frac{\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}-1}{\mathrm{i}(\omega_0-\omega)}\right] \\
c_1^{(1)} &= -\frac{F_0}{2\sqrt{2m\hbar\omega_0}}\left[\frac{\mathrm{e}^{\mathrm{i}(\omega_0+\omega)t}-1}{\mathrm{i}(\omega_0+\omega)}+\frac{\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}-1}{\mathrm{i}(\omega_0-\omega)}\right].
\end{aligned} \tag{9.24}$$

Now we can express the state $|n(t)\rangle$ in the Schrödinger picture:

$$\begin{aligned}
|n(t)\rangle_S &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_0 t}|n(t)\rangle_I = \sum_n c_n(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_0 t}|n\rangle \\
&= \mathrm{e}^{-\frac{\mathrm{i}}{2}\omega_0 t}|0\rangle + \mathrm{e}^{-\mathrm{i}\frac{3}{2}\omega_0 t}c_1^{(1)}(t)\,|1\rangle\,.
\end{aligned} \tag{9.25}$$

Now, we can finally calculate the expectation value of x as

$$\begin{aligned}\langle x\rangle = \langle n(t)|x|n(t)\rangle &= \left(\langle 0|\,\mathrm{e}^{\frac{\mathrm{i}}{2}\omega_0 t} + \langle 1|\,\mathrm{e}^{\mathrm{i}\frac{3}{2}\omega_0 t} c_1^*\right) x\left(\mathrm{e}^{-\frac{\mathrm{i}}{2}\omega_0 t}|0\rangle + \mathrm{e}^{-\mathrm{i}\frac{3}{2}\omega_0 t} c_1^{(1)}(t)\,|1\rangle\right) \\ &= \mathrm{e}^{-\mathrm{i}\omega_0 t} c_1 \langle 0|x|1\rangle + \mathrm{e}^{\mathrm{i}\omega_0 t} c_1^* \langle 1|x|0\rangle = 2\,\mathrm{Re}\left[\mathrm{e}^{-\mathrm{i}\omega_0 t} c_1 \langle 0|x|1\rangle\right]. \end{aligned} \tag{9.26}$$

Again by using (9.22) we obtain $\langle 0|x|1\rangle = \sqrt{\frac{\hbar}{2m\omega}}$ which leads to

$$\begin{aligned}\langle x\rangle &= 2\sqrt{\frac{\hbar}{2m\omega}}\left[\mathrm{e}^{-\mathrm{i}\omega_0 t}\frac{-F_0}{2\sqrt{2m\hbar\omega_0}}\left(\frac{\mathrm{e}^{\mathrm{i}(\omega_0+\omega)t}-1}{\mathrm{i}(\omega_0+\omega)} + \frac{\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}-1}{\mathrm{i}(\omega_0-\omega)}\right)\right] \\ &= -\frac{F_0}{2m\omega_0}\,\mathrm{Re}\left[\frac{\mathrm{e}^{\mathrm{i}\omega t}-\mathrm{e}^{-\mathrm{i}\omega_0 t}}{\omega_0+\omega} + \frac{\mathrm{e}^{-\mathrm{i}\omega t}-\mathrm{e}^{\mathrm{i}\omega_0 t}}{\omega_0-\omega}\right] \\ &= -\frac{F_0}{2m\omega_0}\left[\frac{\cos(\omega t)-\cos(\omega_0 t)}{\omega_0+\omega} + \frac{\cos(\omega t)-\cos(\omega_0 t)}{\omega_0-\omega}\right] \\ &= -\frac{F_0}{2m\omega_0}\frac{(\cos(\omega t)-\cos(\omega_0 t))(\omega_0 - \cancel{\omega} + \omega_0 - \cancel{\omega})}{\omega_0^2-\omega^2} \\ &= -\frac{F_0}{m}\frac{\cos(\omega t)-\cos(\omega_0 t)}{\omega_0^2-\omega^2}. \end{aligned} \tag{9.27}$$

10 Scattering

10.1 Scattering at a potential barrier

Consider a one-dimensional potential barrier with $V \neq 0$ for $-a < x < a$. An incoming wave from the region I is moving to the right:

$$\Psi_k = \begin{cases} e^{ikx} + \rho(k)e^{-ikx}, & x < -a \\ \tau(k)e^{ikx}, & x > a \end{cases}, \tag{10.1}$$

where $k > 0$.

Calculate the solution at $t \to \pm\infty$ for the wave packet

$$\psi(x,t) = \int \phi(k)\Psi_k(x)e^{-\frac{i\hbar k^2}{2m}t}\,dk. \tag{10.2}$$

Use the stationary phase approximation for the integral and then take the limits to show that the final result is

$$\psi(x,t) = \sqrt{\frac{2\pi i m}{\hbar t}}e^{\frac{imx^2}{2\hbar t}} \begin{cases} \phi\left(\frac{mx}{\hbar t}\right), & t \to -\infty \\ \phi\left(-\frac{mx}{\hbar t}\right)\rho\left(-\frac{mx}{\hbar t}\right) + \phi\left(\frac{mx}{\hbar t}\right)\tau\left(\frac{mx}{\hbar t}\right), & t \to +\infty \end{cases} \tag{10.3}$$

where $k = \frac{mx}{\hbar t}$.

- *Interpret physically the result just found.*
- *Show that $|\rho|^2 + |\tau|^2 = 1$ and give a physical interpretation of this result.*
- *What are the velocities of the reflected and transmitted waves? Are they the same?*
- *Does this violate energy conservation? Why?*

Solution: We first want to explain the stationary phase approximation. As we want to apply the limit $t \to \pm\infty$, we see that the phase of the exponential term in the integral (10.2) is rapidly oscillating. The main idea is that only terms contribute to the integral, where the phase is stationary. So we want to expand the phase around the stationary point as a Taylor series and then perform the integration.

Lets first consider the case $t \to -\infty$. We note, that here our solution of the Schrödinger equation only consits of the plane wave of the free particle $\Psi_k = e^{ikx}$. The Integral (10.2) then becomes

$$\psi(x,t) = \int \phi(k)e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\,dk. \tag{10.4}$$

We can now try to find the stationary point of the phase by

$$\left.\frac{d\varphi}{dk}\right|_{k_0} \stackrel{!}{=} 0 \quad \Rightarrow \quad \frac{d\varphi}{dk} = x - \frac{\hbar k_0 t}{2m} \quad \Rightarrow \quad k_0 = \frac{mx}{\hbar t}. \tag{10.5}$$

Now we can expand the phase around k_0 which yields

$$\begin{aligned}\varphi(k) &= \left(k_0 x - \frac{\hbar k_0^2 t}{2m}\right) - \frac{1}{2}\frac{\hbar t}{m}(k-k_0)^2 \\ &= \frac{mx^2}{2\hbar t} - \frac{1}{2}\frac{\hbar t}{m}(k-k_0)^2. \end{aligned} \tag{10.6}$$

When t is relatively large, even a small difference $(k-k_0)$ will generate oscillations within the integral, leading to cancellations. We can therefore extend the integral limits to $\pm\infty$. We can also drag $\phi(k)$ out of the integral by using the fact, that the term inside the integral is practically zero everywhere except at $k = k_0$. Equation (10.4) the becomes

$$\begin{aligned}\psi(x,t) &= \int \phi(k) \mathrm{e}^{\mathrm{i}\left(\frac{mx^2}{2\hbar t} - \frac{1}{2}\frac{\hbar t}{m}(k-k_0)^2\right)} \mathrm{d}k \\ &= \mathrm{e}^{\mathrm{i}\frac{mx^2}{2\hbar t}} \phi(k_0) \int \mathrm{e}^{-\frac{\mathrm{i}}{2}\frac{\hbar t}{m}(k-k_0)^2)} \mathrm{d}k. \end{aligned} \tag{10.7}$$

The integral boils down to a Gaussian integral for which we know the solution

$$\int \mathrm{e}^{-ax^2} \mathrm{d}x = \sqrt{\frac{\pi}{a}}. \tag{10.8}$$

$$\psi(x,t) = \mathrm{e}^{\mathrm{i}\frac{mx^2}{2\hbar t}} \phi\left(\frac{mx}{\hbar t}\right) \sqrt{\frac{2\pi m}{\mathrm{i}\hbar t}}. \tag{10.9}$$

Now let us consider the second case $t \to +\infty$. Here, our solution of the Schrödinger equation consists only of the reflected and transmitted wave. Therefore the integral (10.2) is

$$\psi(x,t) = \int \phi(k)\rho(k) \mathrm{e}^{\mathrm{i}\left(-kx - \frac{\hbar k^2}{2m}t\right)} \mathrm{d}k + \int \phi(k)\tau(k) \mathrm{e}^{\mathrm{i}\left(kx - \frac{\hbar k^2}{2m}t\right)} \mathrm{d}k. \tag{10.10}$$

For the first part, the stationary point of the phase is at $k_0' = -\frac{mx}{\hbar t}$, whereas for the second part we have the same situation as in (10.5). This leads to

$$\begin{aligned}\psi(x,t) &= \mathrm{e}^{\mathrm{i}\frac{mx^2}{2\hbar t}} \left(\phi(k_0')\rho(k_0') \int \mathrm{e}^{-\frac{\mathrm{i}}{2}\frac{\hbar t}{m}(k-k_0)^2} \mathrm{d}k + \phi(k_0)\tau(k_0) \int \mathrm{e}^{-\frac{\mathrm{i}}{2}\frac{\hbar t}{m}(k-k_0)^2} \mathrm{d}k\right) \\ &= \mathrm{e}^{\mathrm{i}\frac{mx^2}{2\hbar t}} \sqrt{\frac{2\pi m}{\mathrm{i}\hbar t}} \left(\phi\left(-\frac{mx}{\hbar t}\right)\rho\left(-\frac{mx}{\hbar t}\right) + \phi\left(\frac{mx}{\hbar t}\right)\tau\left(\frac{mx}{\hbar t}\right)\right). \end{aligned} \tag{10.11}$$

We can show that $|\rho|^2 + |\tau|^2 = 1$ by using the fact, that for this time independent problem the total number of particles in the potential region

$$\int_{-a}^{a} \Psi^* \Psi \, \mathrm{d}x = \text{const.} \tag{10.12}$$

The continuity equation $\dot{\varrho} + \vec{\nabla} \cdot \boldsymbol{j} = 0$ tells us now, that the probability current entering the potential must leave the potential region again. This means that

$$j(x = -a) \stackrel{!}{=} j(x = a). \tag{10.13}$$

The probability current is defined as $\boldsymbol{j} = \frac{\hbar}{m}\mathrm{Im}(\Psi^*\vec{\boldsymbol{\nabla}}\Psi)$. For a plane wave $\mathrm{e}^{\mathrm{i}kx}$ this is

$$j_x = \frac{\hbar}{m}\mathrm{Im}(A^*\mathrm{e}^{-\mathrm{i}kx}\partial_x(A\mathrm{e}^{\mathrm{i}kx})) = \frac{\hbar k}{m}|A|^2. \tag{10.14}$$

For the wave in the region $x < -a : \Psi_{k1} = \mathrm{e}^{\mathrm{i}kx} + \rho(k)\mathrm{e}^{-\mathrm{i}kx}$ the total probability current entering the potential region is

$$j(x=-a) = \frac{\hbar k}{m}(|\mathrm{e}^{\mathrm{i}kx}|^2 - |\rho(k)\mathrm{e}^{-\mathrm{i}kx}|^2) = 1 - |\rho|^2. \tag{10.15}$$

The other wave $x > a : \Psi_{k2} = \tau(k)\mathrm{e}^{-\mathrm{i}kx}$ the current leaving the potential region is

$$j(x=a) = |\tau\mathrm{e}^{-\mathrm{i}kx}|^2 = |\tau|^2. \tag{10.16}$$

Therefore we can conclude

$$1 - |\rho|^2 = |\tau|^2 \quad \Rightarrow \quad |\rho|^2 + |\tau|^2 = 1. \tag{10.17}$$

10.2 S-matrix and transfer matrix

Compute the transfer matrix M and the scattering matrix S for the potential given by:

$$V(x) = \begin{cases} 0, & if\,|x| > a \\ V_0, & if\,|x| < a \end{cases}. \tag{10.18}$$

Describe their relation and properties.

Solution: For this rectangular potential we can write the solutions of the Schrödinger equation as

$$\Psi(x) = \begin{cases} A_1 e^{ikx} + A_1' e^{-ikx} & x < -a \\ A_2 e^{ik'x} + A_2' e^{-ik'x} & -a \le x \le a \\ A_3 e^{ikx} + A_3' e^{-ikx} & x > a \end{cases}. \tag{10.19}$$

Without loss of generality we can assume, that an incoming wave is coming from negative infinity ($A_3' = 0$) with an amplitude $A_1 = 1$.

Now we impose a $\mathscr{C}^1$ condition at the boundary of the potential:

11 Scattering continued

11.1 Differential Cross Section

The differential cross-section $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ is defined as the number of particles per unit time scattered into the solid angle, divided by the incoming particle flux and it quantifies the interaction of the incident flux of particle with the target. However, the differential cross-section can be also seen as the transition rate $R(i \to f) = \frac{2\pi}{\hbar}|T_{fi}|^2\delta(E_f - E_i)$ *integrated on the density of final states $n(E_f) = \frac{mk_f}{\hbar^2}\,\mathrm{d}\Omega$, divided by the incoming flux j_{in} and solid angle. Show the derivation of $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ in this case.*

Solution: Using the hints given in the task the differential cross section can be expressed as

$$\begin{aligned}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{1}{j_{\mathrm{in}}\,\mathrm{d}\Omega}\int R(i\to f)\,n(E_f)\,\mathrm{d}E_f \\ &= \frac{1}{j_{\mathrm{in}}\,\mathrm{d}\Omega}\int \frac{2\pi}{\hbar}|T_{fi}|^2\delta(E_f-E_i)\,n(E_f)\,\mathrm{d}E_f \\ &= \frac{1}{j_{\mathrm{in}}\cancel{\mathrm{d}\Omega}}\frac{2\pi}{\hbar}|T_{fi}|^2 n(E_i), \qquad n(E_i) = \frac{mk_i}{\hbar^2}\cancel{\mathrm{d}\Omega} \\ &= \frac{2\pi}{\hbar}\left(\frac{\hbar k_i}{m}\right)^{-1}\frac{mk_i}{\hbar^2}|T_{fi}|^2 = 2\pi\frac{m^2}{\hbar^4}|T_{fi}|^2. \end{aligned} \tag{11.1}$$

11.2 Scattering amplitude of the spherically symmetric potential

Consider the following symmetrical potential $V(r)$:

$$V(r) = \begin{cases} 0 & \text{if } r > a \\ V_0 & \text{if } r < a \end{cases}. \tag{11.2}$$

Prove that the scattering amplitude $f(\boldsymbol{k},\boldsymbol{k'})$ in the Born approximation is given by

$$f(\boldsymbol{k},\boldsymbol{k'}) = -\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\left[\frac{\sin(qa)}{qa} - \cos(qa)\right], \tag{11.3}$$

where $q = |\boldsymbol{k} - \boldsymbol{k'}|$.

Solution: The scattering amplitude is given in the lecture as

$$f(\boldsymbol{k},\boldsymbol{k'}) = -\frac{m}{2\pi\hbar^2}\left\langle k'|V|\Psi_+^{(k)}\right\rangle. \tag{11.4}$$

In the first Born approximation we can write $\left|\Psi_+^{(k)}\right\rangle$ as

$$\left|\Psi_+^{(k)}\right\rangle \approx (1 + GV + (GV)^2 + \ldots)\,|\Psi_0\rangle \approx |\Psi_0\rangle\,. \tag{11.5}$$

The input wave is assumed to be a plane wave $\langle x|\Psi_0\rangle = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}$ which leads to

$$\begin{aligned}
f(\boldsymbol{k},\boldsymbol{k'}) &= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x \left\langle k'|x\right\rangle \langle x|V|\Psi_0\rangle = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k'}\cdot\boldsymbol{x}} V(\boldsymbol{x}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \\
&= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3r\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}} V_0\, \Theta(a-r), \qquad \boldsymbol{q} = \boldsymbol{k}-\boldsymbol{k'} \propto \hat{\boldsymbol{e}}_z \\
&= -\frac{m}{2\pi\hbar^2}\int_0^{2\pi} \mathrm{d}\varphi \int_0^a \mathrm{d}r\, r^2 \int_0^{\pi} \mathrm{d}\vartheta \sin(\vartheta) \mathrm{e}^{\mathrm{i}|\boldsymbol{q}|r\cos\vartheta} V_0 \\
&= +\frac{m}{\hbar^2} V_0 \int_0^a \mathrm{d}r\, r^2 \int_1^{-1} \mathrm{d}cos(\vartheta)\, \mathrm{e}^{\mathrm{i}qr\cos(\vartheta)} \\
&= \frac{m}{\hbar^2} V_0 \int_0^a \mathrm{d}r\, \frac{r}{q} \underbrace{\frac{1}{\mathrm{i}}\left(\mathrm{e}^{-\mathrm{i}qr} - \mathrm{e}^{\mathrm{i}qr}\right)}_{2\sin(-qr)} = -\frac{m}{\hbar^2} V_0 \int_0^a \mathrm{d}r\, 2r\sin(qr) \\
&= -\frac{2mV_0}{\hbar^2 q}\left(\left[-\cos(qr)\frac{r}{q}\right]_0^a + \int_0^a \frac{1}{q}\cos(qr)\,\mathrm{d}r\right) \\
&= -\frac{2mV_0}{\hbar^2 q}\left(-\frac{a}{q}\cos(aq) + \frac{1}{q^2}\sin(aq)\right) \\
&= -\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\left[\frac{\sin(qa)}{qa} - \cos(qa)\right].
\end{aligned} \tag{11.6}$$

11.3 Radius of the ^{40}Ca nucleus

Estimate the radius of the ^{40}Ca nucleus from the data in Figure 1 (see below) and compare to that expected from the empirical value $\approx 1.4A^{1/3}$fm, where A is the nuclear mass number. Check the validity of using the first-order Born approximation for these data.

Solution: We start this task by noting that the differential cross-section $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ is connected to the scattering amplitude $f(\boldsymbol{k},\boldsymbol{k'})$ by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\boldsymbol{k},\boldsymbol{k'})|^2. \tag{11.7}$$

Here we can see, that the differential cross section vanishes when $f(\boldsymbol{k},\boldsymbol{k'})$ is zero. In theory we could observe, that the cross section will be zero for certain angles ϑ, however, due to diffraction we only observe minima in figure 1. As a first approximation we can model a nucleus by a constant potential for $r < R$ and zero elsewhere. This is the same potential as already discussed in the previous task. We can use the results to find the zero value of the

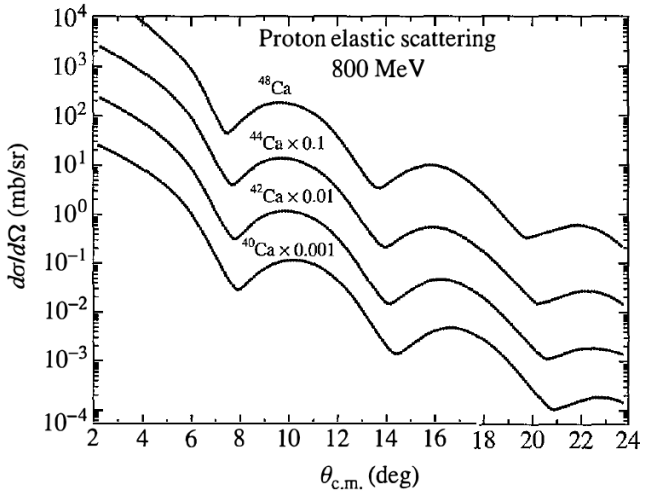


Fig. 1: Data on elastic scattering of protons from the nuclei of four different isotopes of calcium. The angles at which the cross sections show minima decrease consistently with increasing neutron number. Therefore, the radius of the calcium nucleus increases as more neutrons are added, as one expects. From L. Ray et al.,*Phys. Rev* (1980)

corresponding scattering amplitude $f(\boldsymbol{k},\boldsymbol{k'})$

$$f(\boldsymbol{k},\boldsymbol{k}') \overset{(11.6)}{=} -\frac{2m}{\hbar^2}\frac{V_0R^3}{(qR)^2}\left[\frac{\sin(qR)}{qR}-\cos(qR)\right] \overset{!}{=} 0$$
$$\Rightarrow \frac{1}{Rq}\sin(Rq)-\cos(Rq)=0$$
$$\Rightarrow x=\tan(x), \quad x=R\cdot q. \tag{11.8}$$

This is a transcendental equation which can only be solved numerically or graphically. We consider Wolfram|Alpha which gives the following results:

$$x_1=4.493, \quad x_2=7.725, \quad x_3=10.904. \tag{11.9}$$

We now try to find an expression for q. We assume elastic scattering as state in 1, which means $|\boldsymbol{k}|=|\boldsymbol{k'}|$. Using the cosine triangle theorem we find

$$q=|\boldsymbol{q}|=\sqrt{k^2+k'^2-2kk'\cos(\vartheta)}=k\sqrt{2-2\cos(\vartheta)}=2k\sin(\vartheta/2). \tag{11.10}$$

The term k can expressed in terms of proton energy as

$$k=\sqrt{\frac{2m_pE}{\hbar^2}}=6{,}187\cdot10^{16}\,\frac{1}{\mathrm{m}}. \tag{11.11}$$

We can use our results to calculate R

$$R=\frac{x}{q}=\frac{x}{2k\sin(\vartheta/2)}. \tag{11.12}$$

The results of this calculation are summarized in table 1. We can compare this result with the empirical value

$$R\approx1.4\cdot(40)^{1/3}=4{,}79\,\mathrm{fm}. \tag{11.13}$$

We can see, that the Born approximation in first order is indeed valid.

Table 1: Estimated radius of the ^{40}Ca nucleus from the data of figure 1.

	ϑ	R in fm
x_1	7,8°	5.34
x_2	14,4°	4.98
x_3	20,8°	4.88

11.4 Quantum Scattering Cross Section

Consider an arbitrary but localised potential $V(x)$. Recall from your lecture notes, that the formula for the scattering amplitude $f(\vartheta,\varphi) = -\frac{m}{2\pi\hbar^2}\langle k'|T|k\rangle$. The task is now to compute the scattering cross sections from these scattering amplitudes, by employing the "Born series" up to different orders. In the literature, this process is referred to as the "Born approximation".

1. *Find out an expression for $f(\vartheta,\varphi)$ in the first order Born approximation. Integrate the resulting expression of f^2 with respect to $\mathrm{d}\Omega$ over all solid angle $\mathrm{d}\Omega$, to find out the cross section σ. Express your answer as an integral expression.*
2. *Move over now to the second order Born approximation. Once again, find the expression of $f(\vartheta,\varphi)$. Find out an expression for σ using the Optical theorem.*

Compare your answers. Indication: In both cases, your final answer should be:

$$\sigma = \frac{m^2}{\pi\hbar^2}\iint \mathrm{d}^3x\,\mathrm{d}^3x'\,V(x)V(x')\frac{\sin^2(k|\boldsymbol{x}-\boldsymbol{x'}|)}{k^2|\boldsymbol{x}-\boldsymbol{x'}|^2}. \tag{11.14}$$

Solution: In order to compute the total scattering cross-section we first need to evaluate the scattering amplitude $f(k,k')$. As given in the task we have:

$$f(k,k') = \frac{m}{2\pi\hbar^2}\langle k|T|k'\rangle = \frac{m}{2\pi\hbar^2}\langle k|V|k'\rangle. \tag{11.15}$$

The last equality only holds for first order Born approximation

$$T = V + V\frac{1}{E-H_0+\mathrm{i}\varepsilon}V + \ldots. \tag{11.16}$$

with $T \approx V$. So then we obtain the cross-section by integration the square of the scattering ampltiude over the solid angle $\mathrm{d}\Omega_{\boldsymbol{k}'}$

$$\begin{aligned}
\sigma_k = \int \mathrm{d}\Omega_{\boldsymbol{k}'}\,|f(k,k')|^2 &= \left(\frac{m}{2\pi\hbar^2}\right)^2 \int \mathrm{d}\Omega_{k'}\,\langle k'|V|k\rangle\langle k|V|k'\rangle \\
&= \left(\frac{m}{2\pi\hbar^2}\right)^2 \int \mathrm{d}\Omega_{k'}\iint \mathrm{d}^3x\,\mathrm{d}^3x'\,\langle k'|V|x\rangle\langle x|k\rangle\langle k|V|x'\rangle\langle x'|k'\rangle \\
&= \left(\frac{m}{2\pi\hbar^2}\right)^2 \int \mathrm{d}\Omega_{k'}\iint \mathrm{d}^3x\,\mathrm{d}^3x'\,V(x)V(x')\langle k|x'\rangle\langle x|k\rangle\langle k'|x\rangle\langle x'|k'\rangle \\
&= \left(\frac{m}{2\pi\hbar^2}\right)^2 \iint \mathrm{d}^3x\,\mathrm{d}^3x'\,V(x)V(x')\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x'})}\int \mathrm{d}\Omega_{k'}\;\underbrace{\mathrm{e}^{\mathrm{i}\boldsymbol{k'}\cdot(\boldsymbol{x'}-\boldsymbol{x})}}_{4\pi\frac{\sin(k|\boldsymbol{x}-\boldsymbol{x'}|)}{k|\boldsymbol{x}-\boldsymbol{x'}|}}.
\end{aligned} \tag{11.17}$$

This is the cross-section for a given $\boldsymbol{k}$. So in order to obtain the total cross-section we integrate over all possible $\boldsymbol{k}$:

$$\sigma_{\text{total}} = \frac{1}{4\pi}\int \mathrm{d}^3k\,\sigma_{\boldsymbol{k}} = \frac{m^2}{\pi^2\hbar^4}\iint \mathrm{d}^3x\,\mathrm{d}^3x'\,V(x)V(x')\frac{\sin^2(k|\boldsymbol{x}-\boldsymbol{x'}|)}{k^2|\boldsymbol{x}-\boldsymbol{x'}|^2}. \tag{11.18}$$

For the second part we use the optical theorem to compute the total cross section:

$$\sigma_{\text{total}} = \frac{4\pi}{k}\operatorname{Im} f(k,k). \tag{11.19}$$

This is the special case $\boldsymbol{k} = \boldsymbol{k'}$ of forward scattering.

We can see that the first order Born approximation will give a zero, because $\operatorname{Im}(\langle k|V|k\rangle)$ is zero. For the second order instead we will have

$$\begin{aligned}
\sigma_{\text{total}} &= \frac{2m}{\hbar^2 k}\operatorname{Im}\left\langle k|V\frac{1}{E-H_o+\mathrm{i}\varepsilon}|k\right\rangle \\
&= \frac{2m}{\hbar^2 k}\operatorname{Im}\int \mathrm{d}^3x\int \mathrm{d}^3x'\,\langle k|V|x\rangle\underbrace{\left\langle x|\frac{1}{E-H_o+\mathrm{i}\varepsilon}|x'\right\rangle}_{\sim G_+(\boldsymbol{x},\boldsymbol{x'})}\langle x'|k\rangle \\
&= \frac{2m}{\hbar^2 k}\operatorname{Im}\int \mathrm{d}^3x\int \mathrm{d}^3x'\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x'})}V(x)V(x')\frac{2m}{\hbar^2}\quad \underbrace{G_+(\boldsymbol{x},\boldsymbol{x'})}_{-\frac{1}{4\pi}\frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{x}-\boldsymbol{x'}|}}{|\boldsymbol{x}-\boldsymbol{x'}|}} \\
&= \frac{m^2}{\pi\hbar^4}\int \mathrm{d}^3x\int \mathrm{d}^3x'\,V(x)V(x')\frac{\sin^2(k|\boldsymbol{x}-\boldsymbol{x'}|)}{k^2|\boldsymbol{x}-\boldsymbol{x'}|^2}.
\end{aligned}$$

12 Scattering continued

12.1 Born approximation

Calculate the differential cross sections in the Born approximation for scattering for the following potentials:

$$V_1(r) = V_0 \mathrm{e}^{-a^2 r^2}, \quad V_2(r) = V_0 \mathrm{e}^{-ar}. \tag{12.1}$$

Solution: In order to find the differential cross sections in the Born approximation we determine the scattering amplitude $f(k,k')$

$$\begin{aligned} f(\boldsymbol{k},\boldsymbol{k'}) &= -\frac{m}{2\pi\hbar^2}\langle k'|T|k\rangle \approx -\frac{m}{2\pi\hbar^2}\langle k'|V|k\rangle \\ &= -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k'}\cdot\boldsymbol{x}} V(r) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}} V(r) \\ &= -\frac{m}{\hbar^2}\int_0^\infty \mathrm{d}r \underbrace{\int_1^{-1} r^2\, \mathrm{d}(\cos\vartheta)\, \mathrm{e}^{\mathrm{i}qr\cos\vartheta}}_{=\frac{1}{\mathrm{i}qr}\left(\mathrm{e}^{-\mathrm{i}qr}-\mathrm{e}^{\mathrm{i}qr}\right)} V(r) \\ &= +\frac{2m}{q\hbar^2}\int_0^\infty r\sin(qr) V(r)\, \mathrm{d}r\,. \end{aligned} \tag{12.2}$$

Now we can insert the potentials $V_1(r)$ and $V_2(r)$. For the first integral we use Wolfram|Alpha and find:

$$f(\boldsymbol{k},\boldsymbol{k'}) = \frac{2mV_0}{q\hbar^2} \underbrace{\int_0^\infty r\sin(qr)\mathrm{e}^{-a^2r^2}\,\mathrm{d}r}_{\frac{\sqrt{\pi}q\exp\left(-q^2/(4a^2)\right)}{4a^3}} = \frac{mV_0}{2\hbar^2a^3}\sqrt{\pi}\exp\left(-\frac{q^2}{4a^2}\right). \tag{12.3}$$

The second integral can be computed rather straightforwardly. Lets work out the integral part first:

$$\begin{aligned} \int_0^\infty r\sin(qr)\mathrm{e}^{-ar}\,\mathrm{d}r &= \mathrm{Im}\left[\int_0^\infty r\mathrm{e}^{(\mathrm{i}q-a)r}\,\mathrm{d}r\right] \\ &= \mathrm{Im}\Big[\underbrace{\frac{1}{\mathrm{i}q-a} r\mathrm{e}^{(\mathrm{i}q-a)r}\Big|_0^\infty}_{=0} - \int_0^\infty \frac{1}{\mathrm{i}q-a}\mathrm{e}^{(\mathrm{i}q-a)r}\,\mathrm{d}r\Big] \\ &= \mathrm{Im}\left[\frac{1}{(a-\mathrm{i}q)^2}\left(-\mathrm{e}^{(\mathrm{i}q-a)r}\right)\Big|_0^\infty\right] \\ &= \mathrm{Im}\left[\frac{(a+\mathrm{i}q)^2}{(a^2+q^2)^2}\right] = \mathrm{Im}\left[\frac{a^2-q^2+2aq\mathrm{i}}{(a^2+q^2)^2}\right] = \frac{2aq}{(a^2+q^2)^2}. \end{aligned} \tag{12.4}$$

This leads to the scattering amplitude

$$f(\boldsymbol{k},\boldsymbol{k'}) = \frac{2m}{\hbar^2}\frac{V_0}{q}\int_0^\infty r\sin(qr)\mathrm{e}^{-ar}\,\mathrm{d}r = \frac{4maV_0}{\hbar^2}\frac{1}{(a^2+q^2)^2}. \tag{12.5}$$

Now we can find the cross sections by using

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\boldsymbol{k},\boldsymbol{k'})|^2 = \begin{cases} \dfrac{m^2V_0^2}{4\hbar^4a^6}\pi\exp\left(-\dfrac{q^2}{2a^2}\right) & V_1(r) \\ \dfrac{16m^2a^2V_0^2}{\hbar^4}\dfrac{1}{(a^2+q^2)^4} & V_2(r) \end{cases}. \tag{12.6}$$

12.2 Scattering Phase

Determine the scattering phases for scattering at the potential $V = A/r^2$ and calculate the differential cross section for $0 \le \mu A/\hbar^2 \ll 1$, where μ is the reduced mass appearing in the Schrödinger equation.
Hint: *In the radial Schrödinger equation for $U_l = r f_l$ set $u_l = \sqrt{r}g_l$. The differential equation for g_l should be familiar to you. You will probably meet a sum over Legendre polynomials. This can be simplified with the identity*

$$\sum_{l=0}^{\infty} P_l(\cos\theta) = \frac{1}{2\sin(\theta/2)}. \tag{12.7}$$

Solution: For spherically symmetric potentials we can make the ansatz $\Psi(r,\vartheta,\varphi) = R(r)Y_{lm}(\vartheta,\varphi)$. We can write the Schrödinger equation in spherical coordinates as

$$E\Psi(r,\vartheta,\varphi) = \left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\Psi(r,\vartheta,\varphi). \tag{12.8}$$

We can express the Laplace operator as

$$\Delta = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r} - \boldsymbol{L}^2\right)\right], \quad \text{with} \quad \boldsymbol{L}^2Y_{lm}(\vartheta,\varphi) = l(l+1)Y_{lm}(\vartheta,\varphi). \tag{12.9}$$

Therefore we obtain (the spherical harmonics can be divided on both sides)

$$\begin{aligned} ER(r) &= \left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r} - l(l+1)\right)\right] + V(r)\right]R(r) \\ \Rightarrow \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) &- \frac{l(l+1)}{r^2}R(r) + \frac{2m}{\hbar^2}[E - V(r)]R(r) = 0. \end{aligned} \tag{12.10}$$

Now using $u_l = rR$ and $k^2 = \frac{2m}{\hbar^2}E$ we find the radial Schrödinger equation

$$\frac{\mathrm{d}^2u_l}{\mathrm{d}r^2} + \left(k^2 - \frac{2m}{\hbar^2}V - \frac{l(l+1)}{r^2}\right)u_l = 0. \tag{12.11}$$

Now we use the hint given in the task $u_l = \sqrt{r} g_l$ and insert the potential $V = A/r^2$

$$\frac{\mathrm{d}^2(\sqrt{r} g_l)}{\mathrm{d}r^2} + \left(k^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right) \sqrt{r} g_l = 0. \tag{12.12}$$

Using

$$\frac{1}{\sqrt{r}} \frac{\mathrm{d}^2(\sqrt{r} g_l)}{\mathrm{d}r^2} = -\frac{g_l}{4r^2} + \frac{1}{r} \frac{\mathrm{d}g_l}{\mathrm{d}r} + \frac{\mathrm{d}^2 g_l}{\mathrm{d}r^2} \tag{12.13}$$

we can find

$$\begin{aligned} \frac{\mathrm{d}^2 g_l}{\mathrm{d}r^2} + \frac{1}{r} \frac{\mathrm{d}g_l}{\mathrm{d}r} + \left(k^2 - \frac{1}{4r^2} - \frac{2mA}{\hbar^2 r^2} - \frac{l(l+1)}{r^2} \right) g_l = 0 \\ r^2 \frac{\mathrm{d}^2 g_l}{\mathrm{d}r^2} + r \frac{\mathrm{d}g_l}{\mathrm{d}r} + \left(r^2 k^2 - \left(\frac{1}{4} + \frac{2mA}{\hbar} + l(l+1) \right) \right) g_l = 0. \end{aligned} \tag{12.14}$$

This result looks rather similar to the Bessel differential equation

$$x^2 \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + x \frac{\mathrm{d}f}{\mathrm{d}x} + (x^2 - a^2) f = 0. \tag{12.15}$$

12.3 Ensembles of $\frac{1}{2}$ spin systems

1. *Consider a pure ensemble of identically prepared spin $\frac{1}{2}$ systems. Suppose the expectation values $\langle S_x \rangle$ and $\langle S_z \rangle$ and the sign of $\langle S_y \rangle$ are known. Show how we may determine the state vector. Why is it unnecessary to know the magnitude of $\langle S_y \rangle$?*
2. *Consider a mixed ensemble of spin $\frac{1}{2}$ systems. Suppose the ensemble averages $[S_x]$, $[S_y]$ and $[S_z]$ are all known. Show how we may construct the 2×2 density matrix that characterizes the ensemble.*

1.) Solution: A pure ensemble consists only of spin 1/2 systems that are in the same state. A generic state $|\alpha\rangle$ can be described using two angles α, β

$$|\alpha\rangle = \cos\frac{\beta}{2} |+\rangle + \mathrm{e}^{\mathrm{i}\alpha} \sin\frac{\beta}{2} |-\rangle . \tag{12.16}$$

We can now look at the expectation value $\langle S_x \rangle$ using the Pauli two-component formalism

$$\begin{aligned} \langle S_x \rangle = \langle \alpha | S_x | \alpha \rangle &= \left(\langle + | \cos\frac{\beta}{2} + \langle - | \mathrm{e}^{-\mathrm{i}\alpha} \sin\frac{\beta}{2} \right) S_x \left(\cos\frac{\beta}{2} |+\rangle + \mathrm{e}^{\mathrm{i}\alpha} \sin\frac{\beta}{2} |-\rangle \right) \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos\frac{\beta}{2} & \mathrm{e}^{-\mathrm{i}\alpha} \sin\frac{\beta}{2} \end{pmatrix} \sigma_x \begin{pmatrix} \cos\frac{\beta}{2} \\ \mathrm{e}^{\mathrm{i}\alpha} \sin\frac{\beta}{2} \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos\frac{\beta}{2} & \mathrm{e}^{-\mathrm{i}\alpha} \sin\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\frac{\beta}{2} \\ \mathrm{e}^{\mathrm{i}\alpha} \sin\frac{\beta}{2} \end{pmatrix} \\ &= \frac{\hbar}{2} \underbrace{\left(\mathrm{e}^{\mathrm{i}\alpha} + \mathrm{e}^{-\mathrm{i}\alpha} \right)}_{2\cos\alpha} \underbrace{\cos\frac{\beta}{2} \sin\frac{\beta}{2}}_{\frac{1}{2}\sin(\beta)} = \frac{\hbar}{2} \cos\alpha \sin\beta. \end{aligned} \tag{12.17}$$

Analogously we find

$$\begin{aligned}\langle S_y\rangle &= \frac{\hbar}{2}\begin{pmatrix}\cos\frac{\beta}{2} & \mathrm{e}^{-\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\sigma_y\begin{pmatrix}\cos\frac{\beta}{2}\\ \mathrm{e}^{\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\\ &= \frac{\hbar}{2}\begin{pmatrix}\cos\frac{\beta}{2} & \mathrm{e}^{-\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\beta}{2}\\ \mathrm{e}^{\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\\ &= \frac{\hbar}{2}\underbrace{\mathrm{i}\left(-\mathrm{e}^{\mathrm{i}\alpha}+\mathrm{e}^{-\mathrm{i}\alpha}\right)}_{2\sin\alpha}\underbrace{\cos\frac{\beta}{2}\sin\frac{\beta}{2}}_{\frac{1}{2}\sin(\beta)} = \frac{\hbar}{2}\sin\alpha\sin\beta.\end{aligned} \tag{12.18}$$

$$\begin{aligned}\langle S_z\rangle &= \frac{\hbar}{2}\begin{pmatrix}\cos\frac{\beta}{2} & \mathrm{e}^{-\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\sigma_z\begin{pmatrix}\cos\frac{\beta}{2}\\ \mathrm{e}^{\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\\ &= \frac{\hbar}{2}\begin{pmatrix}\cos\frac{\beta}{2} & \mathrm{e}^{-\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}1 & 0\\ -1 & 0\end{pmatrix}\begin{pmatrix}\cos\frac{\beta}{2}\\ \mathrm{e}^{\mathrm{i}\alpha}\sin\frac{\beta}{2}\end{pmatrix}\\ &= \frac{\hbar}{2}\left(\cos^2\frac{\beta}{2}-\sin^2\frac{\beta}{2}\right) = \frac{\hbar}{2}\cos\beta.\end{aligned} \tag{12.19}$$

From the expectation value $\langle S_z\rangle$ we can directly read off

$$\beta = \frac{2}{\hbar}\arccos\langle S_z\rangle. \tag{12.20}$$

Now we can combine $\langle S_x\rangle$ and $\langle S_z\rangle$ to find

$$\begin{aligned}\cos^2\alpha &= \frac{\cos^2\alpha\sin^2\beta}{1-\cos^2\beta} = \frac{4}{\hbar^2}\frac{\langle S_x\rangle^2}{1-\frac{4}{\hbar^2}\langle S_z\rangle^2}\\ \Rightarrow \alpha &= \arccos\left(\pm\sqrt{\frac{\langle S_x\rangle^2}{\frac{\hbar^2}{4}-\langle S_z\rangle^2}}\right).\end{aligned} \tag{12.21}$$

There is a sign ambiguity between α and $\pi-\alpha$ which can be resolved by the sign of $\langle S_y\rangle$.

2.) Solution: We can relate the average expectation values $[S_i]$ to the density operator by

$$[S_i] = \mathrm{Tr}(\rho S_i). \tag{12.22}$$

Therefore we can calculate the average expectation values for a generic density matrix to find its components

$$\begin{aligned}[S_x] &= \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix}a & b\\ c & d\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right] = \frac{\hbar}{2}\mathrm{Tr}\begin{pmatrix}b & a\\ d & c\end{pmatrix} = \frac{\hbar}{2}(b+c)\\ [S_y] &= \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix}a & b\\ c & d\end{pmatrix}\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}\right] = \frac{\mathrm{i}\hbar}{2}\mathrm{Tr}\begin{pmatrix}b & -a\\ d & -c\end{pmatrix} = \frac{\mathrm{i}\hbar}{2}(b-c)\\ [S_z] &= \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix}a & b\\ c & d\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right] = \frac{\hbar}{2}\mathrm{Tr}\begin{pmatrix}a & -b\\ c & -d\end{pmatrix} = \frac{\hbar}{2}(a-d).\end{aligned} \tag{12.23}$$

We also demand, that the trace of the density matrix is one, therefore $a+d=1$.

Using these conditions we can easily determine a and d

$$[S_z] = \frac{\hbar}{2}(2a-1) = \frac{\hbar}{2}(1-2d)$$
$$\Rightarrow a = \frac{1}{2}\left(\frac{2}{\hbar}[S_z]+1\right) \quad d = -\frac{1}{2}\left(\frac{2}{\hbar}[S_z]-1\right). \tag{12.24}$$

Combining $[S_x]$ and $[S_y]$ we can find

$$b = \frac{1}{\hbar}\big([S_x]-\mathrm{i}[S_y]\big) \quad c = \frac{1}{\hbar}\big([S_x]+\mathrm{i}[S_y]\big). \tag{12.25}$$

12.4 Mixed Ensembles

The density matrix is defined as

$$\rho = \sum_i w_i \left|\alpha^i\right\rangle\left\langle\alpha^i\right|. \tag{12.26}$$

If $w_i = 1$ for a given i and 0 elsewhere, then the ensmble is said to be a pure ensemble. Consider a mixed ensemble of spin $\frac{1}{2}$ systems, containing 75 % of S_z^+ systems and 25 % S_x^+. Calculate the resulting ρ and the ensemble average expectation value $[\boldsymbol{S}]$. Consider now that the S_z systems are replaced by systems with $\boldsymbol{S}\cdot\hat{n}(+)$, where $\hat{n} = \cos\theta\,\hat{\boldsymbol{y}} + \sin\theta\,\hat{\boldsymbol{z}}$. Calculate the ensemble average values now.

Solution: The states of the two systems of the ensemble are

$$\left|\alpha^1\right\rangle = |+\rangle, \qquad \left|\alpha^2\right\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle). \tag{12.27}$$

Using (12.26) we can calculate the density matrix as

$$\begin{aligned}\rho &= \frac{3}{4}|+\rangle\langle+| + \frac{1}{4}\left(\frac{1}{\sqrt{2}}(|+\rangle+|-\rangle)\right)\left(\frac{1}{\sqrt{2}}(\langle+|+\langle-|)\right)\\ &= \frac{3}{4}|+\rangle\langle+| + \frac{1}{8}(|+\rangle\langle+| + |+\rangle\langle-| + |+\rangle\langle-| + |-\rangle\langle-|)\\ &= \frac{3}{4}\begin{pmatrix}1&0\\0&0\end{pmatrix} + \frac{1}{8}\begin{pmatrix}1&1\\1&1\end{pmatrix} = \frac{1}{8}\begin{pmatrix}7&1\\1&1\end{pmatrix}.\end{aligned} \tag{12.28}$$

Now we want to compute the ensemble average expectation values. We can use $[S_i] = \mathrm{Tr}(\rho S_i)$

$$\begin{aligned}[S_x] &= \frac{\hbar}{2}\frac{1}{8}\mathrm{Tr}\left[\begin{pmatrix}7&1\\1&1\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\right] = \frac{\hbar}{16}\mathrm{Tr}\begin{pmatrix}1&7\\1&1\end{pmatrix} = \frac{\hbar}{8}\\ [S_y] &= \frac{\hbar}{2}\frac{1}{8}\mathrm{Tr}\left[\begin{pmatrix}7&1\\1&1\end{pmatrix}\begin{pmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{pmatrix}\right] = \frac{\mathrm{i}\hbar}{16}\mathrm{Tr}\begin{pmatrix}1&-7\\1&-1\end{pmatrix} = 0\\ [S_z] &= \frac{\hbar}{2}\frac{1}{8}\mathrm{Tr}\left[\begin{pmatrix}7&1\\1&1\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right] = \frac{\hbar}{16}\mathrm{Tr}\begin{pmatrix}7&-1\\1&-1\end{pmatrix} = \frac{3\hbar}{8}.\end{aligned} \tag{12.29}$$

Therefore we can conclude that $[\boldsymbol{S}]$ is

$$[\boldsymbol{S}] = \begin{pmatrix}[S_x]\\ [S_y]\\ [S_z]\end{pmatrix} = \frac{\hbar}{8}\begin{pmatrix}1\\0\\3\end{pmatrix}. \tag{12.30}$$

Now we consider the case

$$S_z^+ \to \boldsymbol{S}\cdot\hat{n}(+) = S_y^+\cos\theta + S_z^+\sin\theta. \tag{12.31}$$

We can write this new state in the S_z basis as follows using $\left|S_y^+\right\rangle = \frac{1}{\sqrt{2}}(|+\rangle + \mathrm{i}|-\rangle)$

$$S_y^+\cos\theta + S_z^+\sin\theta = \frac{\cos\theta}{\sqrt{2}}\begin{pmatrix}1\\ \mathrm{i}\end{pmatrix} + \begin{pmatrix}\sin\theta\\ 0\end{pmatrix} = \begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta\\ \frac{\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix}. \tag{12.32}$$

We can now use the formula for the average expectation value

$$\begin{aligned}
[S_x] &= \sum_i w_i \langle S_x\rangle_i = \frac{3}{4}\langle \boldsymbol{S}\cdot\hat{n}|S_x|\boldsymbol{S}\cdot\hat{n}\rangle + \frac{1}{4}\underbrace{\left\langle S_x^+|S_x|S_x^+\right\rangle}_{\hbar/2}\\
&= \underbrace{\frac{3}{4}\begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta & \frac{-\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta\\ \frac{\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix}}_{=0} + \frac{\hbar}{8} = \frac{\hbar}{8}. \qquad (12.33)\\
[S_y] &= \frac{3\mathrm{i}}{4}\frac{\hbar}{2}\begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta & \frac{-\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}0&-1\\1&0\end{pmatrix}\begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta\\ \frac{\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix} + \frac{1}{4}\underbrace{\left\langle S_x^+|S_y|S_x^+\right\rangle}_{=0}\\
&= \frac{3\hbar}{8}\cos\theta\Big(\cos\theta + \sqrt{2}\sin\theta\Big) \qquad (12.34)\\
[S_z] &= \frac{3}{4}\frac{\hbar}{2}\begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta & \frac{-\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}\frac{\cos\theta}{\sqrt{2}} + \sin\theta\\ \frac{\mathrm{i}\cos\theta}{\sqrt{2}}\end{pmatrix} + \frac{1}{4}\underbrace{\left\langle S_x^+|S_z|S_x^+\right\rangle}_{=0}\\
&= \frac{3\hbar}{8}\left(\left(\frac{\cos\theta}{\sqrt{2}} + \sin\theta\right)^2 - \frac{\cos^2\theta}{2}\right) = \frac{3\hbar}{8}\sin\theta\Big(\sin\theta + \sqrt{2}\cos\theta\Big). \qquad (12.35)
\end{aligned}$$

$$\Rightarrow [\boldsymbol{S}] = \begin{pmatrix}[S_x]\\ [S_y]\\ [S_z]\end{pmatrix} = \frac{\hbar}{8}\begin{pmatrix}1\\ \cos\theta\big(\cos\theta + \sqrt{2}\sin\theta\big)\\ \sin\theta\big(\sin\theta + \sqrt{2}\cos\theta\big)\end{pmatrix}. \tag{12.36}$$

12.5 Density matrix and maximum entropy (Bonus)

The density matrix of a completely random ensemble is of the form

$$\rho = \frac{1}{N}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{12.37}$$

in any representation. This is due to the fact that all the base states with respect to which the density matrix is written are equally populated. The Von Neumann entropy σ can be defined as

$$\sigma = -Tr(\rho \ln \rho) = -\sum_{k=1}^{N} \rho_{kk} \ln \rho_{kk} \tag{12.38}$$

where the last equality follows if we use the basis in which ρ is diagonal.

- *Prove that for a completely random ensemble $\sigma = \ln N$.*
- *Prove that, subject to the normalization condition $Tr\rho = 1$, the maximum value for σ is $\sigma_{max} = \ln N$.*
  Hint: *use the method of Lagrange multipliers to impose the constraint on the trace of ρ.*

Solution: First we want to calculate the entropy σ for a completely random ensemble. Using the form (12.37) we find

$$\sigma = -\sum_{k=1}^{N} \underbrace{\rho_{kk}}_{1/N} \ln \underbrace{\rho_{kk}}_{1/N} = -\underbrace{\sum_{k=1}^{N} \frac{1}{N}}_{=1} \ln \frac{1}{N} = -\ln \frac{1}{N} = \ln N. \tag{12.39}$$

The second proof requires a bit more work. We now want to maximize σ, keeping the normalization of ρ. As given in the hint we apply the method of Lagrange multipliers:

$$\tilde{\sigma}(\rho) = \sigma(\rho) + \gamma\left[\left(\sum_k \rho_{kk}\right) - 1\right] = \sum_k \rho_{kk} \ln \rho_{kk} + \gamma\left[\left(\sum_k \rho_{kk}\right) - 1\right], \tag{12.40}$$

where γ is the Lagrange multiplier. Now we can impose $\delta\tilde{\sigma}(\rho) = 0$

$$\begin{aligned} \delta\tilde{\sigma}(\rho) &= \sum_k \left(\delta\rho_{kk} \ln \rho_{kk} + \rho_{kk} \frac{1}{\rho_{kk}} \delta\rho_{kk}\right) + \gamma \sum_k \delta\rho_{kk} \\ &= \sum_k \delta\rho_{kk} (\ln \rho_{kk} + 1 + \gamma) = 0. \end{aligned} \tag{12.41}$$

This condition is satisfied, if for any $\delta\rho_{kk}$

$$\ln \rho_{kk} + 1 + \gamma = 0 \quad \Rightarrow \quad \rho_{kk} = \mathrm{e}^{-(1+\gamma)} \tag{12.42}$$

holds. We can now fix the value of γ by using the normalization constraint:

$$\sum_{k=1}^{N} \mathrm{e}^{-(\gamma+1)} = 1 \quad \Rightarrow \gamma = -\left(\ln \frac{1}{N} + 1\right). \tag{12.43}$$

With this we find that the entropy is maximum when the density matrix is a random ensemble with $\rho_{kk} = 1/N$.

13 Many body systems

13.1 Identical particle time-evolution

Explain why an initially completely symmetric or anti-symmetric wave function describing a system of identical particles remains symmetric or anti-symmetric at later times.

Solution: If the initial state vector is symmetric or anti-symmetric it fulfills the following relation:

$$P_{ij}\left|\psi_{\pm}(t_0)\right\rangle = \pm\left|\psi_{\pm}(t_0)\right\rangle, \tag{13.1}$$

where P_{ij} is the transposition operator. For identical particles the Hamiltonian is completely symmetric and therefore commutes with all possible permutations. In particular this implies, that the transposition operator commutes also with the time evolution operator $U(t,t_0) = \exp(-\mathrm{i}/\hbar H_0(t-t_0))$ such that

$$\begin{aligned} P_{ij}\left|\psi_{\pm}(t)\right\rangle &= P_{ij}U(t,t_0)\left|\psi_{\pm}(t_0)\right\rangle \\ &= U(t,t_0)P_{ij}\left|\psi_{\pm}(t_0)\right\rangle = \pm U(t,t_0)\left|\psi_{\pm}(t_0)\right\rangle = \pm\left|\psi_{\pm}(t)\right\rangle. \end{aligned} \tag{13.2}$$

This proves that $\left|\psi_{\pm}(t)\right\rangle$ inherits the anti-symmetry from $\left|\psi_{\pm}(t_0)\right\rangle$.

13.2 Polarization states

We model the phase of a photon as a two-level system (q-bit) whose Hilbert space is spanned by a orthonormal basis of two states: $|1\rangle$ and $|2\rangle$. They correspond, for instance, to two orthogonal linear polarizations with observable polarization operators:

$$P_1 = |1\rangle\langle 1|, \quad P_2 = |2\rangle\langle 2|. \tag{13.3}$$

1. *Provide an example of a normalized pure state for which the expectation value of both P_1 and P_2 equals $1/2$, and a two-by-two matrix representation of the corresponding density-matrix operator in the given basis.*
2. *Find the density matrix for the most general normalized pure state with the properties specified in the previous task.*
3. *The state with partial polarization has the general representation*

   $$\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{\xi}\cdot\boldsymbol{\sigma}), \tag{13.4}$$

   where $\mathbb{1}$ is the 2×2 identity matrix, $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$ is the vector of Pauli matrices, and $\xi \in \boldsymbol{R}^3$. For which $\boldsymbol{\xi}$ is this state a pure state?
4. *For which $\boldsymbol{\xi}$ is $\langle P_1\rangle = 1$? For which $\boldsymbol{\xi}$ is $\langle P_2\rangle = 1$?*
5. *Define the states with circular polarizations:*

   $$|\pm\rangle = \frac{1}{2}(|1\rangle \pm \mathrm{i}|2\rangle). \tag{13.5}$$

   For which $\boldsymbol{\xi}$ is $\langle P_+\rangle = 1$? For which $\boldsymbol{\xi}$ is $\langle P_-\rangle = 1$?

Solution: The generic wavefunction for a two-level system can be written as

$$\left|\psi\right\rangle = c_1 \left|1\right\rangle + c_2 \left|2\right\rangle \quad \text{with} \quad |c_1|^2 + |c_2|^2 = 1. \tag{13.6}$$

The density operator of this system looks like

$$\begin{aligned}\rho = \sum_i w_i \left|\alpha_i\right\rangle \left\langle\alpha_i\right| &= \left|\psi\right\rangle \left\langle\psi\right| \\ &= (c_1 \left|1\right\rangle + c_2 \left|2\right\rangle)(\left\langle 1\right| c_1^* + \left\langle 2\right| c_2^*) \\ &= |c_1|^2 \left|1\right\rangle \left\langle 1\right| + c_2 c_1^* \left|2\right\rangle \left\langle 1\right| + c_2^* c_1 \left|1\right\rangle \left\langle 2\right| + |c_2|^2 \left|2\right\rangle \left\langle 2\right| \\ &= \begin{pmatrix} |c_1|^2 & c_2^* c_1 \\ c_2 c_1^* & |c_2|^2 \end{pmatrix}. \end{aligned} \tag{13.7}$$

The expectation values of P_1 and P_2 can be calculated by using their matrix representation

$$P_1 = \left|1\right\rangle \left\langle 1\right| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P_2 = \left|2\right\rangle \left\langle 2\right| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{13.8}$$

We can calculate the expectation values using $\mathrm{Tr}(\rho \cdot P_i)$

$$\langle P_1 \rangle = \mathrm{Tr}(\rho P_1) = \mathrm{Tr}\begin{pmatrix} |c_1|^2 & 0 \\ 0 & 0 \end{pmatrix} = |c_1|^2 = \frac{1}{2} \Rightarrow c_1 = \frac{1}{\sqrt{2}} \mathrm{e}^{\mathrm{i}\alpha_1} \tag{13.9}$$

$$\langle P_2 \rangle = \mathrm{Tr}(\rho P_2) = \mathrm{Tr}\begin{pmatrix} 0 & 0 \\ 0 & |c_2|^2 \end{pmatrix} = |c_2|^2 = \frac{1}{2} \Rightarrow c_2 = \frac{1}{\sqrt{2}} \mathrm{e}^{\mathrm{i}\alpha_2}. \tag{13.10}$$

The most general normalized pure state looks like

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & \mathrm{e}^{\mathrm{i}(\alpha_1 - \alpha_2)} \\ \mathrm{e}^{\mathrm{i}(\alpha_2 - \alpha_1)} & 1 \end{pmatrix}. \tag{13.11}$$

In order to determine the vectors $\boldsymbol{\xi}$ for which the state (13.4) is a pure state we simply need to demand that $\rho = \rho^2$

$$\rho^2 = \frac{1}{4}(\mathbb{1} + \boldsymbol{\xi}\cdot\boldsymbol{\sigma})(\mathbb{1} + \boldsymbol{\xi}\cdot\boldsymbol{\sigma}) = \frac{1}{4}(\mathbb{1} + 2\cancel{\boldsymbol{\xi}\cdot\boldsymbol{\sigma}} + \boldsymbol{\xi}\cdot\boldsymbol{\sigma}\boldsymbol{\xi}\cdot\boldsymbol{\sigma}) \stackrel{!}{=} \frac{1}{2}(\mathbb{1} + \cancel{\boldsymbol{\xi}\cdot\boldsymbol{\sigma}}). \tag{13.12}$$

We therefore find the condition

$$\begin{aligned}\mathbb{1} = \boldsymbol{\xi}\cdot\boldsymbol{\sigma}\boldsymbol{\xi}\cdot\boldsymbol{\sigma} &= (\xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3)^2 \\ &= \begin{pmatrix} \xi_3 & \xi_1 - \mathrm{i}\xi_2 \\ \xi_1 + \mathrm{i}\xi_2 & -\xi_3 \end{pmatrix}\begin{pmatrix} \xi_3 & \xi_1 - \mathrm{i}\xi_2 \\ \xi_1 + \mathrm{i}\xi_2 & -\xi_3 \end{pmatrix} = \begin{pmatrix} \xi_1^2 + \xi_2^3 + \xi_3^2 & 0 \\ 0 & \xi_1^2 + \xi_2^3 + \xi_3^2 \end{pmatrix}. \end{aligned} \tag{13.13}$$

We find the condition $\xi_1^2 + \xi_2^3 + \xi_3^2 = 1$ meaning that $\boldsymbol{\xi}$ must be normalized.

In order to find for which $\boldsymbol{\xi}$ the expectation value of P_1 or P_2 is one, we just take the trace

$$\langle P_1 \rangle = \mathrm{Tr}(\rho P_1) = \frac{1}{2}(1 + \xi_3) \stackrel{!}{=} 1 \quad \Rightarrow \quad \xi_3 = 1 \tag{13.14}$$

$$\langle P_2 \rangle = \mathrm{Tr}(\rho P_2) = \frac{1}{2}(1 - \xi_3) \stackrel{!}{=} 1 \quad \Rightarrow \quad \xi_3 = -1. \tag{13.15}$$

In the last task we want to find all vectors $\boldsymbol{\xi}$ for which $\langle P_\pm \rangle = 1$ holds. First we determine the matrix representations of $P_\pm$

$$\begin{aligned} |\pm\rangle\langle\pm| &= \frac{1}{2}(|1\rangle \pm \mathrm{i}|2\rangle)(\langle 1| \mp \mathrm{i}\langle 2|) \\ &= \frac{1}{2}(|1\rangle\langle 1| \pm \mathrm{i}|2\rangle\langle 1| \mp \mathrm{i}|1\rangle\langle 2| + |2\rangle\langle 2|) \\ P_\pm &= \frac{1}{2}\begin{pmatrix} 1 & \mp\mathrm{i} \\ \pm\mathrm{i} & 1 \end{pmatrix}. \end{aligned} \tag{13.16}$$

Now we calculate the expectation value

$$\begin{aligned} \langle P_\pm \rangle = \mathrm{Tr}(\rho P_\pm) &= \frac{1}{4}\mathrm{Tr}\begin{pmatrix} 1+\xi_3 & \xi_1 - \mathrm{i}\xi_2 \\ \xi_1 + \mathrm{i}\xi_2 & 1-\xi_3 \end{pmatrix}\begin{pmatrix} 1 & \mp\mathrm{i} \\ \pm\mathrm{i} & 1 \end{pmatrix} \\ &= \frac{1}{4}\mathrm{Tr}\begin{pmatrix} 1+\xi_3 \pm \mathrm{i}\xi_1 \pm x_2 & \cdots \\ \cdots & \mp\mathrm{i}\xi_1 \pm \xi_2 + 1 - \xi_3 \end{pmatrix} = \frac{1}{2}(1 \pm \xi_2) \stackrel{!}{=} 1 \\ \Rightarrow \xi_2 &= \pm 1. \end{aligned} \tag{13.17}$$

13.3 Identical particles addition of angular momentum

It is well known that if we have 2 non-identical spin 1 particles with no orbital angular momentum, then we can have $j = 2, 1, 0$. Discuss what happens if the particles now are identical.

Solution: For two 2 particles we can find the states of total angular momentum by using the Clebsch-Gordan coefficients already calculated in section 5.3. We print again the results:

$m = 0$	$j = 2$	$j = 1$	$j = 0$
$m_1 = 1, m_2 = -1$	$1/\sqrt{6}$	$1/\sqrt{2}$	$1/\sqrt{3}$
$m_1 = 0, m_2 = 0$	$\sqrt{2}/\sqrt{3}$	0	$-1/\sqrt{3}$
$m_1 = -1, m_2 = 1$	$1/\sqrt{6}$	$-1/\sqrt{2}$	$1/\sqrt{3}$

$m = 1$	$j = 2$	$j = 1$
$m_1 = 1, m_2 = 0$	$1/\sqrt{2}$	$1/\sqrt{2}$
$m_1 = 0, m_2 = 1$	$1/\sqrt{2}$	$-1/\sqrt{2}$

Because of the spin statistic theorem, spin 1 particles are considered to be bosons. Therefore their wavefunction must be symmetric under particle exchange $j_{1z} \leftrightarrow j_{2z}$. So the states with $j = 1$ will not survive, as they are antisymmetric unter the exchange, e. g.

$$\frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle) = -\frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle). \tag{13.18}$$