One-dimensional harmonic oscillator

-motivation

-equation, energy levels

-eigenfunctions, Hermite polynomials

-classical analogy
Harmonic oscillator = potential energy depends on square of the space coordinate-force (-gradient of the potential) has a linear dependence on the coordinate.

Many symmetric “potential wells” can be approximated by harmonic oscillator potential close to the potential minimum (lowest order in the Taylor expansion which is symmetric for negative-positive coordinate.)

Thus many physical problems which involve small oscillations of the system not too far from equilibrium are approximated by harmonic oscillator. Out of many examples: oscillations of “electron clouds” of atoms “provoked” by electromagnetic fields or temperature, molecules, electromagnetic fields itself etc etc.

\[
H(p, q) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2
\]

\[
U = \frac{1}{2}m\omega^2 q^2, \quad F = -\frac{dU}{dq} = -m\omega^2 q \overset{\text{def}}{=} -kq \quad \rightarrow \quad k = m\omega^2
\]
The Schrödinger equation is written usually in one of the two forms, depending on which method is used to tackle the problem:

\[
\begin{align*}
-\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \frac{1}{2} m \omega^2 q^2 \Psi(q) &= E \Psi(q) \\
-\frac{\hbar}{m \omega} \frac{d^2}{dq^2} + m \omega q^2 - \frac{E}{\frac{1}{2} \hbar \omega} \Psi(q) &= 0
\end{align*}
\]

\[
\frac{d^2}{dx^2} + x^2 - \varepsilon \Psi(x) = 0
\]  \hspace{1em} \text{(1)}

\[
\frac{1}{2m} \left[ \left( \frac{\hbar}{i} \frac{d}{dq} \right)^2 + (m \omega q)^2 \right] \Psi = E \Psi \hspace{1em} a_\pm \overset{\text{def}}{=} \frac{1}{\sqrt{2m}} \left[ \left( \frac{\hbar}{i} \frac{d}{dq} \right)^\pm (i m \omega q) \right]
\]

we can show that: \( a_- a_+ = \frac{1}{2m} \left[ \left( \frac{\hbar}{i} \frac{d}{dq} \right)^2 + (m \omega q)^2 \right] + \frac{1}{2} \hbar \omega \)

\( a_+ a_- = \frac{1}{2m} \left[ \left( \frac{\hbar}{i} \frac{d}{dq} \right)^2 + (m \omega q)^2 \right] - \frac{1}{2} \hbar \omega \)

and

\[
(a_+ a_- + \frac{1}{2} \hbar \omega) \Psi = E \Psi = (a_- a_+ - \frac{1}{2} \hbar \omega) \Psi
\]  \hspace{1em} \text{(2)}
We spend a very short time now on the second method. We will show that IF: \( \Psi(x) \) is a solution with an energy \( E_0 \), then \( a_+ \Psi(x) \) is also a solution, but with an energy \( E_0 + \hbar \omega \)

\[
(a_+ a_+ + \frac{1}{2} \hbar \omega) a_+ \Psi = (a_+ a_- a_+ + a_+ \frac{1}{2} \hbar \omega) \Psi = a_+ (a_- a_+ + \frac{1}{2} \hbar \omega) \Psi =
\]

\[
= a_+ (a_- a_+ - \frac{1}{2} \hbar \omega + \hbar \omega) \Psi = a_+ (E_0 + \hbar \omega) \Psi = (E_0 + \hbar \omega) a_+ \Psi
\]

So we have proven our point! Now if we find a solution with an energy \( E_0 \) we can construct other solutions and their energies will be of the form:

\[
E_n = E_0 + n \hbar \omega
\]

But what is \( E_0 \) ? and what \( a_- \) operator does?
Writing the equation with “rising” and “lowering” operators $a+$, $a−$ leads to an elegant algebraic method of solving the Schrödinger equation for the oscillator. We will try to start with the “tough” analytical method, using form (1).

\[
\left[ \frac{d^2}{dx^2} - x^2 + \varepsilon \right] \Psi(x) = 0
\]

\[x^2 \overset{\text{def}}{=} q^2 \frac{m \omega}{\hbar} \gg \varepsilon \overset{\text{def}}{=} \frac{E}{\frac{1}{2} \hbar \omega}
\]

lets look first for the solutions which are good for LARGE values of the spacial coordinate thus

\[
\left[ \frac{d^2}{dx^2} - x^2 \right] \Psi(x) = 0
\]

we try \( \Psi(x) = \exp\left( \pm \frac{x^2}{2} \right) \) \( \rightarrow \frac{d^2}{dx^2} \Psi(x) = \frac{d}{dx} \left( \pm x \exp\left( \frac{\pm x^2}{2} \right) \right) \)

\[\rightarrow \frac{d^2}{dx^2} \Psi(x) = \pm \exp\left( \frac{\pm x^2}{2} \right) + x^2 \exp\left( \frac{\pm x^2}{2} \right) = (x^2 \pm 1) \Psi(x)
\]

conclusion-1: our function is an approximate solution for $x \gg 1$ and $x \gg \varepsilon$

\[
\left[ \frac{d^2}{dx^2} - x^2 + 1 \right] \Psi(x) = 0
\]

conclusion -2: if $\varepsilon = 1 = \frac{E}{\frac{1}{2} \hbar \omega}$ \( \rightarrow E = \frac{1}{2} \hbar \omega \)

then : \( \Psi(x) = \exp\left( -\frac{x^2}{2} \right) \) is an EXACT SOLUTION !!
We have shown now that $\Psi(x) = \exp\left(\frac{-x^2}{2}\right)$ is an exact solution with energy $E_0 = \frac{1}{2} \hbar \omega$

We know now that $a_+ \Psi(x)$ will be a solution with $E_1 = \frac{1}{2} \hbar \omega + \hbar \omega$

and we can obtain solutions with higher energies by applying the $a+$ operator. So the energy pattern of our oscillator is:

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

we can also find other eigenfunctions by applying $a+$ operator.

We come back now to our tough analytical way, and try to see what we get.
We have possibly two types of solutions valid for large $x$:

$$\Psi(x) = \exp\left(\frac{\pm x^2}{2}\right)$$

However, we would like to have a solution which we can integrate and normalize -> not divergent at large $x$, thus we chose the one

$$\Psi(x) = \exp\left(-\frac{x^2}{2}\right)$$

Now we postulate general solution in the form

$$\Psi(x) = v(x) \exp\left(-\frac{x^2}{2}\right)$$

$$\frac{d^2}{dx^2} \Psi(x) = \frac{d}{dx} \left[ -x \exp\left(-\frac{x^2}{2}\right) v(x) + v'(x) \exp\left(-\frac{x^2}{2}\right) \right]$$

$$\frac{d^2}{dx^2} \Psi(x) = \left[ -\exp\left(-\frac{x^2}{2}\right) + x^2 \exp\left(-\frac{x^2}{2}\right) \right] v(x) - x \exp\left(-\frac{x^2}{2}\right) v'(x) + v''(x) \exp\left(-\frac{x^2}{2}\right) - x \exp\left(-\frac{x^2}{2}\right) v'(x)$$

$$\frac{d^2}{dx^2} \Psi(x) = \left[ -\exp\left(-\frac{x^2}{2}\right) + x^2 \exp\left(-\frac{x^2}{2}\right) \right] v(x) - 2x \exp\left(-\frac{x^2}{2}\right) v'(x) + v''(x) \exp\left(-\frac{x^2}{2}\right)$$

$$\left[ -\exp\left(-\frac{x^2}{2}\right) + x^2 \exp\left(-\frac{x^2}{2}\right) \right] v(x) - 2x \exp\left(-\frac{x^2}{2}\right) v'(x) + v''(x) \exp\left(-\frac{x^2}{2}\right) - x^2 \exp\left(-\frac{x^2}{2}\right) v(x) + \varepsilon \exp\left(-\frac{x^2}{2}\right) v(x) = 0$$

$$-2x v'(x) + v''(x) + (\varepsilon - 1) v(x) = 0$$

Note that for $\varepsilon = 1$, $v(x) = \text{const}$ is a good solution.
We will try to find now energy levels with analytical method- we will try to find possible functions \( v(x) \) in a polynomial form. we postulate

\[
v(x) = \sum_{k=0}^{\infty} a_k x^k
\]

\[
v'(x) = \sum_{k=0}^{\infty} k a_k x^{(k-1)} \rightarrow xv'(x) = \sum_{k=0}^{\infty} k a_k x^k
\]

\[
v''(x) = \sum_{k=0}^{\infty} k(k-1) a_k x^{(k-2)} = \sum_{k=0}^{\infty} (k+2)(k+1) a_{(k+2)} x^k
\]

inserting \( -2x v'(x) + v''(x) + (\varepsilon - 1) v(x) = 0 \)

\[
[ -2 k a_k + (\varepsilon - 1) a_k + (k+2)(k+1) a_{(k+2)} ] = 0
\]

\[
[ (2 k - \varepsilon + 1) a_k - (k+2)(k+1) a_{(k+2)} ] = 0 \rightarrow a_{(k+2)} = \frac{(2 k - \varepsilon + 1)}{(k+2)(k+1)} a_k
\]

\[
a_2 = \frac{(-\varepsilon + 1)}{2} a_0 ; \quad a_3 = \frac{(2 - \varepsilon + 1)}{3!} a_1
\]
We see that we have two free constants $a_0, a_1$, we expect this from second order equation. We can write $v(x)$ now

$$v(x) = a_0 \left[ 1 + \frac{1 - \varepsilon}{2!} x^2 + \frac{(1 - \varepsilon)(5 - \varepsilon)}{4!} x^4 + \ldots \right] +$$

$$+ a_1 \left[ x + \frac{3 - \varepsilon}{3!} x^5 + \frac{(3 - \varepsilon)(7 - \varepsilon)}{5!} x^7 + \ldots \right]$$

We would not like our $v(x)$ to grow too much so that our total wave function diverges for large $x$. That is why we would like that the series stops somewhere so that

either \hspace{1cm} \begin{align*} a_1 &= 0 \land (\varepsilon = 1 \lor \varepsilon = 5 \lor \varepsilon = 9 \ldots) \\
\text{or} \hspace{1cm} a_0 &= 0 \land (\varepsilon = 3 \lor \varepsilon = 7 \lor \varepsilon = 11 \ldots) \end{align*}

anyway : \hspace{1cm} \begin{align*} \varepsilon &= \frac{E}{\frac{1}{2} \hbar \omega} = 2n + 1 \rightarrow E = (n + \frac{1}{2}) \hbar \omega \\
\frac{1}{2} \hbar \omega & \quad \text{Thus we get the same energy pattern as before.} \end{align*}
The eigenfunctions have the form
\[ \Psi_n(x) = \nu_n(x) \exp\left(\frac{-x^2}{2}\right) \]

\[-2x \nu'(x) + \nu''(x) + (\varepsilon - 1) \nu(x) = 0 \]

\[-2x \nu'_n(x) + \nu''_n(x) + 2n \nu_n(x) = 0 \]

The polynomials fulfilling this equation are called Hermite polynomials
\[ H''_n(x) - 2x H'_n(x) + 2n H_n(x) = 0 \]

we can write some of them explicitly using our calculations (up to a constant)
\[ n=0, \varepsilon = 1 \quad a_1 = 0 \quad , H_0 = a_0... = 1 \]
\[ n=1, \varepsilon = 3 \quad a_0 = 0 \quad , H_1(x) = a_1 x... = 2x \]
\[ n=2, \varepsilon = 5 \quad a_1 = 0 \quad , H_2 = a_0 (1 - 2x^2)... = 4x^2 - 2 \]
\[ n=3, \varepsilon = 7 \quad a_0 = 0 \quad , H_3(x) = a_1 (x - \frac{2}{3}x^3)... = 8x^3 - 12x \]

There are several interesting properties of these polynomials proven on pages 52-54 of your book, which we will just list here ...
Wave functions:

We know that the wave function solutions can be written as

\[ \Psi_n(x) = \text{const} \times H_n(x) \exp\left(-\frac{x^2}{2}\right) \quad \ldots \quad E_n = (n + \frac{1}{2}) \hbar \omega \]

where constant should take care for the proper normalization. From the two properties of the Hermite polynomials:

\[ \int_{-\infty}^{\infty} H_n(x) H_m(x) \exp(-x^2) = 0 \quad \text{if} \quad n \neq m \]

\[ \int_{-\infty}^{\infty} H^2_n(x) \exp(-x^2) = \sqrt{\pi} 2^n n! \]

we know that the wavefunctions corresponding to different energies are orthogonal, and we know how to normalize them, we have to remember however that to normalize them we have to integrate not over \( x \) but over \( q \)

\[ x^2 \overset{\text{def}}{=} q^2 \frac{m \omega}{\hbar} \quad \rightarrow \quad q = x \sqrt{\frac{\hbar}{m \omega}} \]

\[ \Psi_n(q) = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(q \sqrt{\frac{m \omega}{\hbar}}) \exp\left(-m \omega \frac{q^2}{2 \hbar}\right) \]
Classical analogy

Clasically the energy available to the oscillator will be big compared to the minimal oscillator energy, thus

\[ E = (n + \frac{1}{2}) \hbar \omega = (\text{big number} + \frac{1}{2}) \hbar \omega \]

\[ E = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 = \frac{1}{2} m v^2 + \frac{1}{2} m \omega^2 q^2 \rightarrow q_{\text{max}} = \sqrt{\frac{2E}{m \omega^2}} \]

The classical oscillator will swing between \( +q_{\text{max}} \) position.

Quantum solution gives us a probability density (if we take square of the wave function) that the oscillator is in a given position \( q \). What is classically such a probability? We can say that the probability that the oscillator is in between \((q, q + dq)\) is proportional to the time it takes to travel \( dq \) thus

\[ P(q) dq \sim \frac{dt}{\tau} = \frac{\omega}{\pi} \frac{dq}{v} = dq \frac{1}{\sqrt{\frac{2E}{m \omega^2} - q^2}} = dq \frac{1}{\sqrt{q_{\text{max}}^2 - q^2}} \]

we see that the probability density is biggest close to \( q_{\text{max}} \)- we get it also from quantum solutions for large energy.