PHY 304, II-Semester 2021/22, Tutorial 2 solution

Stage 1 Symmetries For the following Hamiltonians, identify all symmetries, write the operators implementing the symmetry transformation and state the resulting conservation laws and degeneracies in the spectrum of the Hamiltonian.

(i) Free particle

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{1}$$

Solution: Translation symmetry for any a. Use Eq. (6.3)

$$[\hat{H}, \hat{T}(a)] = \left[\frac{\hat{p}^2}{2m}, e^{-i\frac{a}{\hbar}\hat{p}}\right] = 0, \tag{2}$$

since any function of the momentum operator commutes with any other function of the momentum operator. Symmetry under parity transformation $\hat{\Pi}$.

$$\hat{\Pi}\hat{H}\hat{\Pi} = \frac{1}{2m}\hat{\Pi}\hat{p}^2\hat{\Pi} = \frac{1}{2m}(\hat{\Pi}\hat{p}\hat{\Pi})(\hat{\Pi}\hat{p}\hat{\Pi}) = \frac{\hat{p}^2}{2m} = \hat{H} \tag{3}$$

where we used $\hat{\Pi}\hat{p}\hat{\Pi} = -\hat{p}$.
Thus parity of the wavefunction is conserved (if it was symmetric initially, it will stay symmetric) and momentum is conserved (see page 148). If we look at section 6.6.5, we have one of those cases where the Hamiltonian has at least two non-commuting symmetries (to find out that Π *and* $T(a)$ *do not commute, sequentially apply each to a Gaussian wavefunction that is not centered on the origin, then do it the other way round.*

$$\hat{\Pi}\hat{T}(a)\psi(x) = \hat{\Pi}\hat{T}(a)e^{-(x-b)^2/(2\sigma)} = \hat{\Pi}e^{-(x-b-a)^2/(2\sigma)} = e^{-(x+b+a)^2/(2\sigma)} \tag{4}$$

$$\hat{T}(a)\hat{\Pi}\psi(x) = \hat{\Pi}\hat{T}(a)e^{-(x-b)^2/(2\sigma)} = \hat{T}(a)e^{-(x+b)^2/(2\sigma)} = e^{-(x+b-a)^2/(2\sigma)} \tag{5}$$

Clearly these are not the same states as is also seen in the plot below.)

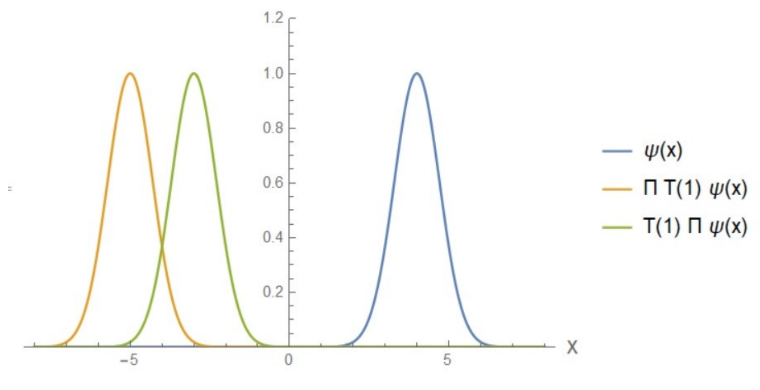

Figure 1: Plots of the gaussian wavefunction under translation and parity transformations. We have taken here $b = 4$, $a = 1$ and $\sigma = 1/2$

Indeed we know from QM-I section 2.1. that all free particle states are twice degenerate, since both $e^{\pm ikx}$ have the same energy $E = \hbar^2 k^2/(2m)$. In the language of QM-II section 6.6.5: We have that $\Pi e^{+ikx} = e^{-ikx}$ is indeed <u>*another*</u> *state with the same energy, not the same state.*

(ii) Mexican hat potential $(\alpha, \beta > 0)$

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m} - \alpha(\hat{x}^2 + \hat{y}^2) + \beta(\hat{x}^2 + \hat{y}^2)^2 \tag{6}$$

Solution: The Hamiltonian is symmetric under the parity transformations Π_x and Π_y. Using

$$\Pi_x \hat{p}_x \Pi_x = -\hat{p}_x \tag{7}$$
$$\Pi_x \hat{p}_y \Pi_x = \hat{p}_y \tag{8}$$
$$\Pi_x \hat{x} \Pi_x = -\hat{x} \tag{9}$$
$$\Pi_x \hat{y} \Pi_x = \hat{y} \tag{10}$$

and similar expressions for $\hat{\Pi}_y$ we can show that

$$\hat{\Pi}_x \hat{H} \hat{\Pi}_x = \hat{\Pi}_y \hat{H} \hat{\Pi}_y = \hat{H} \tag{11}$$

In fact the Hamiltonian is symmetric under reflection on any line passing through the centre as shown in Fig. (3). Another symmetry is rotation about z-axis. The generator of rotation about z-axis is $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$. Consider

$$\begin{aligned}[\hat{x}\hat{p}_y, \hat{H}] &= \frac{1}{2m}[\hat{x}\hat{p}_y, \hat{p}_x^2] + \frac{1}{2m}[\hat{x}\hat{p}_y, \hat{p}_y^2] - \alpha[\hat{x}\hat{p}_y, \hat{x}^2] - \alpha[\hat{x}\hat{p}_y, \hat{y}^2] \\ &\quad + \beta[\hat{x}\hat{p}_y, \hat{x}^4] + 2\beta[\hat{x}\hat{p}_y, \hat{x}^2\hat{y}^2] + \beta[\hat{x}\hat{p}_y, \hat{y}^4] &(12) \\ &= \frac{i\hbar}{m}\hat{p}_x\hat{p}_y - 2i\hbar\alpha\hat{x}\hat{y} - 4i\hbar\beta\hat{x}^3\hat{y} - 4i\hbar\beta\hat{x}\hat{y}^3 &(13)\end{aligned}$$

$$\begin{aligned}[\hat{y}\hat{p}_x, \hat{H}] &= \frac{1}{2m}[\hat{y}\hat{p}_x, \hat{p}_x^2] + \frac{1}{2m}[\hat{y}\hat{p}_x, \hat{p}_y^2] - \alpha[\hat{y}\hat{p}_x, \hat{x}^2] - \alpha[\hat{y}\hat{p}_x, \hat{y}^2] \\ &\quad + \beta[\hat{y}\hat{p}_x, \hat{x}^4] + 2\beta[\hat{y}\hat{p}_x, \hat{x}^2\hat{y}^2] + \beta[\hat{y}\hat{p}_x, \hat{y}^4] &(14) \\ &= \frac{i\hbar}{m}\hat{p}_y\hat{p}_x - 2i\hbar\alpha\hat{y}\hat{x} - 4i\hbar\beta\hat{y}^3\hat{x} - 4i\hbar\beta\hat{y}\hat{x}^3 &(15)\end{aligned}$$

Subtracting these give $[\hat{L}_z, \hat{H}] = 0$. All the symmetries are manifest from the plots given below.

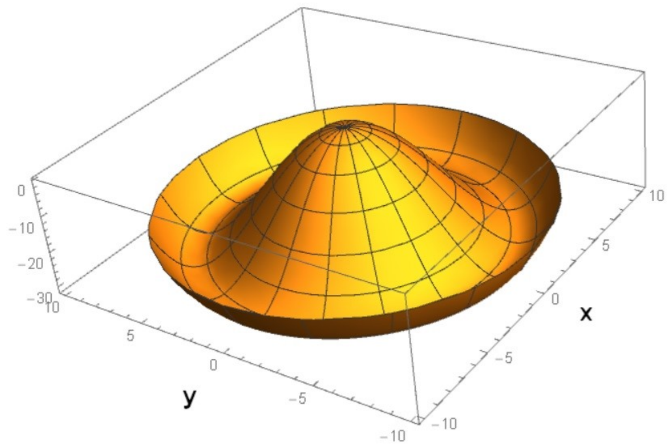

Figure 2: $f(x, y) = -\alpha(x^2 + y^2) + \beta(x^2 + y^2)^2$ for $\alpha = 1$ and $\beta = 0.008$. It is clearly symmetric under rotation about z-axis.

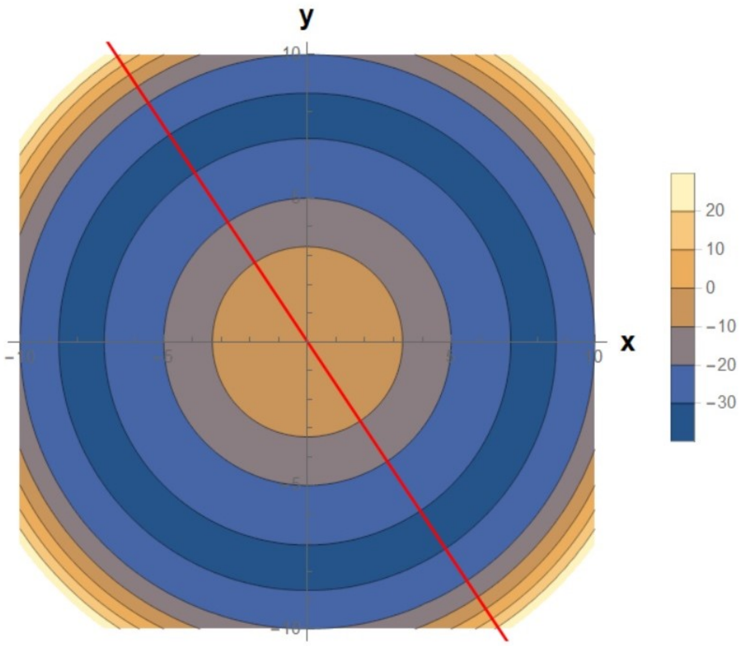

Figure 3: Contour Plot of $f(x, y) = -\alpha(x^2 + y^2) + \beta(x^2 + y^2)^2$ for $\alpha = 1$ and $\beta = 0.008$. It is symmetric under reflection on a line(red) passing through the centre.

Since $\hat{L}_z$ commutes with $\hat{H}$, angular momentum along the z-axis is conserved.

It is easy to see (e.g. using a test-function in spherical polar coordinates) that $\left[\hat{L}_z, \Pi_x\right] \neq 0$, hence we again have a case where we expect degeneracies. For example the first excited state can have either a +/- structure along the x-axis or along the y-axis, both of which are different states but *must have the same energy, by symmetry.*

(iii) Anisotropic 2D oscillator ($\omega_x \neq \omega_y$)

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m} + \frac{1}{2}m(\omega_x^2\hat{x}^2 + \omega_y^2\hat{y}^2) \tag{16}$$

Solution: The symmetries we find here are under the parity transformations $\hat{\Pi}_x$ and $\hat{\Pi}_y$. Using Eq. 7-10 and similar expressions for $\hat{P}_y$ it is easy to show that:

$$\hat{\Pi}_x\hat{H}\hat{\Pi}_x = \hat{\Pi}_y\hat{H}\hat{\Pi}_y = \hat{H} \tag{17}$$

The Hamiltonian is also symmetric under 180 *degrees rotation about z-axis. In contrast to the previous example, this is only a a discrete rotational symmetry, any other angle would not be possible. This is clear from the plots below.*

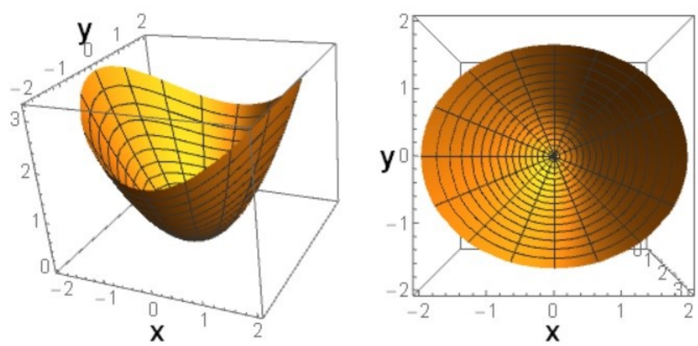

Figure 4: $f(x, y) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2)$ for $m = 2$, $\omega_x = 0.9$ and $\omega_y = 0.6$. The figure on the right is the top view.

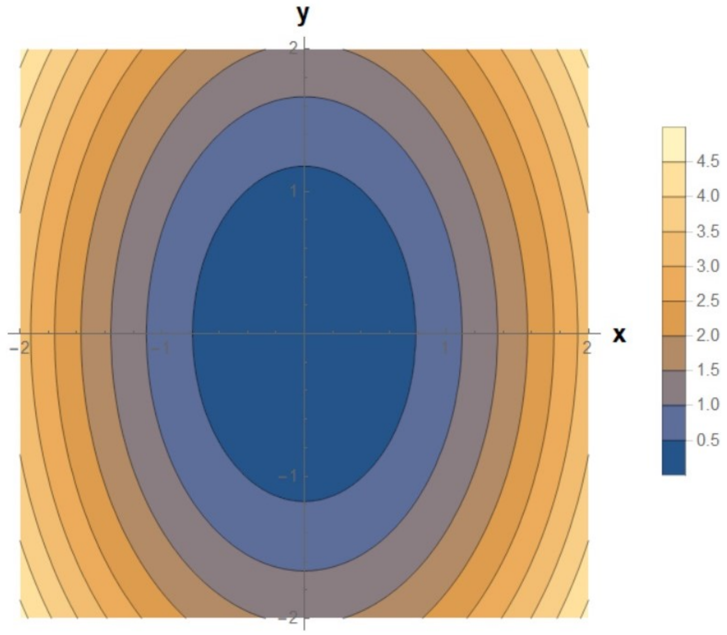

Figure 5: Contour Plot of $f(x,y) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2)$ for $m = 2$, $\omega_x = 0.9$ and $\omega_y = 0.6$. It is symmetric under rotation by 180 deg about z -axis.

However, we can realize that the 180 degrees rotation about z-axis is in fact the same symmetry as $\Pi_x \Pi_y$ (just make a drawing labelling 4 corners by 1,2,3,4, then try this out). Furthermore, $[\Pi_x, \Pi_y] = 0$ (again, make a drawing or use a testfunction $f(x,y)$. Thus here is a scenario where there are two symmetries, but these commute. Thus, in this case we do not expect any degeneracies.

Stage 2 Perturbed particle in the box: Consider a charged particle in an infinite square well potential, subject to an external electric field. The latter causes a an addition $\hat{H}' = q\mathcal{E}_0(x - a/2)$ to the Hamiltonian.

(i) Using perturbation theory, find the first order correction to all energy levels.
Solution: The first order correction to energy levels is given by, Eq.(7.12)

$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle \tag{18}$$

The known solutions of particle in a box are

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{19}$$

We see that all of these are either even or odd with respect to the box centre at $x = a/2$, while the perturbation $\hat{H}'$ is odd. Thus $|\psi(x)|^2 \hat{H}'$ is an odd function of x with respect to $a/2$, and vanishes when integrated over a *symmetric interval centered on $a/2$, such as $[0\ a]$.*

$$E_n^{(1)} = \frac{2q\mathcal{E}_0}{a}\int_0^a dx \sin^2\left(\frac{n\pi x}{a}\right)\left(x-\frac{a}{2}\right) \tag{20}$$

There is no need for explicit calculation. If we transform: $x \to x - a/2$, we get

$$\sin\left(\frac{n\pi x}{a}\right) \to \sin\left(\frac{n\pi(x-\frac{a}{2})}{a}\right) \tag{21}$$

$$= \sin\left(\frac{n\pi x}{a} - \frac{n\pi}{2}\right) \tag{22}$$

$$= \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi}{2}\right) - \sin\left(\frac{n\pi}{2}\right)\cos\left(\frac{n\pi x}{a}\right) \tag{23}$$

$$= \begin{cases} -\sin\left(\frac{n\pi}{2}\right)\cos\left(\frac{n\pi x}{a}\right) & n = \text{odd} \\ \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi}{2}\right) & n = \text{even} \end{cases} \tag{24}$$

The integral 20 becomes

$$E_n^{(1)} = \frac{2q\mathcal{E}}{a} \times \begin{cases} \int_{-a/2}^{a/2} dx\ \sin^2\left(\frac{n\pi}{2}\right)\cos^2\left(\frac{n\pi x}{a}\right)x & n = \text{odd} \\ \int_{-a/2}^{a/2} dx\ \sin^2\left(\frac{n\pi x}{a}\right)\cos^2\left(\frac{n\pi}{2}\right)x & n = \text{even} \end{cases} \tag{25}$$

In both cases the integrand is an odd function. So the integral vanishes. Thus

$$E_n^{(1)} = 0 \tag{26}$$

(ii) Then write down the second order correction to the ground state energy, and without evaluating integrals discuss which is the dominant contribution [assuming $0 < \langle \phi_k | \hat{H}' | \phi_1 \rangle \sim 1/k$ for large k] and what sign the energy shift has. *Bonus: AFTER the tutorial you may confirm the above scaling of matrix elements by explicitly evaluating the integrals.*
Solution: The second order correction to the ground state energy is given by Eq. (7.23)

$$E_1^{(2)} = \sum_{k\neq 1} \frac{|\langle \psi_k^{(0)} | \hat{H}' | \psi_1^{(0)} \rangle|^2}{E_1^{(0)} - E_k^{(0)}} \tag{27}$$

It is clear that the dominant contribution comes from the term corresponding to $k = 2$ i.e. from the first excited state since the absolute value of the energy gap $|E_1 - E_k| = \pi^2\hbar^2(k^2-1)/(2ma^2)$ is the least among that for other values of m, and matrix elements decrease for larger k as was given. The energy will then DECREASE, since $E_1^{(0)} - E_2^{(0)} < 0$.
BONUS: Let us now evaluate the expression on the L.H.S. of 27. Consider the numerator part.

$$\langle \psi_k^{(0)} | \hat{H}' | \psi_1^{(0)} \rangle = \frac{2q\mathcal{E}}{a}\int_0^a dx \sin\left(\frac{k\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\left(x - \frac{a}{2}\right) \tag{28}$$

$$= \frac{q\mathcal{E}}{a}\int_0^a dx\left(\cos\left(\frac{(k-1)\pi x}{a}\right) - \cos\left(\frac{(k+1)\pi x}{a}\right)\right)\left(x-\frac{a}{2}\right) \tag{29}$$

Using the standard integral result

$$\int dx\; x\cos(\alpha x) = \frac{\sin\alpha x}{\alpha} + \frac{\cos\alpha x}{\alpha^2} \tag{30}$$

We get

$$\langle\, \psi_k^{(0)}\, |\hat{H}'|\, \psi_1^{(0)}\,\rangle = \frac{q\mathcal{E}a}{\pi^2(k^2-1)^2}(4k(1+(-1)^k) \tag{31}$$

which gives the second order correction to the ground state energy of the unperturbed system:

$$E_1^{(2)} = -\left(\frac{32mq^2\mathcal{E}_0^2a^4}{\hbar^2\pi^6}\right)\sum_{k\neq 1}\frac{k^2(1+(-1)^k)^2}{(k^2-1)^5} \tag{32}$$

(iii) Also write the first order correction to the wavefunction, again discuss which is the dominant contribution and what it qualitatively does to the ground-state of the particle.
Solution: The first order correction to the ground state is given by Eq. (7.21). Contracting the expression in Eq. (7.21) from the left with position eigenstates $\langle\, x\,|$ we get the first order correction to position space wavefunction

$$\psi_1^{(1)}(x) = \sum_{k\neq 1}\frac{\langle\, \psi_k^{(0)}\, |\hat{H}'|\, \psi_1^{(0)}\,\rangle}{E_1^{(0)} - E_k^{(0)}}\psi_k^{(0)}(x) \tag{33}$$

Again we expect the dominant contribution to come from the term corresponding to first excited state $k = 2$ based on the argument presented earlier in part(ii), thus approximately

$$\psi_1^{(1)}(x) \approx \psi_1^{(0)}(x) + \underbrace{\frac{\langle\, \psi_2^{(0)}\, |\hat{H}'|\, \psi_1^{(0)}\,\rangle}{E_1^{(0)} - E_2^{(0)}}}_{<0}\psi_2^{(0)}(x) \tag{34}$$

This looks approximately as shown in Fig. 6 and when added to $\psi_1^{(0)}(x)$ will thus shift it to the left, as shown in Fig. 7.
BONUS: Explicitly inserting the result Eq. 31 and summing over all terms, we get

$$\psi_1^{(1)}(x) = -\left(\frac{8mq\mathcal{E}_0a^3}{\hbar^2\pi^4}\right)\sqrt{\frac{2}{a}}\sum_{k\neq 1}\frac{k(1+(-1)^k)}{(k^2-1)^3}\sin\left(\frac{k\pi x}{a}\right) \tag{35}$$

$$= -\alpha\sum_{k\neq 1}\frac{k(1+(-1)^k)}{(k^2-1)^3}\sin\left(\frac{k\pi x}{a}\right) \tag{36}$$

The plot below shows how the first few terms up to $k = 20$ modifies the ground state.

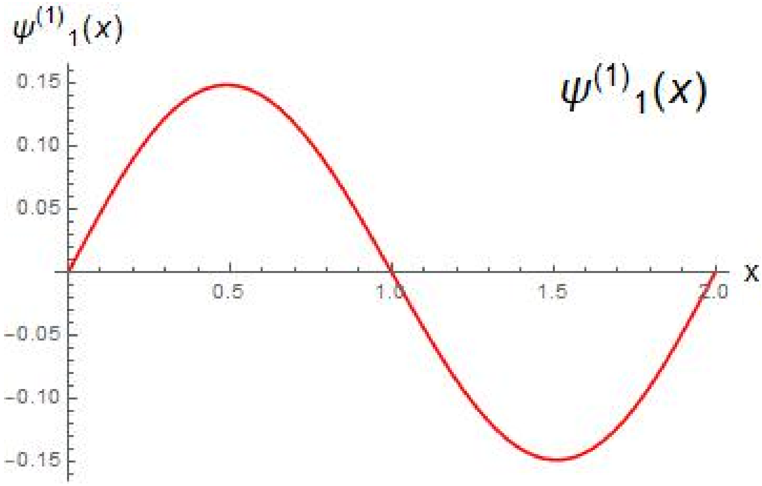

Figure 6: The first order correction to the ground state: $\psi_1^{(1)}(x)$ summing up to $k = 20$. Here $\alpha = 1$ and $a = 2$.

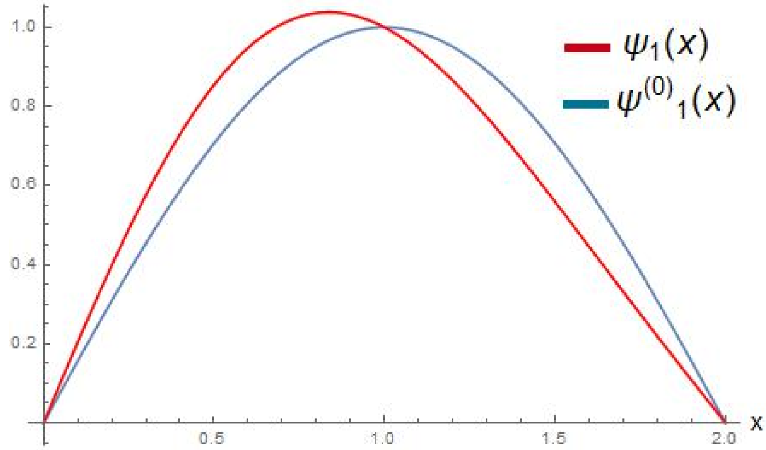

Figure 7: Blue: The unperturbed ground state: $\psi_1^{(0)}(x)$. Red: The first order corrected perturbed ground state: $\psi_1(x) = \psi_1^{(0)}(x) + \psi_1^{(1)}(x)$ summing up to $k = 20$. Here $\alpha = 1$ and $a = 2$.

(iv) Revisit the online app http://www.falstad.com/qm1d/ and select "setup: infinite well + field", particle mass = minimal and well width slider bar at about half, then apply a small field strength to check whether your conclusions for the previous two items were correct.
Solution:

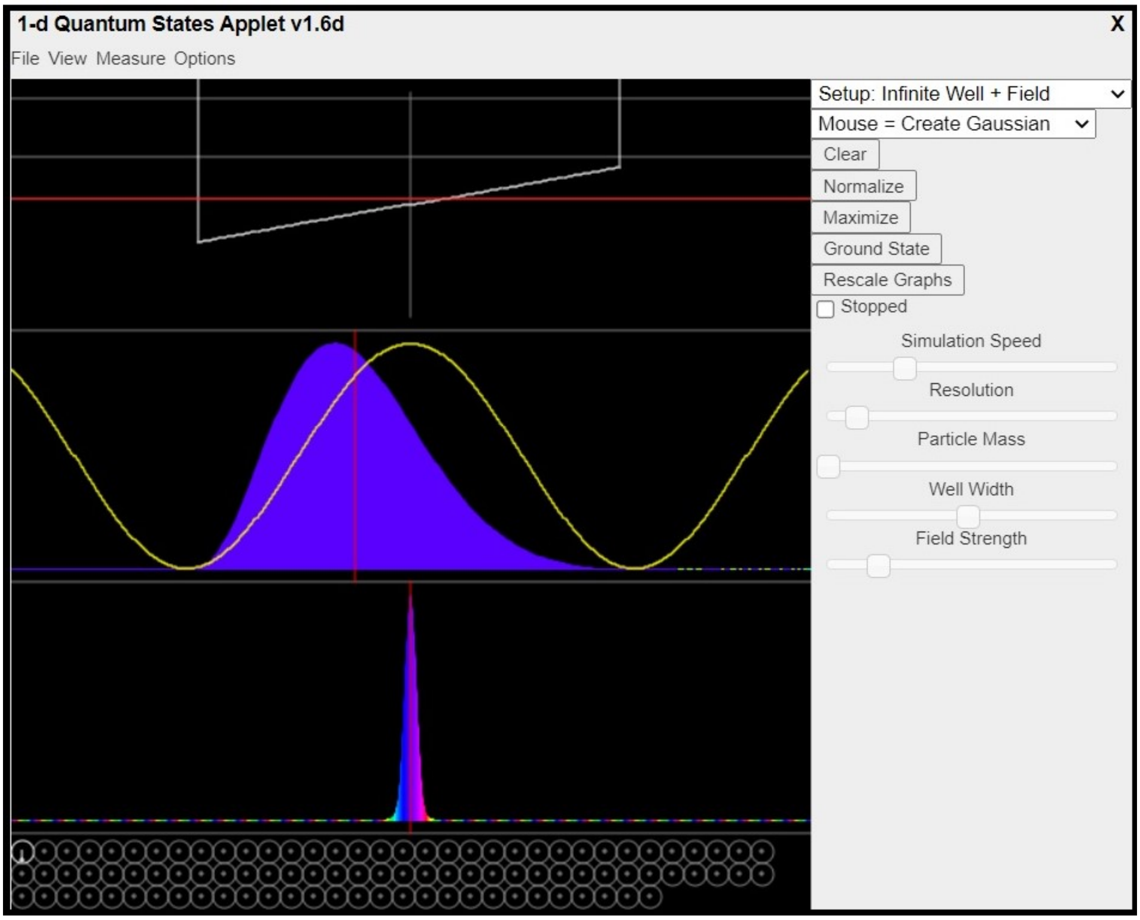

Figure 8: The yellow curve is the unperturbed ground state. The blue one is the perturbed ground state which is shifted towards left just like Fig. (7)

Stage 3 Atom interacting with light: We had heard in PHY106 that light can cause transitions between electronic states of atoms, such as the $|\,\phi_{n\ell m}\,\rangle$ states of the Hydrogen atom in week 10. We had also seen something similar in Example 46. Let us brutally simplify the Hydrogen atom, and consider only two of its internal states, a ground state $|\,g\,\rangle$ and an excited state $|\,e\,\rangle$ and assume this atom is irradiated with laser light.

It turns out (in a preview of PHY402), that with some approximations, this atom can be described by an effective Hamiltonian

$$\hat{H} = \begin{bmatrix} 0 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & -\Delta \end{bmatrix}. \tag{37}$$

We wrote a matrix representation wrt. states $|\,g\,\rangle$ and $|\,e\,\rangle$ in this order. Ω is related to the laser intensity, and $\Delta =$ to the difference between the light frequency and the transition frequency (called a detuning).

We call the light far off resonant if $\Omega \ll |\Delta|$.

(i) Use this conditions to define a suitable splitting of the Hamiltonian to use perturbation theory, and then apply it to find the first and second order corrections to energies and first order correction to states.
Solution: Since $\Omega \ll |\Delta|$ *we split*

$$\hat{H}_0 = \begin{bmatrix} 0 & 0 \\ 0 & -\Delta \end{bmatrix}, \qquad \hat{H}' \qquad = \begin{bmatrix} 0 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & 0 \end{bmatrix}. \tag{38}$$

with "$\hat{H}' \ll \hat{H}_0$*". The eigenstates of* $\hat{H}_0$ *are thus* $|\,g\,\rangle$ *and* $|\,e\,\rangle$ *with (effective*[1]*) energies* 0 *and* $-\Delta$*.*
To see this find out the eigenvalues for $\hat{H}_0$

$$Det \begin{bmatrix} -\lambda & 0 \\ 0 & -\Delta - \lambda \end{bmatrix} = 0 \tag{39}$$

$$\implies \lambda(\Delta + \lambda) = 0 \quad \implies \quad \lambda = 0,\ -\Delta \tag{40}$$

And the eigenstates

$$|\,g\,\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \textit{with} \quad \hat{H}_0|\,g\,\rangle = 0 \tag{41}$$

$$|\,e\,\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \textit{with} \quad \hat{H}_0|\,e\,\rangle = -\Delta|\,e\,\rangle \tag{42}$$

Then the first order energy corrections are zero:

$$E_0^{(1)} = \langle\, g\,|\hat{H}'|\,g\,\rangle = 0 \tag{43}$$

$$E_1^{(1)} = \langle\, e\,|\hat{H}'|\,e\,\rangle = 0 \tag{44}$$

[1] you will learn why in PHY402 why. Think of $|\,g\,\rangle$ as "atom in the ground-state and there is one photon" and $|\,e\,\rangle$ as " atom in the excited state and there is no photon".

The second order correction to the ground state energy is

$$E_0^{(2)} = \frac{|\langle e|\hat{H}'|g\rangle|^2}{0-(-\Delta)} = \frac{1}{\Delta}\left(\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & 0\end{pmatrix}\begin{pmatrix}1 \\ 0\end{pmatrix}\right)^2 = \frac{\Omega^2}{4\Delta} \tag{45}$$

The second order correction to the excited state energy is

$$E_1^{(2)} = \frac{|\langle g|\hat{H}'|e\rangle|^2}{-\Delta-0} = -\frac{1}{\Delta}\left(\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0 & \frac{\Omega}{2} \\ \frac{\Omega}{2} & 0\end{pmatrix}\begin{pmatrix}0 \\ 1\end{pmatrix}\right)^2 = -\frac{\Omega^2}{4\Delta} \tag{46}$$

The first order correction to ground state is

$$|\Psi_0^{(1)}\rangle = \frac{\langle e|\hat{H}'|g\rangle}{0-(-\Delta)}|e\rangle = \frac{\Omega}{2\Delta}|e\rangle = \frac{\Omega}{2\Delta}\begin{pmatrix}0 \\ 1\end{pmatrix} \tag{47}$$

The first order correction to excited state is

$$|\Psi_1^{(1)}\rangle = \frac{\langle g|\hat{H}'|e\rangle}{-\Delta-0}|e\rangle = \frac{-\Omega}{2\Delta}|g\rangle = -\frac{\Omega}{2\Delta}\begin{pmatrix}1 \\ 0\end{pmatrix} \tag{48}$$

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(ii) If the light intensity varies with position $\Omega(\mathbf{r})$ discuss the resultant mechanical effect on the atom for all signs of Δ.
Solution: Let's imagine $\Omega(\mathbf{r}) \sim e^{-|\mathbf{r}|^2/2/\sigma^2}$. *This is not a too bad approximation near the focus of the laser beam. We can read from Eq. (47), that the energy shift of the ground-state atom is* $\Delta E \sim \frac{1}{2\Delta}e^{-|\mathbf{r}|^2/2/\sigma^2}$. *For* $\Delta > 0$ *this is a repulsive potential, and for* $\Delta < 0$ *an attractive potential. This simple model thus offers a first glimpse at optical trapping (and manipulations) of atoms.*