# Introduction to Schrödinger Equation: Harmonic Potential

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## Time-Dependent Schrödinger Equation

For a nonrelativistic particle with mass $m$ moving along the $x$ axis in a potential $V(x,t)$, the time-dependent Schrödinger equation is given by

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t). \tag{1}$$

If the potential $V$ is independent of $t$, the Schrödinger equation can be solved by the method of separation of variables:

$$\Psi(x,t) = \psi(x)f(t). \tag{2}$$

Substituting Eq. (2) into Eq. (1) gives

$$\frac{df}{dt} = -\frac{iE}{\hbar}f \tag{3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi. \tag{4}$$

Eq.(3) is easy to solve; the solution is

$$f(t)=e^{-\frac{iEt}{\hbar}}. \tag{5}$$

Eq.(4) is called the time-independent Schrödinger equation and it can be expressed by

$$\hat{H}\psi=E\psi \tag{6}$$

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x) \tag{7}$$

where $\hat{H}$ is called Hamiltonian operator.

These separable solutions are called stationary states

$$\Psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}}. \tag{8}$$

The eigenvalue $E$ is the energy of the state $\psi(x)$.

Born's statistical interpretation says that $|\Psi(x,t)|^2$ gives the probability of finding the particle at point $x$ at time $t$. Therefore,

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1. \tag{9}$$

Physically realizable states correspond to the square-integrable solutions to the Schrödinger equation. Boundary condition is that $\Psi(x,t)$ must go to zero as $x$ goes to $\pm\infty$.

For stationary states, although the wave function depends on $t$, the probability density does not:

$$|\Psi(x,t)|^2 = \psi e^{-\frac{iEt}{\hbar}} \times \psi^* e^{\frac{iEt}{\hbar}} = |\psi(x)|^2. \tag{10}$$

Principle of Superposition:
The general solution is a linear combination of separable solutions.

$$\Psi_1(x,t) = \psi_1(x) e^{-\frac{iE_1 t}{\hbar}} \tag{11}$$

$$\Psi_2(x,t) = \psi_2(x) e^{-\frac{iE_2 t}{\hbar}} \tag{12}$$

$$\vdots$$

Once we have found the separable solutions, we can construct a much more general solution

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}}. \tag{13}$$

Given the starting wave function $\Psi(x,0)$, the coefficients in the expansion can be determined by

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x) \tag{14}$$

$$c_n = \int_{-\infty}^{\infty} \psi_n(x)^* \times \Psi(x,0) dx. \tag{15}$$

# Harmonic Potential

The harmonic potential is given by

$$V(x) = \frac{1}{2} m\omega^2 x^2 \tag{16}$$

where $m$ is the mass of the particle and $\omega$ is the angular frequency of the oscillation.
We want to solve the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi. \tag{17}$$

If we introduce the dimensionless variable

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

the Schrödinger equation becomes

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi \quad \text{and} \quad K = \frac{2E}{\hbar\omega} \tag{18}$$

where $K$ is the energy.

Our problem is to solve Eq. (18). At very large $\xi$, $\xi^2$ completely dominates over the constant $K$, so in this region

$$\frac{d^2\psi}{d\xi^2} \simeq \xi^2\psi. \tag{19}$$

The approximate solution is

$$\psi(\xi) \simeq Ae^{-\frac{\xi^2}{2}} + Be^{\frac{\xi^2}{2}}. \tag{20}$$

According to the boundary condition,

$$\psi(\xi) \to 0 \text{ as } \xi \to \pm\infty,$$

so $B = 0$. Therefore, the physically acceptable solutions have the asymptotic form

$$\psi(\xi) \to Ae^{-\frac{\xi^2}{2}}, \quad \text{at large } \xi. \tag{21}$$

This suggests that

$$\psi(\xi) = h(\xi)e^{-\frac{\xi^2}{2}}. \tag{22}$$

Then, we substitute Eq. (22) into Eq. (18):

$$\frac{d\psi}{d\xi} = \left(\frac{dh}{d\xi} - \xi h\right) e^{-\frac{\xi^2}{2}} \tag{23}$$

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2 h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right) e^{-\frac{\xi^2}{2}}, \tag{24}$$

so the Schrödinger equation, Eq. (18), becomes

$$\frac{d^2 h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K - 1)h = 0. \tag{25}$$

We use the power expansion method to solve Eq. (25) to look for solutions in the form of power series in $\xi$:

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j. \tag{26}$$

Differentiating the series term by term,

$$\frac{dh}{d\xi} = \sum_{j=0}^{\infty} j a_j \xi^{j-1} \tag{27}$$

$$\frac{d^2h}{d\xi^2} = \sum_{j=0}^{\infty} (j+1)(j+2) a_{j+2} \xi^j. \tag{28}$$

Putting these into Eq. (18), we find

$$\sum_{j=0}^{\infty} \left[ (j+1)(j+2) a_{j+2} - 2j a_j + (K-1) a_j \right] \xi^j = 0. \tag{29}$$

It follows that the coefficient of each power of $\xi$ must vanish,

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

and hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j. \tag{30}$$

This recursion formula is entirely equivalent to the Schrödinger equation. Starting with $a_0$, it generates all the even-numbered coefficients and starting with $a_1$, it generates all the odd coefficients. We write the complete solution as

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

However, not all the solutions so obtained are normalizabled. At very large $j$, the recursion formula becomes (approximately)

$$a_{j+2} \simeq \frac{2}{j} a_j.$$

The approximate solution is

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

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

$$h(\xi) \simeq \sum_j \frac{C}{(j/2)!}\xi^j \simeq C \sum_j \frac{1}{j!}\xi^{2j} \simeq Ce^{\xi^2}.$$

Therefore, if $h$ goes like $\exp(\xi^2)$, the $\psi$ goes like $\exp(\xi^2/2)$:

$$h(\xi) \sim e^{\xi^2} \quad \Rightarrow \quad \psi(\xi) = h(\xi)e^{-\frac{\xi^2}{2}} \sim e^{\frac{\xi^2}{2}} \to \infty \quad \text{as} \quad \xi \to \pm\infty.$$

Therefore, for normalizable solutions, *the power series must terminate*.

There must occur some "highest" $j$ (call it $n$), such that $a_{n+2} = 0$.

$$a_{n+2} = \frac{(2n+1-K)}{(n+1)(n+2)} a_n = 0 \quad \Rightarrow \quad K = 2n+1.$$

For physically acceptable solutions, $K = 2n+1 = 2E/\hbar\omega$. The energy level is

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad \text{for } n = 0, 1, 2, 3, \cdots . \tag{31}$$

For the allowed values of $K$, the recursion formula reads

$$a_{j+2} = \frac{(2j+1-(2n+1))}{(j+1)(j+2)} a_j = \frac{-2(n-j)}{(j+1)(j+2)} a_j. \tag{32}$$

If $n = 0$ $(a_1 = 0)$, there is only one term in the series:

$$h_0(\xi) = a_0 \tag{33}$$

$$\psi_0(\xi) = a_0 e^{-\frac{\xi^2}{2}}. \tag{34}$$

For $n = 1$ we take $a_0 = 0$ and

$$h_1(\xi) = a_1 \xi \tag{35}$$

$$\psi_1(\xi) = a_1 \xi e^{-\frac{\xi^2}{2}}. \tag{36}$$

For $n = 2$ ($a_1 = 0$),

$$a_2 = -2a_0, \quad a_4 = 0, \cdots \tag{37}$$

$$h_2(\xi) = a_0 + a_2\xi^2 = a_0(1 - 2\xi^2) \tag{38}$$

$$\psi_2(\xi) = a_0(1 - 2\xi^2)e^{-\frac{\xi^2}{2}}. \tag{39}$$

In general, $h_n(\xi)$ will be a polynomial of degree $n$ in $\xi$. Apart from the overall factor ($a_0$ or $a_1$), they are the **Hermite polynomials**, $H_n(\xi)$. By tradition, the arbitrary multiplicative factor is chosen so that the coefficient of the highest power of $\xi$ is $2^n$.

# Hermite polynomials

$$H_0 = 1$$

$$H_1 = 2\xi$$

$$H_2 = 4\xi^2 - 2$$

$$H_3 = 8\xi^3 - 12\xi$$

$$H_4 = 16\xi^4 - 48\xi^2 + 12$$

$$H_5 = 32\xi^5 - 160\xi^3 + 120\xi$$

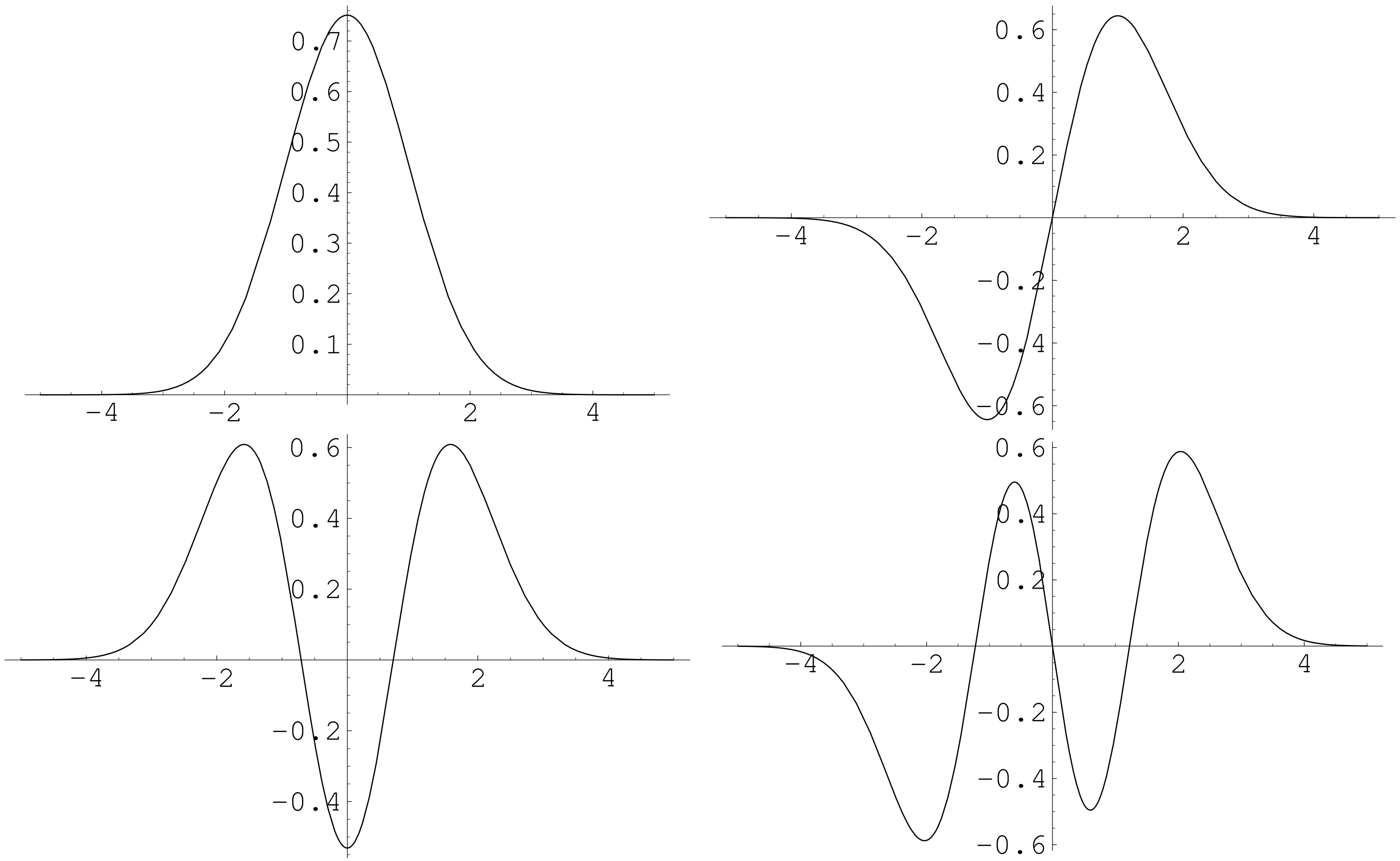
The normalized stationary states for the harmonic potential are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}}. \quad (40)$$

The orthonormality condition of the eigenfunctions $\psi_n(x)$ and $\psi_m(x)$ is

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)dx = \frac{1}{\pi^{1/2}2^n n!} \int_{-\infty}^{\infty} H_n(\xi)H_m(\xi)e^{-\xi^2}d\xi = \delta_{nm}. \quad (41)$$

# First few eignefunctions



# "Energy" Estimate

The time-dependent Schrödinger equation is given by

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) \tag{42}$$

and its complex conjugate is given by

$$-i\hbar\frac{\partial\Psi^*(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*(x,t)}{\partial x^2} + V(x,t)\Psi^*(x,t). \tag{43}$$

We multiply Eq. (42) by $\Psi^*(x,t)$ and multiply Eq. (43) by $\Psi(x,t)$. Then, taking the difference of the two resulting equations gives

$$i\hbar\left(\frac{\partial\Psi}{\partial t}\Psi^* + \frac{\partial\Psi^*}{\partial t}\Psi\right) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\Psi^* - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right). \tag{44}$$

$$\frac{\partial}{\partial t}(\Psi^*\Psi) = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right) \tag{45}$$

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right] \tag{46}$$

We integrate the equation over all space:

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\Psi|^2 dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{\infty} = 0 \tag{47}$$

It follows that

$$\int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx = \text{constant} = \int_{-\infty}^{\infty}|\Psi(x,0)|^2 dx. \tag{48}$$

If $\Psi$ is normalized at $t = 0$, it stays normalized for all future time.

# Reference


- David J. Griffiths, *Introduction to Quantum Mechanics*, Prentice Hall, Englewood Cliffs, N.J., 2005.