HARMONIC OSCILLATOR IN QUANTUM MECHANICS

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Schrödinger's equation

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

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

Here $\hbar$ is the Planck constant, E is the energy of the oscillator.

The solution of Eq. (1) provides 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, the following normalization condition supplements the linear equation (1):

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

Eq. (2) indicates that $\psi(x)$ has the dimension of $[\text{length}]^{-\frac{1}{2}}$.

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. Therefore, 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 that remains in Eq. (4), $\frac{m\omega}{\hbar}$, has the dimension of [length]$^{-2}$. Therefore, the new coordinate variable u,

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

is dimensionless.

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

We can write the Schrödinger's equation Eq. (1) as follows:

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

or

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

The normalization condition Eq. (2) in terms of dimensionless coordinate u is as follows:

$$\int_{-\infty}^{\infty} \left|\psi(u)\right|^2 \mathrm{d}u = 1, \tag{9}$$

where $\psi(u)$ is dimensionless:

$$\psi(u) = \sqrt[4]{\frac{\hbar}{m\omega}}\,\psi(x). \tag{10}$$

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:

$$\psi = e^S, \tag{11}$$

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

$$\frac{\mathrm{d}\,e^S}{\mathrm{d}u} = S' e^S, \quad \frac{\mathrm{d}^2 e^S}{\mathrm{d}u^2} = S'' e^S + S'^2 e^S, \tag{12}$$

where $S' = \frac{\mathrm{d}S}{\mathrm{d}u}$. Substituting Eq. (12) into Eq. (8), arrive at the following nonlinear differential equation:

$$S'' + S'^2 + \varepsilon - u^2 = 0. \tag{13}$$

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

$$\left| S'' \right| \ll S'^2. \tag{14}$$

Therefore, Eq. (13) can be simplified to

$$S'^2 - u^2 = 0 \quad \longrightarrow \quad S' = -u \quad \longrightarrow \quad S = -\frac{u^2}{2}. \tag{15}$$

The choice of 'minus' sign in Eq. (15) is the only one consistent with the requirement Eq. (2). The solution Eq. (15) is also consistent with the assumption Eq. (14).

Thus,

$$\lim_{u \to \pm\infty} \psi(u) = e^{-\frac{u^2}{2}}. \tag{16}$$

Hermite differential equation

Based on the result Eq. (16) we are going to search for a solution of Eq. (8) in the following form:

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

The derivatives of $\psi(u)$ are as follows:

$$\psi' = v'\, e^{-\frac{u^2}{2}} - v\, u\, e^{-\frac{u^2}{2}}, \tag{18}$$

$$\psi'' = v''\, e^{-\frac{u^2}{2}} - 2v'\, u\, e^{-\frac{u^2}{2}} - v\, e^{-\frac{u^2}{2}} + v\, u^2\, e^{-\frac{u^2}{2}}. \tag{19}$$

Substituting Eqs. (17), (19) into Eq. (8) and simplifying, we arrive at the following linear ordinary differential equation:

$$v'' - 2uv' + (\varepsilon - 1)v = 0. \tag{20}$$

For the later convenience, we introduce the notation

$$\varepsilon - 1 \equiv 2n. \tag{21}$$

The equation

$$v'' - 2uv' + 2nv = 0 \tag{22}$$

is called *Hermite equation*.

Solutions of Hermite equation

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

$$v(u) = \int_C e^{ut}\, Y(t)\, \mathrm{d}t, \tag{23}$$

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

The first and the second derivatives of $v(u)$, Eq. (23), are as following:

$$v' = \int_C e^{ut}\, t\, Y(t)\, \mathrm{d}t, \tag{24}$$

$$v'' = \int_C e^{ut}\, t^2\, Y(t)\, \mathrm{d}t. \tag{25}$$

The term with the first derivative in Eq. (22), can be integrated by parts as follows:

$$uv' = \int_C t\, Y(t)\, (u e^{ut} \mathrm{d}t) = \int_C t\, Y(t)\, \mathrm{d}e^{ut} = t\, Y(t)\, e^{ut}\Big|_A^B - \int_C e^{ut} \frac{\mathrm{d}}{\mathrm{d}t}(t\, Y(t)), \tag{26}$$

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

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

$$t\, Y(t)\, e^{ut}\Big|_A^B = 0. \tag{27}$$

In this case,

$$uv' = -\int_C e^{ut} \frac{\mathrm{d}}{\mathrm{d}t}(t\, Y(t)). \tag{28}$$

Substituting Eqs. (23), (25), and (28) into Eq. (22):

$$\int_C e^{ut} \left(2 \frac{\mathrm{d}}{\mathrm{d}t}(t\, Y(t)) + (t^2 + 2n) Y(t) \right) \mathrm{d}t = 0. \tag{29}$$

Hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}(t\, Y) + \left(\frac{t^2}{2} + n \right) Y = 0. \tag{30}$$

Equation (30) is a first order ordinary differential equation that can be integrated separating variables.

To simplify expressions, let's introduce the following notation:

$$Z(t) = t\,Y(t), \quad \longrightarrow \quad Y(t) = \frac{1}{t} Z(t), \tag{31}$$

and write Eq. (30) in the following form:

$$\frac{\mathrm{d}Z}{\mathrm{d}t} + \left(\frac{t}{2} + \frac{n}{t}\right) Z = 0. \tag{32}$$

Separating variables in Eq. (32),

$$\frac{\mathrm{d}Z}{Z} = -\left(\frac{t}{2} + \frac{n}{t}\right)\mathrm{d}t \quad \longrightarrow \quad \ln Z = -\frac{t^2}{4} - n \ln t. \tag{33}$$

Finally,

$$Z(t) = \frac{1}{t^n} e^{-\frac{t^2}{4}} \quad \longrightarrow \quad Y(t) = \frac{1}{t^{n+1}} e^{-\frac{t^2}{4}}, \tag{34}$$

and

$$v(u) = \int_C \frac{1}{t^{n+1}} e^{ut - \frac{t^2}{4}} \mathrm{d}t, \quad \psi(u) = e^{-\frac{u^2}{2}} \int_C \frac{1}{t^{n+1}} e^{ut - \frac{t^2}{4}} \mathrm{d}t. \tag{35}$$

Let's accept, for now without a proof, that Eq. (35) describes a physically acceptable (that is normalizable per Eq. (9)) wave function only if n is a non-negative integer.

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

$$E = \frac{\hbar\omega}{2} \varepsilon = \hbar\omega\left(n + \frac{1}{2}\right), \tag{36}$$

where we used Eqs. (3) and (21).

If n is an integer we can chose an arbitrary closed contour that encircles $t = 0$ as the integration contour C in Eq. (35). Since the integration contour is closed, the requirements Eq. (27) is satisfied automatically.

Hermite polynomials

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

$$v(u) = \oint_C \frac{1}{t^{n+1}} e^{ut - \frac{t^2}{4}} \mathrm{d}t = \oint_C \frac{1}{t^{n+1}} e^{ut - \frac{t^2}{4} - u^2 + u^2} \mathrm{d}t = e^{u^2} \oint_C \frac{1}{t^{n+1}} e^{-\left(u - \frac{t}{2}\right)^2} \mathrm{d}t. \tag{37}$$

Introducing a new integration variable, z,

$$z = u - \frac{t}{2}, \tag{38}$$

and dropping an irrelevant constant factor, obtain:

$$v(u) = e^{u^2} \oint_{C'} \frac{e^{-z^2}}{(z-u)^{n+1}}\,\mathrm{d}z, \tag{39}$$

where C' is an 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. (39) can be rewritten as following:

$$v(u) = e^{u^2} \frac{\mathrm{d}^n}{\mathrm{d}u^n} e^{-u^2}. \tag{40}$$

We can see that $v(u)$ is actually a polynomial of order n. 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	$-8u^3 + 12u$	$(-8u^3+12u)e^{-\frac{u^2}{2}}$

By convention, Hermite polynomials are defined with a factor of $(-1)^n$ to keep positive the coefficient next to the highest power of the argument:

$$H_n(u) = (-1)^n e^{u^2} \frac{\mathrm{d}^n}{\mathrm{d}u^n} e^{-u^2}. \tag{41}$$

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

$$H_n(u) = \sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^m \frac{2^{n-2m}\, n!}{m!\,(n-2m)!}\, u^{n-2m}. \tag{42}$$

The coefficient next to the highest power of the argument is 2^n.

Summarizing, the un-normalized wave function of a harmonic oscillator can be expressed as following:

$$\psi_n(u) = e^{-\frac{u^2}{2}} H_n(u). \tag{43}$$

Normalized wave function

To find the normalized wave function, let's calculate the *normalization integral*:

$$N = \int_{-\infty}^{\infty} \psi_n^2 \, \mathrm{d}u = \int_{-\infty}^{\infty} e^{-u^2} H_n^2(u) \, \mathrm{d}u = \int_{-\infty}^{\infty} (-1)^n H_n(u) \left[\frac{\mathrm{d}^n}{\mathrm{d}u^n} e^{-u^2} \right] \mathrm{d}u, \tag{44}$$

where in the last equality we substituted Eq. (41) for H_n.

Integrating by parts in the last integral n times, we get

$$N = \int_{-\infty}^{\infty} e^{-u^2} \frac{\mathrm{d}^n H_n}{\mathrm{d}u^n} \, \mathrm{d}u. \tag{45}$$

Using Eq. (42),

$$\frac{\mathrm{d}^n H_n}{\mathrm{d}u^n} = 2^n \, n!, \tag{46}$$

therefore

$$N = 2^n \, n! \int_{-\infty}^{\infty} e^{-u^2} \, \mathrm{d}u = 2^n \, n! \sqrt{\pi}. \tag{47}$$

The normalized wave function of quantum harmonic oscillator is as follows:

$$\phi(u) = \frac{1}{\sqrt{N}} \psi_n(u) = \frac{1}{\sqrt{2^n \, n! \sqrt{\pi}}} e^{-\frac{u^2}{2}} H_n(u). \tag{48}$$

References

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