Peeter Joot
peeterjoot@protonmail.com

L_y perturbation

Q: L_y perturbation. [1] pr. 5.17 Find the first non-zero energy shift for the perturbed Hamiltonian

$$\begin{aligned} H &= A\mathbf{L}^2 + BL_z + CL_y \\ &= H_0 + V. \end{aligned} \tag{1.1}$$

A: The energy eigenvalues for state $|l, m\rangle$ prior to perturbation are

$$A\hbar^2 l(l+1) + B\hbar m. \tag{1.2}$$

The first order energy shift is zero

$$\begin{aligned} \Delta^1 &= \langle l, m| CL_y |l, m\rangle \\ &= \frac{C}{2i} \langle l, m| (L_+ - L_-) |l, m\rangle \\ &= 0, \end{aligned} \tag{1.3}$$

so we need the second order shift. Assuming no degeneracy to start, the perturbed state is

$$|l, m\rangle' = {\sum}' \frac{|l', m'\rangle \langle l', m'|}{E_{l,m} - E_{l',m'}} V |l, m\rangle, \tag{1.4}$$

and the next order energy shift is

$$\begin{aligned}
\Delta^2 &= \langle lm| V {\sum}' \frac{|l',m'\rangle \langle l',m'|}{E_{l,m} - E_{l',m'}} V |l,m\rangle \\
&= {\sum}' \frac{\langle l,m| V |l',m'\rangle \langle l',m'|}{E_{l,m} - E_{l',m'}} V |l,m\rangle \\
&= {\sum}' \frac{|\langle l',m'| V |l,m\rangle|^2}{E_{l,m} - E_{l',m'}} \\
&= \sum_{m' \neq m} \frac{|\langle l,m'| V |l,m\rangle|^2}{E_{l,m} - E_{l,m'}} \\
&= \sum_{m' \neq m} \frac{|\langle l,m'| V |l,m\rangle|^2}{\left(A\hbar^2 l(l+1) + B\hbar m\right) - \left(A\hbar^2 l(l+1) + B\hbar m'\right)} \\
&= \frac{1}{B\hbar} \sum_{m' \neq m} \frac{|\langle l,m'| V |l,m\rangle|^2}{m - m'}.
\end{aligned} \tag{1.5}$$

The sum over l' was eliminated because V only changes the m of any state $|l,m\rangle$, so the matrix element $\langle l',m'| V |l,m\rangle$ must includes a $\delta_{l',l}$ factor. Since we are now summing over $m' \neq m$, some of the matrix elements in the numerator should now be non-zero, unlike the case when the zero first order energy shift was calculated in eq. (1.3).

$$\begin{aligned}
\langle l,m'| CL_y |l,m\rangle &= \frac{C}{2i} \langle l,m'| (L_+ - L_-) |l,m\rangle \\
&= \frac{C}{2i} \langle l,m'| (L_+ |l,m\rangle - L_- |l,m\rangle) \\
&= \frac{C\hbar}{2i} \langle l,m'| \left(\sqrt{(l-m)(l+m+1)} |l,m+1\rangle - \sqrt{(l+m)(l-m+1)} |l,m-1\rangle \right) \\
&= \frac{C\hbar}{2i} \left(\sqrt{(l-m)(l+m+1)} \delta_{m',m+1} - \sqrt{(l+m)(l-m+1)} \delta_{m',m-1} \right).
\end{aligned} \tag{1.6}$$

After squaring and summing, the cross terms will be zero since they involve products of delta functions with different indices. That leaves

$$\begin{aligned}
\Delta^2 &= \frac{C^2\hbar}{4B} \sum_{m' \neq m} \frac{(l-m)(l+m+1)\delta_{m',m+1} - (l+m)(l-m+1)\delta_{m',m-1}}{m - m'} \\
&= \frac{C^2\hbar}{4B} \left(\frac{(l-m)(l+m+1)}{m-(m+1)} - \frac{(l+m)(l-m+1)}{m-(m-1)} \right) \\
&= \frac{C^2\hbar}{4B} \left(-(l^2 - m^2 + l - m) - (l^2 - m^2 + l + m) \right) \\
&= -\frac{C^2\hbar}{2B} (l^2 - m^2 + l),
\end{aligned} \tag{1.7}$$

so to first order the energy shift is

$$\boxed{A\hbar^2 l(l+1) + B\hbar m \rightarrow \hbar l(l+1)\left(A\hbar - \frac{C^2}{2B}\right) + B\hbar m + \frac{C^2 m^2 \hbar}{2B}.} \tag{1.8}$$

Exact perturbation equation If we wanted to solve the Hamiltonian exactly, we've have to diagonalize the $2m+1$ dimensional Hamiltonian

$$\begin{aligned} \langle l, m' | H | l, m \rangle = \Big(& A\hbar^2 l(l+1) \\ & + B\hbar m \Big) \delta_{m',m} + \frac{C\hbar}{2i} \left(\sqrt{(l-m)(l+m+1)}\delta_{m',m+1} - \sqrt{(l+m)(l-m+1)}\delta_{m',m-1} \right). \end{aligned} \tag{1.9}$$

This Hamiltonian matrix has a very regular structure

$$\begin{aligned} H &= (Al(l+1)\hbar^2 - B\hbar(l+1))I \\ &+ B\hbar \begin{bmatrix} 1 & & & & \\ & 2 & & & \\ & & 3 & & \\ & & & \ddots & \\ & & & & 2l+1 \end{bmatrix} \\ &+ \frac{C\hbar}{i} \begin{bmatrix} 0 & -\sqrt{(2l-1)(1)} & & & & \\ \sqrt{(2l-1)(1)} & 0 & -\sqrt{(2l-2)(2)} & & & \\ & \sqrt{(2l-2)(2)} & & & & \\ & & & \ddots & & \\ & & & & 0 & -\sqrt{(1)(2l-1)} \\ & & & & \sqrt{(1)(2l-1)} & 0 \end{bmatrix} \end{aligned} \tag{1.10}$$

Solving for the eigenvalues of this Hamiltonian for increasing l in Mathematica (sakuraiProblem5.17a.nb), it appears that the eigenvalues are

$$\lambda_m = A\hbar^2(l)(l+1) + \hbar m B\sqrt{1 + \frac{4C^2}{B^2}}, \tag{1.11}$$

so to first order in C^2, these are

$$\lambda_m = A\hbar^2(l)(l+1) + \hbar m B\left(1 + \frac{2C^2}{B^2}\right). \tag{1.12}$$

We have a $C^2\hbar/B$ term in both the perturbative energy shift eq. (1.7), and the first order expansion of the exact solution eq. (1.11). Comparing this for the $l = 5$ case, the coefficients of $C^2\hbar/B$ in eq. (1.7) are all negative $-17.5, -17., -16.5, -16., -15.5, -15., -14.5, -14., -13.5, -13., -12.5$, whereas the coefficient of $C^2\hbar/B$ in the first order expansion of the exact solution eq. (1.11) are $2m$, ranging from $[-10, 10]$.

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1