6. Harmonic oscillator

In classical physics if we consider the parabolic potential energy (parabolic potential well) $U = kx^2/2$ (elastic force F = - kx elastic forc potential energy), we get harmonic oscillations. Frequency is equal to $\omega = \sqrt{k/M}$, where M is the mass of oscillating body. Classical energy of oscillations is continuous.

Every body oscillating harmonically is called harmonic oscillator. Harmonic oscillator has several applications (small oscillations in twoatomic molecule, in crystal atoms oscillate and so on). In microworld the behaviour of harmonic oscillator is quite different from the classical one: energy is discrete and the probability disribution is different from the classical one. Next we prove it solving the corresponding Schrödinger equation. As we see, it is quite complicated procedure, since the differential equation we have is different from those used in classical physics.

We have the following potential energy

$$U(x) = \frac{M\omega^2 x^2}{2} .$$

Next we must solve the Schrödinger equation

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(x)}{dx^2} + \frac{M\omega^2 x^2}{2}\psi(x) = E\psi(x) .$$

6.1 Change of variables. In order to solve that equation there are several standard steps to follow. The first one is to change variables and write the equation with less constants. In our case we define variables

$$\xi = \sqrt{\frac{M\omega}{\hbar}}\, x , \qquad \lambda = \frac{2E}{\hbar\omega}$$

and write our equation as

$$-\frac{d^2\psi(\xi)}{d\xi^2} + \xi^2\psi(\xi) = \lambda\psi(\xi) \qquad \text{or} \qquad -\psi''(\xi) + \xi^2\psi(\xi) = \lambda\psi(\xi) .$$

6.2 Asymptotical solution. Since the variable ξ is not restricted we must find out whether there exist finite solutions if the variables tend to infinity. If $|\xi| \rightarrow \infty$, we demand that $\psi(\xi) \rightarrow 0$.

If $|\xi| >> \lambda$, we have $-\psi''(\xi) + \xi^2\psi(\xi) = 0$. It is possible to verify that now the possible approximate solution which tends to zero is

$$\psi(\xi) = e^{-\frac{\xi^2}{2}} .$$

Similarly the solution is also $\exp(\xi^2/2)$, but it is unphysical since it infinitely increases.

6.3 Power series. Having asymptotical solution we next try to find the general solution in form

$$\psi(\xi) = v(\xi)e^{-\frac{\xi^2}{2}} ,$$

where $v(\xi)$ is some new function we must find. Substituting the above given solution to our Scrödinger equation we for $v(\xi)$ get the following differential equation

$$\nu'' - 2\xi\nu' + (\lambda - 1)\nu = 0 \ .$$

Next we assume, that $\nu(\xi)$ is expressed as a following power series function

$$\nu(\xi) = \sum_{r=0} a_r \xi^r \quad .$$

Whether the serie is finite or infinite, we analyse later. Calculating derivatives

$$\nu'(\xi) = \sum_{r=0} r a_r \xi^{r-1}$$

and

$$\nu''(\xi) = \sum_{r=0} r(r-1) a_r \xi^{r-2} \equiv \sum_{s=0} (s+2)(s+1) a_{s+2} \xi^s \quad ,$$

(we changed r to $s = r$-2). After substitution to our differential equation, we get

$$\sum_{r=0} (r+2)(r+1) a_{r+2} \xi^r - 2\sum_{r=0} r a_r \xi^r + (\lambda - 1)\sum_{r=0} a_r \xi^r = 0 \quad ,$$

i.e.

$$\sum_{r=0} ((r+2)(r+1) a_{r+2} - 2r\, a_r + (\lambda - 1) a_r) \xi^r = 0$$

Taking the term before ξ^r equal to zero, we have

$$a_{r+2} = \frac{2r + 1 - \lambda}{(r+2)(r+1)} a_r \quad .$$

We got the formula to calculate the coefficients a_r. One of the solutions is given by even series function

$$a_0 \neq 0 \qquad and \qquad a_1 = 0 \ ,$$

and other by odd series function

$$a_1 \neq 0 \qquad ja \qquad a_0 = 0 \ .$$

Now we analyse the large ξ behaviour of $\nu(\xi)$. When $\xi \to \infty$ we see that $\nu(\xi) \to \infty$ and has identical limiting behavior as e^{ξ^2}. For large ξ we have

$$\frac{a_{r+2}}{a_r} \approx \frac{2}{r} \ ,$$

which is the same as for e^{ξ^2} .

Therefore at large values of ξ

$$\nu(\xi) \approx e^{\xi^2}$$

and $\psi(\xi) = \nu(\xi) e^{-\frac{\xi^2}{2}}$ is not finite. Therefore the power series function must be finite. It means that serie terminates on some value n (in other words we have polynomials)

$$a_n \neq 0 \qquad ja \qquad a_{n+2} = 0 \ .$$

From $a_{n+2} = \dfrac{2n + 1 - \lambda}{(n+2)(n+1)} a_n = 0$ we get that

$$\lambda = 2n + 1\,, \quad (n = 0,1,2,...)\,.$$

We got the first important result: to avoid infinities the parameter λ must be discrete and must have the above given values.

6.4 Energy. Since the parameter λ was related with energy, we get that the only possible energy values for harmonic oscillator are as follows

$$E_n = \hbar\omega(n + \frac{1}{2})\,, \quad n = 0,1,2,... \,.$$

Therefore the energy of quantum oscillator is discrete, difference between the neighbour levels is equal to $\hbar\omega$. The minimal energy is nonzero

$$E_0 = \frac{\hbar\omega}{2}\,,$$

therefore the quantum oscillator always „moves" and cannot be at rest.

6.5 Eigenfunctions. Next we try to find eigenfunctions corresponding to the energy E_n. For each $\lambda = 2n + 1$ we get certain polynomial which is called Hermite polynomial

$$v_n(\xi) = H_n(\xi)\,.$$

Hermite polynomials are solutions of the following differential equation

$$H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n(\xi) = 0\,.$$

Eigenfunctions are expressed as

$$\psi_n(\xi) = A_n H_n(\xi) e^{-\frac{\xi^2}{2}}\,,$$

or using the variable x

$$\psi_n(x) = A_n H_n(\sqrt{\frac{M\omega}{\hbar}}\,x) e^{-\frac{M\omega x^2}{2\hbar}}\,.$$

A_n is normalization constant.

6.6 Some properties of Hermite polynomials. Before going to calculations we write down some useful properties of Hermite polynomials. It appears that our calculations simplify if we introduce certain helping function which is called the generating function. It is defined as follows

$$F(s,\xi) = e^{-s^2+2s\xi} \equiv e^{\xi^2-(s-\xi)^2}\,.$$

The use of generating function is that it should be expressed, using Hermite polynomials, as follows

$$F(s,\xi) = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n\,.$$

In order to prove it we at first give some useful relations for $F(s,\xi)$. Calculating

$$\frac{\partial F}{\partial s} = -2(s-\xi) e^{-s^2+2s\xi} \equiv 2(\xi - s)F$$

and

$$\frac{\partial F}{\partial \xi} = 2s\, e^{-s^2+2s\xi} \equiv 2sF$$

we see that $F(s,\xi)$ satisfies the following differential equation

$$\frac{\partial F}{\partial s} + \frac{\partial F}{\partial \xi} = 2\xi\, F \ .$$

Calculating

$$\frac{\partial^2 F}{\partial \xi^2} = 4s^2 F$$

we see that $F(s,\xi)$ satisfies the following second order differential equation

$$\frac{\partial^2 F}{\partial \xi^2} - 2\xi \frac{\partial F}{\partial \xi} + 2s \frac{\partial F}{\partial s} = 0 \ .$$

Proof. Now we shall prove that the power series expansion of $F(s,\xi)$ also satisfies the above given differential equation. Calculating derivatives

$$\frac{\partial^2 F}{\partial \xi^2} = \sum_{n=0}^{\infty} \frac{H_n''(\xi)}{n!} s^n \ , \quad \frac{\partial F}{\partial \xi} = \sum_{n=0}^{\infty} \frac{H_n'(\xi)}{n!} s^n \ , \quad \frac{\partial F}{\partial s} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} n s^{n-1}$$

and substituting them to differential equation, we get

$$\sum_{n=0}^{\infty} \frac{s^n}{n!} (H_n'' - 2\xi\, H_n' + 2nH_n) = 0 \ .$$

The left side is identically equal to zero, if and only if H_n are Hermite polynomials.

Next we derive the general expression for calculating Hermite polynomials. It is possible to verify that

$$H_n(\xi) = \left[\frac{d^n}{ds^n} F(s,\xi)\right]_{s=0} \equiv \left[\frac{d^n}{ds^n} e^{\xi^2-(s-\xi)^2}\right]_{s=0} =$$

$$= e^{\xi^2} \left[\frac{d^n}{ds^n} e^{-(s-\xi)^2}\right]_{s=0} \equiv (-1)^n\, e^{\xi^2}\, \frac{d^n}{d\xi^n}(e^{-\xi^2}) \ ,$$

which gives

$$H_n(\xi) = (-1)^n\, e^{\xi^2}\, \frac{d^n}{d\xi^n}(e^{-\xi^2}) \ .$$

(here the coefficient before ξ^n is always 2^n).

Some examples

$$H_0(\xi) = 1 \ , \quad H_1(\xi) = 2\xi \ , \quad H_2(\xi) = 4\xi^2 - 2 \ ,$$

$$H_3(\xi) = 8\xi^3 - 12\xi \ , \quad H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \ .$$

Some useful relations

$$H_n'(\xi) = 2nH_{n-1}(\xi)\,, \quad \xi H_n(\xi) = \frac{1}{2}H_{n+1}(\xi) + nH_{n-1}(\xi)\ .$$

6.7 Normalization of eigenfunctions. Let us prove that eigenfunctions are orthonormal and find normalization coefficient A_n. Consider the integral

$$\int_{-\infty}^{+\infty} \psi_m{}^*(x)\psi_n(x)\,dx\ .$$

Going to variable ξ and using the general expressions of eigenfunctions via Hermite polynomials, we get

$$\int_{-\infty}^{+\infty} \psi_m{}^*(x)\psi_n(x)\,dx = A_m{}^* A_n \sqrt{\frac{\hbar}{M\omega}} \int_{-\infty}^{+\infty} H_m(\xi)H_n(\xi)e^{-\xi^2}\,d\xi\ .$$

In the next paragraph we prove that

$$\int_{-\infty}^{+\infty} H_m(\xi)H_n(\xi)e^{-\xi^2}\,d\xi = \begin{cases} \sqrt{\pi}\,2^n n!\,, & if \quad m = n, \\ 0 \quad, & if \quad m \neq n. \end{cases}$$

If $m \neq n$, the integraal is zero, therefore the different eigenfunctions are orthogonal.

If $m = n$ we normalize the function to 1. We have

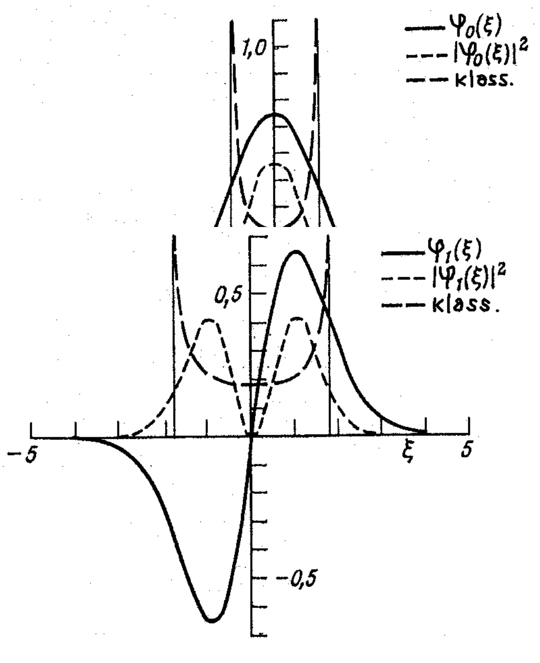
$$|A_n|^2 \sqrt{\frac{\hbar}{M\omega}} \sqrt{\pi}\,2^n n! = 1\ ,$$

which gives (we choose A_n to be real)

$$A_n = \sqrt{\frac{\sqrt{M\omega}}{\sqrt{\pi\hbar}\,2^n n!}} \equiv \left(\frac{M\omega}{\hbar}\right)^{1/4} \frac{1}{\sqrt{\sqrt{\pi}\,2^n n!}}\ .$$

Eigenfunctions in a final form are

$$\psi_n(x) = \left(\frac{M\omega}{\hbar}\right)^{1/4} \frac{1}{\sqrt{\sqrt{\pi}\,2^n n!}} H_n\!\left(\sqrt{\frac{M\omega}{\hbar}}\,x\right) e^{-\frac{M\omega x^2}{2\hbar}}\ .$$



Some special cases. Ground state.

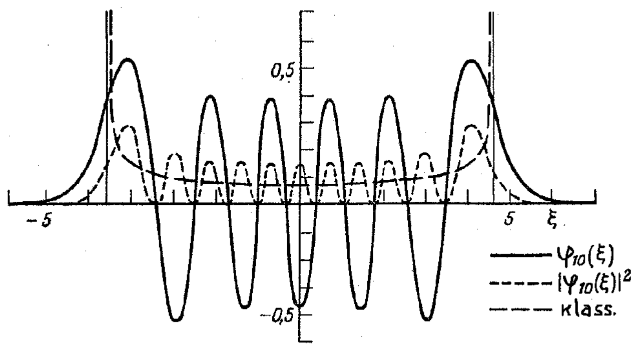
$$E_0 = \hbar\omega/2\,, \quad \psi_0(x) = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{M\omega x^2}{2\hbar}}\ .$$

Behaviour of quantum oscillator is different from the classical one. Probability density is maximal in centre (equilibrium point) and is nonzero outside the classsical region.

First exited state. $E_1 = 3\hbar\omega/2$ and

$$\psi_1(x) = \left(\frac{M\omega}{\hbar}\right)^{3/4}\left(\frac{4}{\pi}\right)^{1/4} x e^{-\frac{M\omega x^2}{2\hbar}} .$$

Behaviour of quantum and classical oscillators are also different.



n = 10. The classical and quantum oscillators behave differently, but in the case of large n we see that the average of quantum probability distribution is practically equal to the probability of classical oscillator. That is the general result, since in the limit of large quantum numbers we have the same results as in classical physics.

7. Harmonic oscillator (integrals)

Here we discuss how to calculate integrals. For each special case there are certain rules and procedures how to do it.

In the previous paragraph we used the integral

$$\int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \begin{cases} \sqrt{\pi}\, 2^n n!\,, & if \quad m = n, \\ 0 \quad , & if \quad m \neq n. \end{cases}$$

Here we demonstrate how it is calculated. The general principle is that using the generating function we try to find such a integral, which is expressed through the above given integrals. In our case it is integral

$$\int_{-\infty}^{+\infty} F(s,\xi)\, F(t,\xi) e^{-\xi^2}\, d\xi \ .$$

We write it down using the direct expressions of generating functions (left hand side of the following equality) and next using the expression via the Hermite polynomials (right side of the following equality)

$$\int_{-\infty}^{+\infty} e^{-s^2+2s\xi-t^2+2t\xi-\xi^2}\, d\xi = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\int_{-\infty}^{+\infty} \frac{H_m(\xi) H_n(\xi)}{m!\, n!} s^m t^n e^{-\xi^2}\, d\xi \ .$$

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$$\int_{-\infty}^{+\infty} e^{-s^2+2s\xi-t^2+2t\xi-\xi^2} \; d\xi = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \int_{-\infty}^{+\infty} \frac{H_m(\xi) H_n(\xi)}{m!\,n!} s^m t^n e^{-\xi^2} \; d\xi \; .$$

As we see, on the right side there are just the integrals we try to calculate. We now must calculate the integral on the right side (which in principle simple, since we must integrate exponents) and then expand the result as series on s and t.

The left hand side integraal gives us

$$\int_{-\infty}^{+\infty} e^{-s^2+2s\xi-t^2+2t\xi-\xi^2} \; d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2} \; d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-u^2} \; du = \sqrt{\pi}\, e^{2st} \; .$$

(We changed the variable: $u = \xi - s - t$ and used the integraal $\int_0^{\infty} e^{-r^2 x^2} \; dx = \frac{\sqrt{\pi}}{2r}\,, \quad r > 0$.)

Expanding the result as series on *s* and *t*, and demanding that it is equal to the right side, we get

$$\sqrt{\pi}\, e^{2st} \equiv \sqrt{\pi} \sum_{m=0}^{\infty} \frac{2^m s^m t^m}{m!} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{s^m t^n}{m!\,n!} \int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} \; d\xi \; .$$

Comparing the expressions on the left and right side we obtain the integrals we have used in the previous paragraph.

Next we give three more useful integrals (proofs are given in Appendix).

First integral.

$$\int_{-\infty}^{+\infty} \psi_n \frac{d\psi_m}{dx} dx = \begin{cases} \sqrt{\frac{M\omega}{\hbar}} \sqrt{\frac{n+1}{2}}\,, & if \quad m = n+1, \\ -\sqrt{\frac{M\omega}{\hbar}} \sqrt{\frac{n}{2}}\,, & if \quad m = n-1, \\ 0\,, & if \quad m \neq n \pm 1. \end{cases}$$

Second integral.

$$\int_{-\infty}^{+\infty} \psi_n x \psi_m \, dx = \begin{cases} \sqrt{\frac{\hbar}{M\omega}} \sqrt{\frac{n+1}{2}}\,, & if \quad m = n+1, \\ \sqrt{\frac{\hbar}{M\omega}} \sqrt{\frac{n}{2}}\,, & if \quad m = n-1, \\ 0\,, & if \quad m \neq n \pm 1. \end{cases}$$

Third integral.

$$\int_{-\infty}^{+\infty} \psi_n x^2 \psi_m \, dx = \begin{cases} \frac{\hbar}{2M\omega}(2n+1)\,, & if \quad m = n, \\ \frac{\hbar}{2M\omega}\sqrt{(n+1)(n+2)}\,, & if \quad m = n+2, \\ \frac{\hbar}{2M\omega}\sqrt{n(n-1)}\,, & if \quad m = n-2, \\ 0\,, & if \quad m \neq n \; and \; m \neq n \pm 2. \end{cases}$$

Example 1. Mean value of energy. Mean value of potential energy for state $\psi_n(x)$. Using the third integral, we get

$$< U >_n = \int_{-\infty}^{+\infty} \psi_n(x) \frac{M\omega^2 x^2}{2} \psi_n(x) \, dx = \frac{M\omega^2}{2} \int_{-\infty}^{+\infty} x^2 \psi_n^2(x) \, dx = \frac{\hbar\omega}{4}(2n+1) \equiv \frac{E_n}{2} \; .$$

The result is the same as in the classical case.

Since the energy operator is a sum of operators of kinetic and potential energy

$$\hat{H} = \hat{T} + U \; ,$$

we without calculations can say that also

$$< T >_n = \frac{E_n}{2} \; .$$

(Always $< \hat{H} >= E_n$).

Since $\hat{T} = -\frac{\hbar^2}{2M} \frac{d^2}{dx^2} = \frac{\hat{p}^2}{2M}$, we find the mean value of momentum square.

$$<T>_n = \frac{1}{2M} <p^2>_n = \frac{E_n}{2} \ ,$$

therefore

$$<p^2>_n = M\,E_n = \frac{M\,\hbar\omega}{2}(2n+1) \ .$$

Example 2. Uncertainty relations for oscillator. At first we demonstrate that

$$<x>_n = \int_{-\infty}^{+\infty} \psi_n(x)\, x \psi_n(x)\, dx = 0 \ ,$$

$$<p>_n = -i\hbar \int_{-\infty}^{+\infty} \psi_n(x) \frac{d\psi_n(x)}{dx} dx = 0 \ .$$

First result follows from tha fact that under the first integraal there is always an odd function, the second follows from our first integral.

Next we deal with root mean square deviation

$$(\Delta x)^2 \equiv <(x - <x>)^2> = <x^2> - <2x<x>> + <<x>^2> \equiv <x^2> - 2<x>^2 + <x>^2 =$$

$$= <x^2> - <x>^2 \ .$$

Since $<x>_n = 0$ and using the third integral, we get

$$(\Delta x)_n^2 = <x^2>_n = \int_{-\infty}^{+\infty} x^2 \psi_n^2(x)\, dx = \frac{\hbar}{2M\omega}(2n+1) \ .$$

Above we find that

$$<p^2>_n = M\,E_n = \frac{M\,\hbar\omega}{2}(2n+1) \ .$$

Therefore we have

$$(\Delta x)_n^2 (\Delta p)_n^2 = \frac{\hbar^2}{4}(2n+1)^2 \ ,$$

and the standard form of uncertainty relations is

$$\Delta x_n \cdot \Delta p_n = \frac{\hbar}{2}(2n+1) \ .$$

For the ground state $n = 0$ it is minimal

$$\Delta x \cdot \Delta p = \frac{\hbar}{2} \ ,$$

for other states it increases linearly on n. Here we see that the minimal value of products of uncertinties is indeed $\hbar/2$, but mostly it is greater.

Appendix:

1. First integral. Expressing it with the help of Hermite polynomials we have

$$\int_{-\infty}^{+\infty}\psi_n(x)\frac{d\psi_m(x)}{dx}dx=\int_{-\infty}^{+\infty}\psi_n(\xi)\frac{d\psi_m(\xi)}{d\xi}d\xi=$$

$$=A_nA_m\int_{-\infty}^{+\infty}H_n(\xi)e^{-\frac{\xi^2}{2}}\frac{d}{d\xi}(H_m(\xi)e^{-\frac{\xi^2}{2}})d\xi$$

We calculate the next integral using the following combination of generating function.

$$\int_{-\infty}^{+\infty}F(s,\xi)e^{-\frac{\xi^2}{2}}\frac{\partial}{\partial\xi}(F(t,\xi)e^{-\frac{\xi^2}{2}})d\xi=\int_{-\infty}^{+\infty}e^{-s^2+2s\xi-\frac{\xi^2}{2}}\frac{\partial}{\partial\xi}(e^{-t^2+2t\xi-\frac{\xi^2}{2}})d\xi=$$

$$=\int_{-\infty}^{+\infty}e^{-s^2-t^2-\xi^2+2s\xi+2t\xi}(-\xi+2t)d\xi=e^{2st}\int_{-\infty}^{+\infty}e^{-(\xi-s-t)^2}\left[-(\xi-s-t)+t-s\right]d\xi=$$

$$=(t-s)e^{2st}\int_{-\infty}^{+\infty}e^{-(\xi-s-t)^2}d\xi=\sqrt{\pi}(t-s)e^{2st}\;.$$

Next we express these integrals using Hermite polynomials

$$\int_{-\infty}^{+\infty}F(s,\xi)e^{-\frac{\xi^2}{2}}\frac{\partial}{\partial\xi}(F(t,\xi)e^{-\frac{\xi^2}{2}})d\xi=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{s^nt^m}{n!m!}\int H_n(\xi)e^{-\frac{\xi^2}{2}}\frac{d}{d\xi}\left[H_m(\xi)e^{-\frac{\xi^2}{2}}\right]d\xi=$$

$$=\sqrt{\pi}(t-s)e^{2st}=\sqrt{\pi}(t-s)\sum_{n=0}^{\infty}\frac{(2st)^n}{n!}=\sqrt{\pi}\sum_{n=0}^{\infty}\frac{2^n(s^nt^{n+1}-s^{n+1}t^n)}{n!}\;.$$

Comparing the expressions of both series, we get as a final result

$$\int_{-\infty}^{+\infty}H_n(\xi)e^{-\frac{\xi^2}{2}}\frac{d}{d\xi}\left[H_m(\xi)e^{-\frac{\xi^2}{2}}\right]d\xi=\begin{cases}\sqrt{\pi}\,2^n(n+1)!, & m=n+1\\ -\sqrt{\pi}\,2^{n-1}n!, & m=n-1\\ 0,\ \mathit{other\ cases}\end{cases}$$

Substituting the normalisation coefficient, we get the first integral.

<u>2. Second integral.</u> That integral is calculated without the generating function. We use the properties of Hermite polynomials and express $\xi H_n(\xi)$ as a superposition of other polynomials

$$\int_{-\infty}^{+\infty}\psi_n(x)x\psi_m(x)dx=\frac{\hbar}{M\omega}A_nA_m\int_{-\infty}^{+\infty}H_n(\xi)\,\xi\,H_m(\xi)e^{-\xi^2}d\xi=$$

$$=\frac{\hbar A_nA_m}{M\omega}\int_{-\infty}^{+\infty}H_n(\xi)(\frac{1}{2}H_{m+1}(\xi)+mH_{m-1}(\xi))e^{-\xi^2}d\xi=$$

$$=\frac{\hbar A_nA_m}{M\omega}\left\{\frac{1}{2}\int_{-\infty}^{+\infty}H_n(\xi)H_{m+1}(\xi)e^{-\xi^2}d\xi+m\int_{-\infty}^{+\infty}H_n(\xi)H_{m-1}(\xi)e^{-\xi^2}d\xi\right\}\;.$$

To obtain the final result we must use integrals we calculated at first.

<u>3. Third integral.</u> Third integral

$$\int_{-\infty}^{+\infty}\psi_n(x)x^2\psi_m(x)dx=(\frac{\hbar}{M\omega})^{\frac{3}{2}}A_nA_m\int_{-\infty}^{+\infty}H_n(\xi)\xi^2H_m(\xi)e^{-\xi^2}d\xi$$

is calculated with the help of generating function. We start with the integral

$$\int_{-\infty}^{+\infty} F(s,\xi)\,F(t,\xi)\,\xi^2 e^{-\xi^2}\,d\xi = e^{2st}\int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2}\xi^2\,d\xi = \sqrt{\pi}\,e^{2st}\left[\frac{1}{2}+(s+t)^2\right] =$$

$$= \sqrt{\pi}\left\{\sum_{n=0}^{\infty}\frac{2^n(s^{n+2}t^n + s^n t^{n+2})}{n!} + \sum_{n=0}^{\infty}\frac{2^{n-1}s^n t^n(2n+1)}{n!}\right\} .$$

On the other hand

$$\int_{-\infty}^{+\infty} F(s,\xi)\,F(t,\xi)\,\xi^2 e^{-\xi^2}\,d\xi = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{s^n t^m}{n!m!}\int_{-\infty}^{+\infty} H_n(\xi)H_m(\xi)\,\xi^2 e^{-\xi^2}\,d\xi \;,$$

which finally gets

$$\int_{-\infty}^{+\infty} H_n(\xi)H_m(\xi)\xi^2 e^{-\xi^2}\,d\xi = \begin{cases} \sqrt{\pi}\,2^{n-1}n!(2n+1), & m=n \\ \sqrt{\pi}\,2^n(n+2)!, & m=n+2 \\ \sqrt{\pi}\,2^{n-2}n!, & m=n-2 \\ 0, & \textit{other cases} \end{cases}$$

and leads to third integral.