Quantum Simple Harmonic Oscillator

$$\frac{P^2}{2m} + \frac{1}{2}(k = m\omega^2)X^2|E\rangle = E|E\rangle$$

$\Downarrow$ rep. in $|x\rangle$

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi(x) = E\psi(x)$$

$\Downarrow$

$$y \equiv bx$$
$$b \equiv \sqrt{\frac{\hbar}{m\omega}}$$
$$\varepsilon \equiv \frac{E}{\hbar\omega}$$

$$\frac{d^2\psi}{dy^2} + (2\varepsilon - y^2)\psi = 0$$

Split this into two limiting cases:

I. $y^2 \gg 2\varepsilon$

$$\frac{d^2\psi}{dy^2} - y^2\psi = 0$$

usual trick: $\psi = Ae^{f(y)}$

$$\frac{d\psi}{dy} = Af'(y)e^{f(y)}$$

$$\frac{d^2\psi}{dy^2} = A\left(f''(y) + (f'(y))^2\right)e^{f(y)}$$

so want

$$\ast \quad A\left(f''(y) + [f'(y)]^2 - y^2\right)e^{f(y)} = 0$$

a pretty obvious ansatz:

$$[f'(y)]^2 = y^2$$

$$f'(y) = \pm y \Rightarrow \underline{f(y) = \pm\tfrac{1}{2}y^2} + \begin{pmatrix}\text{constant}\\ \text{absorbed}\\ \text{into } A\end{pmatrix}$$

then

$$A(\pm 1 + \underbrace{y^2 - y^2}_{\substack{\text{highest order in } y,\\ \text{cancelling}}})e^{\pm\frac{1}{2}y^2} = 0$$

relatively negligible as $y \to \infty$ (as justified in ignoring as we were in ignoring 2ε!)

Turns out, at this level of accuracy, a more general φ works too:

$$\varphi(y) = Ay^m e^{\pm y^2/2}$$

$$\frac{d\varphi}{dy} = Amy^{m-1}e^{\pm y^2/2} \pm Ay^{m+1}e^{\pm y^2/2}$$

$$\frac{d^2\varphi}{dy^2} = (Am(m-1)y^{m-2} \pm 2Amy^m + Ay^{m+2})e^{\pm y^2/2}$$

$$-y^2\varphi = -(\qquad\qquad Ay^{m+2})e^{\pm y^2/2}$$

$$= 0$$

these terms, as $y \to \infty$, are negligible relative to y^{m+2}

(to same approx as ignoring 2ε gave).

II $y \to 0$

$$\frac{d^2\psi}{dy^2} + 2\varepsilon\psi = 0 \qquad \psi = \alpha e^{f(x)}$$

$$\alpha\left(\underbrace{f''(y)}_{\to 0} + [f'(y)]^2 + 2\varepsilon\right)e^{f(y)} = 0$$

$$f'(y) = \pm\sqrt{2\varepsilon}\, i$$

$$f(y) = \pm\sqrt{2\varepsilon}\, iy \quad \left(+ \text{constant absorbed in } \alpha\right)$$

$$\psi(y) = \alpha e^{+\sqrt{2\varepsilon}\, iy} + \beta e^{-\sqrt{2\varepsilon}\, iy}$$

as $y \to 0$ $\psi(y) \to \underbrace{(\alpha+\beta)}_{A} + \underbrace{(\alpha-\beta)\sqrt{2\varepsilon}\, i}_{C}\, y$

$$\to A + cy + O(y^2)$$ (p. 192 above 7.3.10)

Combine I and II for general y

$$\psi(y) = \underline{u(y)}\, e^{-y^2/2}$$

only solution; other solution blows up as $|y| \to \infty$; not a bound state.

$u(y) \to A + cy \quad y \to 0$

$\to y^m \quad |y| \to \infty$

$$\frac{d\psi}{dy} = u' e^{-y^2/2} - yu e^{-y^2/2}$$

$$\frac{d^2\psi}{dy^2} = u'' e^{-y^2/2} - 2yu' e^{-y^2/2} + y^2 u e^{-y^2/2} - u e^{-y^2/2}$$

$$\frac{d^2\psi}{dy^2} + (2\varepsilon - y^2)\psi = (u'' - 2yu' + \cancel{y^2}u + 2\varepsilon u - \cancel{y^2}u - u)e^{-y^2/2}$$

$$= \underline{(u'' - 2yu' + (2\varepsilon - 1)u)\, e^{-y^2/2} = 0}$$

or $\boxed{u'' - 2yu' + (2\varepsilon - 1)u = 0 \qquad 7.3.11 \text{ p.192}}$

another ansatz consistent with the limiting behavior of $u(y)$:

$$u(y) = \sum_{n=0}^{\infty} C_n y^n$$

- $y \to 0$, $u \propto A + cy$ gives $n=0$ lower lim.
- $y \to \infty$, $n \to \infty$ OK, although $n < \infty$ OK too

$$u'(y) = \sum_{n=0}^{\infty} C_n n y^{n-1} = \sum_{n=1}^{\infty} C_n n y^{n-1}$$

$$yu'(y) = \sum_{n=0 \text{ or } 1}^{\infty} C_n n y^n$$

$$u''(y) = \sum_{n=0}^{\infty} C_n n(n-1) y^{n-2} = \sum_{\substack{n=0 \text{ or } 1 \\ \text{or } 2}} C_n n(n-1) y^{n-2}$$

"Index Shift": since y^0 (when $n=2$) is first power, set

$$m = n - 2$$
$$m+1 = n - 1$$
$$m+2 = n$$

$$u''(y) = \sum_{m=0}^{\infty} C_{m+2}(m+2)(m+1) y^m$$

but now m is just a symbol; let's recycle $\underline{n} = m$ (not the old n!)

$$u''(y) = \sum_{n=0}^{\infty} C_{n+2}(n+2)(n+1) y^n$$

plug into 7,3,11 :

$$\underbrace{\sum_{n=0}^{\infty} C_{n+2}(n+2)(n+1)y^n}_{u''(y)} \underbrace{-2\sum_{n=0 \text{ or } 1}^{\infty} C_n n y^n}_{-2y\,u'(y)} \underbrace{+(2\varepsilon-1)\sum_{n=0}^{\infty} C_n y^n}_{u(y)} = 0$$

$$\sum_{n=0}^{\infty} \Big\{ \underbrace{C_{n+2}(n+2)(n+1) - 2C_n n + (2\varepsilon-1)C_n}_{\text{this term must zero for all } n} \Big\} y^n = 0$$

so, $\boxed{C_{n+2} = \frac{(2n+1-2\varepsilon)}{(n+2)(n+1)} C_n \quad \begin{matrix} 7.3.14 \\ \text{p. } 193 \end{matrix}}$

means that given C_0, can compute C_2, C_4, C_6, ...

given C_1, can compute C_3, C_5, C_7, ...

So, given 3 numbers: ε, C_0, C_1, can compute $u(y)$:

$$u(y) = C_0\left[1 + \frac{(1-2\varepsilon)}{2}y^2 + \frac{(5-2\varepsilon)(1-2\varepsilon)}{4\cdot 3\cdot 2}y^4 + \frac{(9-2\varepsilon)(5-2\varepsilon)(1-2\varepsilon)}{6\cdot 5\cdot 4\cdot 3\cdot 2}y^6 + \ldots\right]$$

$$+ C_1\left[y + \frac{(3-2\varepsilon)}{3\cdot 2}y^3 + \frac{(7-2\varepsilon)(3-2\varepsilon)}{5\cdot 4\cdot 3\cdot 2}y^5 + \frac{(11-2\varepsilon)(7-2\varepsilon)(3-2\varepsilon)}{7\cdot 6\cdot 5\cdot 4\cdot 3\cdot 2}y^7 + \ldots\right]$$

notice now ... the factor $\frac{y^n}{n!}$

this means that, if the series really is infinite (doesn't terminate), then

$$u(y) \underset{y\to\infty}{\longrightarrow} e^{y^2}$$

but then $\psi(y) = u(y)e^{-y^2/2} \rightarrow e^{+y^2/2}$

and, that is not a bound state!

For bound states, then, the series must terminate, which means that for <u>some</u> integer n, must have:

$$2n+1-2\varepsilon_n = 0$$

$$\boxed{\varepsilon_n = n+\tfrac{1}{2}}$$

$$\boxed{E_n = \varepsilon_n \hbar\omega = (n+\tfrac{1}{2})\hbar\omega}$$

p. 194
7.3.18
7.3.20

<u>Eigenfunctions</u> (omitting $e^{-y^2/2}$) convention

$C_0 \neq 0$ $\quad n=0 \quad u_0(y) = C_0 = 1 \quad E_0 = \frac{1}{2}\hbar\omega$

$C_1 = 0$ $\quad n=2 \quad u_2(y) = C_0[1-2y^2] \quad E_2 = \frac{5}{2}\hbar\omega$

even $\quad C_0 = -2\cdot 1$ (convention)

$n=4 \quad u_4(y) = C_0[1-4y^2+\frac{4}{3}y^4] \quad E_4 = \frac{9}{2}\hbar\omega$

$C_0 = -4\cdot 3$ (convention)

with these conventions, called "Hermite Polynomials"

$c_0 = 0$ $\quad n=1 \quad E_1 = \frac{3}{2}\hbar\omega \quad u_1(y) = c_1 y$

$c_1 = +2$ (convention).

$c_1 \neq 0$ $\quad n=3 \quad E_3 = \frac{7}{2}\hbar\omega \quad U_3 = c_1(y - \frac{2}{3}y^3)$

$\boxed{\text{coefficient of highest power } n \text{ is } 2^n}$ $\quad c_1 = -4 \cdot 3$ (convention)

Putting things together $\quad \psi_E(x) = \psi_{(n+\frac{1}{2})\hbar\omega}(x) = \psi_n(x)$

$$x = by \qquad y = \frac{1}{b}x$$

with normalizations chosen above,

$$\boxed{\psi_n(x) = \underbrace{\left(\frac{m\omega}{\pi\hbar\, 2^{2n}(n!)^2}\right)^{1/4}}_{\substack{\text{normalization,}\\ \text{not computed here}\\ \text{(will get later)}}} \underbrace{e^{-\left(\frac{m\omega^2 x^2}{2\hbar}\right)}}_{e^{-y^2/2}} \underbrace{H_n\left(\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right)}_{\substack{\text{earlier called}\\ U_n(y)}}}$$

$$\int_{-\infty}^{\infty} H_n(y) H_{n'}(y) e^{-y^2} dy = \sqrt{\pi}\, 2^n n!\, \delta_{nn'}$$

"orthogonal polynomials" under weight e^{-y^2}

QSHO comments (p. 197 + on)

① "macroscopic" oscillator: say

$m = 2 \text{ grams} = 2\cdot 10^{-3}\text{ kg}$

$w = 1 \text{ rad/sec}$

$x_0 = \text{max displacement} = 1\text{ cm} = 10^{-2}\text{ m}$

ⓐ $E = \frac{1}{2}kx_0^2 = \frac{1}{2}m\omega_0^2 x_0^2$

$= \frac{1}{2}\cdot 2\cdot 10^{-3}\cdot 1^2 \cdot 10^{-4}$ Joules

$\simeq 10^{-7}$ Joules.

ⓑ $\hbar\omega = (6.6\cdot 10^{-34}\text{ J}\cdot\text{s})\cdot 1\,\frac{1}{s}$

$\simeq 6.6\cdot 10^{-34}$ Joules.

ⓒ $n \simeq \frac{E}{\hbar\omega} - \frac{1}{2} \simeq \frac{10^{-7}}{6.6\cdot 10^{-34}} - \frac{1}{2} \simeq 10^{26}$

$n \simeq 10^{26} \gg 1$ <u>not quantum at all</u>.

② This problem's results are adapted to describe lots of boson's quantum properties: photons, phonons, ...

③ "zero point energy" of $\frac{1}{2}\hbar\omega$
Not 0 by uncertainty principle (p. 199)

④ n even $\psi_n(-x) = \psi_n(x)$ (even powers of x, y)

n odd $\psi_n(-x) = -\psi_n(x)$ (odd powers of x, Y)

define "Parity Operator" $\underset{\sim}{\Pi}$

By definition $|\psi\rangle \doteq \psi(x)$

$$\underset{\sim}{\Pi}|\psi\rangle \doteq \psi(-x)$$

a.k.a. $\underset{\sim}{\Pi}\,\psi(x) = \psi(-x)$

The eigenstates of the QSHO are also eigenstates of $\underset{\sim}{\Pi}$ with eigenvalues ± 1:

$$\underset{\sim}{\Pi}\,\psi_n(x) = (-1)^n \psi_n(x)$$

⑤ QSHO states tunnel past the classical turning points

⑥ $P_n(x) = |\psi_n(x)|^2$ unlike classical, where

$$P(x) \propto dt \propto \frac{dx}{v(x)} \propto \frac{1}{\omega(x_0^2 - x^2)^{1/2}}$$

but as $n \to \infty$ the average value of $P_n(x)$ does resemble classical probability.