Harmonic oscillator in quantum mechanics

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Dimensionless Schrödinger's equation

in quantum mechanics a harmonic oscillator with mass m and frequency ω is described by the following Schrödinger's equation:

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

The solution of Eq. (1) supply both the energy spectrum of the oscillator $E=E_n$ and its wave function, $\psi=\psi_n(x)$; $|\psi(x)|^2$ is a probability density to find the oscillator at the position x. Since the probability to find the oscillator somewhere is one,

$$\int_{-\infty}^{\infty}|\psi(x)|^2\mathrm{d}x=1. \tag{2}$$

As a first step in solving Eq. (1) we switch to dimensionless units: $\hbar\omega$ has the dimension of energy, hence $\frac{E}{\hbar\omega}$ is dimensionless. Hence we introduce the parameter, ε,

$$\varepsilon\equiv\frac{2E}{\hbar\omega}. \tag{3}$$

We divide Eq. (1) by $\frac{\hbar\omega}{2}$:

$$-\frac{\hbar}{m\omega}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{m\omega}{\hbar}x^2\psi(x)=\varepsilon\psi(x). \tag{4}$$

The only dimensional parameter combination remaining in Eq. (4), $\frac{m\omega}{\hbar}$, has the dimension of $[\text{length}]^{-2}$. Therefore, the new variable u,

$$u\equiv\sqrt{\frac{m\omega}{\hbar}}x \tag{5}$$

is dimensionless.

$$\frac{m\omega}{\hbar}x^2=u^2,\quad \frac{\hbar}{m\omega}\frac{\mathrm{d}^2}{\mathrm{d}x^2}=\frac{\mathrm{d}^2}{\mathrm{d}u^2}. \tag{6}$$

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}u^2} + u^2\psi(x) = \varepsilon\psi(x), \tag{7}$$

or

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}u^2} + \left(\varepsilon - u^2\right)\psi = 0. \tag{8}$$

Asymptotics of the wave function as $u \to \pm\infty$

How $\psi(u)$ behave when $u \to \pm\infty$? Let's search for the solution of Eq. (8) in the following form:

$$\psi = e^S, \tag{9}$$

where $S(u)$ is a new unknown function.

$$\frac{\mathrm{d}\, e^S}{\mathrm{d}u} = S' e^S, \quad \frac{\mathrm{d}^2 e^S}{\mathrm{d}u^2} = S'' e^S + S'^2 e^S, \tag{10}$$

where $S' = \frac{\mathrm{d}S}{\mathrm{d}u}$. Substituting Eq. (10) into Eq. (8), arrive at the following nonlinear differential equation:

$$S'' + S'^2 + \varepsilon - u^2 = 0. \tag{11}$$

In the limit $u \to \pm\infty$, $\varepsilon \ll u^2$. In addition, as we see shortly,

$$S'' \ll S'^2. \tag{12}$$

Therefore, Eq. (11) can be simplified to

$$S'^2 - u^2 = 0 \quad \longrightarrow \quad S' = -u \quad \longrightarrow \quad S = -\frac{u^2}{2}. \tag{13}$$

The choice of 'minus' sign in Eq. (13) is the only one consistent with the requirement Eq. (2). The solution Eq. (13) is also consistent with the assumption Eq. (12).

Thus,

$$\lim_{u\to\pm\infty} \psi(u) = e^{-\frac{u^2}{2}}. \tag{14}$$

Hermite differential equation

Based on the result Eq. (14) we are going to search for a solution of Eq. (8) in the following form:

$$\psi(u) = v(u)\, e^{-\frac{u^2}{2}}. \tag{15}$$

$$\psi' = v'\, e^{-\frac{u^2}{2}} - v\, u\, e^{-\frac{u^2}{2}} \tag{16}$$

$$\psi'' = v''\, e^{-\frac{u^2}{2}} - 2v'\, u\, e^{-\frac{u^2}{2}} - v\, e^{-\frac{u^2}{2}} + v\, u^2\, e^{-\frac{u^2}{2}}. \tag{17}$$

Substituting Eqs. (15), (17) into Eq. (8) and simplifying, we arrive at the following equation:

$$v'' - 2uv' + (\varepsilon - 1)v = 0. \tag{18}$$

For the later convenience, we introduce the notation

$$\varepsilon - 1 \equiv 2n. \tag{19}$$

The equation

$$v'' - 2uv' + 2nv = 0 \tag{20}$$

is called *Hermite equation*.

Solutions of Hermite equation

Let's search for the solution of Hermite equation in the following definite integral form,

$$v(u) = \int\limits_C e^{ut}\, Y(t)\, \mathrm{d}t, \tag{21}$$

where the contour integral in the complex plane is taken over yet unspecified contour C and $Y(t)$ is a yet unknown function.

The derivatives of $v(u)$, Eq. (21), are as following:

$$v' = \int\limits_C e^{ut}\, t\, Y(t)\, \mathrm{d}t, \tag{22}$$

$$v'' = \int\limits_C e^{ut}\, t^2\, Y(t)\, \mathrm{d}t. \tag{23}$$

$$uv' = \int\limits_C t\, Y(t)\, (ue^{ut}\mathrm{d}t) = \int\limits_C t\, Y(t)\, \mathrm{d}e^{ut} = t\, Y(t)\, e^{ut}\big|_A^B - \int\limits_C e^{ut}\, \frac{\mathrm{d}}{\mathrm{d}t}\, (t\, Y(t))\,, \tag{24}$$

where A and B denote the end points of the contour C.

Let's impose the following restriction on the contour C:

$$t\, Y(t)\, e^{ut}\big|_A^B = 0. \tag{25}$$

In this case,

$$uv' = -\int\limits_C e^{ut}\, \frac{\mathrm{d}}{\mathrm{d}t}\, (t\, Y(t))\,. \tag{26}$$

Substituting Eqs. (21), (23), and (26) into Eq. (20):

$$\int\limits_C e^{ut} \left(2\frac{\mathrm{d}}{\mathrm{d}t}\, (t\, Y(t)) + (t^2 + 2n) Y(t) \right) \mathrm{d}t = 0. \tag{27}$$

Hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(t\,Y\right) + \left(\frac{t^2}{2} + n\right)\,Y = 0. \tag{28}$$

Equation (28) can be integrated as following. To simplify notations, let's introduce the following notation:

$$Z(t) = t\,Y(t), \quad \longrightarrow \quad Y(t) = \frac{1}{t}Z(t). \tag{29}$$

Separating variables in Eq. (28),

$$\frac{\mathrm{d}Z}{\mathrm{d}t} + \left(\frac{t}{2} + \frac{n}{t}\right)\,Z = 0 \quad \longrightarrow \quad \frac{\mathrm{d}Z}{Z} = -\left(\frac{t}{2} + \frac{n}{t}\right)\mathrm{d}t \quad \longrightarrow \quad \ln Z = -\frac{t^2}{4} - n\ln t. \tag{30}$$

Finally,

$$Z(t) = \frac{1}{t^n}e^{-\frac{t^2}{4}} \quad \longrightarrow \quad Y(t) = \frac{1}{t^{n+1}}e^{-\frac{t^2}{4}}, \tag{31}$$

and

$$v(u) = \int\limits_C \frac{1}{t^{n+1}}e^{ut-\frac{t^2}{4}}\mathrm{d}t, \quad \psi(u) = e^{-\frac{u^2}{2}}\int\limits_C \frac{1}{t^{n+1}}e^{ut-\frac{t^2}{4}}\mathrm{d}t. \tag{32}$$

Let's accept, for now without a proof, that Eq. (32) describes a physically acceptable, normalizable per Eq. (2), wave function only if n is a non-negative integer.

In particular that means that the energy spectrum of a harmonic oscillator

$$E = \frac{\hbar\omega}{2}\varepsilon = \hbar\omega\left(n + \frac{1}{2}\right), \tag{33}$$

where we used Eqs. (3) and (19).

If n is an integer we can chose an arbitrary closed contour that encircles $t = 0$ as the integration contour C in Eq. (32).

Hermite polynomials

Let's have a closer look at $v(u)$.

$$v(u) = \oint\limits_C \frac{1}{t^{n+1}}e^{ut-\frac{t^2}{4}}\mathrm{d}t = \oint\limits_C \frac{1}{t^{n+1}}e^{ut-\frac{t^2}{4}-u^2+u^2}\mathrm{d}t = e^{u^2}\oint\limits_C \frac{1}{t^{n+1}}e^{-\left(u-\frac{t}{2}\right)^2}\mathrm{d}t. \tag{34}$$

Introducing a new integration variable, z,

$$z = u - \frac{t}{2}, \tag{35}$$

and dropping an irrelevant factor, obtain:

$$v(u) = e^{u^2}\oint\limits_{C'} \frac{e^{-z^2}}{(z-u)^{n+1}}\,\mathrm{d}z, \tag{36}$$

where we abandoned an irrelevant constant and where C' is an arbitrary closed contour encircling the point $z = u$.

Using Cauchy's formula for derivatives of analytic functions,

$$\frac{\mathrm{d}^k f(u)}{\mathrm{d}u^k} = \frac{k!}{2\pi i} \oint \frac{f(z)}{(z-u)^{k+1}}\, \mathrm{d}z,$$

the expression Eq. (36) can be rewritten as following:

$$v(u) = e^{u^2} \frac{\mathrm{d}^n}{\mathrm{d}u^n} e^{-u^2}. \tag{37}$$

We can see that $v(u)$ is actually a polynomial. The first few non-normalized wave functions are as following:

n	$v_n(u)$	$\psi_n(u)$
0	1	$e^{-\frac{u^2}{2}}$
1	$-2u$	$-2ue^{-\frac{u^2}{2}}$
2	$4u^2 - 2$	$(4u^2 - 2)e^{-\frac{u^2}{2}}$
3	$-8u^3 + 12u$	$(-8u^3 + 12u)e^{-\frac{u^2}{2}}$

Hermite's polynomials define with a factor of $(-1)^n$ to keep positive the coefficient next to the highest power of the argument:

$$H_n(u) = (-1)^n e^{u^2} \frac{\mathrm{d}^n}{\mathrm{d}u^n} e^{-u^2}. \tag{38}$$

For the reference, the explicit expression for Hermite polynomials is as following:

$$H_n(x) = \sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^m \frac{2^{n-2m}\, n!}{m!\,(n-2m)!}\, x^{n-2m}. \tag{39}$$

A wave function in quantum mechanics defined up to an arbitrary constant, hence the wave function of a harmonic oscillator can be expressed as following:

$$\psi_n(u) = e^{-\frac{u^2}{2}} H_n(u). \tag{40}$$

References

[1] Lev D. Landau and Evgeny M. Lifshitz. *Quantum Mechanics Non-Relativistic Theory*, volume III of *Course of Theoretical Physics*. Butterworth-Heinemann, 3 edition, 1981.