Brute - Force Treatment of Quantum HO

Simple Harmonic Motion

One of the most commonly encountered problems in quantum mechanics is that of the HARMONIC OSCILLATOR

* This is equivalent to the problem of SIMPLE HARMONIC MOTION in classical systems
* Such harmonic motion is known to be described by a SECOND ORDER differential equation of the form

$$\frac{d^2x}{dt^2} = -\omega^2 x \qquad (13.1)$$

⇒ In this equation *w* is the FREQUENCY of the harmonic motion and the solutions to Equation 13.1 correspond to OSCILLATORY behavior

⇒ Examples of CLASSICAL systems that exhibit simple harmonic motion include an oscillating mass on a SPRING and the motion of a simple PENDULUM

⇒ Examples of QUANTUM harmonic oscillators include the VIBRATING ATOMS in crystals and the motion of ELECTRONS in a magnetic field

Simple Harmonic Motion

For a particle of mass *m* Equation 13.1 implies that the particle moves under the influence of a POSITION-DEPENDENT force

$$F(x) = -m\omega^2 x \qquad (13.2)$$

* By INTEGRATING this equation we obtain the corresponding POTENTIAL-ENERGY variation of the particle

$$V(x) = V(x_o = 0) - \int_{x_o=0}^{x} F(x)dx = \frac{1}{2}m\omega^2 x^2 \qquad (13.3)$$

* A particle that moves in this PARABOLIC potential does so with a CONSTANT total energy (*E*) while its potential energy and momentum (*p*) vary according to

$$E = \frac{1}{2m}p(x)^2 + \frac{1}{2}m\omega^2 x^2 \qquad (13.4)$$

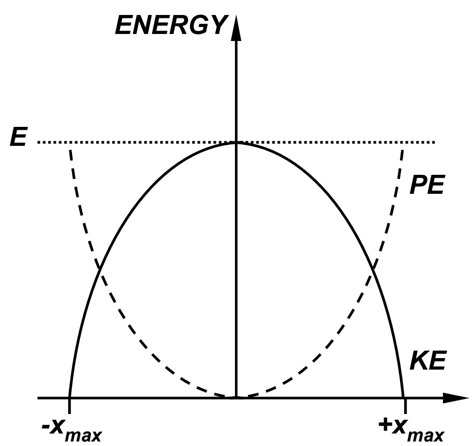
Simple Harmonic Motion

• Equation 13.4 shows that at the ORIGIN of the motion the potential energy is equal to ZERO and the momentum is MAXIMAL

$$E = \frac{1}{2m} p(x=0)^2 \qquad (13.5)$$

* As the particle moves away from the origin however its potential energy INCREASES while at the same time its momentum DECREASES and eventually reaches zero

$\Rightarrow$ These TWO points define the MAXIMAL extent of oscillation which increases as the total energy of the particle increases



• ***POSITION-DEPENDENT ENERGY VARIATIONS FOR THE SIMPLE HARMONIC OSCILLATOR***

• ***THE TOTAL ENERGY OF THE PARTICLE IS CONSTANT AND INDEPENDENT OF POSITION***

• ***THE KINETIC-ENERGY TERM IS MAXIMAL AT THE ORIGIN (x = 0) WHILE THE POTENTIAL ENERGY IS MAXIMAL AT THE EXTREMAL ENDS OF THE MOTION*** $\pm x_{max}$

• ***THE VALUE OF*** x_{max} ***INCREASES WITH INCREASING TOTAL ENERGY***

Strategy for solving the quantum harmonic oscillator problem with the brute-force method

- Clean up the TISWE
- Find the solution in the asymptotic limit $X(\xi)$
- Factor out the asymptotic behavior: $AH(\xi)X(\xi)$
- Derive differential equation for $H(\xi)$
- Expand $H(\xi)$ in the power series
- Put series in the diferential equation and derive recurrence relation
- Enforce boundary condition: Quantize *E*

The Quantum Harmonic Oscillator

To study the QUANTUM-MECHANICAL properties of the harmonic oscillator we need to solve the following form of the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+\frac{1}{2}m\omega^2x^2\psi(x)=E\psi(x) \qquad (13.6)$$

* To make our discussion a little easier we introduce the CHANGE OF VARIABLES

$$\zeta \equiv \sqrt{\frac{m\omega}{\hbar}}x \qquad (13.7) \qquad\qquad K \equiv \frac{2E}{\hbar\omega} \qquad (13.8)$$

* With this change the Schrödinger equation now becomes

$$\frac{\partial^2\psi(\zeta)}{\partial\zeta^2}=(\zeta^2-K)\psi(\zeta) \qquad (13.9)$$

The Quantum Harmonic Oscillator

To begin with we note that for large values of *z* (*x*) Equation 13.9 may be approximated as

$$\frac{\partial^2 \psi(\zeta)}{\partial \zeta^2} \approx \zeta^2 \psi(\zeta) \qquad (13.10)$$

* The corresponding wavefunction solutions to this equation are

$$\psi(\zeta) \approx A e^{-\zeta^2/2} \cancel{+ B e^{\zeta^2/2}} \qquad (13.11)$$

⇒ The second term in this equation can be NEGLECTED since it DIVERGES for large *z* while we know that the range of the particle should be FINITE

* The ASYMPTOTIC form to Equation 13.11 suggests that we write the FULL solutions to the wavefunction (valid for ALL values of *z*) as

$$\psi(\zeta) = h(\zeta) e^{-\zeta^2/2} \qquad (13.12)$$

The Quantum Harmonic Oscillator

By introducing the wavefunction solution of Equation 13.12 into Equation 13.9 the Schrödinger equation now becomes

$$\frac{\partial^2 h(\zeta)}{\partial \zeta^2} - 2\zeta \frac{\partial h(\zeta)}{\partial \zeta} + (K-1)h(\zeta) = 0 \qquad (13.13)$$

* We PROPOSE to look for solutions to $h(z)$ of the POWER-SERIES form

$$h(\zeta) = a_0 + a_1\zeta + a_2\zeta^2 + \ldots = \sum_{i=0}^{\infty} a_i \zeta^i \qquad (13.14)$$

* Successive DIFFERENTIATION of this power series yields

$$\frac{\partial h(\zeta)}{\partial \zeta} = \sum_{i=0}^{\infty} i a_i \zeta^{i-1} \qquad (13.15)$$

$$\frac{\partial^2 h(\zeta)}{\partial \zeta^2} = \sum_{i=0}^{\infty} i(i-1) a_i \zeta^{i-2} \qquad (13.16)$$

The Quantum Harmonic Oscillator

Through substitution of Equations 13.15 & 13.6 our Schrödinger equation now becomes

$$\sum_{i=0}^{\infty}((i+1)(i+2)a_{i+2} - 2ia_i + (K-1)a_i)\zeta^i = 0 \qquad (13.17)$$

* The only way in which this equation can be satisfied for ALL values of *i* is if the coefficient of EACH power of *z* VANISHES

$$(i+1)(i+2)a_{i+2} - 2ia_i + (K-1)a_i = 0 \qquad (13.18)$$

* In this way we arrive at a RECURSION FORMULA

$$a_{i+2} = \frac{(2i+1-K)}{(i+1)(i+2)}a_i \qquad (13.19)$$

⇒ From a knowledge of a_0 we can use this formula to obtain all *i*-EVEN coefficients while a knowledge of a_1 allows us to obtain all *i*-ODD coefficients

The Quantum Harmonic Oscillator

Based on the above we write our wavefunction solutions as

$$h(\zeta) = h_{odd}(\zeta) + h_{even}(\zeta) \qquad (13.20)$$

$$h_{odd}(\zeta) = a_1\zeta + a_3\zeta^3 + a_5\zeta^5 + \dots \qquad (13.21)$$

$$h_{even}(\zeta) = a_0 + a_2\zeta^2 + a_4\zeta^4 + \dots \qquad (13.22)$$

* There is a PROBLEM with our discussion however since NOT all the solutions obtained in this way can be normalized!

$\Rightarrow$ At LARGE *i* the recursion formula becomes

$$a_{i+2} \approx \frac{2}{i} a_i \quad \Rightarrow \quad a_i = \frac{c}{(i/2)!} \qquad (13.23)$$

c IS A CONSTANT

The Quantum Harmonic Oscillator

• When the above approximation holds our wavefunction solutions become

$$h(\zeta) \approx c\sum \frac{1}{(i/2)!}\zeta^{i} \approx c\sum \frac{1}{(k)!}\zeta^{2k} \approx ce^{\zeta^2} \qquad (13.24)$$

* These solutions have exactly the form that we DON'T want however since the exponential term DIVERGES in the limit of infinite z (x)

* The only way out of this problem is to require that our recursion formula (Equation 13.19) TERMINATES at some given value of n

$$a_{n+2} = \frac{(2n+1-K)}{(n+1)(n+2)}a_n \qquad (13.19)$$

⇒ That is we require some value of n for which $a_{n+2} = 0$ which leads us to (if n is odd then all coefficients with even values of n must vanish and vice versa)

$$K = 2n+1 \qquad (13.25)$$

The Quantum Harmonic Oscillator

• Equation 13.25 is a QUANTIZATION CONDITION on the energy of the particle

$$E_n = \left[n + \frac{1}{2}\right]\hbar\omega\,, \quad n = 0, 1, 2, \ldots \qquad (13.27)$$

* This CRUCIAL equation tells us that the modes of vibration of the quantum oscillator are QUANTIZED

* For these quantized energies our RECURSION FORMULA may now be written as

$$a_{i+2} = \frac{(2i + 1 - K)}{(i+1)(i+2)} a_i = \frac{-2(n-i)}{(i+1)(i+2)} a_i \qquad (13.28)$$

$$n = 0: \quad h_0(\zeta) = a_0 \quad \therefore \quad \psi_0(\zeta) = a_0 e^{-\zeta^2/2} \qquad (13.29)$$

$$n = 1: \quad h_1(\zeta) = a_1\zeta \quad \therefore \quad \psi_1(\zeta) = a_1 \zeta e^{-\zeta^2/2} \qquad (13.30)$$

$$n = 2: \quad h_2(\zeta) = a_0(1 - 2\zeta^2) \quad \therefore \quad \psi_2(\zeta) = a_0(1 - 2\zeta^2) e^{-\zeta^2/2} \qquad (13.31)$$

The Quantum Harmonic Oscillator

In general the function $h_n(z)$ will be a POLYNOMIAL of degree n in z involving ONLY either odd or even powers

* Apart from the overall factor (a_0 or a_1) they are known as HERMITE POLYNOMIALS $H_n(z)$

* The arbitrary multiplicative factor is chosen so that the coefficient of the highest power of z is 2^n and the NORMALIZED wavefunctions are given as (see Appendix)

$$\psi_n(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\zeta) e^{-\zeta^2/2}, \quad \zeta \equiv \sqrt{\frac{m\omega}{\hbar}}x \qquad (13.32)$$

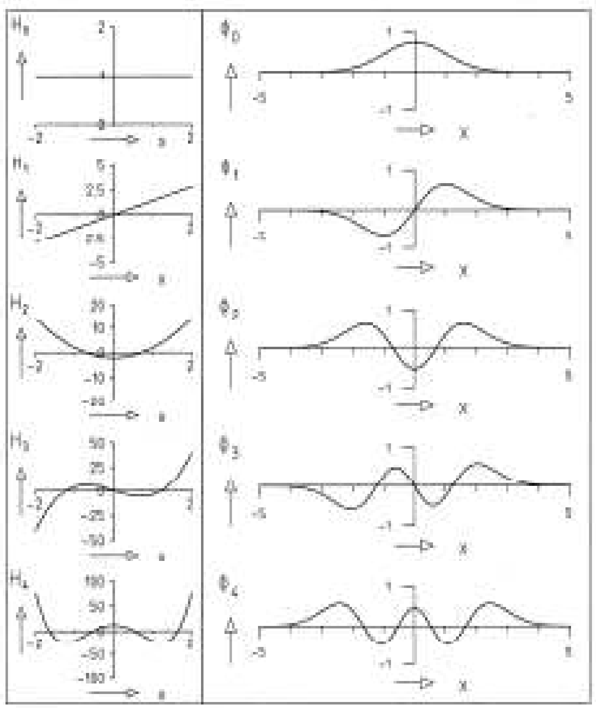
$H_0 = 1$	$H_4 = 16x^4 - 48x^2 + 12$
$H_1 = 2x$	$H_5 = 32x^5 - 160x^3 + 120x$
$H_2 = 4x^2 - 2$	
$H_3 = 8x^3 - 12x$	

THE FIRST FEW HERMITE POLYNOMIALS $H_n(x)$

The Quantum Harmonic Oscillator

Some oscillator wavefunctions are shown below and from their form we see that the behavior of the quantum oscillator is vary DIFFERENT to that of its classical counterpart

* The probability of finding the particle outside the classically allowed range is NOT zero since the particle can TUNNEL into the classically-forbidden region
* For the ODD wavefunctions the probability of finding the particle at the center of the parabolic potential is ZERO



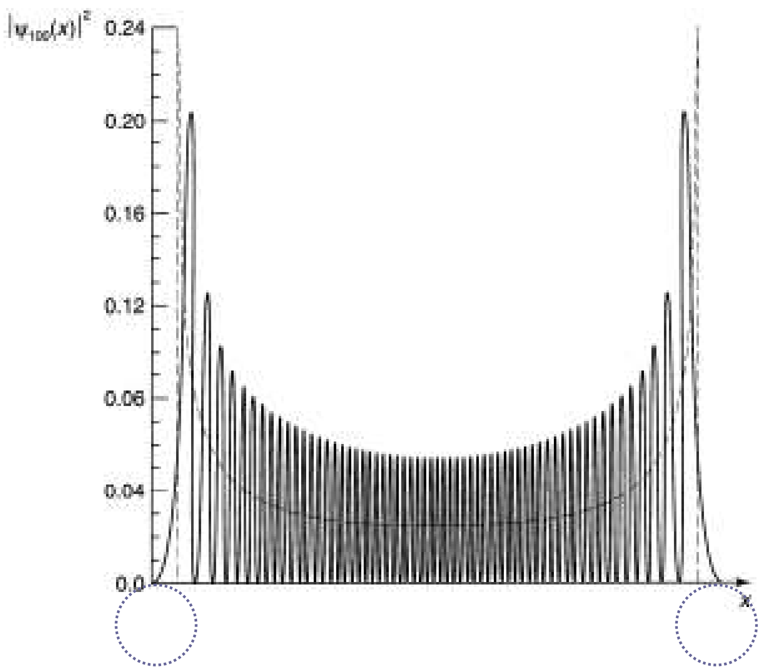
- ***THE FIRST FOUR WAVEFUNCTIONS FOR THE HARMONIC OSCILLATOR***
- ***NOTE THAT THE WAVEFUNCTIONS DECAY WITH INCREASING MAGNITUDE OF x AS WE WOULD EXPECT FOR A CLASSICAL OSCILLATOR***
- ***THE EFFECTIVE RANGE OF THE WAVEFUNCTION INCREASES WITH INCREASING ENERGY AS WE WOULD EXPECT CLASSICALLY***
- ***THE RANGE OF THE WAVEFUNCTION EXTENDS BEYOND THAT ALLOWED CLASSICALLY HOWEVER SINCE THE PARTICLE CAN TUNNEL INTO THE CLASSICALLY-FORBIDDEN REGIONS***
- ***THE PICTURE BOOK OF QUANTUM MECHANICS***
  S. BRANDT and H-D. DAHMEN, SPRINGER-VERLAG, NEW YORK (1995)

The Quantum Harmonic Oscillator

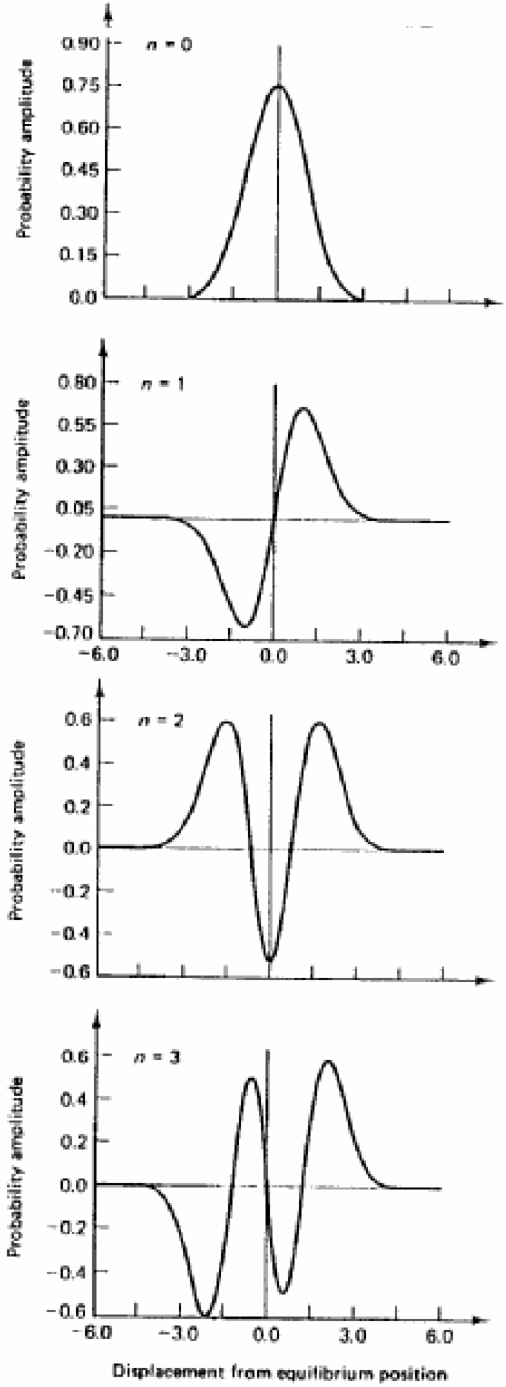
With increasing quantum number *n* the quantum-mechanical probability density begins to MATCH that expected for a CLASSICAL particle

* The probability is MAXIMAL at the ENDS of the motion where the velocity is ZERO and MINIMAL at the CENTER of motion where the velocity is MAXIMAL

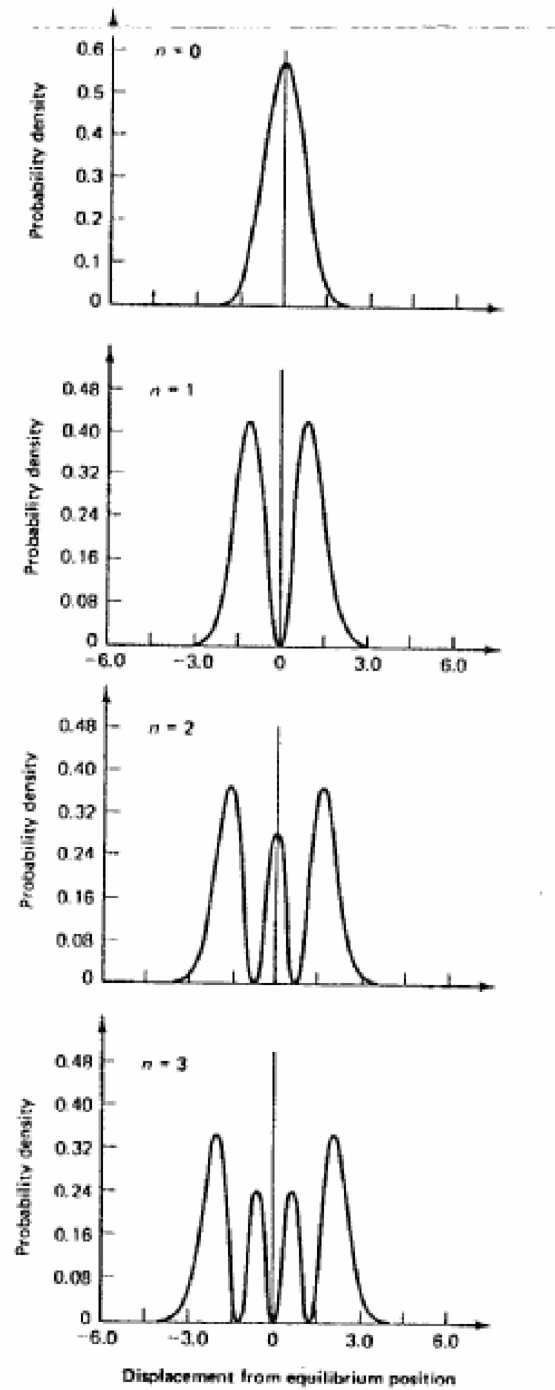
* This is an example of the CORRESPONDENCE PRINCIPLE which requires quantum mechanics to yield the results of classical physics in the limit of LARGE quantum number



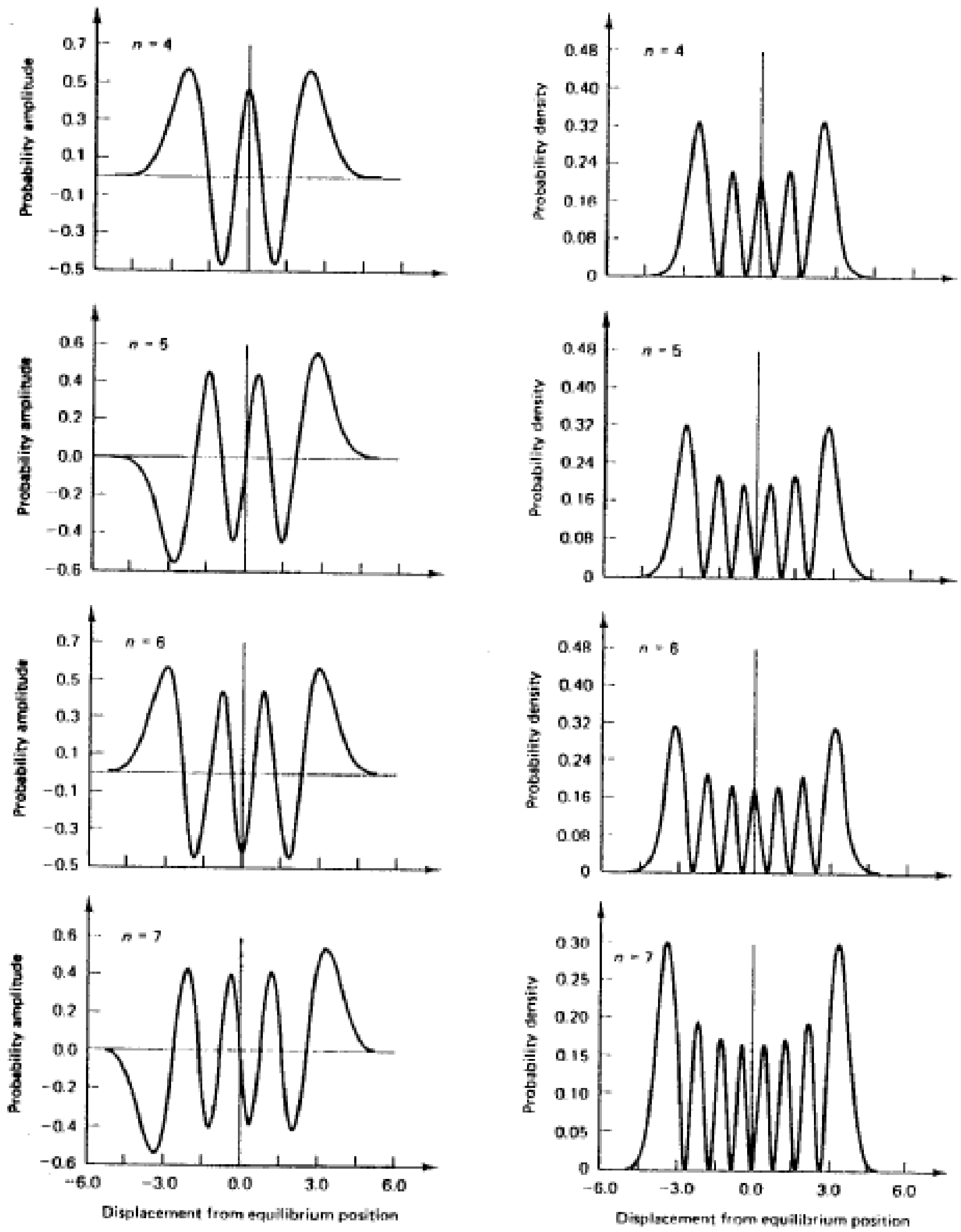
- *THE SOLID LINE SHOWS THE PROBABILITY DENSITY FOR THE HUNDREDTH ENERGY LEVEL OF THE HARMONIC OSCILLATOR*
- *THE DASHED LINE SHOWS THE CORRESPONDING DENSITY FOR A CLASSICAL PARTICLE WITH THE SAME ENERGY*
- *FOR THE LARGE QUANTUM NUMBER CONSIDERED HERE WE SEE A CORRESPONDENCE BETWEEN THE QUANTUM AND CLASSICAL PROBABILITY DENSITIES*
- *NOTE THAT THE QUANTUM PARTICLE CAN TUNNEL BEYOND THE RANGE OF THE CLASSICAL PARTICLE HOWEVER (CIRCLED REGIONS)*
- *INTRODUCTION TO QUANTUM MECHANICS D. J. GRIFFITHS, PRENTICE HALL, NEW JERSEY (1995)*


n = 0
n = 1
n = 2
n = 3
Probability amplitude
0.90
0.75
0.60
0.45
0.30
0.15
0.0
0.80
0.55
0.30
0.05
-0.20
-0.45
-0.70
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-6.0
-3.0
0.0
3.0
6.0
Displacement from equilibrium position

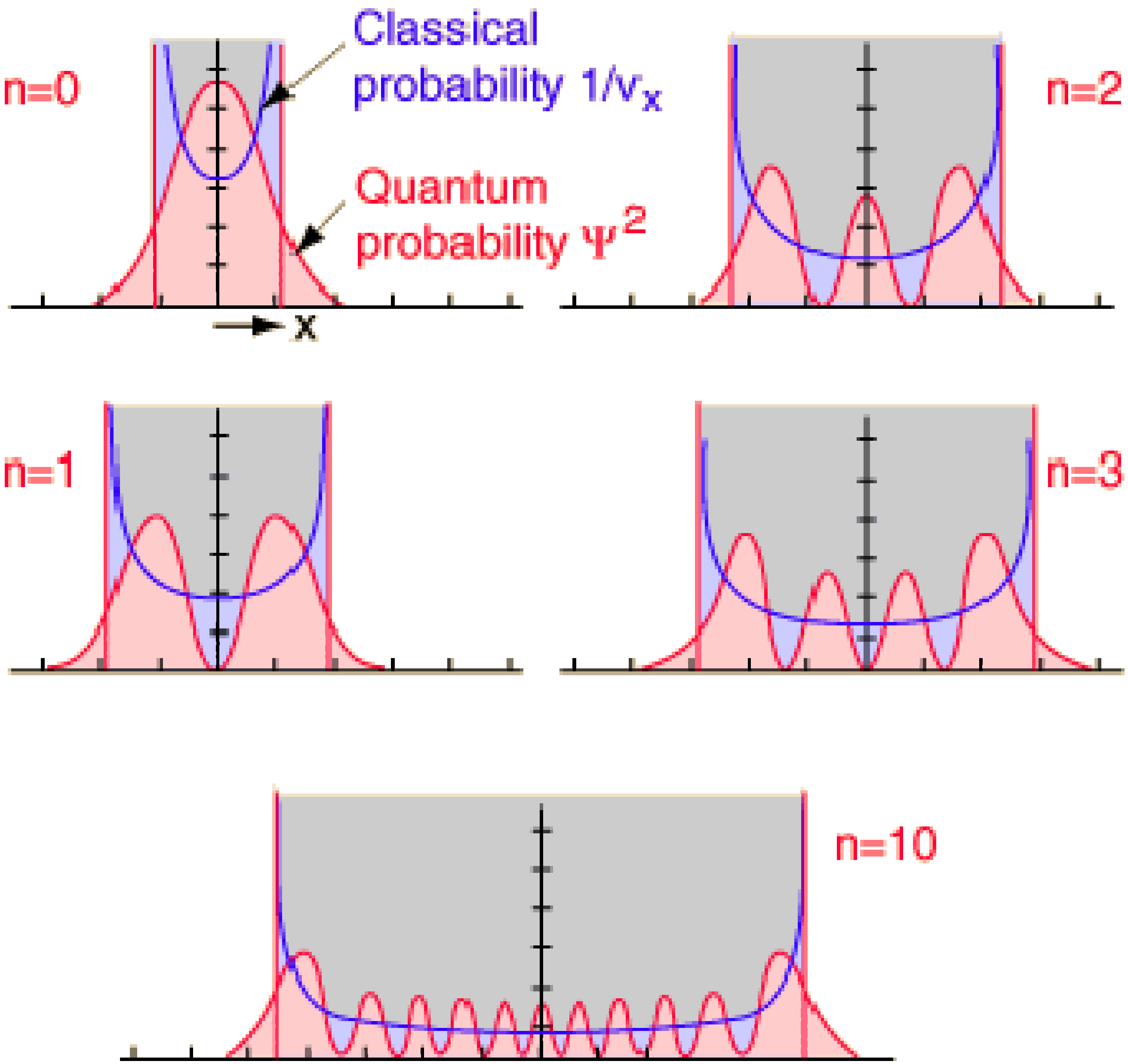
(a)


n = 0
n = 1
n = 2
n = 3
Probability density
0.6
0.5
0.4
0.3
0.2
0.1
0
0.48
0.40
0.32
0.24
0.16
0.08
-6.0
-3.0
3.0
6.0
Displacement from equilibrium position

(b)


n = 4
n = 5
n = 6
n = 7
Probability amplitude
Probability density
-6.0
-3.0
0.0
3.0
6.0
Displacement from equilibrium position

(a) (b)



n=0
Classical
probability 1/v$_x$
Quantum
probability ψ^2
x
n=2
n=1
n=3
n=10

n	$H_n(y)$	E_n
0	1	$\frac{1}{2}\hbar\omega$
1	$2y$	$\frac{3}{2}\hbar\omega$
2	$4y^2 - 2$	$\frac{5}{2}\hbar\omega$
3	$8y^3 - 12y$	$\frac{7}{2}\hbar\omega$
4	$16y^4 - 48y^2 + 12$	$\frac{9}{2}\hbar\omega$
5	$32y^5 - 160y^3 + 120y$	$\frac{11}{2}\hbar\omega$

First four harmonic oscillator normalized wavefunctions

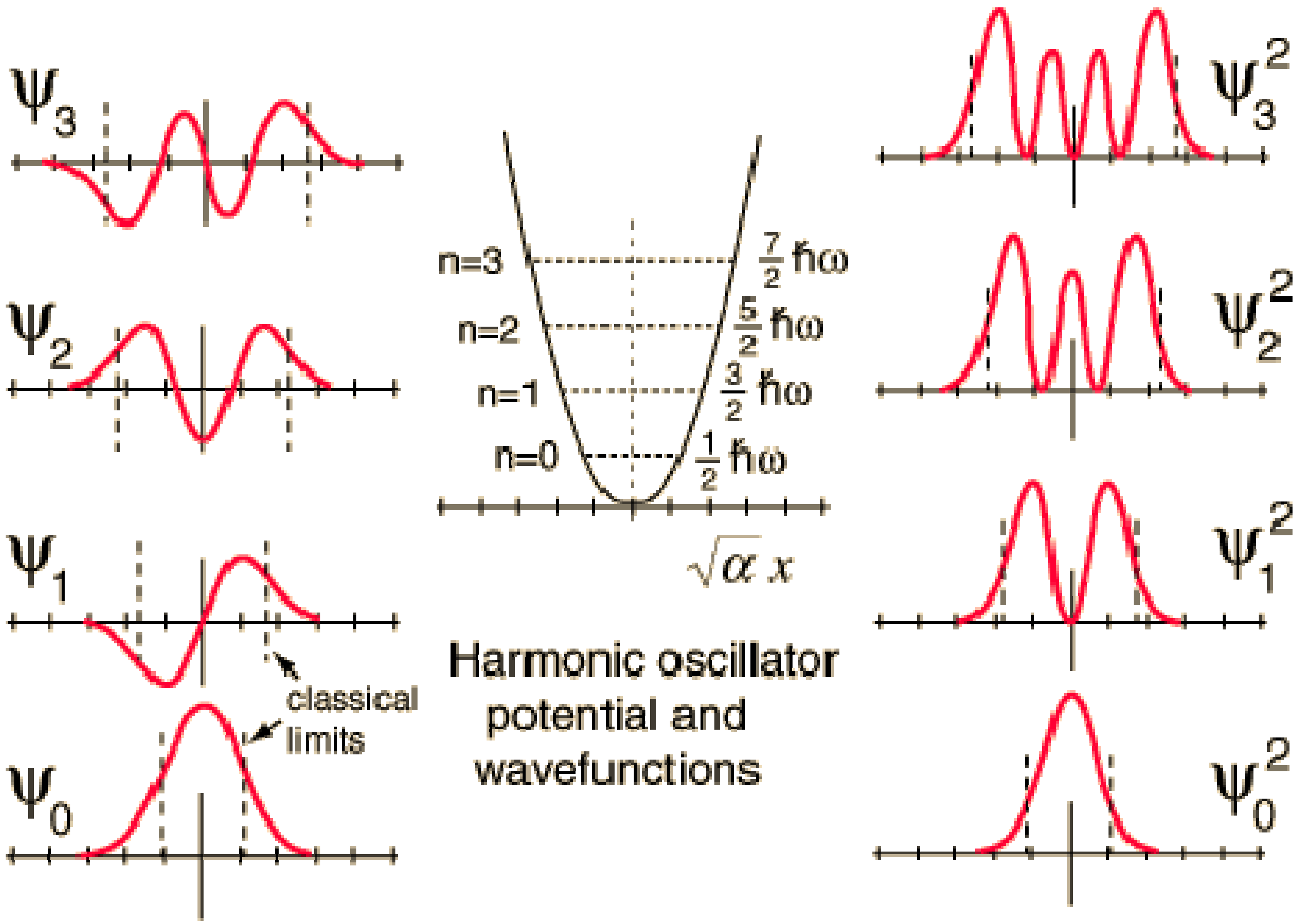
$$\Psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-y^2/2}$$

$$\Psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2}y\, e^{-y^2/2}$$

$$\Psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2y^2 - 1)\, e^{-y^2/2}$$

$$\Psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}}(2y^3 - 3y)\, e^{-y^2/2}$$

$$\alpha = \frac{m\omega}{\hbar} \qquad y = \sqrt{\alpha}\, x$$



Ψ_3
Ψ_2
Ψ_1
Ψ_0
classical limits
n=3
n=2
n=1
n=0
$\frac{7}{2}\hbar\omega$
$\frac{5}{2}\hbar\omega$
$\frac{3}{2}\hbar\omega$
$\frac{1}{2}\hbar\omega$
$\sqrt{\alpha}\,x$
Harmonic oscillator potential and wavefunctions
Ψ_3^2
Ψ_2^2
Ψ_1^2
Ψ_0^2

Some General Conclusions

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

$$\psi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\beta x) \exp\left[-\frac{\beta^2 x^2}{2}\right], \quad \beta = \sqrt{\frac{m\omega_0}{\hbar}}$$

The classical Turning point is found from the condition:

$$(n + 1/2)\hbar\omega_0 = \frac{1}{2} m\omega_0^2 x_n^2 \rightarrow x_n = \pm\sqrt{\frac{2n+1}{\beta^2}}$$

Handy integrals of Eigenfunctions of the SHO

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}$$

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

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

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

Position and momentum expectation values

$$\langle x \rangle_n = 0 \rightarrow (\Delta x)_n = \sqrt{\langle x^2 \rangle_n} = \sqrt{\frac{E_n}{m\omega_0^2}}$$

$$\langle p \rangle_n = 0 \rightarrow (\Delta p)_n = \sqrt{\langle p^2 \rangle_n} = \sqrt{mE_n}$$

$$(\Delta x)_n (\Delta p)_n = E_n / \omega_0 = (n + 1/2)\hbar$$

Appendix

• **Prior to their normalization solution of the Schrödinger equation yields allowed wavefunctions for the harmonic oscillator that take the form**

$$\psi_n(x) = c_n H_n(\zeta) e^{-\zeta^2/2} \qquad (A13.1)$$

*** Here c_n is an as yet undetermined NORMALIZATION CONSTANT and to determine this we define the GENERATING FUNCTION**

$$F(s,\zeta) = \sum_{n=0}^{\infty} H_n(\zeta) \frac{s^n}{n!} \qquad (A13.2)$$

⇒ This function is a power series in *s* with coefficients given by Hermite polynomials of the appropriate order

*** DIFFERENTIATING both sides of Equation A13.2 with respect to ζ yields**

$$\frac{\partial F(s,\zeta)}{\partial \zeta} = \sum_{n=0}^{\infty} \frac{\partial H_n(\zeta)}{\partial \zeta} \frac{s^n}{n!} \qquad (A13.3)$$

Appendix

• To determine the derivative on the RHS of Equation A13.3 we note that the derivatives of the Hermite polynomials satisfy

$$\frac{\partial H_n(\zeta)}{\partial \zeta} = 2nH_{n-1}(\zeta) \qquad (A13.4)$$

* With this relation Equation A13.3 can now be rewritten as

$$\frac{\partial F(s,\zeta)}{\partial \zeta} = 2sF(s,\zeta) \qquad (A13.5)$$

* Solution of this differential equation yields

$$F(s,\zeta) = F(s,0)e^{2s\zeta} = \left[\sum_{n=0}^{\infty} H_n(0)\frac{s^n}{n!}\right]e^{2s\zeta} \qquad (A13.6)$$

⇒ We have used Equation A13.2 in the final step of this equation

Appendix

- We have seen that $H_n(0) = 0$ for ODD values of n while for EVEN values

$$H_n(0) = (-1)^{n/2} \frac{n!}{(n/2)!} \qquad (A13.7)$$

* With this form Equation A13.6 can now be rewritten as

$$F(s,0) = \sum_{k=0}^{\infty} (-1)^k \frac{s^{2k}}{k!} = e^{-s^2} \qquad (A13.8)$$

* This leads to the FINAL simple form for the GENERATING FUNCTION

$$F(s,\zeta) = e^{-s^2} e^{-2s\zeta} = e^{\zeta^2 - (s-\zeta)^2} \qquad (A13.9)$$

Appendix

• We now note that the generating function has been defined such that

$$H_n(\zeta) = \left[\frac{\partial^n}{\partial s^n} F(s,\zeta) \right]_{s=0} \qquad (A13.10)$$

* Substituting Equation A13.10 for the generating function this becomes

$$H_n(\zeta) = (-1)^n e^{\zeta^2} \frac{\partial^n}{\partial \zeta^n} e^{-\zeta^2} \qquad (A13.11)$$

* Now consider the integral

$$I = \int_{-\infty}^{\infty} F(s,\zeta)\, F(t,\zeta) e^{-\zeta^2} d\zeta \qquad (A13.12)$$

Appendix

• **From Equation A13.9 it is straightforward to show that Equation A13.12 reduces to**

$$I = \sqrt{\pi} \sum_n \frac{2^n s^n t^n}{n!} \qquad (A13.13)$$

*** On the other hand we could use our original definition of the generating function (Equation A13.4) to write the integral *I* as**

$$I = \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} H_n(\zeta) \frac{s^n}{n!} \sum_{n=0}^{\infty} H_n(\zeta) \frac{t^n}{n!} e^{-\zeta^2} d\zeta$$

$$= \sum_{n=0}^{\infty} \frac{s^n}{n!} \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{-\infty}^{\infty} H_n(\zeta) H_n(\zeta) e^{-\zeta^2} d\zeta \qquad (A13.14)$$

$\Rightarrow$ **By definition Equations A13.13 & A13.14 must be EQUAL**

Appendix

- **Equating Equations A13.13 & A13.14 yields the following result**

$$\int_{-\infty}^{\infty} H_n(\zeta) H_n(\zeta) e^{-\zeta^2} d\zeta = \sqrt{\pi}\, 2^n n! \qquad (A13.15)$$

*** NORMALIZATION of the wavefunction of Equation A13.1 requires**

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_n(x)dx = c_n^* c_n \int_{-\infty}^{\infty} H_n^*(\zeta) H_n(\zeta) e^{-\zeta^2} d\zeta = 1 \qquad (A13.16)$$

⇒ Comparison of Equations A13.15 & A13.16 reveals

$$c_n^* c_n = \frac{1}{\sqrt{\pi}\, 2^n n!} \quad \therefore \quad c_n = \frac{1}{(\sqrt{\pi}\, 2^n n!)^{1/2}} \qquad (A13.15)$$

⇒ In this way we finally (!) arrive at the NORMALIZED wavefunctions

$$\psi_n(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\zeta) e^{-\zeta^2/2}, \quad \zeta \equiv \sqrt{\frac{m\omega}{\hbar}}\, x \qquad (13.32)$$