Notes on Schrödinger's equation

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1 Eigenfunctions of the continuous problem

Consider the 1-D Schrödinger equation governing the wave function $\Psi(x,t)$,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + V(x)\Psi, \quad t \geq 0, \quad \|\Psi\| < \infty \tag{1}$$

subject to appropriate initial conditions. Here, $V(x)$ is a potential function. For a harmonic oscillator, the potential function satisfies

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

We can solve (1) using separation of variables. We make the ansatz

$$\Psi(x,t) = \phi(t)\psi(x),$$

which we insert into (1). In the standard way, we obtain

$$e := \frac{i\hbar\phi'}{\phi} = \frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi\right). \tag{2}$$

Because $\phi = \phi(t)$ and $\psi = \psi(x)$, the coefficient e must be constant for all x and t. This observation leads to the eigenvalue problem

$$e\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi := \hat{H}\psi. \tag{3}$$

Here, e is the eigenvalue, ψ is the eigenfunction, and $\hat{H}$ is called the Hamiltonian operator. The right hand side can be factored according to

$$\hat{H}\psi = \frac{\hbar\omega}{2}\left(\sqrt{\frac{m\omega}{\hbar}}x - \frac{\hbar}{\sqrt{m\omega}}\frac{\partial}{\partial x}\right)\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{\hbar}{\sqrt{m\omega}}\frac{\partial}{\partial x}\right)\psi + \frac{\hbar\omega}{2}\psi.$$

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Thus, the Hamiltonian operator can written as

$$\hat{H}\psi = \hbar\omega \left(a^\dagger a + \frac{1}{2} I \right) \psi, \tag{4}$$

where we have introduced the lowering operator a,

$$a = \frac{1}{\sqrt{2}} \left(\frac{x}{x_0} + x_0 \frac{\partial}{\partial x} \right), \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}, \tag{5}$$

and its adjoint, the raising operator, $a^\dagger$,

$$a^\dagger = \frac{1}{\sqrt{2}} \left(\frac{x}{x_0} - x_0 \frac{\partial}{\partial x} \right). \tag{6}$$

The factorization of the Hamiltonian operator allows the eigenvalues and eigenfunctions to be computed in a very elegant way. The fundamental eigenfunction corresponds to the ground state and is denoted $\psi_0(x)$. It satisfies

$$a\psi_0 = 0.$$

This equation is solved by the normalized Gaussian function

$$\psi_0(x) = \frac{e^{-x^2/(2x_0^2)}}{\pi^{1/4} x_0^{1/2}}, \quad \int_{-\infty}^{\infty} |\psi_0|^2 \, dx = 1.$$

The corresponding eigenvalue follows from (4),

$$\hat{H}\psi_0 = \hbar\omega \left(a^\dagger a + \frac{1}{2} I \right) \psi_0 = \frac{\hbar\omega}{2} \psi_0, \quad e_0 = \frac{\hbar\omega}{2}.$$

To derive the higher eigenfunctions, we start by studying the commutator

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = \ldots = I. \tag{7}$$

Therefore,

$$[\hat{H} a^\dagger] = \hat{H} a^\dagger - a^\dagger \hat{H} = \hbar\omega (a^\dagger a a^\dagger - a^\dagger a^\dagger a) = \hbar\omega a^\dagger [a, a^\dagger] = \hbar\omega a^\dagger.$$

We conclude that

$$\hat{H} a^\dagger = a^\dagger \hat{H} + \hbar\omega a^\dagger. \tag{8}$$

Assume we know the normalized eigenfunction $\psi_n(x)$ with eigenvalue e_n. From (8),

$$\hat{H} a^\dagger \psi_n = a^\dagger \hat{H} \psi_n + \hbar\omega a^\dagger \psi_n = (e_n + \hbar\omega) a^\dagger \psi_n.$$

We conclude that $a^\dagger\psi_n$ is an (unnormalized) eigenfunction with eigenvalue $e_{n+1} = e_n + \hbar\omega$. We write the normalized eigenfunction as $\psi_{n+1} = \beta^{-1}a^\dagger\psi_n$, where the normalization factor β will be determined below. Because ψ_0 has eigenvalue $e_0 = \hbar\omega/2$,

$$\begin{aligned} e_1 &= e_0 + \hbar\omega = \hbar\omega\left(1 + \frac{1}{2}\right), \\ e_2 &= e_1 + \hbar\omega = e_0 + 2\hbar\omega = \left(2 + \frac{1}{2}\right), \\ &\vdots \\ e_n &= \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \dots. \end{aligned}$$

From the definition of the eigenvalue problem (3) and the factorization (4),

$$\hbar\omega\left(a^\dagger a + \frac{1}{2}I\right)\psi_n = e_n\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n.$$

We define the number operator by

$$\hat{N} = a^\dagger a. \tag{9}$$

It has the same eigenfunctions as $\hat{H}$ and non-negative integer eigenvalues,

$$\hat{N}\psi_n = n\psi_n, \quad n = 0, 1, 2, \dots$$

To normalize the eigenfunction $\psi_{n+1}(x) = \beta^{-1}a^\dagger\psi_n$, we start by defining $u(x) = a^\dagger\psi_n(x)$. Its norm is defined by

$$\|u\|^2 = \langle u, u\rangle = \int_{-\infty}^{\infty} \bar{u}(x)u(x)\,dx.$$

From the definition of the adjoint of an operator,

$$\langle a^\dagger\psi_n, a^\dagger\psi_n\rangle = \langle\psi_n, aa^\dagger\psi_n\rangle$$

From (7) and (9), $aa^\dagger = \hat{N} + I$. Therefore,

$$\langle a^\dagger\psi_n, a^\dagger\psi_n\rangle = \langle\psi_n, (\hat{N} + I)\psi_n\rangle = (n+1)\|\psi_n\|^2.$$

Because $\|\psi_n\| = 1$, the normalized eigenfunction becomes

$$\psi_{n+1}(x) = \frac{1}{\sqrt{n+1}}a^\dagger\psi_n(x), \quad n = 0, 1, 2, \dots. \tag{10}$$

This relation can also be written

$$\sqrt{n+1}\,\psi_{n+1} = a^\dagger\psi_n.$$

By applying the lowering operator a to the above equation,

$$\sqrt{n+1}a\psi_{n+1} = aa^\dagger\psi_n = (\hat{N}+I)\psi_n = (n+1)\psi_n.$$

Thus, $a\psi_{n+1} = \sqrt{n+1}\psi_n$, i.e.,

$$a\psi_n = \sqrt{n}\psi_{n-1}.$$

By applying (10) recursively,

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\,(a^\dagger)^n\psi_0(x), \quad n = 1, 2, 3, \ldots.$$

The eigenfunctions can be expressed in terms of the n^{th} order Hermite polynomials,

$$\kappa_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}.$$

By using Rodrigues formulae,

$$\psi_n(x) = \frac{1}{\pi^{1/4}x_0^{n+1/2}\sqrt{2^n n!}}\kappa_n(x/x_0)e^{-x^2/(2x_0^2)}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}. \tag{11}$$

We summarize the most important relations in the following lemma.

Lemma 1. *The eigenvalue problem for the 1-D Schrödinger equation is*

$$e\psi = \frac{\hbar\omega}{2}\left(-x_0^2\frac{\partial^2\psi}{\partial x^2} + \frac{x^2}{x_0^2}\psi\right) := \hat{H}\psi.$$

Here, x_0 and ω are real constants, e is the eigenvalue, ψ is the eigenfunction, and $\hat{H}$ is called the Hamiltonian operator. It can be factored into

$$\hat{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right),$$

where a and $a^\dagger$ are called the lowering and raising operators, respectively,

$$a = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + x_0\frac{\partial}{\partial x}\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} - x_0\frac{\partial}{\partial x}\right), \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

The smallest eigenvalue of H and the corresponding normalized eigenfunction are

$$e_0 = \frac{1}{2}\hbar\omega, \quad \psi_0(x) = \frac{e^{-x^2/(2x_0^2)}}{\pi^{1/4}x_0^{1/2}}.$$

The higher eigenvalues satisfy

$$e_n = \hbar\omega\left(n + \frac{1}{2}\right),$$

and the eigenfunctions are given by (11). The normalized eigenfunctions satisfy the recursive relations

$$a\psi_n = \sqrt{n}\psi_{n-1}, \quad a^\dagger\psi_n(x) = \sqrt{n+1}\,\psi_{n+1}.$$

From (2), the time dependence corresponding to the eigenfunction $\psi_n(x)$ with eigenvalue e_n satisfies

$$i\hbar\phi_n' = e_n\phi = \hbar\omega(n+1/2)\phi,$$

which is solved by

$$\phi_n(t) = c_n e^{-i(n+1/2)\omega t}.$$

Thus, a general solution of the time-dependent Schrödinger equation can be written as an eigenfunction expansion

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-i(n+1/2)\omega t},$$

where the coefficients c_n are determined by the initial data.

2 Matrix formulation