Harmonic Oscillator

In this notes we will be focusing on the nuclear motion of a diatomic system rather than the familiar electronic Hamiltonian we have been working with lately. For the particular case of a diatomic we will show how the nuclei describe an oscillatory motion around its equilibrium position. Then, this will lead naturally to the discussion of the Quantum Harmonic Oscillator.

A. The nuclear motion for a diatomic.

Previously we introduced the molecular Hamiltonian for a molecular system of M nuclei and N atoms. In that case the Hamiltonian look like

$$\hat{H} = \sum_{i=1}^{N} -\frac{1}{2}\nabla_i^2 + \sum_{\alpha=1}^{M} -\frac{1}{2M_\alpha}\nabla_\alpha^2 + \sum_{\alpha=1}^{M}\sum_{\beta>\alpha} \frac{Z_\alpha Z_\beta}{\left|\mathbf{R}_\alpha - \mathbf{R}_\beta\right|} + \sum_{i=1}^{N}\sum_{j>i}\frac{1}{\left|\mathbf{r}_i - \mathbf{r}_j\right|} - \sum_{\alpha=1}^{M}\sum_{i=1}^{N}\frac{Z_\alpha}{\left|\mathbf{R}_\alpha - \mathbf{r}_i\right|} \quad (1.1)$$

We have studied how within the Born-Oppenheimer approximation (nuclei fixed) the previous problem is separated into two Hamiltonians: one for the electronic motion and the other for the nuclear motion.

For the nuclear motion the Hamiltonian takes the following form

$$.\hat{H}_N = \sum_{\alpha=1}^{M} -\frac{1}{2M_\alpha}\nabla_\alpha^2 + U\left(\{\mathbf{R}_\alpha\}\right). \quad (1.2)$$

and therefore the Schrodinger equation looks like

$$\left[\sum_{\alpha=1}^{M} -\frac{1}{2M_\alpha}\nabla_\alpha^2 + U\left(\{\mathbf{R}_\alpha\}\right)\right]\Psi_N\left(\mathbf{R}_1, \mathbf{R}_2, ..., \mathbf{R}_M\right) = E_N\Psi_N\left(\mathbf{R}_1, \mathbf{R}_2, ..., \mathbf{R}_M\right) \quad (1.3)$$

For simplicity purposes we will focus on a diatomic system. Equation (1.3) then reduces to

$$\left[-\frac{1}{2M_1}\nabla_1^2 - \frac{1}{2M_2}\nabla_2^2 + U\left(\mathbf{R}_1, \mathbf{R}_2\right)\right]\Psi_N\left(\mathbf{R}_1, \mathbf{R}_2\right) = E_N\Psi_N\left(\mathbf{R}_1, \mathbf{R}_2\right) \quad (1.4)$$

Let us recall that $U\left(\{\mathbf{R}_\alpha\}\right)$ is the potential energy surfaces determined by the geometry of the system (that is by the position of the nuclei). In the particular case of a diatomic such a potential energy surface depends only on the relative position of the two nuclei $R = \left|\mathbf{R}_1 - \mathbf{R}_2\right|$. The general form of this potential is presented in Fig. 1. (taken from *Quantum Chemistry,* Levine I. N. 5th ed).

The value of $R = R_e$ at which the potential reaches it minimum is known as the *equilibrium internuclear distance.*
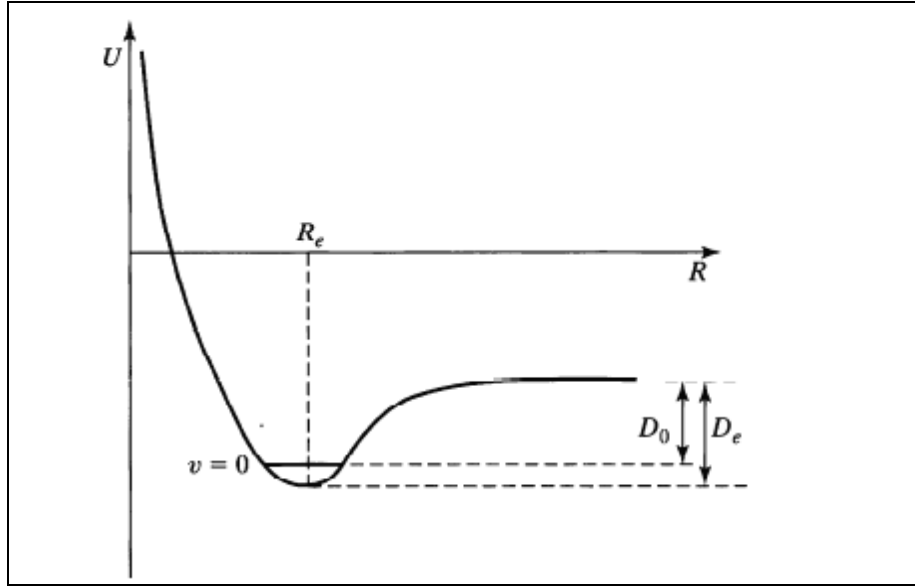
Fig. 1. Electronic energy including internuclear repulsion as a function of the internuclear distance R for a diatomic-molecule bound electronic state.

We mentioned earlier this potential has a finite value when the separation between nuclei is very big. Let us denote such a value by U_∞. Then

$$U_\infty = \lim_{R \to \infty} U(R) \tag{1.5}$$

If we pull apart the two nuclei that compose the system until the point in which there is no bond anymore, then the energy that would take to break it can be expressed as

$$D_e = U_\infty - U(R_e) \tag{1.6}$$

The fact that for a diatomic the potential depends only on the relative position of the nuclei is very convenient for further development. This will permit us to make a convenient change of variables in the Schrodinger equation of interest. Indeed, for this sort of systems it is very standard to introduce the center of mass system. This change of coordinates is given by

$$\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1$$
$$\mathbf{r} = \frac{M_1 \mathbf{R}_1 + M_2 \mathbf{R}_2}{M_1 + M_2} \tag{1.7}$$

and therefore the nuclear coordinates can be expressed in terms of the relative position and the center of mass vector as

$$\mathbf{R}_1 = \mathbf{r} - \frac{M_2}{M_1 + M_2}\mathbf{R}$$

$$\mathbf{R}_2 = \mathbf{r} - \frac{M_1}{M_1 + M_2}\mathbf{R} \tag{1.8}$$
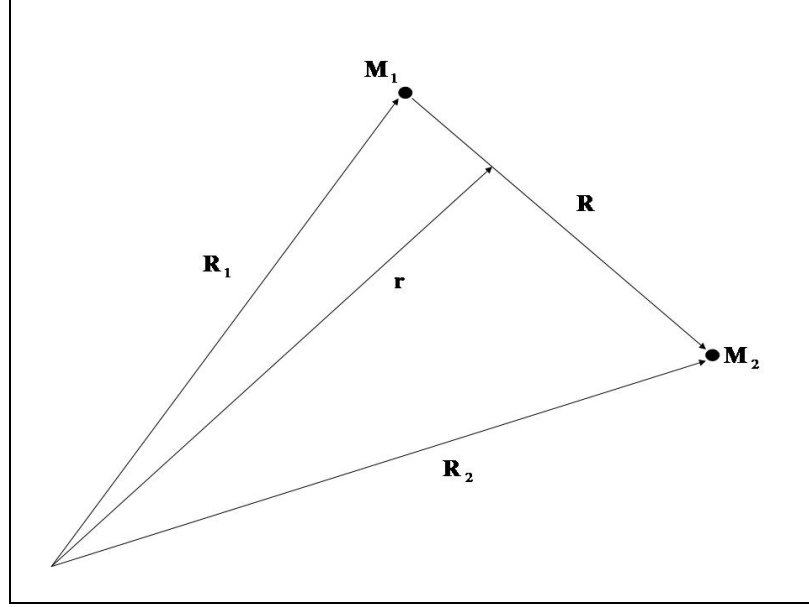

Fig. 2. The two-nuclei system with its corresponding center of mass system of coordinates.

With this change of coordinates the Laplacians that appear in (1.4) are given in terms of the new coordinates as

$$\nabla_1^2 = \frac{M_1^2}{\left(M_1 + M_2\right)^2}\nabla_r^2 - 2\frac{M_1}{M_1 + M_2}\nabla_r \cdot \nabla_R + \nabla_R^2$$

$$\nabla_2^2 = \frac{M_2^2}{\left(M_1 + M_2\right)^2}\nabla_r^2 + 2\frac{M_1}{M_1 + M_2}\nabla_r \cdot \nabla_R + \nabla_R^2 \tag{1.9}$$

After substituting (1.9) in (1.4) we obtain

$$\left[-\frac{1}{2}\frac{1}{\left(M_1 + M_2\right)}\nabla_r^2 - \frac{1}{2}\frac{M_1 + M_2}{M_1 M_2}\nabla_R^2 + U\left(R\right)\right]\Psi_N\left(\mathbf{R}_1, \mathbf{R}_2\right) = E_N \Psi_N\left(\mathbf{R}_1, \mathbf{R}_2\right) \tag{1.10}$$

As we can notice, changing into center of mass coordinates is advantageous since the two-body problem is now turned into two one particle problems. One of the equations represents translational motion of the entire molecule while the other one

represents relative motion between the nuclei. Then this suggest to propose the wave function that solves eq. (1.10) as

$$\Psi_N\left(\mathbf{R}_1,\mathbf{R}_2\right)=\psi_{N,tr}\left(\mathbf{r}\right)\psi_{N,\mathrm{int}}\left(\mathbf{R}\right) \tag{1.11}$$

This separation of variables takes (1.10) to the following couple of equations

$$\left[\frac{1}{2}\frac{M_1+M_2}{M_1M_2}\nabla_R^2+U\left(R\right)\right]\psi_{N,\mathrm{int}}\left(\mathbf{R}\right)=E_{N,\mathrm{int}}\psi_{N,\mathrm{int}}\left(\mathbf{R}\right)$$

$$\left[-\frac{1}{2}\frac{1}{\left(M_1+M_2\right)}\nabla_r^2\right]\psi_{N,tr}\left(\mathbf{r}\right)=E_{N,tr}\psi_{N,tr}\left(\mathbf{r}\right) \tag{1.12}$$

We notice that the second equation in (1.12) looks like the Hamiltonian of a particle in a three dimensional box whose dimensions are those of a container holding the gas of diatomic molecules. Then the wave function $\psi_{N,tr}\left(\mathbf{r}\right)$ is related to the three dimensional particle in a box system. The wave function $\psi_{N,\mathrm{int}}\left(\mathbf{R}\right)$ will be related to the quantum harmonic oscillator which is precisely the discussion we will be focusing on in this notes.

Rewriting the first equation of (1.12) we obtain

$$\left[-\frac{1}{2\mu}\nabla_R^2+U\left(\mathbf{R}\right)\right]\psi_{N,\mathrm{int}}\left(\mathbf{R}\right)=E_N\psi_{N,\mathrm{int}}\left(\mathbf{R}\right) \tag{1.13}$$

with the *reduced mass* given by

$$\mu=\frac{M_1M_2}{M_1+M_2} \tag{1.14}$$

If we fix one of the nuclei at the origin of coordinates we will notice that (1.10) takes the form of the hydrogen-like Schrodinger equation studied before. So, by doing so the equation can be solved by proposing the same separation of variables it was proposed back then

$$\psi_{N,\mathrm{int}}\left(\mathbf{R}\right)=P\left(R\right)Y_J^M\left(\theta_N,\phi_N\right) \tag{1.15}$$

where the subindex *N* has been included to specify we are dealing with nuclear coordinates and $Y_J^M\left(\theta_N,\phi_N\right)$ are the usual spherical coordinates. Let us recall that $J=0,1,2,...$ and $M=-J,-J+1,...,-1,0,1,...,J-1,J$.

Just like in the Hydrogen-like atom, after this separation of variables the radial equation takes the following form

$$-\frac{\hbar^2}{2\mu}\left[\frac{d^2P}{dR^2}+2\frac{dP}{dR}\right]+\frac{J(J+1)\hbar^2}{2\mu R^2}P(R)+U(R)P(R)=E_{int,R}P(R) \qquad (1.16)$$

In order to simplify (1.16) we apply the following change of variables

$$P(R)=\frac{F(R)}{R} \qquad (1.17)$$

which transforms (1.16) into

$$-\frac{\hbar^2}{2\mu}\frac{d^2F}{dR^2}+\left[U(R)+\frac{J(J+1)\hbar^2}{2\mu R^2}\right]F(R)=E_{int,R}F(R) \qquad (1.18)$$

We can recognize the term in square brackets as an effective potential. That is

$$V_{eff}(R)=U(R)+\frac{J(J+1)\hbar^2}{2\mu R^2} \qquad (1.19)$$

With this effective potential (1.19) takes the form of a typical Schrodinger equation. In order to solve it we will approximate (1.19) through a couple of Taylor series.

The first Taylor series will be applied on the $U(R)$ term around the equilibrium position R_e. That is

$$U(R)=U(R_e)+U'(R_e)\cdot(R-R_e)+\frac{1}{2}U''(R_e)\cdot(R-R_e)^2+... \qquad (1.20)$$

Since R_e is the position at which the potential reaches its minimum, the second term of the right side of (1.19) is zero. By denoting $k_e=U''(R_e)$ we have then

$$U(R)\simeq U(R_e)+\frac{1}{2}k_e(R-R_e)^2+... \qquad (1.21)$$

After substituting (1.21) in (1.18) we obtain

$$-\frac{\hbar^2}{2\mu}\frac{d^2F}{dR^2}+\left[U(R_e)+\frac{1}{2}k_e(R-R_e)^2+\frac{J(J+1)\hbar^2}{2\mu R^2}\right]F(R)=E_{int,R}F(R) \qquad (1.22)$$

It is convenient to make a new change of variables in (1.22). Such a change I given by

$$x=R-R_e \qquad (1.23)$$

Then (1.22) takes the form

$$-\frac{\hbar^2}{2\mu}\frac{d^2G}{dx^2}+\left[U(R_e)+\frac{1}{2}k_ex^2+\frac{J(J+1)\hbar^2}{2\mu(x+R_e)^2}\right]G(x)=E_{int,R}G(x) \qquad (1.24)$$

where

$$G(x)=F(R) \qquad (1.25)$$

The second Taylor series will be applied in the second term in square brackets in eq. (1.24). This development looks like

$$\frac{1}{(x+R_e)^2}=\frac{1}{\left[R_e\left(1+\dfrac{x}{R_e}\right)\right]^2}=\frac{1}{R_e^2\left(1+\dfrac{x}{R_e}\right)^2}=\frac{1}{R_e^2}\left[1-2\frac{x}{R_e}+3\frac{x^2}{R_e^2}-...\right] \qquad (1.26)$$

Since we are assuming that $R\simeq R_e$ then $x\ll 1$ (that is, very small). Therefore we neglect all powers of $\dfrac{x}{R_e}$ and we keep only the constant term. Therefore

$$\frac{1}{(x+R_e)^2}\simeq\frac{1}{R_e^2} \qquad (1.27)$$

After substituting (1.27) into (1.24) we obtain the following equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2G}{dx^2}+\left[U(R_e)+\frac{1}{2}k_ex^2+\frac{J(J+1)\hbar^2}{2\mu R_e^2}\right]G(x)=E_{int,R}G(x) \qquad (1.28)$$

or equivalently

$$-\frac{\hbar^2}{2\mu}\frac{d^2G}{dx^2}+\frac{1}{2}k_ex^2G(x)=\left[E_{int,R}-U(R_e)-\frac{J(J+1)\hbar^2}{2\mu R_e^2}\right]G(x) \qquad (1.29)$$

We notice that eq. (1.29) is the equation of a quantum harmonic oscillator (see section B of these notes). The energy spectrum of this system are given by $\left(n+\dfrac{1}{2} \right)h\nu$.

Therefore

$$E_{\text{int},R} - U\left(R_e \right) - \frac{J\left(J+1 \right)\hbar^2}{2\mu R_e^2} = \left(n+\frac{1}{2} \right)h\nu \tag{1.30}$$

and finally

$$E_{\text{int},R} = U\left(R_e \right) + \frac{J\left(J+1 \right)\hbar^2}{2\mu R_e^2} + \left(n+\frac{1}{2} \right)h\nu \tag{1.31}$$

Working backwards (equations 1.15, 1.17 and 1.25) and considering the solutions to the harmonic oscillator (equation 1.48), it can be verified that (1.15) takes the form

$$\psi_{N,\text{int}}\left(R,\theta_N,\phi_N \right) = \frac{1}{\sqrt{2^n}\sqrt{\pi}n!} e^{-y^2/2} \frac{H_n\left(y \right)}{R} Y_J^M\left(\theta_N,\phi_N \right)$$

$$y = \frac{\mu\nu}{h}\left(R - R_e \right) \tag{1.32}$$

Then we have showed how the nuclei of a diatomic will describe a harmonic oscillatory motion around its equilibrium point. The details about the quantum harmonic oscillator are presented in the following section.

B. The Quantum Harmonic Oscillator.

From first year physics we remember that the simplest picture of a harmonic oscillator is that of a point mass μ attached to a spring with elastic constant k_e. The force that the mass experiences is given by Hooke's law

$$F_{Hooke} = -k_e x \tag{1.33}$$

with the following potential energy

$$U\left(x \right) = \frac{1}{2}k_e x^2 \tag{1.34}$$

Then the total energy of this system is given by

$$E = \frac{p^2}{2\mu} + \frac{1}{2}k_e x^2 \tag{1.35}$$

One of the important conclusions about this system is that the natural frequency of the oscillations performed by the point mass is given in terms of its mass μ and the elastic constant k_e. The frequency and angular frequencies are given, respectively, by

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k_e}{\mu}} \tag{1.36}$$

$$\omega = \sqrt{\frac{k_e}{\mu}} \tag{1.37}$$

Taking this into a Quantum Mechanical context (that is replacing the dynamic variables by the corresponding operators) it is easily verified that the Schrodinger equation for the harmonic oscillator system is given by

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{1}{2}k_e x^2\psi = E\psi \tag{1.38}$$

or considering the angular frequency can be expressed as

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{1}{2}\mu\omega^2 x^2\psi = E\psi \tag{1.39}$$

Now we do some work on the equation before attempting to solve it. We perform the following change of variables

$$y = \alpha x \tag{1.40}$$

where

$$\alpha^4 = \frac{\mu k_e}{\hbar^2} = \frac{\mu^2\omega^2}{\hbar^2}$$

After using the chain rule to express the second derivative with respect of x in terms of the second derivative respect to y the previous differential equation takes the following form

$$\frac{d^2\psi}{dy^2} + \left(\lambda - y^2\right)\psi = 0 \tag{1.41}$$

with $\lambda = \dfrac{2E}{\hbar\omega} = \dfrac{2E}{h\nu}$

This is a very standard differential equation in the field of Mathematical-Physics. Indeed, the differential equation:

$$\varphi_n''(z) + \left(2n + 1 - z^2\right)\varphi_n(z) = 0 \qquad (1.42)$$

has known solutions given by

$$\varphi_n(x) = e^{-x^2/2} H_n(x) \qquad (1.43)$$

where the functions $H_n(x)$ are the *Hermite polynomials.* These polynomials can be obtained by the use of the Rodrigues' formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right) \qquad (1.44)$$

We present a few of these polynomials

$$
\begin{aligned}
H_0(z) &= 1 \\
H_1(z) &= 2z \\
H_2(z) &= 4z^2 - 2 \\
H_3(z) &= 8z^3 - 12z
\end{aligned}
\qquad (1.45)
$$

Based on these it is possible to obtain Hermite polynomials of higher order by the use of the following recurrence relationships

$$
\begin{aligned}
H_{n+1}(z) &= 2zH_n(z) - 2nH_{n-1}(z) \\
\frac{dH_n}{dz}(z) &= 2nH_{n-1}(z)
\end{aligned}
\qquad (1.46)
$$

Hermite polynomials are orthogonal,

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x)\,dx = 2^n \sqrt{\pi}\, n!\, \delta_{mn} \qquad (1.47)$$

Based on (1.41), (1.42), (1.43) and (1.47) we conclude that the normalized wave function for the harmonic oscillator is given by

$$\psi_n(y) = \frac{1}{\sqrt{2^n \sqrt{\pi} n!}} e^{-y^2/2} H_n(y)$$

$$y = \sqrt{\frac{\mu\omega}{\hbar}} x$$

(1.48)

with energies

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)h\nu$$

(1.49)

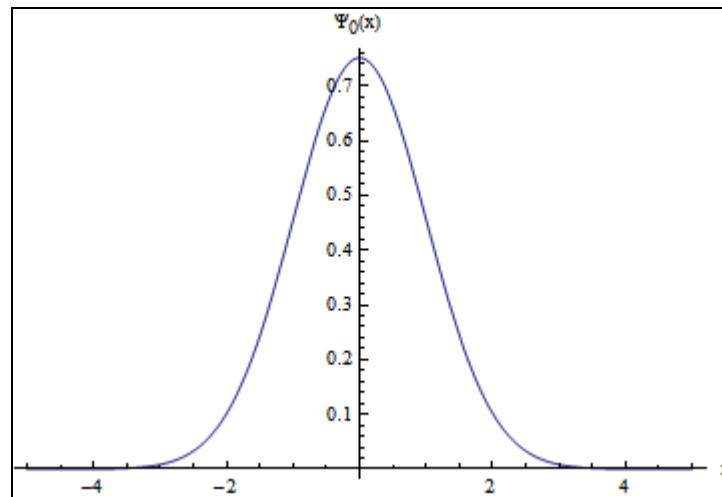Below we present some of the wave functions for the harmonic oscillator

Fig. 1. Ground state harmonic oscillator wave function

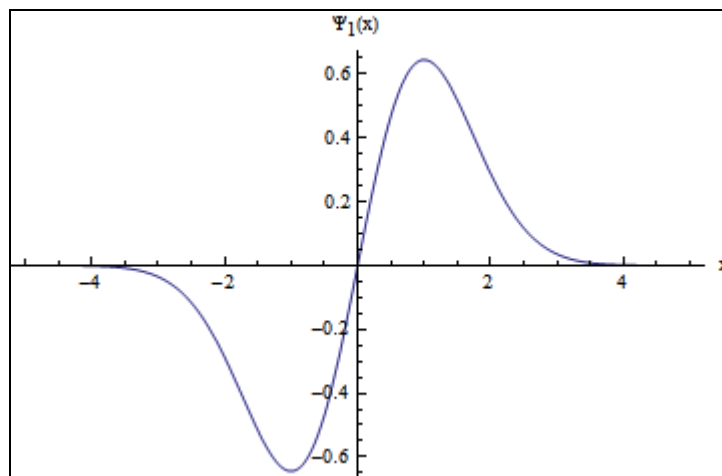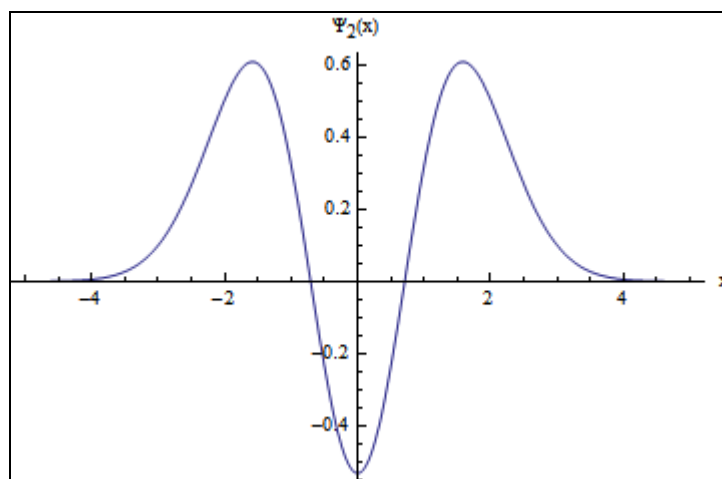Fig. 2. First excited state harmonic oscillator wave function

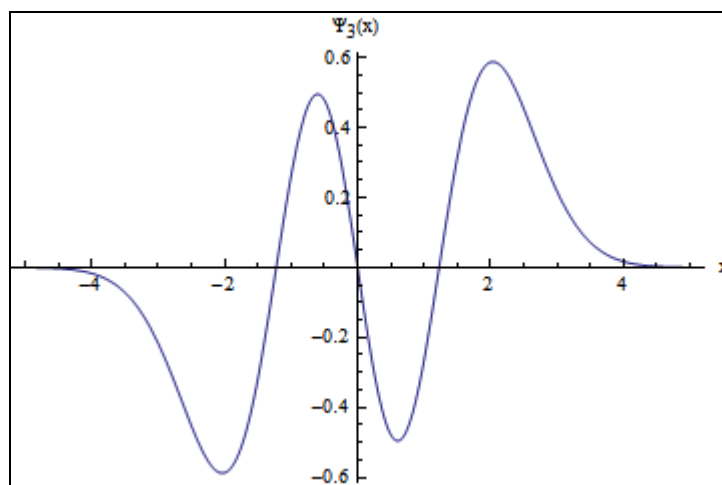Fig. 3. Second excited state harmonic oscillator wave function

Fig. 4. Third excited state harmonic oscillator wave function

Additionally it can be mentioned there is an equivalent treatment for the quantum harmonic oscillator based on *creation and annihilation operators.* This is a powerful technique that will permit to compute expectation values easily without any explicit computation of integrals.

This approach is presented in the next section of these notes.

C. Creation and Annihilation Operators

We have presented in the previous section the solution to the Schrodinger equation for the harmonic oscillator. They are given in terms of the Hermite polynomials in a very complicated way. Then they are not the best we can wish for to perform calculations with. Nevertheless there is an alternative treatment for the harmonic oscillator through *creation and annihilation* operators.

This section is devoted to the introduction of this useful technique.

We start with equation (1.39), which is the Hamiltonian for the harmonic oscillator. Let us express it in terms of the momentum operator. That is

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2\hat{x}^2$$
$$= \hbar\omega\left[\frac{1}{2\mu\hbar\omega}\hat{p}^2 + \frac{\mu\omega^2}{2\hbar\omega}\hat{x}^2\right]$$

(1.50)

Let us do some mathematical manipulation on (1.50)

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2\hat{x}^2$$
$$= \hbar\omega\left[\frac{1}{2\mu\hbar\omega}\hat{p}^2 + \frac{\mu\omega^2}{2\hbar\omega}\hat{x}^2\right]$$
$$= \hbar\omega\left\{\frac{\mu\omega^2}{2\hbar\omega}\left[\hat{x}^2 + \frac{2\hbar\omega}{2\mu^2\hbar\omega^3}\hat{p}^2\right]\right\}$$
$$= \hbar\omega\left\{\frac{\mu\omega}{2\hbar}\left[\hat{x}^2 + \frac{1}{\mu^2\omega^2}\hat{p}^2\right]\right\}$$
$$= \hbar\omega\left\{\left(\sqrt{\frac{\mu\omega}{2\hbar}}\right)^2\left[\hat{x}^2 + \frac{1}{\mu^2\omega^2}\hat{p}^2\right]\right\}$$

(1.51)

Let us notice that the term in square brackets is a sum of two squares. Clearly these expressions can be factorized using complex numbers as a product

of conjugate binomials. However, in this particular case we should be careful since the objects we are dealing with are operators and they do not commute. A useful identity for the further development is the commutation relation between the position and momentum operator

$$[\hat{x},\hat{p}]=i\hbar \tag{1.52}$$

Equipped with this identity we continue with the development of (1.51). It can be verified that

$$
\begin{aligned}
\hat{H} &= \hbar\omega\left\{\left(\sqrt{\frac{\mu\omega}{2\hbar}}\right)^2\left[\hat{x}^2+\frac{1}{\mu^2\omega^2}\hat{p}^2\right]\right\} \\
&= \hbar\omega\left\{\left(\sqrt{\frac{\mu\omega}{2\hbar}}\right)^2\left[\left(\hat{x}-\frac{i}{\mu\omega}\hat{p}\right)\left(\hat{x}+\frac{i}{\mu\omega}\hat{p}\right)-\frac{i}{\mu\omega}(\hat{x}\hat{p}-\hat{p}\hat{x})\right]\right\} \\
&= \hbar\omega\left\{\left(\sqrt{\frac{\mu\omega}{2\hbar}}\right)^2\left[\left(\hat{x}-\frac{i}{\mu\omega}\hat{p}\right)\left(\hat{x}+\frac{i}{\mu\omega}\hat{p}\right)\right]-\left(\sqrt{\frac{\mu\omega}{2\hbar}}\right)^2\left[\frac{i}{\mu\omega}[\hat{x},\hat{p}]\right]\right\} \quad (1.53) \\
&= \hbar\omega\left\{\left[\sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x}-\frac{i}{\mu\omega}\hat{p}\right)\sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x}+\frac{i}{\mu\omega}\hat{p}\right)\right]+\left(\sqrt{\frac{\mu\omega}{2\hbar}}\right)^2\left[\frac{\hbar}{\mu\omega}\right]\right\} \\
&= \hbar\omega\left\{\left[\sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x}-\frac{i}{\mu\omega}\hat{p}\right)\sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x}+\frac{i}{\mu\omega}\hat{p}\right)\right]+\frac{1}{2}\right\}
\end{aligned}
$$

Introducing the notation

$$
\begin{aligned}
\hat{a}^+ &= \sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x}-\frac{i}{\mu\omega}\hat{p}\right) \\
\hat{a} &= \sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x}+\frac{i}{\mu\omega}\hat{p}\right)
\end{aligned} \tag{1.54}
$$

the Hamiltonian (1.53) takes the following form

$$\hat{H}=\hbar\omega\left(\hat{a}^+\hat{a}+\frac{1}{2}\right) \tag{1.55}$$

Operators (1.54) are called, respectively, *creation and annihilation* operators and expression (1.55) sometimes is referred to as the *factorization of the Hamiltonian*.

In order to understand the name given to these operators we state that it can directly verified that they have the following properties

$$\hat{a}^+\psi_n = \sqrt{n+1}\,\psi_{n+1}$$
$$\hat{a}\psi_n = \sqrt{n}\,\psi_{n-1}$$

(1.56)

These identities can be obtained by means of (1.46) and by recalling that the momentum operator is essentially the derivative operator and the position operator is just a product by position.

From (1.56) clearly we can interpret $\hat{a}^+$, $\hat{a}$ as operators that enable us to obtain states with higher or lower energy with respect to the original state taken.

These operators, as mentioned before, are very convenient when computing matrix elements of operators related to position and momentum. That is, from (1.54) we can solve for position and momentum operators in terms of the creation and annihilation ones

$$\hat{x} = \sqrt{\frac{\hbar}{2\mu\omega}}\left(\hat{a} + \hat{a}^+\right)$$
$$\hat{p} = i\sqrt{\frac{\mu\hbar\omega}{2}}\left(-\hat{a} + \hat{a}^+\right)$$

(1.57)

Since we know (from 1.56) what the effect of the creation and annihilation operators are on the wave functions of the harmonic oscillator, it is easy to verify that

$$\langle\psi_m|\hat{x}|\psi_n\rangle = \sqrt{\frac{\hbar}{2\mu\omega}}\left(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right)$$
$$\langle\psi_m|\hat{p}|\psi_n\rangle = i\sqrt{\frac{\mu\hbar\omega}{2}}\left(-\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right)$$

(1.58)

The matrix elements (1.58) are useful particularly when we are dealing with selection rules (electric dipole at least). The conclusion is that the only transitions allowed for the harmonic oscillator are $\Delta n = n_f - n_i = \pm 1$.