1 Harmonic Oscillator

Harmonic oscillators are useful models of complicated potentials in a variety of disciplines including:

– quantum theory of electromagnetic radiation
– study of lattice vibrations in crystalline solids
– infrared spectra of diatomic molecules

Actually, classical systems rarely execute simple oscillatory motion; more often they undergo damped or forced harmonic motion. Even if particles execute complicated harmonic motion, their small excursion about equilibrium can be accurately approximated by the simple harmonic oscillator. Hence, the SHO (simple harmonic oscillator) is a starting point for study of any system whose particles oscillate about equilibrium positions.

Example 1

Consider a point moving along the circumference of a circle at a constant angular frequency ω_0. The projection of the point $x(t)$ is then given by

$$x(t) = A\cos(\omega_0 t + \phi) \tag{1}$$

where ω_0 is the so called natural frequency. The second derivative is

$$\begin{aligned} \frac{d^2x}{dt^2} &= -\omega_0^2 A\cos(\omega_0 t + \phi) && (2) \\ &= -\omega_0^2 x(t) && (3) \end{aligned}$$

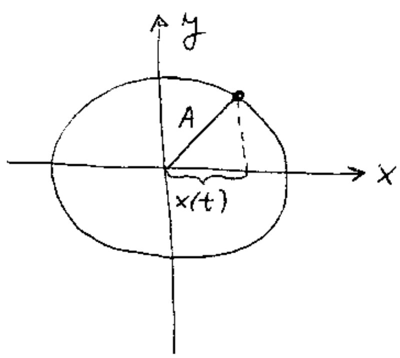

Figure 1: A point moving in a circular path

The above expression is the famous differential equation of SIMPLE harmonic motion.

Example 2

Consider now mass on a spring. If the wall is immovable and the spring is ideal, and if friction and gravity are negligible, then the force on the mass trying to restore it to its equilibrium position x_E is

$$F = m\frac{d^2x}{dt^2} \tag{4}$$
$$= -k_f(x - x_E) \tag{5}$$

where k_f is the force constant.

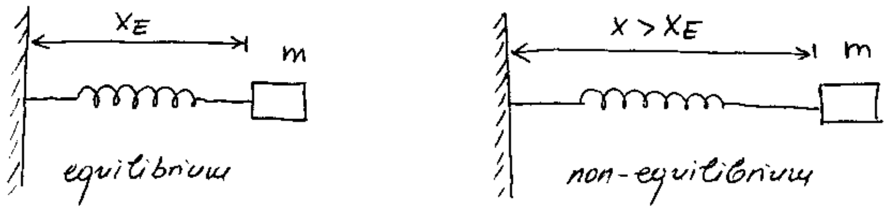

Figure 2: Spring system.

The trajectory of the mass object is then

$$\frac{d^2x}{dt^2} = -\frac{k_f}{m}(x - x_E) \tag{6}$$
$$= -\omega_0^2(x - x_E) \tag{7}$$

where

$$\omega_0 = \sqrt{\frac{k_f}{m}} \tag{8}$$

is the natural frequency that is related to the physical properties of the system (the mass and the force constant of the spring).

The potential energy of the particle is simple given by

$$V(x) = -\int F dx \tag{9}$$
$$= +k_F \int x dx \tag{10}$$
$$= \frac{1}{2}k_F x^2 \tag{11}$$
$$= \frac{1}{2}m\omega_0^2 x^2 \tag{12}$$

The total energy is just $V(x)+$kinetic energy, i.e.,

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 \tag{13}$$

$$= \text{const (conserved)} \tag{14}$$

As the particle oscillates back and forth, its kinetic energy and speed change because its potential energy changes. To understand this, we need rigorous derivation for $V(x)$

$$V(x) = \frac{1}{2}m\omega_0^2(x-x_E)^2 \tag{15}$$

$$\rightarrow \text{At equilibrium, potential energy is zero and k.e. is maximum}$$

At the classical turning point, k.e. is zero, and the p.e. is maximum, i.e.,

$$E = \frac{1}{2}m\omega_0^2(x_m-x_E)^2 \tag{16}$$

$$\Rightarrow x_m - x_E = \delta x_m$$

$$= \sqrt{\frac{2E}{m\omega_0^2}} \tag{17}$$

Near these points, the particle slows down, stops and turns around.

From the above observations, we can predict the outcome of a measurement of the position of a classical SHO. During one period of oscillations, it is most likely to find the particle at positions where its speed is the smallest, i.e., near the CLASSICAL TURNING POINT. Later on, we will compare this prediction with what quantum physics predicts for a microscopic oscillator.

Classical Probability Density

To define a probability, we must identify an ensemble, i.e., a large number of identical, non-interacting systems, all in the same state. For macroscopic systems, in a position measurement at a fixed time, all the members of the ensemble would yield the same result. Thus, we will assume that the positions of the members of the ensemble are measured at random times. We thus define classical probability density

$$P_{\text{cl}}(x)dx = \text{probability of finding the particle in the interval } x \text{ to } x+dx \tag{18}$$

If $T_0 = \frac{2\pi}{\omega_0}$ is the time required for the particle to carry out one cycle of simple harmonic motion then

$$
\begin{aligned}
P_{\text{cl}}(x)dx &= \frac{dt}{T_0} && (19)\\
&\rightarrow \text{fraction of the period that the} \\
&\quad\ \text{particle spends in the interval } x \text{ at } x && (20)
\end{aligned}
$$

Now, consider EXAMPLE 1 assuming $\phi = -\pi/2$. For this particular case

$$x(t) = A\sin(\omega_0 t) \tag{21}$$

The time dt is related to the velocity v by

$$
\begin{aligned}
v &= \frac{dx}{dt} && (22)\\
&\Rightarrow \quad dt = \frac{dx}{v} && (23)
\end{aligned}
$$

which leads to

$$P_{\text{cl}}(x)dx = \frac{\omega_0}{2\pi}\frac{1}{v}dx \tag{24}$$

Since

$$
\begin{aligned}
v &= \frac{dx}{dt} && (25)\\
&= \omega_0 A\cos(\omega_0)\sqrt{A^2 - x^2(t)} && (26)\\
&= \omega_0\sqrt{A^2 - A^2\sin^2(\omega_0 t)} && (27)\\
&= \omega_0\sqrt{A^2 - x^2(t)} && (28)
\end{aligned}
$$

we arrive at

$$
\begin{aligned}
P_{\text{cl}}(x)dx &= \frac{\omega_0}{2\pi}\frac{1}{\sqrt{A^2 - x^2(t)}} && (29)\\
&= \frac{1}{2\pi}\frac{1}{\sqrt{A^2 - x^2(t)}} && (30)
\end{aligned}
$$

This function is the relative probability that in a measurement at a random time of the position of a macroscopic simple harmonic oscillator with energy E, we will obtain a value in the infinitesimal range dx at x.

To find the normalized classical probability density, we must normalize it, i.e.,

$$\int_{-\infty}^{\infty} P_{\text{cl}}(x)dx = 1 \tag{31}$$

which leads to

$$P_{\rm cl}(x)dx = \frac{1}{\pi\sqrt{A^2 - x^2}} \tag{32}$$

If the energy of the particle is E, we must have

$$\begin{aligned} E &= \underbrace{\frac{mv^2}{2}}_{\text{k.e.}} + \underbrace{\frac{1}{2}m\omega_0^2 x^2}_{\text{p.e.}} & (33) \\ &= \frac{1}{2}m\omega_0^2 A^2 \cos^2(\omega_0 t) + \frac{1}{2}m\omega_0^2 A \sin^2(\omega_0 t) \\ &= \frac{1}{2}m\omega_0^2 A^2 & (34) \end{aligned}$$

Thus

$$A^2 = \frac{2E}{m\omega_0^2} \tag{35}$$

or

$$\begin{aligned} P_{\rm cl}(x)dx &= \frac{1}{\pi\sqrt{\frac{2E}{m\omega_0^2} - x^2}} \\ &= \frac{\sqrt{m\omega_0^2}}{\pi} \frac{1}{\sqrt{2E - m\omega_0^2 x^2}} & (36) \end{aligned}$$

$P_{\rm cl}(x)$ predicts that the macroscopic simple harmonic oscillator is least likely to be found at equilibrium ($x = 0$), where it is moving most rapidly, and most likely to be found near the classical turning points, at which it will stop and turn around.

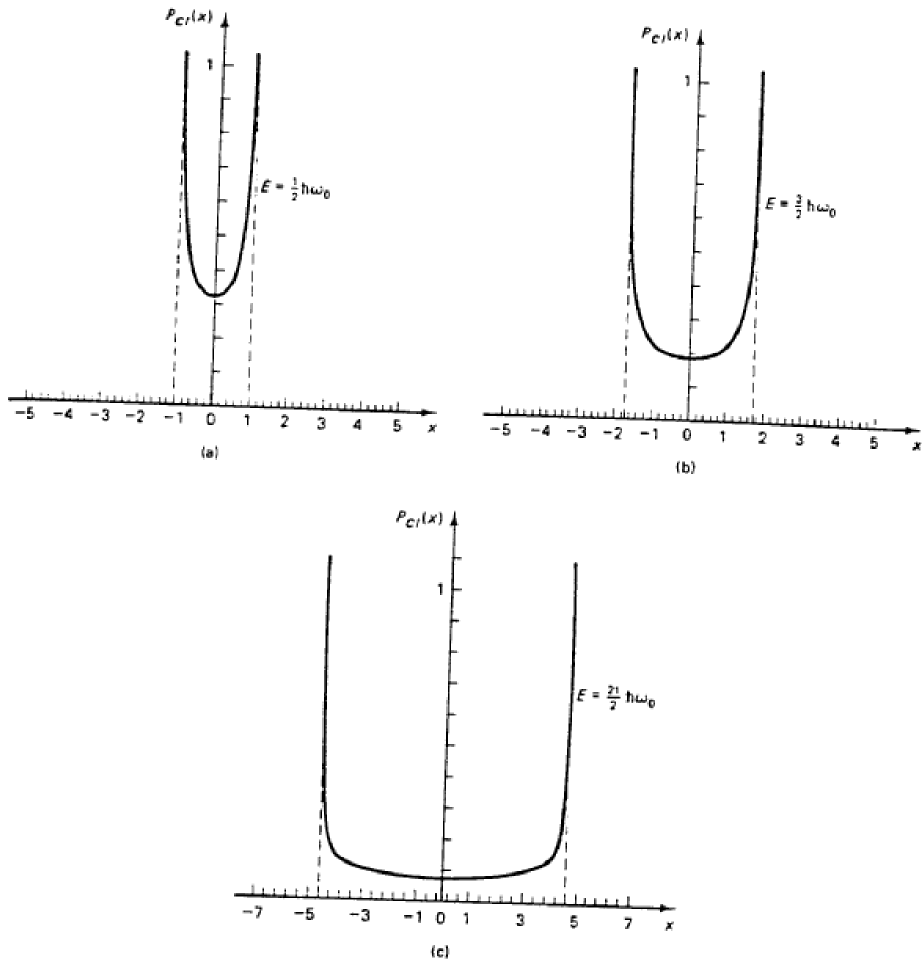

Figure 3: The classical probability function for three energies. These energies correspond to those of the ground state ($n = 0$), the first excited state ($n = 1$), and the tenth excited state ($n = 10$) of a microscopic oscillator with mass m and natural frequency ω_0.

The Quantum Simple Harmonic Oscillator

The Hamiltonian operator is

$$\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\hat{T}(x)} + \underbrace{\frac{1}{2}m\omega_0^2 x^2}_{V(x)} \tag{37}$$

(1) Because $V(x)$ increases without limit, it supports an infinite number of bound states, but no continuum states.

(2) Because $V(x)$ is symmetric, its eigenfunctions have definite parity.

We need to solve the time-independent SWE

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega_0^2 x^2\psi = E\psi \tag{38}$$

using the method of power series using the following game plan:

A CLEAN up TISE using intermediate quantities $\psi(x) \to \psi(\xi)$

B FIND THE SOLUTION IN THE asymptotic limit $\xi \to \infty$, $\psi(\xi) \to \chi(\xi)$

C FACTOR OUT THE ASYMPTOTIC BEHAVIOR: $\psi(\xi) - AH(\xi)\chi(\xi)$

D DERIVE A DIFFERENTIAL EQUATION FOR $H(\xi)$

E EXPAND THE UNKNOWN FUNCTION IN A POWER SERIES, i.e.,

$$H(\xi) = \sum_j c_j \xi^j \tag{39}$$

F PUT SERIES IN THE DE AND DERIVE RECURRENCE RELATION c_j in terms of c_{j-1}

G ENFORCE BOUNDARY CONDITIONS : QUANTIZE E

(A) Cleaning up of the TISE

We need to clean up the equation to minimize the number of symbols we must manipulate. Start with

$$\frac{d^2\psi}{dx^2} - \frac{m\omega_0^2}{\hbar^2}x^2\psi + \frac{2mE}{\hbar^2}\psi = 0 \tag{40}$$

Define

$$\boxed{\beta = \sqrt{\frac{m\omega_0}{\hbar}}} \tag{41}$$

and

$$\boxed{\xi = \beta x} \tag{42}$$

Then

$$\frac{d}{dx} \rightarrow \frac{d}{d\xi}\frac{d\xi}{dx} = \beta\frac{d}{d\xi} \tag{43}$$

$$\frac{d^2}{dx^2} = \frac{d}{dx}\left(\frac{d}{dx}\right) = \frac{d}{d\xi}\left(\beta\frac{d}{d\xi}\right)\frac{d\xi}{dx} = \beta^2\frac{d^2}{d\xi^2} \tag{44}$$

or

$$\begin{aligned}\left[\frac{m\omega_0}{\hbar}\frac{d^2}{d\xi^2} - \frac{m^2\omega_0^2}{\hbar^2}\frac{\xi^2}{\beta^2} + \frac{2mE}{\hbar^2}\right]\psi(\xi) &= 0 \\ \left[\frac{m\omega_0}{\hbar}\frac{d^2}{d\xi^2} - \frac{m^2\omega_0^2}{\hbar^2}\frac{\hbar}{m\omega_0}\xi^2 + \frac{2mE}{\hbar^2}\right]\psi(\xi) &= 0 \\ \left[\frac{d^2}{d\xi^2} - \xi^2 + \frac{\not{\hbar}}{\not{m}\hbar\omega_0}\frac{2\not{m}\not{\hbar}E}{\hbar^{\not{2}}}\right]\psi(\xi) &= 0\end{aligned} \tag{45}$$

$$\boxed{\left[\frac{d^2}{d\xi^2} - \xi^2 + \epsilon\right]\psi(\xi) = 0} \tag{46}$$

where

$$\boxed{\epsilon = \frac{2E}{\hbar\omega_0}} \tag{47}$$

This last equation is known as *Weber*'s equation. Since the solutions of this equation are known, we can simply write it down, but we won't learn anything about the physics behind it.

(B) Asymptotic limit

When confronted with an unfamiliar DE, the first thing that one needs to check is its asymptotic limit, i.e., when $\xi \rightarrow \infty$. In this limit $\xi^2 \gg \epsilon$ and we might ignore this term, to arrive at:

$$\left(\frac{d^2}{dx^2} - \xi^2\right)\chi(\xi) = 0 \tag{48}$$

We used the fact that as $\xi \rightarrow \infty, \psi(\xi) \rightarrow \chi(\xi)$.

The general solution of this equation is of the form

$$Ae^{-\xi^2/2} + Be^{\xi^2/2} \tag{49}$$

As $\xi \rightarrow$, one of the terms, the term $e^{\xi^2/2}$ blows up. To get an admissible solution to the TISE, we exploit the arbitrariness of the constants and assume that $B = 0$. Hence

$$\chi(\xi) = A^{-\xi^2/2} \tag{50}$$

which means that

$$\begin{aligned} \psi(\xi) &= AH(\xi)\chi(\xi) && (51) \\ &= AH(\xi)e^{-\xi^2/2} && (52) \end{aligned}$$

(C) Factor out Asymptotic Behavior and Find DE for $H(\xi)$
If we substitute the result for $\psi(\xi)$ into Weber's equation, we get

$$\begin{aligned} \frac{d}{d\xi}\psi &= A\frac{dH}{d\xi}e^{-\xi^2/2} - A\xi H(\xi)e^{-\xi^2/2} && (53) \\ \frac{d^2\psi}{s\xi^2} &= A\frac{d^2H}{d\xi^2}e^{-\xi^2/2} - A\xi\frac{dH}{d\xi}e^{-\xi^2/2} \\ &- AH(\xi)e^{-\xi^2/2} - A\xi\frac{dH}{d\xi}e^{-\xi^2/2} + A\xi^2H(\xi)e^{-\xi^2/2} && (54) \\ &= A\frac{d^2H}{d\xi^2}e^{-\xi^2/2} - 2A\xi\frac{dH}{d\xi}e^{-\xi^2/2} \\ &- AH(\xi)e^{-\xi^2/2} + A\xi^2H(\xi)e^{-\xi^2/2} && (55) \end{aligned}$$

Hence

$$\begin{aligned} &\cancel{A}\frac{d^2H}{d\xi^2}\cancel{e^{-\xi^2/2}} - 2\cancel{A}\xi\frac{dH}{d\xi}\cancel{e^{-\xi^2/2}} \\ &-\cancel{A}H\cancel{e^{-\xi^2/2}} + \cancel{A}\cancel{\xi^2He^{-\xi^2/2}} - \cancel{A}\cancel{\xi^2He^{-\xi^2/2}} + \cancel{A}\epsilon H\cancel{e^{-\xi^2/2}} = 0 && (56) \end{aligned}$$

or

$$\boxed{\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\epsilon - 1)H(\xi) = 0} \tag{57}$$

This last equation is called *Hermite differential equation.*
(E) Expand $H(\xi)$ in a Power Series
We will try to find a solution for this equation be expanding $H(\xi)$ in a power series, i.e., assuming

$$H(\xi) = \sum_{j=0}^{\infty} c_j \xi^j \tag{58}$$

We need to find the coefficients c_j to obtain $H(\xi)$. We can achieve this by substituting $H(\xi)$ in the DE, i.e., using that

$$\begin{aligned} \frac{dH}{d\xi} &= \sum_{j=1}^{\infty} j c_j \xi^{j-1} \\ &= \sum_{j=0}^{\infty} (j+1) c_{j+1} \xi^j \end{aligned} \tag{59}$$

$$\begin{aligned} \frac{d^2H}{d\xi^2} &= \sum_{j=2}^{\infty} j(j-1) c_j \xi^{j-2} \\ &= \sum_{j=0}^{\infty} (j+2)(j+1) c_{j+2} \xi^j \end{aligned} \tag{60}$$

Hence

$$\sum_{j=0}^{\infty} (j+2)(j+1) c_{j+2} \xi^j - 2\xi \sum_{j=1}^{\infty} j c_j \xi^{j-1} + (\epsilon - 1) \sum_{j=0}^{\infty} c_j \xi^j = 0 \tag{61}$$

$$\sum_{j=0}^{\infty} (j+2)(j+1) c_{j+2} \xi^j - 2 \sum_{j=1}^{\infty} j c_j \xi^j + (\epsilon - 1) \sum_{j=0}^{\infty} c_j \xi^j = 0 \tag{62}$$

$$c_2 + (\epsilon - 1) c_0 + \sum_{j=0}^{\infty} \left[(j+2)(j+1) c_{j+2} - 2 j c_j + (\epsilon - 1) c_j \right] \xi^j \tag{63}$$

For this expression to be zero, we must have that

$$c_2 + (\epsilon - 1) = 0 \tag{64}$$

$$(j+2)(j+1) c_{j+2} - 2 j c_j + (\epsilon - 1) c_j = 0 \tag{65}$$

or

$$\begin{aligned} c_2 &= (1-\epsilon) c_0, & j = 0 \\ c_{j+2} &= \frac{2j + (1-\epsilon)}{(j+1)(j+2)} c_j, & j = 1, 2, \cdots \end{aligned} \tag{66}$$

$$\boxed{\frac{c_{j+2}}{c_j} = \frac{2j + (1-\epsilon)}{(j+1)(j+2)}} \rightarrow \text{point (F)} \tag{67}$$

(a) Successive coefficients c_{j+2} and c_j are related through a recurrence relation.

(b) The energy variable appears in the recurrence relation (very important).

We can use the recurrence relation to determine terms in the Hermite series from the arbitrary coefficients c_0 and c_1, i.e.,

$$H(\xi) = \begin{cases} c_0 \left[1 + \frac{c_2}{c_0}\xi^2 + \frac{c_4}{c_2}\frac{c_2}{c_0}\xi^4 + \cdots\right] & \text{even parity function} \\ c_1 \left[\xi + \frac{c_3}{c_1}\xi^3 + \frac{c_5}{c_3}\frac{c_3}{c_1}\xi^5 + \cdots\right] & \text{odd parity function} \end{cases} \tag{68}$$

It looks like that we are done. We can calculate the arbitrary coefficients from the normalization of the eigenfunctions, but there is a major problem. The problem is not the convergence of the series, since

$$\frac{c_{j+2}\xi^{j+1}}{c_j\xi^j} = \frac{2j+1-\epsilon}{(j+1)(j+2)}\xi^2 \xrightarrow[j \to \infty]{} \frac{2\xi^2}{j} \to 0 \quad \text{d'Alembert ratio test} \tag{69}$$

The problem is what the series converges to, which brings us to the last point of our plan of attack.

(F) Enforce boundary conditions

For $|\xi| \to \infty$, the series converges to e^{ξ^2} which means that

$$\psi(\xi) = AH(\xi)e^{-\xi^2/2} \tag{70}$$

$$\xrightarrow[|\xi| \to \infty]{} Ae^{\xi^2}e^{-\xi^2/2} \tag{71}$$

$$\to Ae^{\xi^2/2} \tag{72}$$

Since the product is not bounded, it cannot be normalized and is thus not physically admissible.

We can eliminate this problem by enforcing all the coefficients larger than $c_{j_{\max}}$ to be zero by enforcing $c_{j_{\max}+2} = 0$. Then

$$2j_{\max} + 1 - \epsilon = 0 \qquad \text{or} \qquad \epsilon = 1 + 2j_{\max} \tag{73}$$

For any value of $j_{\max} > 0$, the above condition forces the Hermite series to be finite, and the resulting function is called *Hermite polynomial*, i.e.,

$$H(\xi) = \sum_{j=0}^{j_{\max}} c_j\xi^j, \qquad \epsilon = 2j_{\max} + 1 \tag{74}$$

$$\begin{array}{lllllllll} j_{\max} & = & 0 & \Rightarrow & \epsilon & = & 1 & H_0(\xi) & = & c_0 \\ j_{\max} & = & 1 & \Rightarrow & \epsilon & = & 3 & H_1(\xi) & = & c_1\xi \\ j_{\max} & = & 2 & \Rightarrow & \epsilon & = & 5 & H_2(\xi) & = & c_0 + c_2\xi^2 \\ j_{\max} & = & 3 & \Rightarrow & \epsilon & = & 7 & H_3(\xi) & = & c_1\xi + c_3\xi^3 \end{array} \tag{75}$$

where

$$
\begin{aligned}
c_2 &= \frac{1-\epsilon}{2} c_0 && (76)\\
&= \frac{1-5}{2} c_0 && (77)\\
&= -2c_0 && (78)
\end{aligned}
$$

$$
\begin{aligned}
c_3 &= \frac{2+(1-\epsilon)}{2\times 3} c_1 && (79)\\
&= \frac{2+1-7}{6} c_1 && (80)\\
&= -\frac{4}{6} c_1 && (81)\\
&= -\frac{2}{3} c_1 && (82)
\end{aligned}
$$

Here we have labeled the Hermite polynomials with the index $n = j_{\max}$. The energy variables is then

$$
\begin{aligned}
\epsilon_n &= 2n+1 && (83)\\
&= \frac{E_n}{\hbar\omega_0} && (84)
\end{aligned}
$$

or

$$\boxed{E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega_0} \qquad (85)$$

The requirement that $H_n(\xi)$ is a finite polynomial restricts the energies of the simple harmonic oscillator to $E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0$

Again, we have uncovered a subtile relation between mathematics and physics, the latter limiting the solutions provided by the former:

$$\boxed{\text{boundary conditions}} \Rightarrow \boxed{\text{energy quantization}} \qquad (86)$$

Choosing c_0 and c_1 to be equal to 1, we can now construct the first four Hermite polynomials, i.e.,

$$
\begin{array}{lcllc}
H_0(\xi) & = & 1 & & \\
H_1(\xi) & = & \xi & \rightarrow & 2\xi \\
H_2(\xi) & = & 1-2\xi^2 & \rightarrow & 4\xi^2-2 \\
H_3(\xi) & = & \xi - \frac{2}{3}\xi^3 & \rightarrow & 8\xi^3 - 12\xi
\end{array}
\qquad (87)
$$

The Hamiltonian eigenfunction $\psi_n(x)$ of the SHO is now

$$\psi_n(x) = A_n H_n(\beta x) e^{-\beta^2 x^2/2} \tag{88}$$

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}, \qquad n = 0, 1, 2\cdots \tag{89}$$

The corresponding eigenstates are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0, \qquad n = 0, 1, 2, \cdots \tag{90}$$

The only parts that need to be worked out are the normalization constant, for which it can be shown that

$$A_n = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \tag{91}$$

The corresponding wave function is then

$$\psi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\beta x) e^{-\beta^2 x^2/2} \tag{92}$$

Here is a summary

$$H_0(\xi) = 1 \tag{93}$$

$$H_1(\xi) = 2\xi \tag{94}$$

$$H_2(\xi) = 4\xi^2 - 2 \tag{95}$$

$$H_3(\xi) = 8\xi^3 - 12\xi \tag{96}$$

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \tag{97}$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi \tag{98}$$

$$H_6(\xi) = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \tag{99}$$

$$H_7(\xi) = 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi \tag{100}$$

$$H_8(\xi) = 256\xi^8 - 3584\xi^6 + 12440\xi^4 - 13440\xi^2 + 1680 \tag{101}$$

$$H_9(\xi) = 512\xi^9 - 9216\xi^7 + 48384\xi^5 - 80640\xi^3 + 30240\xi \tag{102}$$

$$\begin{array}{lll}
n & E_n & \psi_n(x) \\
0 & \frac{1}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-\beta^2x^2/2} \\
1 & \frac{3}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{2}} 2\beta x e^{-\beta^2x^2/2} \\
2 & \frac{5}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{8}} \left(4\beta^2x^2-2\right) e^{-\beta^2x^2/2} \\
3 & \frac{7}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{48}} \left(8\beta^3x^3-12\beta x\right) e^{-\beta^2x^2/2} \\
4 & \frac{9}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{384}} \left(16\beta^4x^4-48\beta^2x^2+12\right) e^{-\beta^2x^2/2} \\
5 & \frac{11}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{3840}} \left(32\beta^5x^5-160\beta^3x^3+120\beta x\right) e^{-\beta^2x^2/2}
\end{array} \tag{103}$$

The SHO - The Physics

In the previous section we derived the mathematical properties of the SHO - the eigenfunctions and the corresponding eigenvalues. Here, since our ultimate goal is the physical insight, we will focus on the statistical properties of this system.

(a) Classical turning point

The classical turning point is defined as the point where $E_n = V(x_n)$ or

$$\left(n + \frac{1}{2}\hbar\omega_0 = \frac{1}{2}m\omega_0^2 x_n^2\right) \tag{104}$$

Hence

$$\begin{aligned}
x_n^2 &= \frac{(2n+1)\hbar\omega_0}{m\omega_0^2} && (105) \\
&= \frac{(2n+1)\hbar}{m\omega_0} && (106) \\
&= \frac{2n+1}{\beta^2} && (107) \\
x_n &= \pm\sqrt{\frac{2n+1}{\beta^2}} && (108)
\end{aligned}$$

(b) Probability density $P_n(x)$

$P_n(x)$ tells us what to expect in a position measurement on an ensemble of SHO's in the n'th stationary state. There are several differences between the classical and quantum oscillator.

(1) The classical oscillator cannot penetrate into a forbidden region. No matter what state is in, the quantum oscillator does not penetrate into the classically forbidden regions.

(2) For small energies, the quantum physics predicts that the particle is most likely to be found in the center. Contrary to this, classical physics predicts that it is most likely to be found near the classical turning points. At higher energies, the two essentially predict the same result.

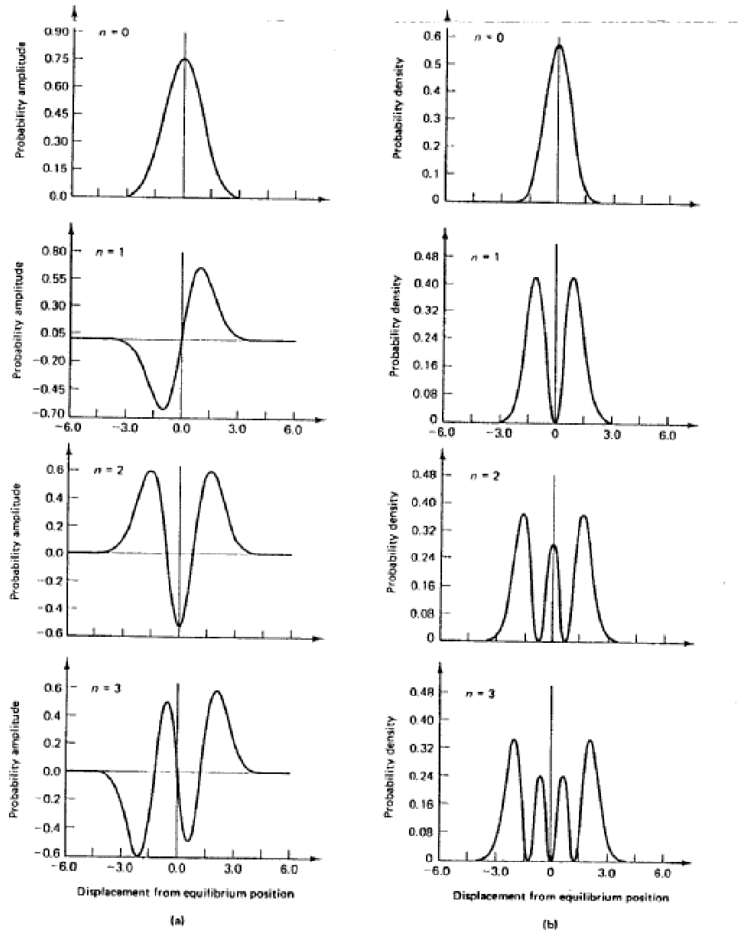

Figure 4: Eigen functions for the stationary states of the SHO with $n = 4, 5, 6$ and 7

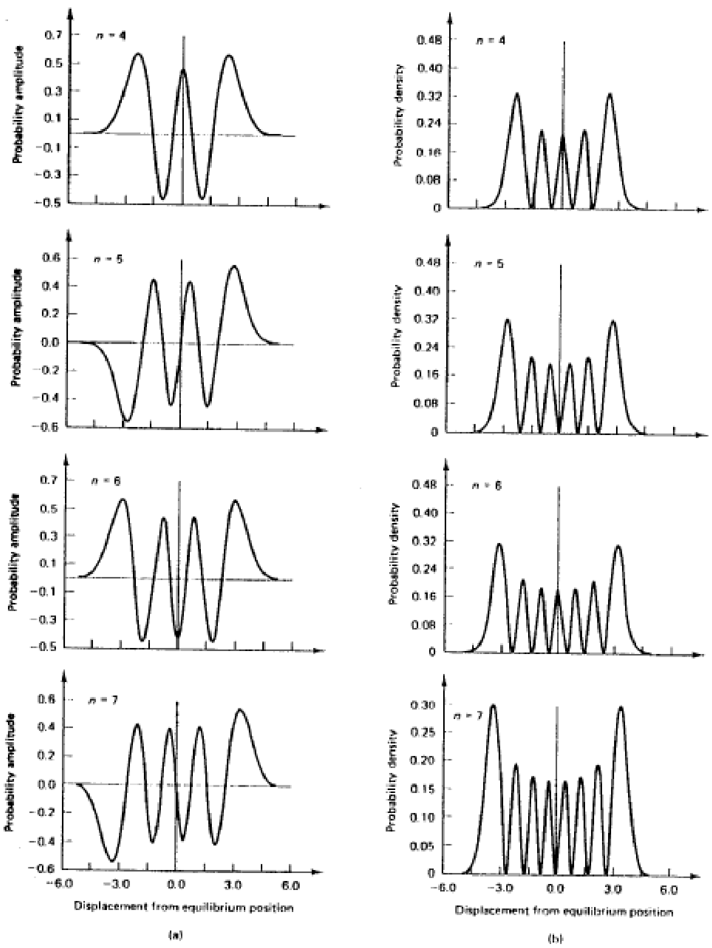

Figure 5: Probability densities for the stationary states of the SHO with $n = 4, 5, 6$ and 7

The following are handy integrals of eigenfunctions of the SHO.

$$\begin{aligned}
\beta &= \sqrt{\frac{m\omega_0}{\hbar}} \\
\int_{-\infty}^{\infty} \psi_n^*(x)\frac{d}{dx}\psi_m(x)dx &= \begin{cases} \beta\sqrt{\frac{n+1}{2}} & m = n+1 \\ -\beta\sqrt{\frac{n}{2}} & m = n-1 \\ 0 & \text{otherwise} \end{cases} \\
\int_{-\infty}^{\infty} \psi_n^*(x)x\frac{d}{dx}\psi_m(x)dx &= \begin{cases} \frac{1}{\beta}\sqrt{\frac{n+1}{2}} & m = n+1 \\ \frac{1}{\beta}\sqrt{\frac{n}{2}} & m = n-1 \\ 0 & \text{otherwise} \end{cases} \\
\int_{-\infty}^{\infty} \psi_n^*(x)x^2\frac{d}{dx}\psi_m(x)dx &= \begin{cases} \frac{2n+1}{2\beta^2} & m = n \\ \frac{\sqrt{(n+1)(n+2)}}{2\beta^2} & m = n+2 \\ 0 & \text{otherwise} \end{cases}
\end{aligned} \tag{109}$$

(c) Position and momentum expectation values and uncertainties

$$\langle x\rangle_n = \int_{-\infty}^{\infty} \psi_n^*(x)x\psi_n(x)dx = 0 \tag{110}$$

↖↗

even or odd functions
the product is an even
number

$$\langle p\rangle_n = \frac{\hbar}{i}\int_{-\infty}^{\infty} \psi_n^*(x)\frac{\partial\psi_n}{\partial x}dx = 0 \tag{111}$$

⟶ even → odd
odd → even

knowing the expectation values of position and momentum makes the evaluation of their uncertainties easier. For example

$$(\Delta x)_n = \sqrt{\langle x^2\rangle_n - \langle x\rangle_n^2} \tag{112}$$

$$= \sqrt{\langle x^2\rangle_n} \tag{113}$$

$$
\begin{aligned}
(\Delta p)_n &= \sqrt{\langle p^2\rangle_n - \langle p\rangle_n^2} &(114)\\
&= \sqrt{\langle p^2\rangle_n} &(115)
\end{aligned}
$$

where

$$
\begin{aligned}
\langle x^2\rangle_n &= \int_{\infty}^{\infty} \psi_n^*(x)x^2\psi_n(x)dx &(116)\\
\langle p^2\rangle_n &= -\hbar^2 \int_{\infty}^{\infty} \psi_n^*(x)\frac{d^2\psi_n}{dx^2}dx &(117)
\end{aligned}
$$

Using the results given in the Table, we have that

$$
\begin{aligned}
\langle x^2\rangle_n &= \frac{2n+1}{2\beta^2} &(118)\\
&= \frac{2n+1}{2m\omega_0/\hbar} &(119)\\
&= \frac{\left(n+\frac{1}{2}\right)\hbar\omega_0}{m\omega_0^2} &(120)\\
&= \frac{E_n}{m\omega_0^2} &(121)
\end{aligned}
$$

Thus

$$
(\Delta x)_n = \sqrt{\frac{E_n}{m\omega_0^2}} \qquad (122)
$$

$\rightarrow$ The position uncertainty increases with increasing energy (i.e., with increasing n)

At first glance, the evaluation of the momentum uncertainty looks very difficult since, in the position representation, $p^2 = -\hbar^2 d^2/dx^2$. We can avoid this complication by taking advantage of the TISE

$$
-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = \left[E_n - V(x)\right]\psi_n(x) \qquad (123)
$$

or

$$
\begin{aligned}
-\hbar^2\frac{d^2\psi_n}{dx^2} &= 2m\left[E_n - V(x)\right]\psi_n(x) &(124)\\
&= p^2\psi_n &(125)
\end{aligned}
$$

Using the above, we can get much simpler expression for this expectation value, i.e.,

$$\begin{aligned}
\langle p^2 \rangle &= \langle E_n - V(x) \rangle 2m & (126)\\
&= 2m \left[E_n - \frac{1}{2} m\omega_0^2 \langle x^2 \rangle_n \right] & (127)\\
&= 2m \left[E_n - \frac{1}{2} m\omega_0^2 \frac{E_n}{m\omega_0^2} \right] & (128)\\
&= 2m \left[E_n - \frac{1}{2} E_n \right] & (129)\\
&= mE_n & (130)
\end{aligned}$$

This simple result gives the equally simple momentum uncertainty

$$\begin{aligned}
(\Delta p)_n &= \sqrt{mE_n} & (131)\\
&= \sqrt{\left(n + \frac{1}{2}\right) \hbar\omega_0 m} & (132)
\end{aligned}$$

(d) The Heisenberg Uncertainty Principle for the SHO

Using the expressions for the position and momentum uncertainties for the n^{th} state (stationary) for a SHO, we can calculate the uncertainty product, i.e.,

$$\begin{aligned}
(\Delta x)_n (\Delta p)_n &= \sqrt{\frac{E_n}{m\omega_0^2}} \sqrt{mE_n} & (133)\\
&= \frac{E_n}{\omega_0} & (134)\\
&= \left(n + \frac{1}{2}\right) \hbar & (135)
\end{aligned}$$

The uncertainty product satisfies the uncertainty principle in a special way: for the ground state ($n = 0$) it is equal to $\hbar/2$, identically what we obtained for a Gaussian function.

A Simpler Approach with Operators

The normalized eigenfunctions of the harmonic oscillator all take the form

$$\psi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \tag{136}$$

where $\xi = \beta x$.

For the Hermit polynomials $H_n(\xi)$, the following two recurrence relations hold

$$
\begin{aligned}
\xi H_n &= n H_{n-1} + \frac{1}{2} H_{n+1} && (137)\\
\frac{d}{d\xi} H_n &= 2n H_{n-1} && (138)
\end{aligned}
$$

Using the above two equations, one can obtain a relationship between eigenfunctions of the harmonic oscillator, which belong to neighboring quantum numbers

$$
\begin{aligned}
H_n(\xi) &= \left(\frac{\pi}{\beta^2}\right)^{1/4} \psi_n(\xi) e^{\xi^2/2} \sqrt{2^n n!} && (139)\\
H_{n-1}(\xi) &= \left(\frac{\pi}{\beta^2}\right)^{1/4} \sqrt{2^{n-1}(n-1)!}\psi_{n-1}(\xi) e^{\xi^2/2} && (140)\\
H_{n+1}(\xi) &= \left(\frac{\pi}{\beta^2}\right)^{1/4} \sqrt{2^{n+1}(n-1)!}\psi_{n-1}(\xi) e^{\xi^2/2} && (141)
\end{aligned}
$$

Thus

$$
\begin{aligned}
\xi \cancel{\left(\frac{\pi}{\beta^2}\right)^{1/4}} \psi_n(\xi) \cancel{e^{\xi^2/2}} \sqrt{2^n n!} &= n \cancel{\left(\frac{\pi}{\beta^2}\right)^{1/4}} \sqrt{2^{n-1}(n-1)!}\psi_{n-1}(\xi) \cancel{e^{\xi^2/2}} \\
&+ \frac{1}{2} \cancel{\left(\frac{\pi}{\beta^2}\right)^{1/4}} \sqrt{2^{n+1}(n+1)!}\psi_{n+1}(\xi) \cancel{e^{\xi^2/2}}
\end{aligned} \qquad (142)
$$

$$
\xi \psi_n(\xi) \sqrt{\cancel{n} \cdot 2} = \overset{\sqrt{n}}{\cancel{n}} \psi_{n-1}(\xi) + \frac{1}{\cancel{2}} \sqrt{\cancel{4}\cancel{n}(n+1)}\psi_{n+1}(\xi) \qquad (143)
$$

or

$$
\boxed{\xi \psi_n(\xi) = \sqrt{\frac{n}{2}}\psi_{n-1}(\xi) + \sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi)} \qquad (144)
$$

From the above we get

$$
\frac{d}{d\xi}\left[\cancel{\left(\frac{\pi}{\beta^2}\right)^{1/4}} e^{\xi^2/2} \sqrt{\cancel{2}^n n!}\psi_n(\xi)\right] = 2n \cancel{\left(\frac{\pi}{\beta^2}\right)^{1/4}} e^{\xi^2/2} \sqrt{2^{n-\cancel{1}}(n-1)!} \;\; \psi_{n-1}(\xi) \qquad (145)
$$

$$\sqrt{2n}\left[\xi \cancel{e^{\xi^2/2}}\,\psi_n(\xi) + \cancel{e^{\xi^2/2}}\,\frac{d\psi_n}{d\xi}\right] = 2n\cancel{e^{\xi^2/2}}\,\psi_{n-1}(\xi) \tag{146}$$

$$\boxed{\frac{d\psi_n}{d\xi} = 2\sqrt{\frac{n}{2}}\psi_{n-1}(\xi) - \xi\psi_n(\xi)} \tag{147}$$

We can now rearrange the above equation so that both sides of the above two equations look alike

$$\frac{d\psi_n}{d\xi} = 2\sqrt{\frac{n}{2}}\psi_{n-1}(\xi) - \sqrt{\frac{n}{2}}\psi_{n-1}(\xi) - \sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi) \tag{148}$$

$$\boxed{\frac{d\psi_n}{d\xi} = \sqrt{\frac{n}{2}}\psi_{n-1}(\xi) - \sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi)} \tag{149}$$

Adding and subtracting gives

$$\begin{aligned}
\xi\psi_n(\xi) + \frac{d\psi_n}{d\xi} &= \sqrt{\frac{n}{2}}\psi_{n-1}(\xi) + \cancel{\sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi)} \\
&+ \sqrt{\frac{n}{2}}\psi_{n-1}(\xi) - \cancel{\sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi)} \\
&= \sqrt{2n}\psi_{n-1}(\xi)
\end{aligned} \tag{150}$$

$$\begin{aligned}
\xi\psi_n(\xi) - \frac{d\psi_n}{d\xi} &= \cancel{\sqrt{\frac{n}{2}}\psi_{n-1}(\xi)} + \sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi) \\
&- \cancel{\sqrt{\frac{n}{2}}\psi_{n-1}(\xi)} + \sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi) \\
&= 2\sqrt{\frac{n+1}{2}}\psi_{n+1}(\xi) \\
&= \sqrt{2}\sqrt{n+1}\psi_{n+1}(\xi)
\end{aligned} \tag{151}$$

or

$$\boxed{\begin{aligned}
\frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right)\psi_n(\xi) &= \sqrt{n}\psi_{n-1}(\xi) \\
\frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right)\psi_n(\xi) &= \sqrt{n+1}\psi_{n+1}(\xi)
\end{aligned}} \tag{152}$$

With the above two equations, we can evaluate the neighboring eigenfunctions ψ_{n-1} and ψ_{n+1}, provided that $\psi_n(\xi)$ is known. We can define the operators (for brevity)

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial \xi}\right) \tag{153}$$

$\uparrow$

lowering operator (154)

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial \xi}\right) \tag{155}$$

$\uparrow$

raising operator (156)

Now using the result previously derived $\frac{\partial}{\partial x} = \beta \frac{\partial}{\partial \xi}$, we can express $\hat{a}$ and $\hat{a}^\dagger$ as

$$\begin{aligned}
\hat{a} &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} + \sqrt{\frac{\hbar}{m\omega_0}}\frac{\partial}{\partial x}\right) && (157)\\
&= \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} + \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x}\right) && (158)\\
&= \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) && (159)
\end{aligned}$$

$$\begin{aligned}
\hat{a}^\dagger &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} - \sqrt{\frac{\hbar}{m\omega_0}}\frac{\partial}{\partial x}\right) && (160)\\
&= \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right) && (161)
\end{aligned}$$

With the introduction of these operators, we can simply write

$$\hat{a}\psi_n = \sqrt{n}\psi_{n-1} \tag{162}$$

and

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1} \tag{163}$$

We now want to turn to the properties of these two operators

(1) The wave functions ψ_n is an eigenfunction of the operator product $\hat{a}^\dagger\hat{a}$ because

$$\begin{aligned}
\hat{a}^\dagger\hat{a}\psi_n &= \hat{a}^\dagger\sqrt{n}\psi_{n-1} && (164)\\
&= \sqrt{n}\sqrt{n}\psi_n && (165)\\
&= n\psi_n && (166)
\end{aligned}$$

We therefore can define a number operator $\hat{N} = \hat{a}\hat{a}^\dagger$ such that

$$\hat{N}\psi_n = n\psi_n \tag{167}$$

Hence the eigenvalues of $\hat{N}$ are n, and the eigenfunctions are ψ_n.

(2) From the definitions of $\hat{a}^\dagger$ and $\hat{a}$, it also follows that they satisfy the commutator relation, i.e.,

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 \tag{168}$$

$$\begin{aligned}
[\hat{a}, \hat{a}^\dagger]\psi_n &= (\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a})\psi_n && (169)\\
&= \hat{a}\sqrt{n+1}\psi_{n+1} - \hat{a}^\dagger\sqrt{n}\psi_{n-1} && (170)\\
&= (n+1)\psi_n - n\psi_n && (171)\\
&= \psi_n && (172)\\
&\Rightarrow [\hat{a}, \hat{a}^\dagger] = 1 && (173)
\end{aligned}$$

(3) By successfully applying $\hat{a}^\dagger$ on ψ, one is able to calculate all eigenfunctions starting from the ground state ψ_0 for which $\hat{a}\psi_0 = 0$. Thus, we can use

$$\hat{a}\psi_0 = 0 \tag{174}$$

and

$$\begin{aligned}
\hat{a}^\dagger\psi_n &= \sqrt{n+1}\psi_{n+1} && (175)\\
& && (176)
\end{aligned}$$

$$\Rightarrow \psi_{n+1} = \frac{1}{\sqrt{n+1}}a^\dagger\psi_n \tag{177}$$

to generate all the eigenfunctions. This is much simpler than using the brute - force method, which we described previously. If we iteratively apply the above, we will get

$$\begin{aligned}
\psi_1 &= \frac{1}{\sqrt{1}}a^\dagger\psi_0 && (178)\\
\psi_2 &= \frac{1}{\sqrt{2}}a^\dagger\psi_1 && (179)\\
&= \frac{1}{\sqrt{2}}a^\dagger\frac{1}{\sqrt{1}}a^\dagger\psi_0 && (180)\\
&= \frac{(a^\dagger)^2}{\sqrt{2!}}\psi_0 && (181)
\end{aligned}$$

and

$$\psi_n = \frac{(a^\dagger)^2}{\sqrt{n!}}\psi_0 \tag{182}$$

The differential equation for the ground state is

$$\hat{a}\psi_0 = 0 \Rightarrow \tag{183}$$

$$\xi\psi_0 + \frac{\psi_0}{\partial\xi} = 0 \tag{184}$$

$$\frac{d\psi_0}{\psi_0} = -\xi d\xi \Rightarrow \tag{185}$$

$$\psi_0 = A^{-\xi^2/2} \tag{186}$$

If we normalize it, we will get

$$\psi_0 = \left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-\xi^2/2} \tag{187}$$

which coincides with our earlier results.

(4) We can also represent the Hamiltonian of the system in terms of $\hat{a}$ and $\hat{a}^\dagger$. We know that

$$\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 \tag{188}$$

and

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega_0}\right) \tag{189}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega_0}\right) \tag{190}$$

$$\tag{191}$$

Now if we calculate the product

$$\hat{a}\hat{a}^\dagger = \frac{m\omega_0}{2\hbar}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \tag{192}$$

$$= \frac{m\omega_0}{2\hbar}\left(\hat{x}^2 - i\frac{\hat{p}\hat{x}}{m\omega_0} + i\frac{\hat{x}\hat{p}}{m\omega_0} + \frac{p^2}{(m\omega_0)^2}\right) \tag{193}$$

$$= \frac{m\omega_0\hat{x}^2}{2\hbar} + \frac{\hat{p}^2}{2m\omega_0\hbar} - \frac{i}{2\hbar}\underbrace{(\hat{p}\hat{x} - \hat{x}\hat{p})}_{-i\hbar} \Rightarrow \tag{194}$$

$$\hat{a}^\dagger\hat{a} = \frac{m\omega_0\hat{x}^2}{2\hbar} + \frac{\hat{p}^2}{2m\omega_0\hbar} - \frac{i}{2\not{\hbar}}(-i\not{\hbar}) \tag{195}$$

or

$$\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\hbar\omega_0 = \frac{1}{2}m\omega_0^2\hat{x}^2+\frac{\hat{p}^2}{2m} \quad (196)$$

$$= \hat{H} \quad (197)$$

i.e.,

$$\boxed{\hat{H}=\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\hbar\omega_0} \quad (198)$$

The energy eigenvalues are then

$$\hat{H}\psi_n = E_n\psi_n \quad (199)$$

$$= \left(\hat{a}^\dagger\hat{a}\dagger\frac{1}{2}\right)\hbar\omega_0\psi_n \quad (200)$$

$$= \left(n+\frac{1}{2}\right)\hbar\omega_0\psi_n \quad (201)$$

i.e.,

$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega_0 \quad (202)$$

Interpretation of $\hat{a}^\dagger$ and $\hat{a}$

The ground state ($n=0$) has the zero-point energy $E_0=\frac{\hbar\omega_0}{2}$. Since the energy spectrum of a harmonic oscillator is equidistant, the state ψ_n posseses and energy value that is larger by the term $n\hbar\omega_0$. If we distribute this energy to n energy quanta $\hbar\omega_0$ (quanta of the oscillator field), we will call these energy quanta PHONONS. Then ψ_n is called an n - phonon state which in Dirac's notation is

$$\psi_n=|n\rangle \quad (203)$$

The "ket" contains the number of phonons in that state. The zero-point state $|0\rangle$ is called VACUUM. In this notation

$$\hat{a}|n\rangle=\sqrt{n}|n-1\rangle \quad (204)$$

and

$$\hat{a}^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle \quad (205)$$

Now, the following interpretation is appropriate:

– if acting on the wave function, the operator $\hat{a}$ annihilates one phonon at a time, whereas $\hat{a}^\dagger$ creates one. Therefore, we can call $\hat{a}^\dagger$ and $\hat{a}$, creation and annihilation operators. $\hat{N}$ os termed the phonon number operator since

$$\hat{N}|n\rangle = n|n\rangle \tag{206}$$

where n is the number of phonons of the corresponding states.

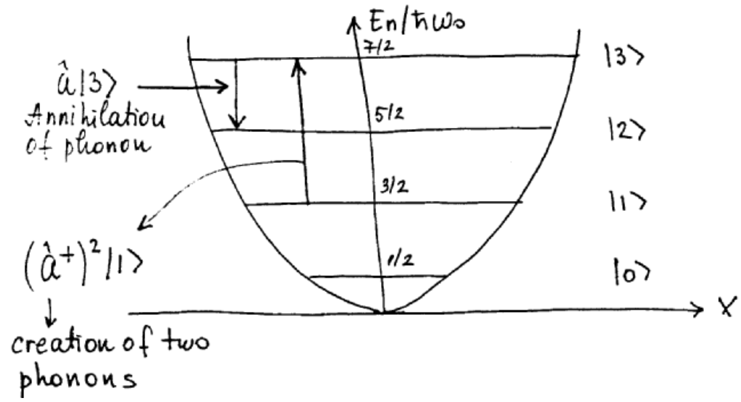

Figure 6: Energy levels of the harmonic oscillator

The introduction of the phonon representation is often referred to as SECOND QUANTIZATION.

<u>Example</u>

Using the creation and annihilation operators, compute $\langle x^2 \rangle$ and $\langle p^2 \rangle$.

The operators $\hat{a}$ and $\hat{a}^\dagger$ are defined as

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega_0} \right) \tag{207}$$

and

$$\hat{a}^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega_0} \right) \tag{208}$$

where

$$\hat{a}\psi_n = \sqrt{n}\psi_{n-1} \tag{209}$$

and

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1} \tag{210}$$

or in Dirac notation

$$\hat{a}|n\rangle = \sqrt{n}|n\rangle \tag{211}$$

and

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{212}$$

We can calculate $\hat{x}$ and $\hat{p}$ by adding and subtracting the expressions for $\hat{a}$ and $\hat{a}^\dagger$

$$\hat{a} + \hat{a}^\dagger = 2\sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} \tag{213}$$

$$= \sqrt{\frac{2m\omega_0}{\hbar}}\hat{x} \Rightarrow \tag{214}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}}(\hat{a} + \hat{a}^\dagger) \tag{215}$$

$$\hat{a} - \hat{a}^\dagger = 2\sqrt{\frac{m\omega_0}{2\hbar}}\frac{1}{m\omega_0}i\hat{p} \tag{216}$$

$$= \sqrt{\frac{2}{m\omega_0\hbar}}i\hat{p} \Rightarrow \tag{217}$$

$$\hat{p} = i\sqrt{\frac{m\omega_0\hbar}{2}}(\hat{a}^\dagger - \hat{a}) \tag{218}$$

Now

$$\langle x_n^2\rangle = \langle n|x^2|n\rangle \tag{219}$$

$$= \frac{\hbar}{2m\omega_0}\langle n|(\hat{a} + \hat{a}^\dagger)^2|n\rangle \tag{220}$$

$$= \frac{\hbar}{2m\omega_0}\langle n|\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}|n\rangle \tag{221}$$

$$= \frac{\hbar}{2m\omega_0}\left[\langle n|\hat{a}^2|n\rangle + \langle n|\hat{a}\hat{a}^\dagger|n\rangle + \langle n|\hat{a}^\dagger\hat{a}|n\rangle + \langle n|\hat{a}^{\dagger 2}|n\rangle\right] \tag{222}$$

where

$$\langle n|\hat{a}^2|n\rangle = \langle n|\hat{a}\sqrt{n}|n-1\rangle \tag{223}$$

$$= \sqrt{n}\sqrt{n-1}\langle n|n-2\rangle \tag{224}$$

$$= 0 \tag{225}$$

$$\begin{aligned}
\langle n|\hat{a}\hat{a}^\dagger|n\rangle &= \sqrt{n+1}\langle n|\hat{a}|n+1\rangle & (226)\\
&= \sqrt{n+1}\sqrt{n+1}\langle n|n\rangle & (227)\\
&= (n+1) & (228)
\end{aligned}$$

$$\begin{aligned}
\langle n|\hat{a}^\dagger\hat{a}|n\rangle &= \sqrt{n}\langle n|\hat{a}^\dagger|n-1\rangle & (229)\\
&= \sqrt{n}\sqrt{n}\langle n|n\rangle & (230)\\
&= n & (231)
\end{aligned}$$

$$\begin{aligned}
\langle n|\hat{a}^{\dagger 2}|n\rangle &= \sqrt{n+1}\langle n|\hat{a}^\dagger|n+1\rangle & (232)\\
&= \sqrt{n+1}\sqrt{n+2}[\langle n|n+2\rangle] & (233)\\
&= 0 & (234)
\end{aligned}$$

Thus

$$\begin{aligned}
\langle x_n^2\rangle &= \frac{\hbar}{2m\omega_0}(n+1+n) & (235)\\
&= \frac{\hbar}{2m\omega_0}(2n+1) & (236)\\
&= \frac{\hbar\omega_0(n+1/2)}{m\omega_0^2} & (237)\\
&= \frac{E_n}{m\omega_0^2} & (238)
\end{aligned}$$

For the expectation value of the momentum squared, we have that

$$\begin{aligned}
\langle p^2\rangle_n &= -\frac{m\omega_0\hbar}{2}\langle n|(\hat{a}^\dagger-\hat{a})^2|n\rangle & (239)\\
&= -\frac{m\omega_0\hbar}{2}\langle n|\hat{a}^{\dagger 2}-\hat{a}^\dagger\hat{a}-\hat{a}\hat{a}^\dagger+\hat{a}^2|n\rangle & (240)\\
&= -\frac{m\omega_0\hbar}{2}[-n-n-1] & (241)\\
&= \frac{m\omega_0\hbar}{2}(2n+1) & (242)\\
&= m\omega_0\hbar(n+1/2) & (243)\\
&= mE_n & (244)
\end{aligned}$$

Hence

$$\langle x^2 \rangle_n = \frac{E_n}{m\omega_0^2} \tag{245}$$

and

$$\langle p^2 \rangle_n = mE_n \tag{246}$$

We also can calculate

$$\begin{aligned}
\langle x \rangle &= \sqrt{\frac{\hbar}{2m\omega_0}} \langle n|\hat{a} + \hat{a}^\dagger|n\rangle && (247)\\
&= \sqrt{\frac{\hbar}{2m\omega_0}} \left[\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^\dagger|n\rangle\right] && (248)\\
&= 0 && (249)
\end{aligned}$$

$$\begin{aligned}
\langle p \rangle &= i\sqrt{\frac{m\omega_0\hbar}{2}} \langle n|\hat{a}^\dagger - \hat{a}|n\rangle && (250)\\
&= i\sqrt{\frac{m\omega_0\hbar}{2}} \left[\langle n|\hat{a}^\dagger|n\rangle - \langle n|\hat{a}|n\rangle\right] && (251)\\
&= 0 && (252)
\end{aligned}$$

Hence

$$\begin{aligned}
\Delta x_n \Delta p_n &= \sqrt{\langle x^2 \rangle_n} \sqrt{\langle p^2 \rangle_2} && (253)\\
&= \sqrt{\frac{E_n}{m\omega_0^2}} \sqrt{mE_n} && (254)\\
&= \frac{E_n}{\omega_0} && (255)
\end{aligned}$$

$$\Delta x_n \Delta p_n = \hbar(n + 1/2) \rightarrow \text{identical to what we had earlier} \tag{256}$$

Motion in a Magnetic Field

An interesting example to consider is the motion of an electron orbiting around magnetic field lies. Classically, when the electron moves in an electromagnetic field, the Lorentz force acts on the particle

$$\begin{aligned}
\mathbf{F} &= -e\left[\mathbf{E} + \mathbf{v} \times \mathbf{B}\right] && (257)\\
&= -e\left[\mathbf{E} + \mathbf{E}_{\text{ind}}\right] && (258)
\end{aligned}$$

The electric and magnetic field strengths can be expressed by the corresponding potentials ϕ and $\mathbf{A}$ according to

$$\mathbf{F} = -e\left[-\nabla\phi + \mathbf{E}_{\text{ind}}\right] \tag{259}$$
$$= \frac{\hbar d\mathbf{k}}{dt} \tag{260}$$
$$= \frac{d\mathbf{p}}{dt} \tag{261}$$

The induced field $\mathbf{E}_{\text{ind}}$ can be found from the Faraday's law, under the assumptions that $\mathbf{E} = \mathbf{0}$, i.e., $\phi = 0$, or

$$\nabla \times \mathbf{E}_{\text{ind}} = -\frac{\partial \mathbf{B}}{\partial t} \tag{262}$$
$$= -\frac{\partial}{\partial t}(\nabla \times \mathbf{A}) \tag{263}$$
$$= -\nabla \times \frac{\partial \mathbf{A}}{\partial t} \tag{264}$$

Thus

$$\mathbf{E}_{\text{ind}} = -\frac{\partial \mathbf{A}}{\partial t} \tag{265}$$

This means that

$$\frac{d\mathbf{p}}{dt} = -e\left(-\frac{\partial \mathbf{A}}{\partial t}\right) \tag{266}$$
$$= e\frac{\partial \mathbf{A}}{\partial t} \Rightarrow \tag{267}$$

$$\frac{d}{dt}(\mathbf{p} - e\mathbf{A}) = 0 \tag{268}$$

The last expression suggests that the proper total momentum to use in the Hamiltonian is just

$$\mathbf{p} \rightarrow \hbar\mathbf{k} - e\mathbf{A} \qquad \text{Pierls substitution} \tag{269}$$

We want to find the solution of the TISE (stationary Schroedinger equation) in the absence of any external potential, i.e.,

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \tag{270}$$

$$\Rightarrow \frac{(\mathbf{p} - e\mathbf{A})^2}{2m}\psi = E\psi \tag{271}$$

Assuming that the magnetic field is along the z - axis we can choose the vector potential to be of the form

$$\mathbf{A} = \mathbf{B} \times \hat{a}_y \tag{272}$$
$$= A_y \hat{a}_y \tag{273}$$

where $\hat{a}_y$ is the unit vector along the y - direction. This particular choice of the vector potential is known as the Landau gauge. The $\mathbf{B}$ will be oriented along the z - axis can be proven from the definition of the vector potential, i.e.,

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{274}$$

Thus

$$\mathbf{B} = \begin{vmatrix} \hat{a}_x & \hat{a}_y & \hat{a}_z \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} \tag{275}$$
$$= \hat{a}_x \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) - \hat{a}_y \left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) + \hat{a}_z \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \tag{276}$$

or

$$B_x = \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \tag{277}$$
$$B_y = \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \tag{278}$$
$$B_z = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \tag{279}$$

Since $A_x = A_y = 0$ and $A_y = xB$ we have that $B_x = B_y = 0$, $B_z = \frac{\partial}{\partial x} A_y = \frac{\partial}{\partial x}(xB) = B$. This completes our proof that $\mathbf{B} = (0, 0, B)$.

Now let's go back to the solution of the TISE, which can also be written im the form

$$\frac{(\mathbf{p} - e\mathbf{A})^2}{2m} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} - \frac{e}{2m}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \underset{\displaystyle \frac{e^2 A_y^2}{2m}}{\underset{\Downarrow}{\frac{e^2 A^2}{2m}}} \tag{280}$$

$$\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p} = p_y A_y + A_y p_y \tag{281}$$

$$
\begin{aligned}
&= \frac{\hbar}{i}\frac{\partial}{\partial y}xB + xB\frac{\hbar}{i}\frac{\partial}{\partial y} && (282)\\
&= 2xB\frac{\hbar}{i}\frac{\partial}{\partial y} && (283)\\
&= 2xBp_y && (284)\\
&= \frac{2xBk_y}{\hbar}\hbar^2 && (285)\\
&= 2xB\hbar k_y && (286)
\end{aligned}
$$

Hence

$$
\begin{aligned}
\hat{H} &= \frac{p_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{p_z^2}{2m} - \frac{exB}{\hbar m}k_y\hbar^2 + \frac{e^2x^2B^2}{2m} && (287)\\
&= \frac{p_x^2}{2m} + \frac{p_z^2}{2m} + \frac{e^2x^2B^2}{2m} - \hbar^2\frac{exB}{\hbar m}k_y + \frac{\hbar^2 k_y^2}{2m} && (288)\\
&= \frac{p_x^2}{2m} + \frac{p_z^2}{2m} + \frac{1}{2m}(eB)^2\left[x^2 - 2\frac{xk_y\hbar^2}{\hbar eB} + \left(\frac{\hbar k_y}{eB}\right)^2\right] && (289)\\
&= \frac{p_x^2}{2m} + \frac{p_z^2}{2m} + \frac{1}{2}m\left(\frac{eB}{m}\right)^2\left[x^2 - 2x\left(\frac{\hbar k_y}{eB}\right) + \left(\frac{\hbar k_y}{eB}\right)^2\right] && (290)
\end{aligned}
$$

At this point we may introduce the following two important quantities

$$\omega_c = \frac{eB}{m} \qquad \text{cyclotron frequency} \qquad (291)$$

$$
\begin{aligned}
x_0 &= \frac{\hbar k_y}{eB}\\
&= k_y l_B^2 && (292)
\end{aligned}
$$

$$l_B = \left(\frac{\hbar}{eB}\right)^{1/2} \qquad \text{magnetic length} \qquad (293)$$

With this new set of variables, the Hamiltonian of the system simplifies to

$$
\begin{aligned}
\hat{H} &= \frac{p_z^2}{2m} + \frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2(x^2 - 2xx_0 + x_0^2) && (294)\\
&= \frac{p_z^2}{2m} + \frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2(x - x_0)^2 && (295)
\end{aligned}
$$

If the wave function $\psi(x, y, z)$ has the general solution

$$\psi(x, y, z) = e^{i(yk_y + zk_z)}\phi(x) \qquad (296)$$

then

$$\frac{p_z^2}{2m}\psi(x,y,z) = \frac{\hbar^2 k_z^2}{2m}\psi(x,y,z) \tag{297}$$
$$= E_z\psi(x,y,z) \tag{298}$$

which leads to

$$E_z\psi(x,y,z) + \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega_c^2(x-x_0)^2\right]\psi(x,y,z)$$
$$= E\psi(x,y,z) \tag{299}$$

or

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega_c^2(x-x_0)^2\right]\phi(x) = \epsilon\phi(x) \tag{300}$$

where $\epsilon = E - E_0$. With the substitution $x' = x - x_0$, we arive at

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2} + \frac{1}{2}m\omega_c^2 x'^2\right]\phi(x') = \epsilon\phi(x')} \tag{301}$$

Once again, we have the equation of a harmonic oscillator. From the above equation, we can immediately write down the energy eigenvalues

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_c, \quad n = 0, 1, 2, \cdots \tag{302}$$

and the corresponding wave functions

$$\phi_n(x') = \frac{1}{\sqrt{2^n n!}}\sqrt[4]{\frac{m\omega_c}{\hbar\pi}}e^{-m\omega_c(x-x_0)^2/2\hbar}H_n\left(\sqrt{\frac{m\omega_c}{\hbar}}(x-x_0)\right) \tag{303}$$

The total energy is then given by

$$E_n = \epsilon_n + \frac{\hbar^2 k_z^2}{2m} \tag{304}$$
$$= \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m} \tag{305}$$

Neglecting the motion in the z - direction ($z_z = 0$), the energy E_n is quantized.

Now let's turn our attention to $\psi_n(x)$. For a given k_y, $\phi_n(x')$ os localized in the x -direction, but not in the y-direction. This result is unexpected, for both directions should be equally represented. However, as we have seen above, the energy is independent of k_y, so that we have infinite degeneracy. It can be shown that wave packets of the form

$$\psi_{n,k_z}(x,y,z) = \int_{-\infty}^{\infty} c_n(k_y) e^{i(yk_y+zk_z)} \phi_{k_y}(x) dk_y \tag{306}$$

where $c(k_y)$ can be chosen so that the solution is localized in the y-direction as well. Such bound states in the xy - plane are unrestricted in the z - direction, i.e., along the direction of the magnetic field **B**. They correspond classically to electrons orbiting perpendicular to **B**, but moving with a constant velocity along **B** and are called Landau states; the energy levels

$$\epsilon_n = \hbar\omega_c \left(n + \frac{1}{2}\right) \tag{307}$$

are called Landau levels.

The classical turning point is given by

$$\frac{1}{2} m\omega_c^2 (x_n - x_0)^2 = \epsilon_n \tag{308}$$

i.e., it is found under the assumption that the kinetic energy is zero. Then

$$\begin{aligned} x_n - x_0 &= r_n & (309) \\ &= \sqrt{\frac{2\epsilon_n}{m\omega_c^2}} & (310) \\ &= \sqrt{\frac{2\hbar\not{\omega_c}(n+1/2)}{m\omega_c^{\not{2}}}} & (311) \end{aligned}$$

where r_n is the natural cyclotron radius of the harmonic motion (classically)

$$\begin{aligned} r_n &= \sqrt{\frac{2\hbar(n+1/2)}{m\omega_c}} & (312) \\ &= \sqrt{\frac{\hbar(2n+1)}{meB/m}} & (313) \\ &= \sqrt{\frac{\hbar}{eB}}\sqrt{2n+1} & (314) \\ &= l_B\sqrt{2n+1} & (315) \end{aligned}$$

$r_n = \sqrt{2n+1} l_B \rightarrow$ radius of the harmonic motion of the electrons in the n-th level.

<u>3D Systems</u>

As previously described, in the 3D system, the motion of the electrons in the presence of a magnetic fields is described by the Harmonic oscillator model and in the plane perpendicular to the magnetic field, the energy is quantized into Landau levels, i.e.,

$$E_n = \hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{\hbar^2k_z^2}{2m} \tag{316}$$

The wave functions ϕ_n are centered at a point

$$x_0 = k_y l_B^2 \tag{317}$$
$$= \frac{\hbar}{eB}k_y \tag{318}$$

From the equation for E_n, it is easily seen that the quantum states in the k - space are located on cylinders, with the symmetry axes along the z-direction. For the $x-y$motion, states are characterized with the cyclotron energy $(n+1/2)\hbar\omega_c$, located on circles with radii

$$\frac{\hbar^2}{2m}(k_x^2+k_y^2) = \left(n+\frac{1}{2}\right)\hbar\omega_c \tag{319}$$

or

$$k_x^2+k_y^2 = \frac{2m}{\hbar^2}\left[\left(n+\frac{1}{2}\right)\hbar\omega_c\right] \tag{320}$$

The degeneracy of a simple - spin Landau level can be found from the number of possible cyclotron orbits in the crystal. The assumption is that the center of th quantum state is within sample boundaries

$$0 < x_0 < L_x \Rightarrow 0 < k_y l_B^2 < L < x \Rightarrow 0 < \frac{\hbar k_y}{eB} < L_x \tag{321}$$

or

$$0 < k_y < \frac{eB}{\hbar}L_x \tag{322}$$

That means that the number of possible states in the range $\left[0, \frac{eB}{\hbar}L_x\right]$ is

$$g = \frac{\frac{eB}{\hbar}L_x}{\frac{2\pi}{L_y}} \tag{323}$$
$$= \frac{eB}{2\pi\hbar}L_xL_y \tag{324}$$
$$= \frac{eB}{h}L_xL_y \tag{325}$$

i.e., the DOS per unit area is $eB/\hbar$.

Now if we assume that in the 2D - plane we have the single spin DOS - function $m^*/2\pi\hbar^2$, then in the energy range $\hbar\omega_c$, the number of states is

$$\hbar\omega_c \frac{m^*}{2\pi\hbar^2} = \frac{eB}{m^*} \cdot \frac{m^*}{h} \tag{326}$$

$$= \frac{eB}{h} \tag{327}$$

This is identical to what we previously calculated, i.e., the average density of states in a quantized magnetic field is unaffected. Instead of having a 2D continuum of states, these states are collapsed in a single degenerate Landau state.

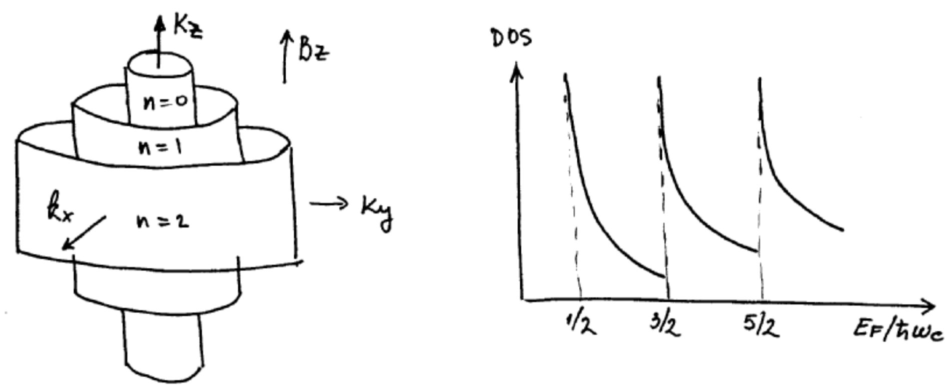

Figure 7: Landau States

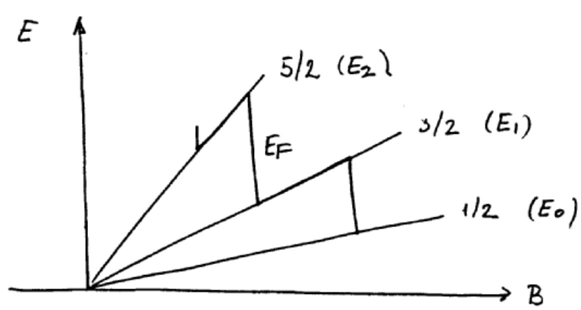

Figure 8: Low Temperature

2D - system

In 2 D hereto-structures, with a magnetic field perpendicular to the layer plane, the same Landau quantization occurs. However, the effect is even more pronounced as the z-motion of the carriers is also frozen by the confining potential leading to a "completely confined quantum limit"

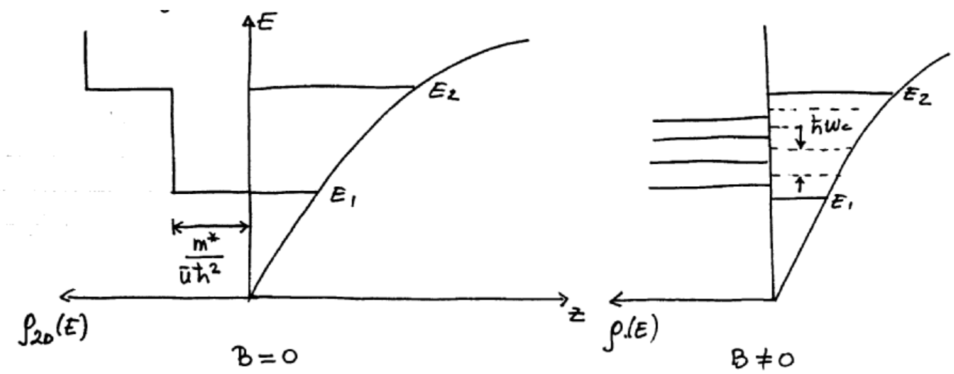

Figure 9: The energy level structure is made up of a ladder of cyclotron levels for each confined state, each level having a singular DOS with a degeneracy eB/h