Physics 711: Assignment 3

(to be submitted by Wednesday, October 1, 2025)

1. The commutator of operators $\hat{A}$ and $\hat{B}$ is defined as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. (Note that version 14.3 of Mathematica introduces the commands `Commutator` and `NonCommutativeExpand`.)

   (a) Prove that $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$ and $[\hat{A}, \hat{A}] = 0$.

   The commutator is antisymmetric:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = -(\hat{B}\hat{A} - \hat{A}\hat{B}) = -[\hat{B}, \hat{A}].$$

   Moreover, setting $\hat{A} = \hat{B}$ implies that $[\hat{A}, \hat{A}] = -[\hat{A}, \hat{A}] = 0$.

   (b) For operators $\hat{A}$, $\hat{B}$, and $\hat{C}$ and complex numbers α and β, show that

$$[\alpha\hat{A} + \beta\hat{B}, \hat{C}] = \alpha[\hat{A}, \hat{C}] + \beta[\hat{B}, \hat{C}].$$

   Expand out and recollect terms to show linearity and the distributive property.

   (c) Prove that the commutator distributes over an operator product as follows:

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}].$$

$$\begin{aligned}
[\hat{A}, \hat{B}\hat{C}] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{C} + \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A}) = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]
\end{aligned}$$

   (d) Prove the famous Jacobi identity:

$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0.$$

   Expand the nested commutator to get

$$\begin{aligned}
[\hat{A}, [\hat{B}, \hat{C}]] &= \hat{A}(\hat{B}\hat{C} - \hat{C}\hat{B}) - (\hat{B}\hat{C} - \hat{C}\hat{B})\hat{A} \\
&= \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} - \hat{B}\hat{C}\hat{A} + \hat{C}\hat{B}\hat{A} \\
&= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} + \hat{C}\hat{B}\hat{A} - \hat{A}\hat{C}\hat{B}.
\end{aligned}$$

   Looking at the 3 cyclic permutations of this expression, we see that there are $3! = 6$ unique terms that cancel in pairs:

$$\begin{aligned}
[\hat{A}, [\hat{B}, \hat{C}]] &= \underbrace{\hat{A}\hat{B}\hat{C}}_{1} - \underbrace{\hat{B}\hat{C}\hat{A}}_{2} + \underbrace{\hat{C}\hat{B}\hat{A}}_{3} - \underbrace{\hat{A}\hat{C}\hat{B}}_{4} \\
[\hat{B}, [\hat{C}, \hat{A}]] &= \underbrace{\hat{B}\hat{C}\hat{A}}_{2} - \underbrace{\hat{C}\hat{A}\hat{B}}_{5} + \underbrace{\hat{A}\hat{C}\hat{B}}_{4} - \underbrace{\hat{B}\hat{A}\hat{C}}_{6} \\
[\hat{C}, [\hat{A}, \hat{B}]] &= \underbrace{\hat{C}\hat{A}\hat{B}}_{5} - \underbrace{\hat{A}\hat{B}\hat{C}}_{1} + \underbrace{\hat{B}\hat{A}\hat{C}}_{6} - \underbrace{\hat{C}\hat{B}\hat{A}}_{3}
\end{aligned}$$

   (e) Consider operators $\hat{x}$ and $\hat{p}$ satisfying $[\hat{x}, \hat{p}] = i\hbar$. Argue that $[\hat{x}, \hat{p}^2] = 2i\hbar\hat{p}$, $[\hat{x}, \hat{p}^3] = 3i\hbar\hat{p}^2$, and more generally, $[\hat{x}, \hat{p}^n] = ni\hbar\hat{p}^{n-1}$. Use this result to show that

$$[\hat{x}, f(\hat{p})] = i\hbar f'(\hat{p}),$$

   where f is any smooth function.

You can show that $[\hat{x}, \hat{p}^n] = ni\hbar\hat{p}^{n-1}$ by recursion. With this result in hand, observe that

$$[\hat{x}, f(\hat{p})] = \left[\hat{x}, \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f(x)}{dx^n}\bigg|_{x=0} \hat{p}^n\right] = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f(x)}{dx^n}\bigg|_{x=0} [\hat{x}, \hat{p}^n]$$
$$= \sum_{n=1}^{\infty} \frac{1}{n!} \frac{d^n f(x)}{dx^n}\bigg|_{x=0} ni\hbar\hat{p}^{n-1} = i\hbar \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \frac{d^{n-1} f'(x)}{dx^{n-1}}\bigg|_{x=0} \hat{p}^{n-1} = i\hbar f'(\hat{p}).$$

2. In class we considered a planar quantum rotor model with a symmetry-breaking term that favours angular orientation near $\phi = 0$:

$$\hat{H} = \frac{\hat{L}^2}{2I} - I\Omega^2 \cos\hat{\phi}.$$

Here, I is the moment of inertia, and Ω is the natural frequency of the corresponding classical problem in the small-amplitude-oscillation limit. The operators $\hat{\phi}$ and $\hat{L}$ obey the canonical commutation relationship $[\hat{\phi}, \hat{L}] = i\hbar$. We made the decision to work in the ϕ-representation, so that the operators take the form ϕ and $L = (\hbar/i)\partial/\partial\phi$ and act on a wave function $\psi(\phi)$.

(a) Show that states $\chi_m(\phi) \sim \exp(im\phi)$ are eigenstates of the angular momentum operator with eigenvalue $\hbar m$. Determine the proper normalization of the states. Here's a Mathematica version of the solution:

```
\[Chi][\[Phi]_] = Exp[I m \[Phi]]/Sqrt[2 \[Pi]]
Assuming[m \[Element] Integers, Integrate[Conjugate[\[Chi][\[Phi]]] \[Chi][\[Phi]],
    {\[Phi], 0, 2 \[Pi]}]]
L = (\[HBar]/I) D[#, \[Phi]] &
L[\[Chi][\[Phi]]]/\[Chi][\[Phi]]
```

Acting with $\hat{L} = (\hbar/i)(\partial/\partial\phi)$ on $\chi_m(\phi)$ gives the eigenvalue relation

$$\hat{L}\chi_m(\phi) = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\exp(im\phi) = \frac{\hbar}{i}(im)\exp(im\phi) = \hbar m\chi_m(\phi).$$

This says that $\chi_m(\phi)$ is a state of definite angular momentum $L = \hbar m$.
To get a properly normalized wave function $\chi_m(\phi) = C\exp(im\phi)$, we have to fix the normalization constant according to

$$\int_{-\pi}^{\pi} d\phi\, \chi_m(\phi)^*\chi_m(\phi) = |C|^2 \int_{-\pi}^{\pi} d\phi\, e^{-im\phi}e^{im\phi} = 2\pi|C|^2 = 1.$$

The phase of C is arbitrary, so we're free to choose $\chi_m(\phi) = (2\pi)^{-1/2}\exp(im\phi)$.

(b) Argue that the parity operation (reflection across the preferred axis, $\phi \to -\phi$) is a symmetry of the Hamiltonian. Construct a basis of states of definite even ($P = +1$) and odd ($P = -1$) parity from linear combinations of the angular momentum states $\chi_m(\phi)$. Explain how this basis can be used to block diagonalize the Hamiltonian.
The Hamiltonian is

$$\hat{H} = \frac{\hat{L}^2}{2I} - I\Omega^2\cos\hat{\phi} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi.$$

It's invariant under reflection since it only involves terms that are even in the angular variable:

$$\hat{H} \xrightarrow{\phi\to-\phi} -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial(-\phi)^2} - I\Omega^2\cos(-\phi)$$
$$= -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi = \hat{H}.$$

Let's build states of definite parity. The parity operation on $\chi_m(\phi) = (2\pi)^{-1/2}\exp(im\phi)$ is equivalent to changing the sign of m:

$$\hat{P}\chi_m(\phi) = (2\pi)^{-1/2}\hat{P}\exp(im\phi) = (2\pi)^{-1/2}\exp[im(-\phi)] = (2\pi)^{-1/2}\exp[i(-m)\phi] = \chi_{-m}(\phi).$$

Hence, the following are states of definite parity.

$$\begin{aligned}\chi_0^{(+)} &= \frac{1}{\sqrt{2\pi}}\\ \chi_{m\geq 1}^{(+)} &= \frac{1}{\sqrt{2}}(\chi_m + \chi_{-m})\\ \chi_{m\geq 1}^{(-)} &= \frac{1}{\sqrt{2}}(\chi_m - \chi_{-m})\end{aligned}$$

We can check that the eigenvalues are $P = 1$ and $P = -1$, respectively.

$$\begin{aligned}\hat{P}\chi_0^{(+)} &= \hat{P}\frac{1}{\sqrt{2\pi}} = \frac{1}{\sqrt{2\pi}} = (+1)\chi_0^{(+)}\\ \hat{P}\chi_{m\geq 1}^{(+)} &= \frac{1}{\sqrt{2}}(\hat{P}\chi_m + \hat{P}\chi_{-m}) = \frac{1}{\sqrt{2}}(\chi_{-m} + \chi_m) = \frac{1}{\sqrt{2}}(\chi_m + \chi_{-m}) = (+1)\chi_{m\geq 1}^{(+)}\\ \hat{P}\chi_{m\geq 1}^{(-)} &= \frac{1}{\sqrt{2}}(\hat{P}\chi_m - \hat{P}\chi_{-m}) = \frac{1}{\sqrt{2}}(\chi_{-m} - \chi_m) = -\frac{1}{\sqrt{2}}(\chi_m - \chi_{-m}) = (-1)\chi_{m\geq 1}^{(-)}\end{aligned}$$

States carrying different parity quantum numbers are guaranteed to have zero overlap (i.e., they're orthogonal), since

$$\int_{-\pi}^{\pi} d\phi\, \chi_m^{(+)}(\phi)^*\chi_{m'}^{(-)}(\phi) = \int_{-\pi}^{\pi} d\phi\, \chi_m^{(+)}(-\phi)^*\chi_{m'}^{(-)}(-\phi) = -\int_{-\pi}^{\pi} d\phi\, \chi_m^{(+)}(\phi)^*\chi_{m'}^{(-)}(\phi) = 0.$$

Then we can take advantage of the fact that $\hat{H}\hat{P} = \hat{P}\hat{H}$. The difference between these two matrix elements must vanish:

$$\begin{aligned}\int_{-\pi}^{\pi} d\phi\, \chi_m^{(P)}(\phi)^*\hat{H}\hat{P}\chi_{m'}^{(P')}(\phi) &= P'\int_{-\pi}^{\pi} d\phi\, \chi_m^{(P)}(\phi)^*\hat{H}\chi_{m'}^{(P')}(\phi),\\ \int_{-\pi}^{\pi} d\phi\, \chi_m^{(P)}(\phi)^*\hat{P}\hat{H}\chi_{m'}^{(P')}(\phi) &= P\int_{-\pi}^{\pi} d\phi\, \chi_m^{(P)}(\phi)^*\hat{H}\chi_{m'}^{(P')}(\phi).\end{aligned}$$

Hence,

$$(P - P')\int_{-\pi}^{\pi} d\phi\, \chi_m^{(P)}(\phi)^*\hat{H}\chi_{m'}^{(P')}(\phi) = 0,$$

which says that the matrix elements are ncessarily zero if the parity quantum numbers P and P' are not the same. In other words, the Hamiltonian has the block diagonal form

$$\int_{-\pi}^{\pi} d\phi\, \chi_m^{(P)}(\phi)^*\hat{H}\chi_{m'}^{(P')}(\phi) = H_{m,m'}^{(P)}\delta_{P,P'}.$$

(c) Consider a truncated basis that contains only the two lowest-lying states in each of the even- and odd-parity sectors. Write the time-independent Schrödinger equation as two 2×2 matrix eigenvector problems.

Note that

$$\chi_0^{(+)} = \frac{1}{\sqrt{2\pi}}$$
$$\chi_{m\geq 1}^{(+)} = \frac{1}{\sqrt{2}}(\chi_m + \chi_{-m}) = \frac{1}{2\sqrt{\pi}}[\exp(im\phi) + \exp(-im\phi)] = \frac{1}{\sqrt{\pi}}\cos m\phi$$
$$-i\chi_{m\geq 1}^{(-)} = \frac{-i}{\sqrt{2}}(\chi_m - \chi_{-m}) = \frac{1}{2i\sqrt{\pi}}[\exp(im\phi) - \exp(-im\phi)] = \frac{1}{\sqrt{\pi}}\sin m\phi$$

So the even and odd parity sectors are spanned by

$$\{\chi_m^{(+)} : m \geq 0\} = \left\{\frac{1}{\sqrt{2\pi}}, \frac{\cos\phi}{\sqrt{\pi}}, \frac{\cos 2\phi}{\sqrt{\pi}}, \frac{\cos 3\phi}{\sqrt{\pi}}, \ldots\right\}$$
$$\{\chi_m^{(-)} : m \geq 1\} = \left\{\frac{\sin\phi}{\sqrt{\pi}}, \frac{\sin 2\phi}{\sqrt{\pi}}, \frac{\sin 3\phi}{\sqrt{\pi}}, \frac{\sin 4\phi}{\sqrt{\pi}}, \ldots\right\}$$

Computed with respect to the first two basis functions is each set, we get the following Hamiltonian blocks:

$$H^{(+)} = \begin{pmatrix} H_{1,1}^{(+)} & H_{1,2}^{(+)} \\ H_{2,1}^{(+)} & H_{2,2}^{(+)} \end{pmatrix} = \int_{-\pi}^{\pi} d\phi \begin{pmatrix} \chi_0^{(+)}\hat{H}\chi_0^{(+)} & \chi_0^{(+)}\hat{H}\chi_1^{(+)} \\ \chi_1^{(+)}\hat{H}\chi_0^{(+)} & \chi_1^{(+)}\hat{H}\chi_1^{(+)} \end{pmatrix} = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$
$$H^{(-)} = \begin{pmatrix} H_{1,1}^{(-)} & H_{1,2}^{(-)} \\ H_{2,1}^{(-)} & H_{2,2}^{(-)} \end{pmatrix} = \int_{-\pi}^{\pi} d\phi \begin{pmatrix} \chi_1^{(-)}\hat{H}\chi_1^{(-)} & \chi_1^{(-)}\hat{H}\chi_2^{(-)} \\ \chi_2^{(-)}\hat{H}\chi_1^{(-)} & \chi_2^{(-)}\hat{H}\chi_2^{(-)} \end{pmatrix} = \begin{pmatrix} d & e \\ e & f \end{pmatrix}$$

We must evaluate the integral expressions for even-parity

$$a = \int_{-\pi}^{\pi} d\phi \, \frac{1}{\sqrt{2\pi}}\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\frac{1}{\sqrt{2\pi}} = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi \left(0 - I\Omega^2\cos\phi\right) = 0$$
$$b = \int_{-\pi}^{\pi} d\phi \, \frac{\cos\phi}{\sqrt{\pi}}\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\frac{1}{\sqrt{2\pi}} = -\frac{I\Omega^2}{\sqrt{2}\pi}\int_{-\pi}^{\pi} d\phi \, \cos^2\phi = -\frac{I\Omega^2}{\sqrt{2}}$$
$$c = \int_{-\pi}^{\pi} d\phi \, \frac{\cos\phi}{\sqrt{\pi}}\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\frac{\cos\phi}{\sqrt{\pi}} = \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi \left(\frac{\hbar^2}{2I}\cos^2\phi - I\Omega^2\cos^3\phi\right) = \frac{\hbar^2}{2I}$$

and odd-parity coefficients

$$d = \int_{-\pi}^{\pi} d\phi \, \frac{\sin\phi}{\sqrt{\pi}}\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\frac{\sin\phi}{\sqrt{\pi}} = \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi \left(\frac{\hbar^2}{2I}\sin^2\phi - I\Omega^2\cos\phi\sin^2\phi\right) = \frac{\hbar^2}{2I}$$
$$e = \int_{-\pi}^{\pi} d\phi \, \frac{\sin\phi}{\sqrt{\pi}}\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\frac{\sin 2\phi}{\sqrt{\pi}} = \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi \left(\frac{2\hbar^2}{I}\sin\phi\sin 2\phi - I\Omega^2\cos\phi\sin\phi\sin 2\phi\right) = -\frac{I\Omega^2}{2}$$
$$f = \int_{-\pi}^{\pi} d\phi \, \frac{\sin 2\phi}{\sqrt{\pi}}\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\frac{\sin 2\phi}{\sqrt{\pi}} = \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi \left(\frac{2\hbar^2}{I}\sin^2 2\phi - I\Omega^2\cos\phi\sin^2 2\phi\right) = \frac{2\hbar^2}{I}$$

Expressed in terms of an energy scale $\epsilon_0 = \hbar^2/2I$ and dimensionless coupling $g = (I\Omega/\hbar)^2$, the matrix blocks are

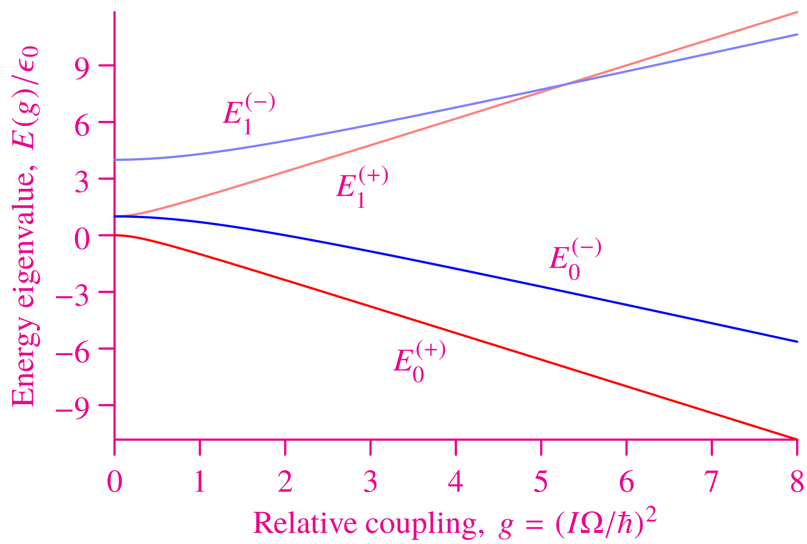
$$H^{(+)} = \begin{pmatrix} 0 & \frac{I\Omega^2}{\sqrt{2}} \\ \frac{I\Omega^2}{\sqrt{2}} & \frac{\hbar^2}{2I} \end{pmatrix} = \epsilon_0 \begin{pmatrix} 0 & -\sqrt{2}g \\ -\sqrt{2}g & 1 \end{pmatrix}$$
$$H^{(-)} = \begin{pmatrix} \frac{\hbar^2}{2I} & \frac{I\Omega^2}{2} \\ \frac{I\Omega^2}{2} & \frac{2\hbar^2}{I} \end{pmatrix} = \epsilon_0 \begin{pmatrix} 1 & -g \\ -g & 4 \end{pmatrix}$$

(d) Solve the even-parity 2×2 eigenproblem. (You are welcome to make use of Mathematica's `Eigensystem` or its `Eigenvectors` and `Eigenvalues` commands.) For the ground state, plot the probability density $|\psi(\phi)|^2$ of finding the rotor in the vicinity of angle ϕ. Do this for small, intermediate, and large values of Ω.

Here are the solutions to the eigenproblem in the even and odd sector:

$$E_0^{(+)} = \frac{1}{2}\left(1 - \sqrt{1+8g^2}\right) \qquad \psi_0^{(+)} \sim (1+\sqrt{1+8g^2}, 2\sqrt{2}g)$$
$$E_1^{(+)} = \frac{1}{2}\left(1 + \sqrt{1+8g^2}\right) \qquad \psi_1^{(+)} \sim (1-\sqrt{1+8g^2}, 2\sqrt{2}g)$$
$$E_0^{(-)} = \frac{1}{2}\left(5 - \sqrt{9+4g^2}\right) \qquad \psi_0^{(-)} \sim (3+\sqrt{9+4g^2}, 2g)$$
$$E_1^{(-)} = \frac{1}{2}\left(5 + \sqrt{9+4g^2}\right) \qquad \psi_1^{(-)} \sim (3-\sqrt{9+4g^2}, 2g)$$

Over the full range of couplings, the lowest energy is $E_0^{(+)}$, which means that the even-parity state with coefficients $\psi_0^{(+)} \sim (1+\sqrt{1+8g^2}, 2\sqrt{2}g)$ is the ground state.



The corresponding (non-normalized) wave function is

$$\psi_0^{(+)}(\phi) = (1+\sqrt{1+8g^2})\chi_0^{(+)}(\phi) + 2\sqrt{2}g\chi_1^{(+)}(\phi).$$

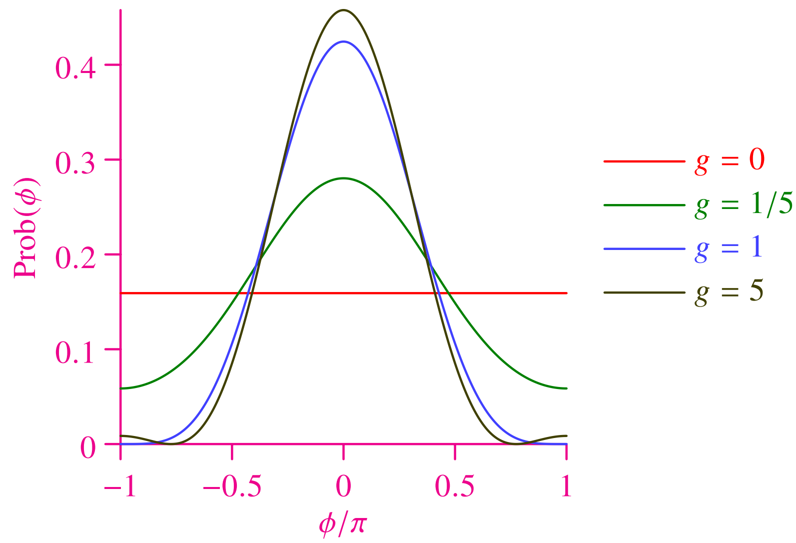
Since $\chi_0^{(+)}$ and $\chi_1^{(+)}$ are orthogonormal, the normalization factor is

$$\begin{aligned}\mathcal{N} = \int_{-\pi}^{\pi} d\phi\, |\psi_0^{(+)}(\phi)|^2 &= \left(1+\sqrt{1+8g^2}\right)^2 + \left(2\sqrt{2}g\right)^2 \\ &= \left(1 + 2\sqrt{1+8g^2} + 1 + 8g^2\right) + 8g^2 \\ &= 2(1+8g^2) + 2\sqrt{1+8g^2}\end{aligned}$$

$$\text{Prob}(\phi) = \frac{1}{\mathcal{N}}\left|\psi_0^{(+)}\right|^2 = \frac{\left|(1+\sqrt{1+8g^2})\chi_0^{(+)}(\phi) + 2\sqrt{2}g\chi_1^{(+)}(\phi)\right|^2}{2(1+8g^2)+2\sqrt{1+8g^2}}$$

$$= \frac{\left|(1+\sqrt{1+8g^2})\frac{1}{\sqrt{2\pi}} + 2\sqrt{2}g\frac{\cos\phi}{\sqrt{\pi}}\right|^2}{2(1+8g^2)+2\sqrt{1+8g^2}}$$

$$= \frac{\left[1+\sqrt{1+8g^2}+4g\cos\phi\right]^2}{4\pi\left[1+8g^2+\sqrt{1+8g^2}\right]}$$



$$\text{Prob}(\phi) \xrightarrow{g\to 0} \frac{1}{2\pi}\left(1+4g\cos\phi+2g^2\cos 2\phi\right)+O(g^3)$$
$$\xrightarrow{g\to\infty} \frac{1}{4\pi}\left(2+2\sqrt{2}\cos\phi+\cos 2\phi\right)+O(g^{-1})$$

(e) Compute the expectation values of $\hat{H}$ with respect to the next-lowest-lying states in each sector. Based on energy comparisons, comment on the appropriateness of the basis truncation.

$$\int_{-\pi}^{\pi} d\phi\,\frac{\cos 2\phi}{\sqrt{\pi}}\hat{H}\frac{\cos 2\phi}{\sqrt{\pi}} = \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi\,\cos 2\phi\left(-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} - I\Omega^2\cos\phi\right)\cos 2\phi$$

$$= \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi\,\cos 2\phi\left(\frac{4\hbar^2}{2I} - I\Omega^2\cos\phi\right)\cos 2\phi$$

$$= \frac{1}{\pi}\int_{-\pi}^{\pi} d\phi\left(\frac{2\hbar^2}{I}\cos^2 2\phi - I\Omega^2\cos\phi\cos^2 2\phi\right) = \frac{2\hbar^2}{I} = 4\epsilon_0$$

$$
\begin{aligned}
\int_{-\pi}^{\pi} d\phi \, \frac{\sin 3\phi}{\sqrt{\pi}} \hat{H} \frac{\sin 3\phi}{\sqrt{\pi}} &= \frac{1}{\pi} \int_{-\pi}^{\pi} d\phi \, \sin 3\phi \left(-\frac{\hbar^2}{2I} \frac{\partial^2}{\partial \phi^2} - I\Omega^2 \cos\phi \right) \sin 3\phi \\
&= \frac{1}{\pi} \int_{-\pi}^{\pi} d\phi \, \sin 3\phi \left(\frac{9\hbar^2}{2I} - I\Omega^2 \cos\phi \right) \sin 3\phi \\
&= \frac{1}{\pi} \int_{-\pi}^{\pi} d\phi \left(\frac{2\hbar^2}{I} \sin^2 3\phi - I\Omega^2 \cos\phi \sin^2 3\phi \right) = \frac{9\hbar^2}{2I} = 9\epsilon_0
\end{aligned}
$$

More generally, the level-m expectation value is $m^2\epsilon_0$. So if the basis is cut off such that level M is the highest state included, then the gap to the neglected state is $2M + 1$ times greater than the level spacing between the lowest two levels:

$$
\frac{\epsilon_0 (M+1)^2 - \epsilon_0 M^2}{\epsilon_0 - 0} = 2M + 1.
$$

If the neglected states are sufficiently gapped out, they can't effectively hybridize with the low-energy states. To get well converged results, we'd probably want M to be on the order of at least 10 or 100.