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Chapter 6

The Schrodinger Equation.

Lecture 1

Wave function
Probability interpretation
Normalization conditions

"Derivation" of Schrodinger equation.
$\cos(kx-\omega t)$, $\sin(kx-\omega t)$ plane wave

Comments on Schrodinger equation

Normalization Go to 0 fast

Expectation value

$\langle f(x)\rangle$ $\langle x^2\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\, x^2\, \psi(x)\, dx$

$\langle g(p)\rangle$ $\langle p^2\rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \left[-\hbar^2 \frac{\partial^2}{\partial x^2}\right] \psi(x,t)\, dx$

Seperation of variable.

Lecture 2

Example 1 Infinite potential well

Example 2 Simple harmonic oscillator

Meaning of eigenfunctions and eigenvalues

Outline of the course.

Chapter 6
The Schrodinger Equation

$\psi(x,t)$ one dimensional wave function

$\downarrow$ complex

$\psi(\vec{r},t)$ three dimensional wave function.

$= U(x,t) + iV(x,t)$

$= R(x,t)\, e^{iS(x,t)}$

$U(x,t)$, $V(x,t)$; $R(x,t)$, $S(x,t)$ are real functions

$\psi^*(x,t) = U(x,t) - iV(x,t) = R(x,t)\, e^{-iS(x,t)}$

$|\psi(x,t)|^2 = \psi^*(x,t)\,\psi(x,t)$

$= (U(x,t))^2 + (V(x,t))^2$

$= [R(x,t)]^2 \geq 0$

In double slit experiment,

$\psi = \psi_1 + \psi_2$

$|\psi|^2 = |\psi_1 + \psi_2|^2$

$= |\psi_1|^2 + |\psi_2|^2 + \overbrace{\underbrace{\psi_1^* \psi_2}_{\text{interference}} + \psi_2^* \psi_1}^{\text{real}}$

$|\psi(x,t)|^2 dx$ probability of finding the "electron" between x and $x+dx$ at time t (M. Born)

$|\psi|^2$ is positive definite

$\downarrow$ allow the probability interpretation.

Normalization condition

$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$

If the equation that ψ obeys is linear, then a complex constant C multiply the ψ is also a solution of the equation

↓

we can always multiply the wave function we found originally by a constant to ensure the function satisfies the normalization conditions

↓

normalization procedure.

Next we shall discuss the equation obeyed by $\psi(x,t)$ i.e., the Schrodinger equation.

Note. we shall not derive the Schrodinger equation. The equation cannot be derived any more than Newton's equation of motion could be

A complex plane wave function can be written as

$$A\, e^{ikx - i\omega t}$$

$$i\hbar \frac{\partial}{\partial t}\psi = \hbar\omega\psi = E\psi \qquad E = h\nu = \hbar\omega$$

$$-i\hbar \frac{\partial}{\partial x}\psi = \hbar k\psi = p\psi \qquad k = \frac{2\pi}{\lambda}$$

$$p = \frac{h}{\lambda}$$

These equations has the general form

$$(\text{differential operator})\,\psi = \text{constant}\ \psi$$

For free particle $\quad E = \dfrac{p^2}{2m}$

$$\Rightarrow \quad i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

↓

Schrodinger equation for free particle

For an "electron" moving under the influence of potential $V(x)$

$$\frac{p^2}{2m} + V(x) = E$$

Hint $\quad E_{op} \rightarrow i\hbar \frac{\partial}{\partial t}$

$\quad\quad P_{op} \rightarrow -i\hbar \frac{\partial}{\partial x}$

Multiple by $\psi(x,t)$

$$\Rightarrow \quad i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x,t)\psi(x,t)$$

Schrodinger equation
(time - dependent)
in one dimension.

- The equation is linear.
- The equation is complex
- The equation is first order derivative in t.
  Given $\psi(x,0) \Rightarrow \psi(x,t)$
- The equation is first order derivative in t,
  second order derivative in x
  $\Rightarrow$ the equation is not relativistic

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi \qquad (1)$$

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V^*\psi \qquad (2)$$

$V^* = V$ for real potential

$\psi^* \cdot (1) - \psi \cdot (2)$

$$i\hbar\, \psi^* \frac{\partial \psi}{\partial t} + i\hbar \frac{\partial \psi^*}{\partial t}\psi = -\frac{\hbar^2}{2m}\left[\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2}{\partial x^2}\psi^*\right]$$

$$= -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$$

$$\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{i\hbar 2m}\frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$$

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty} \psi^*\psi \, dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial x}\frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right] dx$$

$$\frac{d}{dt} \qquad = -\int_{-\infty}^{\infty} \frac{\partial}{\partial x} S \, dx \rightarrow 0$$

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Erwin Schrödinger. [*Courtesy of the Niels Bohr Library, American Institute of Physics.*]

Max Born

(1882–1970, German–British)

Born is best known for his work on the mathematical structure of quantum mechanics and the interpretation of the wave function. After getting his doctorate, he worked with J. J. Thomson at Cambridge and lectured in Chicago for Michelson. He subsequently became professor at Berlin and then Göttingen. When Hitler came to power, Born left Germany and became a professor at Edinburgh University. He won the Nobel Prize in physics in 1954 for his contributions to quantum theory.

B I O G R A P H Y

ERWIN SCHRÖDINGER
(1887–1961)

Erwin Schrödinger was an Austrian theoretical physicist best known as the creator of wave mechanics. As a young man he was a good student who liked mathematics and physics, but also Latin and Greek for their logical grammar. He received a doctorate in physics from the University of Vienna. Although his work in physics was interrupted by World War I, by 1920 he had produced important papers on statistical mechanics, color vision, and general relativity, which he at first found quite difficult to understand. Expressing his feelings about a scientific theory in the remarkably open and outspoken way he maintained throughout his life, Schrödinger found general relativity initially "depressing" and "unnecessarily complicated." Other Schrödinger remarks in this vein, with which some readers will enthusiastically agree, are as follows: The Bohr–Sommerfeld quantum theory was "unsatisfactory, even disagreeable." "I . . . feel intimidated, not to say repelled, by what seem to me the very difficult methods [of matrix mechanics] and by the lack of clarity."

Shortly after de Broglie introduced the concept of matter waves in 1924, Schrödinger began to develop a new relativistic atomic theory based on de Broglie's ideas, but his failure to include electron spin led to the failure of this theory for hydrogen. By January of 1926, by treating the electron as a nonrelativistic particle, however, Schrödinger had introduced his famous wave equation and successfully obtained the energy values and wavefunctions for hydrogen. As Schrödinger himself pointed out, an outstanding feature of his approach was that the discrete energy values emerged from his wave equation in a natural way (as in the case of standing waves on a string), and in a way superior to the artificial postulate approach of Bohr. Another outstanding feature of Schrödinger's wave mechanics was that it was easier to apply to physical problems than Heisenberg's matrix mechanics, because it involved a partial differential equation very similar to the classical wave equation. Intrigued by the remarkable differences in conception and mathematical method of wave and matrix mechanics, Schrödinger did much to hasten the universal acceptance of all of quantum theory by demonstrating the mathematical equivalence of the two theories in 1926.

Although Schrödinger's wave theory was generally based on clear physical ideas, one of its major problems in 1926 was the physical interpretation of the wavefunction Ψ. Schrödinger felt that the electron was ultimately a wave, Ψ was the vibration amplitude of this wave, and $\Psi^*\Psi$ was the electric charge density. As mentioned in Chapter 4, Born, Bohr, Heisenberg, and others pointed out the problems with this interpretation and presented the currently accepted view that $\Psi^*\Psi$ is a probability, and that the electron is ultimately no more a wave than a particle. Schrödinger never accepted this view, but registered his "concern and disappointment" that this "transcendental, almost psychical interpretation" had become "universally accepted dogma."

In 1927 Schrödinger, at the invitation of Max Planck, accepted the chair of theoretical physics at the University of Berlin, where he formed a close friendship with Planck and experienced six stable and productive years. In 1933, disgusted with the Nazis like so many of his colleagues, he left Germany. After several moves reflecting the political instability of Europe, he eventually settled at the Dublin Institute for Advanced Studies. Here he spent 17 happy, creative years working on problems in general relativity, cosmology, and the application of quantum physics to biology. This last effort resulted in a fascinating short book, *What is Life?*, which induced many young physicists to investigate biological processes with chemical and physical methods. In 1956, he returned home to his beloved Tyrolean mountains. He died there in 1961.

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B I O G R A P H Y

MAX BORN
(1882–1970)

Max Born was a German theoretical physicist who made major contributions in many areas of physics, including relativity, atomic and solid-state physics, matrix mechanics, the quantum mechanical treatment of particle scattering ("Born approximation"), the foundations of quantum mechanics (Born interpretation of Ψ), optics, and the kinetic theory of liquids. Born received the doctorate in physics from the University of Göttingen in 1907, and he acquired an extensive knowledge of mathematics as the private assistant to the great German mathematician David Hilbert. This strong mathematical background proved a great asset when he was quickly able to reformulate Heisenberg's quantum theory in a more consistent way with matrices.

In 1921, Born was offered a post at the University of Göttingen, where he helped build one of the strongest physics centers of the twentieth century. This group consisted, at one time or another, of the mathematicians Hilbert, Courant, Klein, and Runge and the physicists Born, Jordan, Heisenberg, Franck, Pohl, Heitler, Herzberg, Nordheim, and Wigner, among others. In 1926, shortly after Schrödinger's publication of wave mechanics, Born applied Schrödinger's methods to atomic scattering and developed the Born approximation method for carrying out calculations of the probability of scattering of a particle into a given solid angle. This work furnished the basis for Born's startling (in 1926) interpretation of $|\Psi|^2$ as the probability density. For this so-called statistical interpretation of $|\Psi|^2$ he was awarded the Nobel prize in 1954.

Fired by the Nazis, Born left Germany in 1933 for Cambridge and eventually the University of Edinburgh, where he again became the leader of a large group investigating the statistical mechanics of condensed matter. In his later years Born campaigned against atomic weapons, wrote an autobiography, and translated German humorists into English.

(AIP Emilio Segrè Visual Archives)

$\Rightarrow$ the normalization is preserved.

Normalization

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = N$$

Define $\psi' = \frac{1}{\sqrt{N}} \psi$

$$\Rightarrow \int_{-\infty}^{\infty} |\psi'|^2 dx = 1$$

$$P(x,t) = \psi'^*(x,t)\psi'(x,t)$$

probability density

Expectation value

$$\langle x \rangle_t = \int_{-\infty}^{\infty} \psi'^*(x,t)\, x\, \psi'(x,t)\, dx$$

expectation value of x at time t

$$= \frac{\int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\, dx}$$

More generally

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \psi^*(x) f(x) \psi(x)\, dx.$$

Now we want to calculate $\langle p \rangle$

expectation of the momentum.

From earlier discussion

$$p = -i\hbar \frac{\partial}{\partial x}$$

$$\int ⓒ \psi^* ⓑ \psi ⓐ dx$$

ⓐ is not defined

ⓒ clearly gives a pure imaginary answer

is not acceptable.

ⓑ is the only possible choice.

Next we want to prove

$$\frac{d\langle x \rangle}{dt} = \frac{\langle p \rangle}{m}$$

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int \psi^* x \psi \, dx$$

$$= \int \left[\frac{\partial \psi^*}{\partial t} x\psi + \psi^* x \psi\right] dx$$

$$\frac{\partial \psi}{\partial t} = i\frac{\hbar}{m}\frac{\partial^2}{\partial x^2}\psi(x,t) - \frac{i}{\hbar}V(x)\psi(x,t)$$

This is the Schrodinger equation

$$\frac{\partial \psi^*}{\partial t} = -i\frac{\hbar}{m}\frac{\partial^2}{\partial x^2}\psi^*(x,t) + \frac{i}{\hbar}V(x)\psi^*(x,t)$$

$V(x) = V^*(x)$ is used

$$\Rightarrow \frac{\partial \psi^*}{\partial t}x\psi + \psi^* x\frac{\partial \psi}{\partial t} = -\frac{i\hbar}{2m}\left(\frac{\partial^2\psi^*}{\partial x^2}x\psi - \psi^* x\frac{\partial^2\psi}{\partial x^2}\right)$$

$$= -\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}x\psi - \psi^* x\frac{\partial\psi}{\partial x} - \psi^*\psi\right) - \frac{i\hbar}{m}\psi^*\frac{\partial}{\partial x}\psi$$

this can be shown readily by work out the algebra.

Integrate both side from $-\infty$ to ∞

$$LHS = \frac{d\langle x\rangle}{dt}$$

The first term in the RHS $\Rightarrow$ vanishes

since $\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx$ is finite

$\psi(x)$ goes to zero faster than $x^{-\frac{1}{2}}$

$$\Rightarrow \quad RHS = -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\psi\,dx = \frac{\langle p\rangle}{m}$$

· This is the Ehrenfest theorem

One can show $\frac{d\langle p\rangle}{dt} = \langle -\frac{\partial V}{\partial x}\rangle$

· Support the identification $P_{op} \to -i\hbar\frac{\partial}{\partial x}$

· $\langle p\rangle$ is real

In more mathematical language, P_{op} is Hermitian.

· Note, the role played by the boundary condition.
normalization

Time dependent Schrodinger equation.

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi = i\hbar\frac{\partial}{\partial t}\psi$$

Define $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) = H_{op}$

$V(x,t)$

Hamiltonian operator

The Schrodinger equation can be written as

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}$$

If V is time-independent, i.e., $V(x,t) = V(x)$ then the problem can be solved by method of seperation of variables.

Ansatz, $\psi(x,t) = u(x)T(t)$

Substitute into the time-dependent Schrodinger equation

$$\Rightarrow \quad i\hbar u(x) \frac{dT(t)}{dt} = T(t)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)u(x)\right)$$

Divide by $T(t)u(x)$

$$\underbrace{i\hbar \frac{1}{T(t)}\frac{dT(t)}{dt}}_{\text{function of } t \text{ only}} = \underbrace{\frac{1}{u(x)}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)u(x)\right)}_{\text{function of } x \text{ only}}$$

the only possibility
it is a constant
(known as seperation
constant) E

$$\Rightarrow \quad i\hbar \frac{dT(t)}{dt} = E\,T(t) \quad \Rightarrow \quad T(t) = e^{-iEt/\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)u(x) = E\,u(x)$$

$$[H_{op}u(x) = E\,u(x)]$$

time independent Schrodinger equation.

If $u_E(x)$ is found, then

$$\psi(x,t) = u_E(x)e^{-iEt/\hbar}$$

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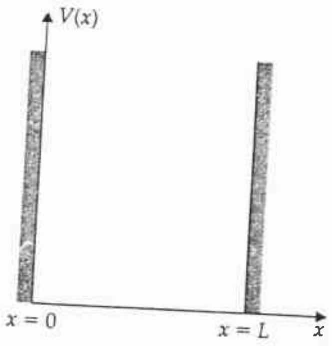
Example: The infinite well. (See the textbook)

$$V(x) = \begin{cases} \infty & \text{for } x > L \\ 0 & \text{for } 0 < x < L \\ \infty & \text{for } x < 0 \end{cases}$$



The infinite-well potential has infinitely high potential-energy "walls" that confine a particle under its influence to the region $0 < x < L$. It is convenient to choose the bottom of the well to correspond to zero potential energy.

In the region $0 < x < L$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) = E\,u(x)$$

Boundary condition

$u(0) = u(L) = 0$

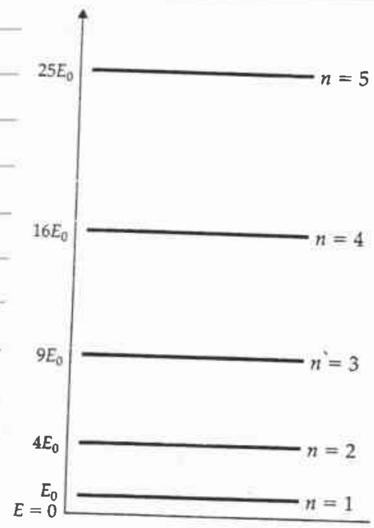
$u(x) = A \sin kx$ $\quad$ ($u = 0$ at $x = 0$)

$kL = n\pi$ $\quad$ $n = 1, 2, \cdots$

$\downarrow$

$k = \frac{n\pi}{k}$

$\Rightarrow \quad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$ $\quad$ $n = 1, 2, \cdots$



The energy spectrum (i.e., the allowed, or possible, energy values) for a particle of mass m in the infinite well of •Fig. 6–5. The ground-state energy is $E_0 = \frac{\hbar^2\pi^2}{2mL^2}$.

Normalization

$|A|^2 \int_0^L \sin^2 kx \, dx = 1$

$\Rightarrow \quad A = \frac{\sqrt{2}}{L} e^{i\varphi}$

$\downarrow$

does not appear in physical probabilities

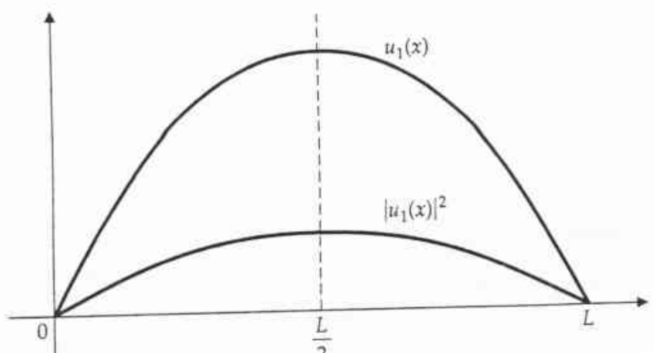
$\int \psi^* \; L \; \psi \, dx$

linear operator

the result is independent of φ

Ground state wave function

$u_1(x) = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$



The ground-state wave function $u_1(x)$, as well as the associated probability distribution $|u_1(x)|^2$, for the infinite well is symmetric about the midpoint $x = L/2$.

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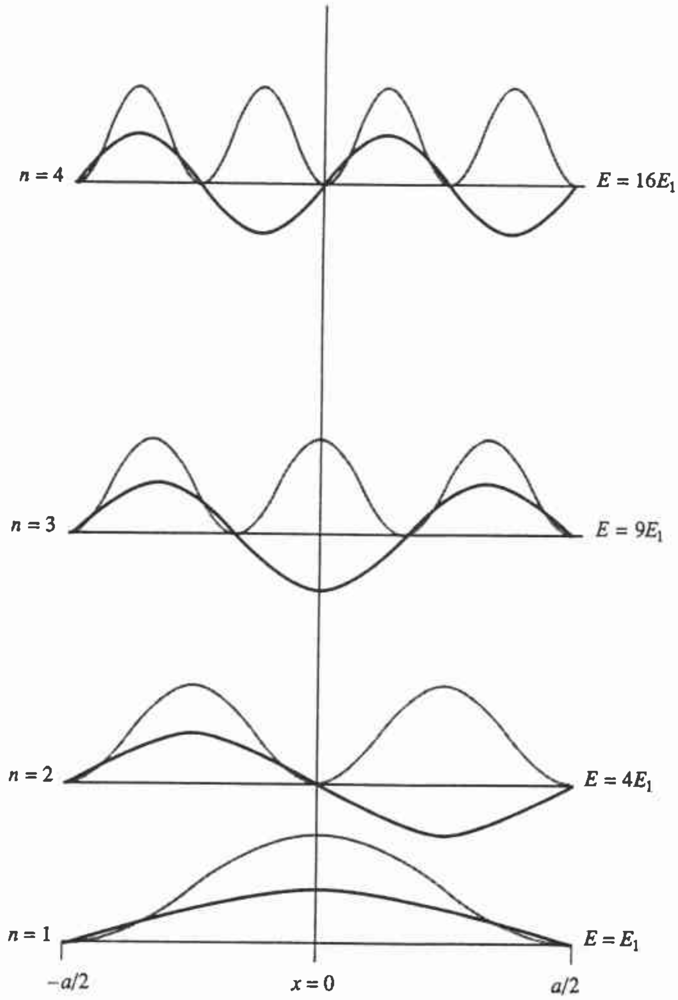

The wave functions (solid color) and probability densities (light color) for the ground state (n = 1) and first three excited states (n = 2, 3, and 4) of a particle confined to an infinite one-dimensional potential well of width a. Note that the wave functions are either odd or even functions of x.

Example: Simple harmonic oscillator

$$V(x) = \frac{1}{2} k x^2$$

(See Griffiths' "Introduction to Quantum Mechanics" P. 37 to 43 ; and the textbook P. 143 - 144)

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

$$m\omega^2 = k$$

Let $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$ (changing variable to simplify the equation)

$$\Rightarrow \quad \frac{d^2\psi}{d^2\xi} = (\xi^2 - K)\psi \qquad K = \frac{2E}{\hbar\omega}$$

For large ξ

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2} \cong \xi^2\psi$$

$\Rightarrow$ approximate solution $\psi(\xi) \simeq A e^{-\xi^2/2} + B e^{+\xi^2/2}$

not normalizable

$$\psi(\xi) = h(\xi) e^{-\xi^2/2}$$

(hoping $h(\xi)$ has simpler functional form than $\psi(x)$)

$$\Rightarrow \quad \frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0$$

Solve the equation using the series expansion method

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j \xi^j$$

Task is to find $a_0, a_1, \cdots$

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{j=0}^{\infty} j a_j \xi^{j-1}$$

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4 a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j$$

Put back into the differential equation

$$\sum_{j=0}^{\infty}[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j]\xi^j = 0$$

$$\Rightarrow \quad (j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0$$

$$\Rightarrow \quad a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j$$

recursion relation

$a_0 \Rightarrow a_2, a_4, \cdots$ can be calculated
$a_1 \Rightarrow a_1, a_2, \cdots$ can be calculated

$$h(\xi) = h_{even}(\xi) + h_{odd}$$

$$h_{even}(\xi) = a_0 + a_2\xi^2 + a_4\xi^4 + \cdots \qquad \text{built on } a_0$$

$$h_{odd}(\xi) = a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots \qquad \text{built on } a_1$$

However, not all the solutions so obtained are normalizable

For large j, $\quad a_{j+2} \simeq \frac{2}{j} a_j$

$$\downarrow$$

$$a_j \sim \frac{C}{(j/2)!}$$

$$h(\xi) \simeq C \sum \frac{1}{(j/2)!} \xi^j \simeq C \sum \frac{1}{k!} \xi^{2k} \simeq C e^{\xi^2/2}$$

$$\downarrow$$

not acceptable

Therefore, the series must be terminate

$\downarrow$

There must occur some "highest" j (call it n)

$$K = 2n+1$$

$$\Downarrow$$

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

$$\updownarrow$$

$$\psi_n(x) = \underbrace{\left(\frac{m\omega}{n\hbar}\right)^{1/4}}_{\text{normalization constant}} \frac{1}{\sqrt{2^n n!}} \underbrace{H_n(\xi)}_{\text{Hermite polynomial}} e^{-\xi^2/2}$$

We return now to the Schrödinger equation for the harmonic oscillator (Equation 2.39):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi.$$

Things look a little cleaner if we introduce the dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x; \qquad [2.55]$$

in terms of ξ, the Schrödinger equation reads

$$\frac{d^2\psi}{d\xi^2}=(\xi^2-K)\psi, \qquad [2.56]$$

where K is the energy, in units of $(1/2)\hbar\omega$:

$$K \equiv \frac{2E}{\hbar\omega}. \qquad [2.57]$$

Our problem is to solve Equation 2.56, and in the process obtain the "allowed" values of K (and hence of E).

To begin with, note that at very large ξ (which is to say, at very large x), ξ^2 completely dominates over the constant K, so in this regime

$$\frac{d^2\psi}{d\xi^2}\approx \xi^2\psi, \qquad [2.58]$$

which has the approximate solution (check it!)

$$\psi(\xi)\approx Ae^{-\xi^2/2}+Be^{+\xi^2/2}. \qquad [2.59]$$

The B term is clearly not normalizable (it blows up as $|x|\to\infty$); the physically acceptable solutions, then, have the asymptotic form

$$\psi(\xi)\to (\ \ )e^{-\xi^2/2}, \quad \text{at large } \xi. \qquad [2.60]$$

This suggests that we "peel off" the exponential part,

$$\psi(\xi)=h(\xi)e^{-\xi^2/2}, \qquad [2.61]$$

in hopes that what remains $[h(\xi)]$ has a simpler functional form than $\psi(\xi)$ itself.[14] Differentiating Equation 2.61, we have

$$\frac{d\psi}{d\xi}=\left(\frac{dh}{d\xi}-\xi h\right)e^{-\xi^2/2}$$

and

$$\frac{d^2\psi}{d\xi^2}=\left(\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(\xi^2-1)h\right)e^{-\xi^2/2},$$

so the Schrödinger equation (Equation 2.56) becomes

$$\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(K-1)h=0. \qquad [2.62]$$

I propose to look for a solution to Equation 2.62 in the form of a power series in ξ[15]:

$$h(\xi)=a_0+a_1\xi+a_2\xi^2+\cdots=\sum_{j=0}^{\infty}a_j\xi^j. \qquad [2.63]$$

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[14]Note that although we invoked some approximations to *motivate* Equation 2.61, what follows is *exact*. The device of stripping off the asymptotic behavior is the standard first step in the power series method for solving differential equations—see, for example, Boas (cited in footnote 8), Chapter 12.

[15]According to Taylor's theorem, any reasonably well-behaved function can be expressed as a power series, so Equation 2.63 involves no real loss of generality. For conditions on the applicability of the series method, see Boas (cited in footnote 8) or George Arfken, *Mathematical Methods for Physicists*, 3rd ed. (Orlando, FL: Academic Press, 1985), Section 8.5.

Differentiating the series term by term,

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{j=0}^{\infty} ja_j\xi^{j-1},$$

and

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j.$$

Putting these into Equation 2.62, we find

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right]\xi^j = 0. \qquad [2.64]$$

It follows (from the uniqueness of power series expansions[16]) that the coefficient of *each power* of ξ must vanish,

$$(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0,$$

and hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j. \qquad [2.65]$$

This **recursion formula** is entirely equivalent to the Schrödinger equation itself. Given a_0 it enables us (in principle) to generate $a_2, a_4, a_6, \ldots$, and given a_1 it generates $a_3, a_5, a_7, \ldots$. Let us write

$$h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi), \qquad [2.66]$$

where

$$h_{\text{even}}(\xi) \equiv a_0 + a_2\xi^2 + a_4\xi^4 + \cdots$$

is an *even* function of ξ (since it involves only even powers), built on a_0, and

$$h_{\text{odd}}(\xi) \equiv a_1\xi + a_3\xi^3 + a_5\xi^5 + \cdots$$

is an *odd* function, built on a_1. Thus Equation 2.65 determines $h(\xi)$ in terms of two arbitrary constants (a_0 and a_1)—which is just what we would expect, for a second-order differential equation.

However, not all the solutions so obtained are normalizable. For at very large j, the recursion formula becomes (approximately)

$$a_{j+2} \approx \frac{2}{j}a_j,$$

[16] See, for example, Arfken (footnote 15), Section 5.7.

with the (approximate) solution

$$a_j \approx \frac{C}{(j/2)!},$$

for some constant C, and this yields (at large ξ, where the higher powers dominate)

$$h(\xi) \approx C \sum \frac{1}{(j/2)!}\xi^j \approx C \sum \frac{1}{k!}\xi^{2k} \approx Ce^{\xi^2}.$$

Now, if h goes like $\exp(\xi^2)$, then ψ (remember ψ?—that's what we're trying to calculate) goes like $\exp(\xi^2/2)$ (Equation 2.61), which is precisely the asymptotic behavior we *don't* want.[17] There is only one way to wiggle out of this: For normalizable solutions *the power series must terminate*. There must occur some "highest" j (call it n) such that the recursion formula spits out $a_{n+2} = 0$ (this will truncate *either* the series h_{even} *or* the series h_{odd}; the *other* one must be zero from the start). For physically acceptable solutions, then, we must have

$$K = 2n + 1,$$

for some positive integer n, which is to say (referring to Equation 2.57) that the *energy* must be of the form

$$E_n = (n + \frac{1}{2})\hbar\omega, \quad \text{for } n = 0, 1, 2, \ldots. \qquad [2.67]$$

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in Equation 2.50.

For the allowed values of K, the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j. \qquad [2.68]$$

If $n = 0$, there is only one term in the series (we must pick $a_1 = 0$ to kill h_{odd}, and $j = 0$ in Equation 2.68 yields $a_2 = 0$):

$$h_0(\xi) = a_0,$$

and hence

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

(which reproduces Equation 2.48). For $n = 1$ we pick $a_0 = 0$,[18] and Equation 2.68 with $j = 1$ yields $a_3 = 0$, so

$$h_1(\xi) = a_1\xi,$$

[17] It's no surprise that the ill-behaved solutions are still contained in Equation 2.65; this recursion relation is equivalent to the Schrödinger equation, so it's got to include both the asymptotic forms we found in Equation 2.59.

[18] Note that there is a completely different set of coefficients a_j for each value of n.

and hence

$$\psi_1(\xi) = a_1 \xi e^{-\xi^2/2}$$

(confirming Equation 2.51). For $n = 2$, $j = 0$ yields $a_2 = -2a_0$, and $j = 2$ gives $a_4 = 0$, so

$$h_2(\xi) = a_0(1 - 2\xi^2)$$

and

$$\psi_2(\xi) = a_0(1 - 2\xi^2)e^{-\xi^2/2},$$

and so on. (Compare Problem 2.13, where the same result was obtained by algebraic means.)

In general, $h_n(\xi)$ will be a polynomial of degree n in ξ, involving even powers only, if n is an even integer, and odd powers only, if n is an odd integer. Apart from the overall factor (a_0 or a_1) they are the so-called **Hermite polynomials**, $H_n(\xi)$.[19] The first few of them are listed in Table 2.1. By tradition, the arbitrary multiplicative factor is chosen so that the coefficient of the highest power of ξ is 2^n. With this convention, the normalized[20] stationary states for the harmonic oscillator are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)e^{-\xi^2/2}. \qquad [2.69]$$

They are identical (of course) to the ones we obtained algebraically in Equation 2.50. In Figure 2.5a I have plotted $\psi_n(x)$ for the first few n's.

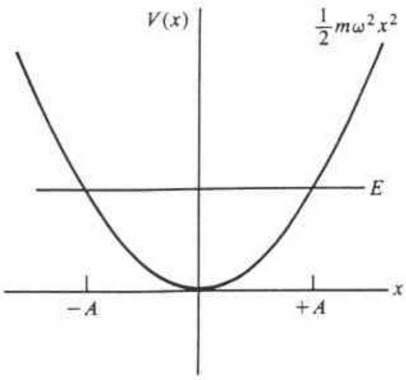
The quantum oscillator is strikingly different from its classical counterpart—not only are the energies quantized, but the position distributions have some bizarre features. For instance, the probability of finding the particle outside the classically allowed range (that is, with x greater than the classical amplitude for the energy in question) is *not* zero (see Problem 2.15), and in all odd states the probability of finding the particle at the center of the potential well is zero. Only at relatively large n do we begin to see some resemblance to the classical case. In Figure 2.5b I have superimposed the classical position distribution on the quantum one (for $n = 100$); if you smoothed out the bumps in the latter, the two would fit pretty well (however, in the classical case we are talking about the distribution of positions over *time* for *one* oscillator, whereas in the quantum case we are talking about the distribution over an *ensemble* of identically-prepared systems).[21]

Table 2.1: The first few Hermite polynomials, $H_n(x)$.

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

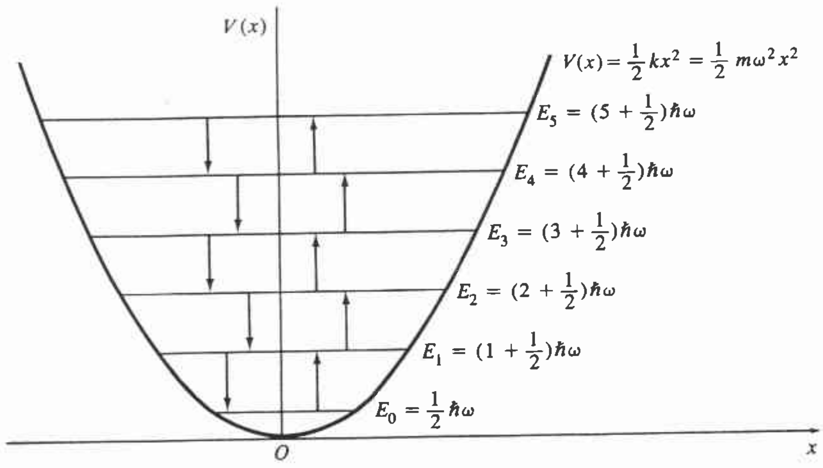
[19]The Hermite polynomials have been studied extensively in the mathematical literature, and there are many tools and tricks for working with them. A few of these are explored in Problem 2.18.

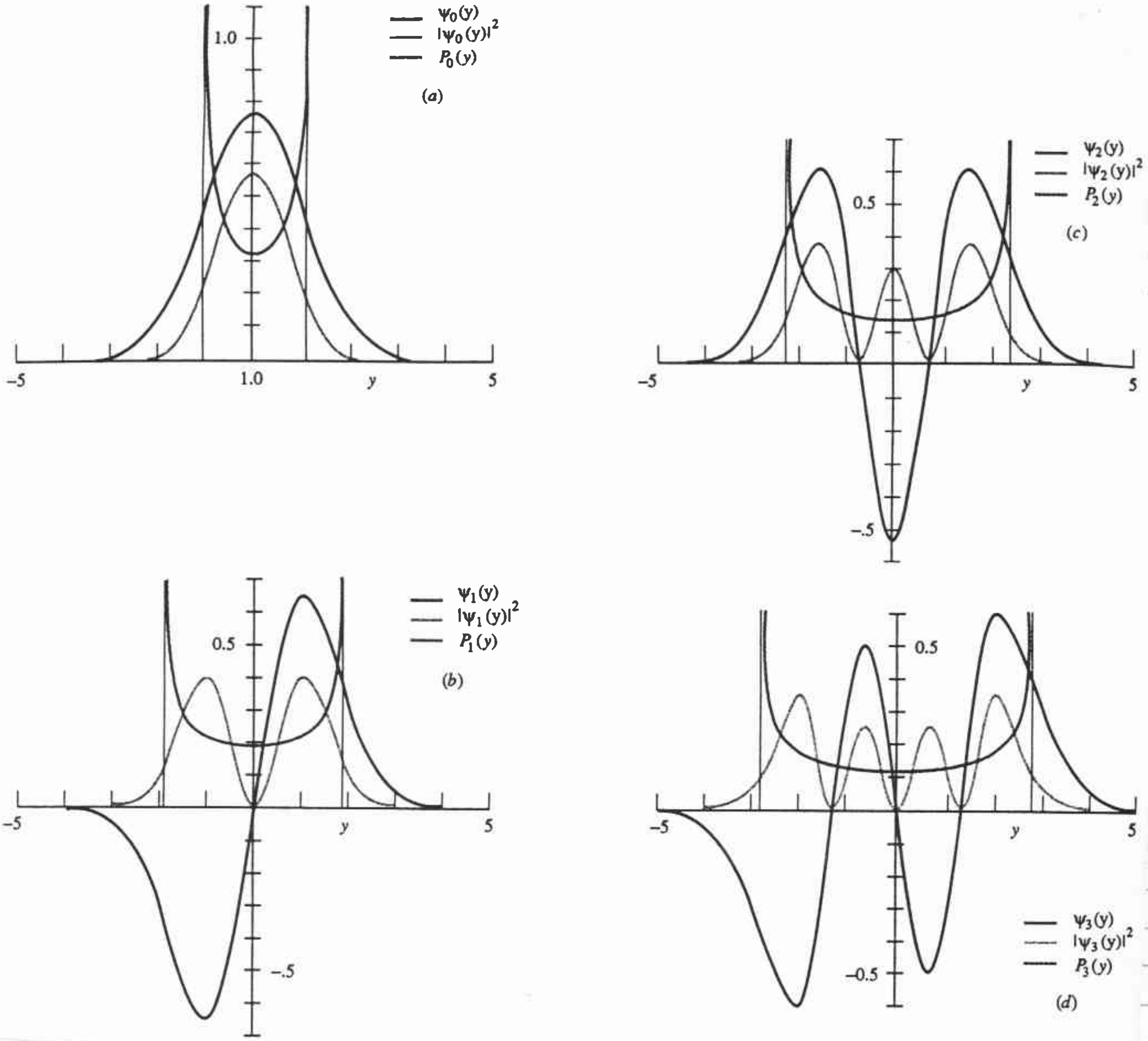
[20]I shall not work out the normalization constant here; if you are interested in knowing how it is done, see, for example, Leonard Schiff, *Quantum Mechanics*, 3rd ed. (New York: McGraw-Hill, 1968), Section 13.

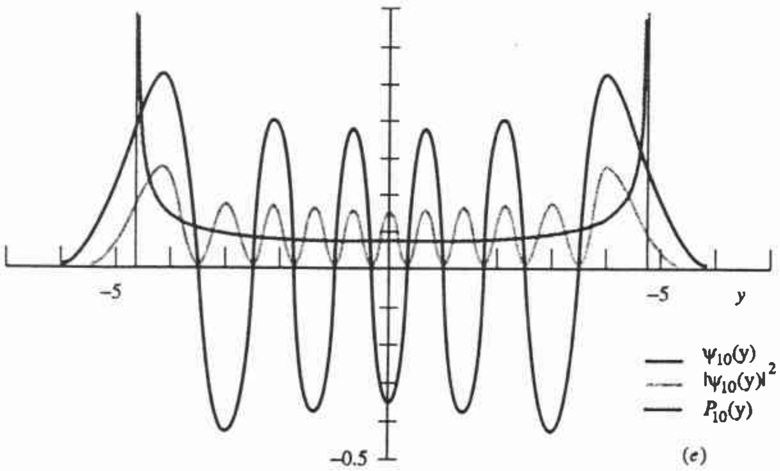


The potential function $V(x)$ of a one-dimensional harmonic oscillator. Classically, a particle of energy E oscillates between the turning points at $x = \pm A$.

The energy levels of the harmonic oscillator. Note that the difference between adjacent energy levels is independent of n and equal to $\Delta E = \hbar\omega_0$. Transitions corresponding to $\Delta n = \pm 1$ are indicated by arrows.







The harmonic oscillator wave functions for $n = 0, 1, 2, 3$, and 10. Shown in each of the drawings are the wave function $\psi(y)$; the probability density $|\psi(y)|^2$; and $P(y)$, the probability distribution for a classical particle of the same energy. The turning points are indicated by the vertical lines; the abscissa is the dimensionless variable y.

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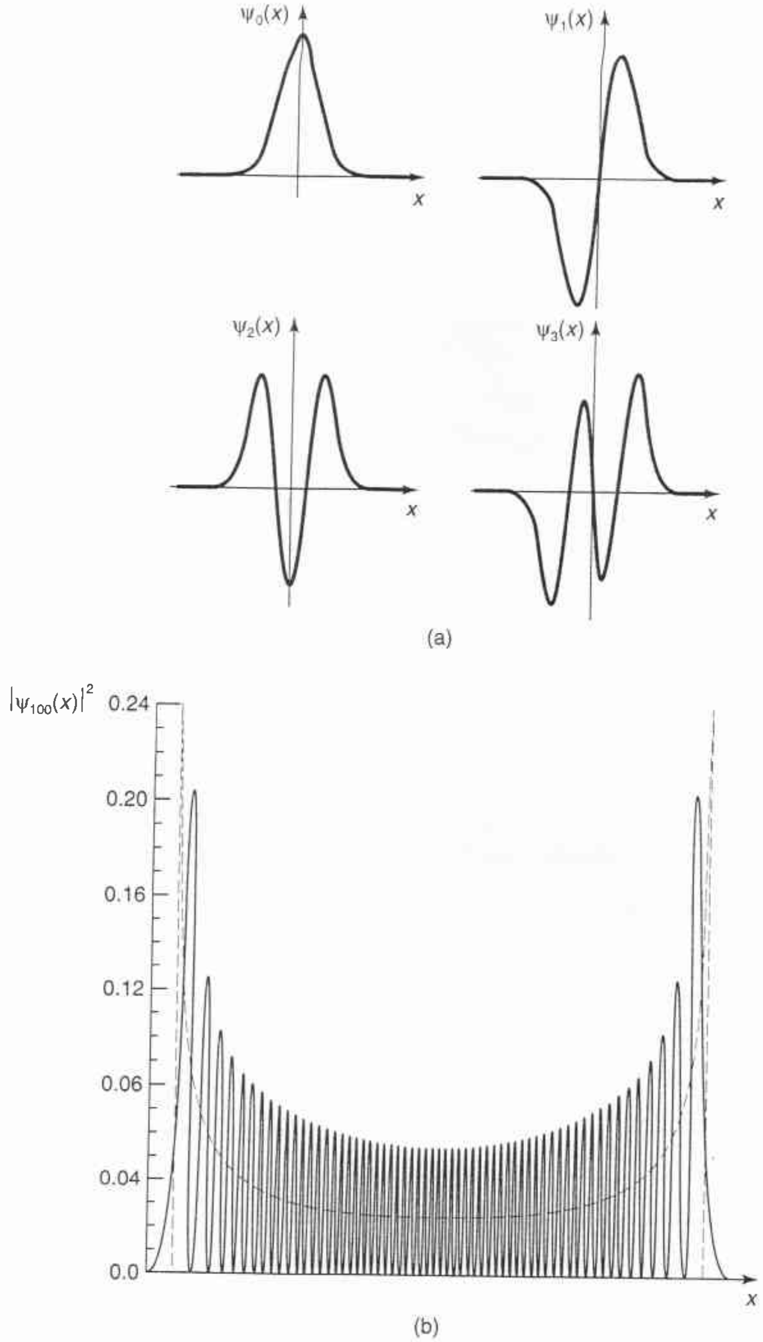

(a) The first four stationary states of the harmonic oscillator.
(b) Graph of $|\psi_{100}|^2$, with the classical distribution (dashed curve) superimposed.

Chapter 8 Wave Functions

Let us go back to the simple harmonic oscillator case

$$\underset{\substack{\downarrow \\ \text{Hamiltonian}}}{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$$

$$\psi(x,t) = \psi(x)\, e^{-iEt/\hbar} \Leftarrow \underbrace{H\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)}_{\text{time-dependent Schrodinger equation}}$$

$$\underbrace{H\psi(x) = E\,\psi(x)}_{\text{time-independent Schrodinger equation}}$$

$$H\,\psi_n(x) = E_n\,\psi_n(x)$$

$$\psi_n(x) = \underbrace{\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n n!}}}_{\text{normalization}}\,\underbrace{H_n(\xi)}_{\text{Hermite polynomials}}\,e^{-\xi^2/2}$$

A short review on Hermite polynomials are given in Appendix A

$$\int_{-\infty}^{\infty}|\psi_n(x)|^2\,dx = 1$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\,x \qquad \omega = \sqrt{\frac{k}{m}}$$

$\psi_n(x)$ is the eigenfunction of the time-independent Schrodinger equation corresponds to eigenvalues $(n+\frac{1}{2})\hbar\omega$ respectively

$$\psi_l^* \qquad \frac{-\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} + V\psi_n = E_n\psi_n \qquad H\psi_n = E_n\psi_n$$

$$\psi_n \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi_l^*}{dx^2} + V\psi_l^* = E_l\psi_l^*$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\psi_l^*\frac{d^2\psi_n}{dx} - \psi_n\frac{d^2\psi_l^*}{dx}\right) = (E_n - E_l)\psi_n\psi_l^*$$

$$\frac{2m}{\hbar^2}(E_l - E_n)\int_{-\infty}^{\infty}\psi_l^*\psi_n\,dx = \int_{-\infty}^{\infty}\frac{d}{dx}\left(\psi_l^*\frac{d\psi_n}{dx} - \psi_n\frac{d\psi_l^*}{dx}\right)dx$$

$$= \left[\psi_l^*\frac{d\psi_n}{dx} - \psi_n\frac{d\psi_l^*}{dx}\right]\Big|_{-\infty}^{\infty}$$

$$\underbrace{\int_{-\infty}^{\infty}\psi_n^*\psi_n\,dx < \infty}_{\text{normalization requirement}} \Rightarrow \psi_n(x) \to 0 \text{ faster than } \frac{1}{\sqrt{x}}$$

$$\Rightarrow \frac{2m}{\hbar^2}(E_l - E_n)\int_{-\infty}^{\infty}\psi_l^*\psi_n\,dx = 0$$

$$E_l \neq E_n$$

$$\Rightarrow \int \psi_l^*(x)\psi_n(x)\,dx = 0$$

If $E_n = E_\ell$, then the eigenfunctions are said to be degenerate.

If $\psi_\ell'(x)$, $\psi_n'(x)$ are eigenfunctions, i.e., are solutions of the time independent Schrodinger equation, with the same eigenvalue $E_n = E_\ell$

Then. $\psi_a = \psi_\ell' + \alpha \psi_n'$ is also an eigenfunction.

$$\int \psi_n'^* \psi_a \, dx = \int \psi_n'^* \psi_\ell' \, dx + \alpha \int \psi_n'^* \psi_n \, dx$$

If we choose $\alpha = -\dfrac{\int \psi_n'^* \psi_\ell \, dx}{\int \psi_n'^* \psi_n \, dx}$, then ψ_n', ψ_a are orthogonal

Choose $\psi_n = \psi_n'$, $\psi_\ell = \psi_a$, then ψ_n, ψ_ℓ will be orthogonal.

The idea can clearly be extended to cases where there are more than two independent eigenfunctions having the same energy.

This is known as Schmidt orthogonalization procedure.

$\{\psi_n(x)\}$ forms a orthonormal set

$$\Rightarrow \quad \int \psi_n^*(x)\, \psi_\ell(x)\, dx = \delta_{n\ell}$$

Expand $\Psi(x,t)$ in terms of above orthonormal set

$$\Psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x,t)$$

completeness

$E_n \neq E_m$, we have $\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x)\,dx = 0$

the wave function being normalized

$$\Rightarrow \quad \underbrace{\int_{-\infty}^{\infty} \psi_m^*(x)\,\psi_n(x)\,dx = \delta_{mn}}_{\text{orthonormality condition}}$$

$\{\psi_n(x)\}$ forms an orthonormal set of functions

$$\psi_n(x)\,e^{-iE_nt/\hbar} = \psi_n(x)\,e^{-i(n+\frac{1}{2})\omega t}$$

is a solution of the time-dependent Schrodinger equation.

The Schrodinger equation is linear

$$\psi(x,t) = \sum_{n=0}^{\infty} a_n\,\psi_n(x)\,e^{-iE_nt/\hbar}$$

is again a solution of the time-dependent Schrodinger equation

a_n can be determined by specifying the initial wave function $\psi(x,0)$

$$\psi(x,0) = \sum_n a_n\psi_n(x) \qquad \int \psi^*(x,0)\psi(x,0)\,dx = \sum_{n=0}^{\infty}|a_n|^2 = 1$$

$$\int_{-\infty}^{\infty} \psi_m^*(x)\,\psi(x,0)\,dx = \sum_n \int \psi_m^*(x)\,a_n\,\psi_n(x)$$

$$= \sum_n a_n\,\delta_{mn} = a_m$$

We have solved the Schrodinger equation, i.e., given the Hamiltonian H and the initial condition $\psi(x,0)$, $\psi(x,t)$ can be found.

If $\psi(x,t)$ is found, then

$$\langle E\rangle_t = \langle H\rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\,H\,\psi(x,t)\,dx$$

$$= \int_{-\infty}^{\infty} \sum_n a_n^*\,\psi_n^*(x)\,e^{+iE_nt/\hbar} \sum_m E_m\,\psi_m(x)\,e^{-iE_mt/\hbar}\,dx$$

$$= \sum_n\sum_m a_n^* a_m E_m\,e^{i(E_n-E_m)t/\hbar}\,\delta_{nm} = \sum_m E_m\,|a_m|^2$$

$$a_m = \int_{-\infty}^{\infty} \psi_m^*(x)\,\psi(x,0)\,dx$$

Normalization condition

$$\int \Psi^*(x,t)\,\Psi(x,t)\,dx = 1$$

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = \sum_n a_n a_n^* \underbrace{\int_{-\infty}^{\infty} \psi_n^*(x)\psi_n(x)dx}_{=1}$$

$$+ \sum_\ell \sum_n a_\ell^* a_n\, e^{-i(E_n - E_\ell)t/\hbar} \underbrace{\int_{-\infty}^{\infty} \psi_\ell^*(x)\,\psi_n(x)\,dx}_{=0}$$

$$= \sum_n a_n a_n^* = 1$$

The normalization condition is independent of time
$\Rightarrow$ if we normalize the wave function at time $t = t_0$ then it will remain normalized.

If $\Psi(x,0)$ is given $\Rightarrow$ $\Psi(x,t) = \sum_n a_n \Psi_n(x,t)$

specified if a_n, $\psi_n(x)$, E_n are given

$$\Psi(x,0) = \sum_{n=1}^{\infty} a_n \psi_n(x)$$

$$\int_{-\infty}^{\infty} \psi_\ell^*(x)\,\Psi(x,0)dx = \sum_{n=1}^{\infty} a_n \int_{-\infty}^{\infty} \psi_\ell^*(x)\,\psi_n(x)\,dx$$

$$= a_\ell$$

$$\Rightarrow \quad a_n = \int_{-\infty}^{\infty} \psi_n^*(x')\,\Psi(x',0)\,dx'$$

$$\Rightarrow \quad \Psi(x,t) = \sum_n \left\{ \int_{-\infty}^{\infty} \psi_n^*(x')\,\Psi(x',0)\,dx' \right\} e^{-iE_n t/\hbar} \psi_n(x)$$

$\psi(x,t)$ can be obtained:

(i) H is specified

(ii) $H\psi_n = E_n\psi_n$ is solved

time-independent Schrodinger equation is solved.

(iii) Initial condition is known.

Now if $\psi_n(x,0) = \psi_n(x)$

$\qquad\downarrow$ eigenfunction of time independent Schrodinger equation for simple harmonic oscillator with eigenvalues $(n+\frac{1}{2})\hbar\omega$

$$\psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$$

$\downarrow$ this wave function satisfies the time dependent Schrodinger equation and the initial condition

$$\langle A\rangle_t = \int_{-\infty}^{\infty} \psi_n^*(x)\, A\, \psi_n(x)\, dx = \int_{-\infty}^{\infty} \psi_n^*(x,t)\, A\, \psi_n(x,t)\, dx$$

independent of t.

$$\psi_n(x) = A_n \underbrace{H_n(\xi)}_{\text{Hermite polynomial}} e^{-\xi^2/2}$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\, x \quad , \quad \omega = \sqrt{\frac{k}{\omega}}$$
$$= \sqrt{\lambda}\, x$$

Normalization

$$\int_{-\infty}^{\infty} \psi_n^*(x)\, \psi_n(x)\, dx = 1$$
$$\parallel$$
$$\int_{-\infty}^{\infty} |A_n|^2 [H_n(\xi)]^2 e^{-\xi^2} dx = 1$$

$$\Rightarrow \quad A_n = \left[\frac{1}{2^n\, n!}\left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}}\right]^{\frac{1}{2}}$$

See the derivation in A-4 of Appendix A

Now we shall calculate the expectation values

(i) $\langle x\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, x\, \psi_n(x)\, dx = 0$

$\downarrow$ the integrand is an odd function of x

(ii) $\langle x^2\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, x^2\, \psi_n(x)\, dx$

$$= |A_n|^2 \int_{-\infty}^{\infty} [H_n(\xi)]^2\, x^2 e^{-\xi^2}\, dx$$

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$y \to \xi$, $\quad \xi = \sqrt{\lambda}\, x \qquad dx \to \frac{d\xi}{\sqrt{\lambda}} \qquad \lambda \to \alpha$

$$\langle x^2 \rangle = |A_n|^2 \frac{1}{\alpha} \int_{-\infty}^{\infty} [H_n(\xi)]^2 e^{-\xi^2} \xi^2 \, dx$$

$$\updownarrow$$

$$\frac{A_n^2}{\alpha} \int_{-\infty}^{\infty} e^{-y^2} [H_n(y)]^2 y^2 \, dx$$

$y H_n(y) = \frac{1}{2}[H_{n+1}(y) + 2n H_{n-1}(y)]$ Equation (6) of Appendix A

$$y^2 H_n(y) = \frac{1}{2}[y H_{n+1}(y) + 2ny H_{n-1}(y)]$$

$$= \frac{1}{2}[\frac{1}{2} H_{n+2}(y) + (n+\frac{1}{2}) H_n(y) + 2n\frac{1}{2} H_n(y) + \frac{1}{2} 2n\, 2(n-1) H_{n-2}(y)]$$

$$= \frac{1}{4} H_{n+2}(y) + (n+\frac{1}{2}) H_n(y) + n(n-1) H_{n-2}(y)$$

$$\langle x^2 \rangle = \frac{n+\frac{1}{2}}{\alpha} \underbrace{A_n^2 \int_{-\infty}^{\infty} e^{-y^2} [H_n(y)]^2 dy}_{=1}$$

normalization condition

$$= \frac{n+\frac{1}{2}}{\alpha}$$

(iii) $\langle p_x \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \frac{\hbar}{i}\frac{d}{dx} \psi_n(x)\, dx$

$$= \frac{\hbar}{i} A_n^2 \sqrt{\alpha} \int_{-\infty}^{\infty} e^{-y^2/2} H_n(y) \frac{d}{dy} (e^{-y^2/2} H_n(y)) dx$$

$$\frac{d}{dy} e^{-y^2/2} H_n(y) = e^{-y^2/2} \frac{dH_n(y)}{dy} - y H_n(y) e^{-y^2/2}$$

$$= e^{-y^2/2} [2n H_{n-1}(y) - \frac{1}{2} H_{n+1}(y) - \frac{1}{2} 2n H_{n-1}(y)]$$

$$= e^{-y^2/2} [n H_{n-1}(y) - \frac{1}{2} H_{n+1}(y)]$$

Clearly, $\langle p_x \rangle = 0$

(iv) $\langle p_x^2 \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) (\frac{\hbar}{i}\frac{d}{dx})^2 \psi_n(x)\, dx$

$$= -\alpha\hbar^2 A_n^2 \int_{-\infty}^{\infty} e^{-y^2/2} H_n(y) \frac{d^2}{dy^2} e^{-y^2/2} H_n(y) dx$$

$$\frac{d^2}{dy^2} e^{-y^2/2} H_n(y) = \frac{d}{dy} \{ e^{-y^2/2} [n H_{n-1}(y) - \frac{1}{2} H_{n+1}(y)] \}$$

$$= e^{-y^2/2} [n \frac{dH_{n-1}(y)}{dy} - \frac{1}{2} \frac{dH_{n+1}(y)}{dy}]$$

Equation (7) of Appendix (A)

$$- e^{-y^2/2} [ny H_{n-1}(y) - \frac{1}{2} y H_{n+1}(y)]$$

$$= e^{-y^2/2} [n \cdot 2(n-1) H_{n-2}(y) - \frac{1}{2} 2(n+1) H_n(y) - n\frac{1}{2} H_n(y) - n\frac{1}{2}\, 2(n-1) H_{n-2}(y) + \frac{1}{2}\cdot\frac{1}{2} H_{n+2} + \frac{1}{2}\cdot\frac{1}{2} 2(n+1) H_n(y)]$$

$$= e^{-y^2/2} [n(n-1) H_{n-2}(y) - (n+\frac{1}{2}) H_n(y) + \frac{1}{4} H_{n+1}(y)]$$

$$\langle p_x^2 \rangle = -\alpha\hbar^2 A_n^2 \int_{-\infty}^{\infty} e^{-y^2} \{-(n+\frac{1}{2})\} [H_n(y)]^2 dx = (n+\frac{1}{2})\alpha\hbar^2$$

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$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{\alpha}(n+\frac{1}{2})$

$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 = (n+\frac{1}{2})\alpha\hbar^2$

$\Rightarrow \quad \Delta x \, \Delta p_x = (n+\frac{1}{2})\hbar$

$$\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1} a^n}\sqrt{\frac{\pi}{a}}$$

For ground state $n=0$, $H_0(\xi)=1$, only Gaussian integrals are needed

Expectation values of some observables for mixed states

$$\psi(x,0) = \frac{1}{\sqrt{2}}\Big(\underbrace{A_0 e^{-y^2/2}}_{\psi_0(x)} H_0(y) + \underbrace{A_1 e^{-y^2/2}}_{\psi_1(x)} H_1(y)\Big)$$

$\psi_0(x)$, $\psi_1(x)$ are properly normalized.

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left[A_0 e^{-y^2/2} H_0(y) e^{-i\omega t/2} + A_1 e^{-y^2/2} H_1(y) e^{-3i\omega t/2}\right]$$

Remember $E_n = (n+\frac{1}{2})\hbar\omega$

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\left(i\hbar\frac{\partial}{\partial t}\right)\psi(x,t)\,dx$$

$$= \frac{1}{2}\int_{-\infty}^{\infty}\left(\psi_0^*(x) e^{i\omega t/2} + \psi_1^*(x) e^{i3\omega t/2}\right)\Big(\hbar\frac{\omega}{2}\psi_0(x) e^{-i\omega t/2} + \hbar\frac{3\omega}{2}\psi_1(x)$$

$$\cdot\, e^{-i3\omega t/2}\Big]dx$$

$$= \frac{1}{2}\hbar\omega\left(\frac{1}{2}+\frac{3}{2}\right) = \hbar\omega$$

$$\langle x \rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\, x\, \psi(x,t)\,dx$$

$$= \frac{1}{2}\int_{-\infty}^{\infty}\left(\psi_0^*(x) e^{i\omega t/2} + \psi_1^*(x) e^{i3\omega t/2}\right) x \left(\psi_0(x) e^{-i\omega t/2} + \psi_1(x) e^{-i3\omega t/2}\right)dx$$

$$= \frac{1}{2}\int_{-\infty}^{\infty}\Big[\psi_0^*(x)\, x\, \psi_0(x) + \psi_1^*(x)\, x\, \psi_1(x) + \psi_0^*(x)\, x\, \psi_1(x) e^{-i\omega t}$$

$$+ \psi_1^*(x)\, x\, \psi_0(x) e^{i\omega t}\Big]dx$$

$$= \left[\int_{-\infty}^{\infty}\psi_0^*(x)\, x\, \psi_1(x)\,dx\right]\cos\omega t$$

$$\int_{-\infty}^{\infty}\psi_0^*(x)\, x\, \psi_1(x)\,dx$$

$$= \frac{1}{\alpha}\int_{-\infty}^{\infty} A_0 A_1 e^{-y^2} H_0(y) H_1(y)\, y\, dy$$

$\frac{1}{\sqrt{\alpha}}$ from $x \to y$, $\frac{1}{\sqrt{\alpha}}$ from $dx \to dy$

$y H_1(y) = \frac{1}{2}H_2(y) + \frac{1}{2}\,2\cdot 1\, H_0(y)$ from recursive relation

$$\int_{-\infty}^{\infty}\psi_0^*(x)\, x\, \psi_1(x) = \frac{1}{\alpha} A_0 A_1 \underbrace{\int_{-\infty}^{\infty} e^{-y^2}dy} = \frac{1}{\alpha}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}}\left(\frac{1}{2}\right)^{\frac{1}{2}}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}}\sqrt{\pi} = \frac{1}{\sqrt{2\alpha}}$$

$\Rightarrow \quad \langle x \rangle = \frac{1}{\sqrt{2}\alpha} \cos \omega t$

Similarily $\quad \langle p_x \rangle = -\sqrt{\frac{\alpha}{2}}\, \hbar \sin \omega t$

(Can be obtained through Ehrenfest theorem)

If $\quad \psi(x,0) = \frac{1}{\sqrt{2}} [e^{i\delta_0} \psi_0(x) + e^{i\delta_1} \psi_1(x)]$

then $\quad \psi(x,t) = e^{i\delta_0} \frac{1}{\sqrt{2}} [\psi_0(x) e^{-i\omega t/2} + e^{i(\delta_1 - \delta_0)} \psi_1(x) e^{-i3\omega t/2}]$

$\Rightarrow \quad \langle x \rangle = \frac{1}{\sqrt{2}\alpha} \cos [\omega t + (\delta_1 - \delta_0)]$

$\langle p_x \rangle = -\sqrt{\frac{\alpha}{2}}\, \hbar \sin [\omega t + (\delta_1 - \delta_0)]$

The relative phase $\delta_1 - \delta_0$ is observable , δ_0 is unimportant.

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Appendix A

Hermite Polynomials

From P. 6-10, we find

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (K-1)H = 0$$

$(h \to H)$

Acceptable solutions can be found only if

$K = 2n+1 \qquad n = 0, 1, 2, \cdots$

$$\Rightarrow \quad \frac{d^2H_n}{d\xi^2} - 2\xi\frac{dH_n(\xi)}{d\xi} + 2n H_n(\xi) = 0$$

this is defining differential equation

Generating function and recursive relations

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

Expanding the exponential function in terms of powers of s and ξ, we see that the coefficients of the powers s^n are polynomials in terms of ξ – the Hermite polynomials. This can be shown as follows: we have

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

$$\frac{\partial S}{\partial s} = (-2s+2\xi)\,e^{-s^2+2s\xi} = \sum_{n=0}^{\infty}\frac{(-2s+2\xi)s^n}{n!}H_n(\xi)$$
$$= \sum_{n=0}^{\infty}\frac{s^{n-1}}{(n-1)!}H_n(\xi) \quad . \tag{5}$$

Equating equal powers of s in the sums of these two equations, we obtain

$$\frac{\partial H_n(\xi)}{\partial \xi} = 2nH_{n-1}(\xi) \quad ,$$
$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \quad . \tag{6}$$

Therefore it follows that

$$\frac{\partial H_n(\xi)}{\partial \xi} = 2\xi H_n(\xi) - H_{n+1}(\xi) \quad , \tag{7}$$

and hence

$$\frac{\partial^2 H_n(\xi)}{\partial \xi^2} = 2H_n(\xi) + 2\xi\frac{\partial H_n(\xi)}{\partial \xi} - \frac{\partial H_{n+1}(\xi)}{\partial \xi}$$
$$= 2\xi\frac{\partial H_n(\xi)}{\partial \xi} + 2H_n(\xi) - (2n+2)H_n(\xi)$$

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$$= 2\xi \frac{\partial H_n(\xi)}{\partial \xi} - 2nH_n(\xi) \quad . \tag{8}$$

This is exactly differential equation (3), proving that the $H_n(\xi)$ appearing in the generating function (4) are indeed Hermite polynomials.

The recurrence formulas (6) may be used to calculate the H_n and their derivatives. Another explicit expression directly obtainable from the generating function is quite useful; let us now establish this important relation. From (4) it follows instantly that

$$\left.\frac{\partial^n S(\xi, s)}{\partial s^n}\right|_{s=0} = H_n(\xi) \quad . \tag{9}$$

Now, for an arbitrary function $f(s-\xi)$, it also holds that

$$\frac{\partial f}{\partial s} = -\frac{\partial f}{\partial \xi} \quad . \tag{10}$$

Thus

$$\begin{aligned} \frac{\partial^n S}{\partial s^n} &= \mathrm{e}^{\xi^2} \frac{\partial^n \mathrm{e}^{-(s-\xi)^2}}{\partial s^n} \\ &= (-1)^n \mathrm{e}^{\xi^2} \frac{\partial^n}{\partial \xi^n} \mathrm{e}^{-(s-\xi)^2} \quad . \end{aligned} \tag{11}$$

Comparing (11) with (9) yields the very useful formula,

$$H_n(\xi) = (-1)^n = \mathrm{e}^{\xi^2} \frac{\partial^n}{\partial \xi^n} \mathrm{e}^{-\xi^2} \quad . \tag{12}$$

$$\lambda = \sqrt{\frac{m\omega}{\hbar}}$$

The $H_n(\xi)$ are polynomials of nth degree in ξ with the dominant term $2^n\xi^n$. The first five $H_n(\xi)$ calculated from (7.22) or (12) of the foregoing example are:

$$\begin{aligned} &H_0(\xi) = 1 \quad , \qquad H_1(\xi) = 2\xi \quad , \\ &H_2(\xi) = 4\xi^2 - 2 \quad , \quad H_3(\xi) = 8\xi^3 - 12\xi \quad , \quad H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \quad . \end{aligned} \tag{7.23}$$

The eigenfunctions (7.21) were combined by introducing the abbreviation $\xi = \sqrt{\lambda}x$ and using the Hermite polynomials in a way that holds for both even and odd n, i.e.

$$\psi_n(x) = N_n \mathrm{e}^{(-1/2)\xi^2} H_n(\xi) \quad , \quad \xi = \sqrt{\lambda}x \quad . \tag{7.24}$$

The constant N_n, which depends on the index n, is determined by the normalization condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = 1 \quad , \tag{7.25}$$

since we require the position probability to be 1 for the particle in the entire configuration space. Thus

$$n = 0 : \psi_0(x) = \sqrt[4]{\frac{\lambda}{\pi}} \exp\left(-\frac{1}{2}\lambda x^2\right) \quad ,$$

$$n = 1 : \psi_1(x) = 2\sqrt{\frac{1}{2}\sqrt{\frac{\lambda}{\pi}}} \exp\left(-\frac{1}{2}\lambda x^2\right) \sqrt{\lambda} x \quad ,$$

$$n = 2 : \psi_2(x) = \sqrt{\frac{1}{8}\sqrt{\frac{\lambda}{\pi}}} \exp\left(-\frac{1}{2}\lambda x^2\right) (4\lambda x^2 - 2) \quad . \tag{7.33}$$

From (7.24) and (7.30) it follows that, for space reflection, the eigenfunctions have the symmetry property

$$\psi_n(-x) = (-1)^n \psi_n(x) \quad . \tag{7.34}$$

This means

n even: $\psi(-x) = \psi(x) \rightarrow$ parity $+1$

n odd: $\psi(-x) = -\psi(x) \rightarrow$ parity -1 .

For the lowest H_n, it can easily be shown that they possess precisely n different real zeros and $n-1$ extremal values (see Fig. 7.1). With respect to (12) in Example 7.2, we have

$$H_{nk+1} = -e^{\xi^2} \frac{d}{d\xi}(e^{-\xi^2} H_n) \quad . \tag{7.35}$$

On the assumption that H_n possesses $n+1$ real extremal values, we can conclude the existence of $n+1$ extremal values for $e^{-\xi^2} H_n$ (since $e^{-\xi^2} \rightarrow 0$ for $\xi \rightarrow \infty$). The extremal values are identical with the zeros of the derivative $d/d\xi$; therefore H_{n+1} has precisely $n+1$ real zeros. This conclusion shows that the Hermite polynomials $H_n(\xi)$ – and, in consequence, the wave functions $\psi_n(\xi)$ – possess n different real zeros. This is a special case of a universally valid theorem which states that the principal quantum number of an eigenfunction is identical with the number of zeros.

In Fig. 7.1, some of the ψ_n are plotted together with an energy diagram. The energy eigenvalues are represented as horizontal lines with the quantum segments $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. For each of the lines there is a corresponding eigenfunction $\psi_n(x)$ drawn on an arbitrary scale.

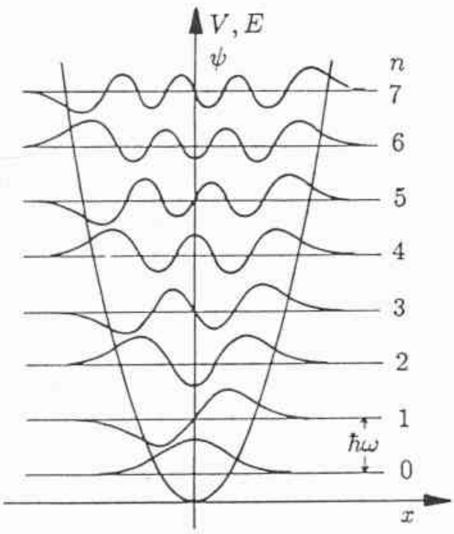

Fig. 7.1. Oscillator potential, energy levels and corresponding wavefunctions

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx = \frac{1}{\sqrt{\lambda}} N_n^2 \int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi)^2\, d\xi = 1 \quad . \tag{7.26}$$

Using relation (12) of Example 7.2 to express one of the Hermite polynomials that appears in the integrand of the normalization integral, the evaluation of this integral becomes simply

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx = (-1)^n \frac{N_n^2}{\sqrt{\lambda}} \int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} e^{-\xi^2}\, d\xi \quad . \tag{7.27}$$

By partial integration we obtain

$$\int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} e^{-\xi^2}\, d\xi$$

$$= \left[\left(\frac{d^{n-1}}{d\xi^{n-1}} e^{-\xi^2} \right) H_n(\xi) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{dH_n}{d\xi} \frac{d^{n-1}}{d\xi^{n-1}} e^{-\xi^2}\, d\xi \quad . \tag{7.28}$$

The first term is, because of (12) in Example 7.2, equal to $(-1)^{n-1} e^{-\xi^2} H_{n-1}(\xi) H_n(\xi)$. It vanishes at infinity, due to the exponential function.

Having carried out partial integration n times, we are left with

$$\int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} e^{-\xi^2}\, d\xi = (-1)^n \int_{-\infty}^{\infty} \frac{d^n H_n}{d\xi^n} e^{-\xi^2}\, d\xi \quad . \tag{7.29}$$

Since $H_n(\xi)$ is a polynomial of nth order with the dominant term $2^n \xi^n$, for the nth derivative,

$$\frac{d^n}{d\xi^n} H_n(\xi) = 2^n n! \tag{7.30}$$

holds.

From this we find that

$$\int_{-\infty}^{\infty} H_n(\xi) \frac{d^n}{d\xi^n} e^{-\xi^2}\, d\xi = (-1)^n (2^n) n! \int_{-\infty}^{\infty} e^{-\xi^2}\, d\xi = (-1)^n (2^n) n! \sqrt{\pi} \quad , \tag{7.31}$$

and for the normalization constant,

$$N_n = \sqrt{\sqrt{\frac{\lambda}{\pi}} \frac{1}{2^n n!}} \quad .$$

The stationary states of the harmonic oscillator in quantum mechanics are therefore

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!} \sqrt{\frac{\lambda}{\pi}}} \exp\left(-\frac{1}{2} \lambda x^2 \right) H_n(\sqrt{\lambda} x) \quad . \tag{7.32}$$

Here we have suppressed the phase factor $(-1)^n$, since it is not essential. To discuss the solution, we take a look at the first three eigenfunctions of the linear harmonic oscillator (see Fig. 7.1):