# Appendix to Approach 1: Series Solution Method[+]

Step 1:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega_0^2 x^2\right)\psi = 0 \qquad (1)$$

becomes

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

where $y \equiv \sqrt{\frac{m\omega_0}{\hbar}}\, x$ and $\alpha \equiv \frac{E}{\left(\frac{1}{2}\hbar\omega_0\right)}$

Problem becomes: Solve for $\psi(y)$ and $\alpha$ together with $\underbrace{\text{B.C.'s}}_{\text{well-behaved } \psi(y)}$

[+] Some steps will be filled in

**Step 2:** Consider limiting behavior for $y \to \pm\infty$ (i.e. $x \to \pm\infty$)

Eq.(1) becomes $\frac{d^2\psi}{dy^2} - y^2\psi = 0$ (for $y \to \pm\infty$ behavior)

$\psi(y) \sim e^{\pm\frac{1}{2}y^2}$ works

Check: $\frac{d\psi}{dy} \sim \pm y\, e^{\pm\frac{1}{2}y^2}$ ; $\frac{d^2\psi}{dy^2} \sim y^2 e^{\pm\frac{1}{2}y^2} \pm e^{\pm\frac{1}{2}y^2}$

$\sim y^2 e^{\pm\frac{1}{2}y^2}$ $(y \to \pm\infty)$

$\sim y^2\psi$ OK!

- But B.C. requires $\psi \to 0$ as $y \to \pm\infty$,

  $\therefore \psi(y) \sim e^{-\frac{1}{2}y^2}$ [$\psi(y) \sim e^{+\frac{1}{2}y^2}$ fails to satisfy B.C.'s]

- In general, for $y \to \pm\infty$ (large $|y|$)

  $\psi(y) \sim y^m \cdot e^{-\frac{1}{2}y^2}$ [Check: Ex]

**Step 3:** Consider $y \to 0$ behavior ($x \to 0$ behavior)

Eq.(1) becomes $\dfrac{d^2\psi}{dy^2} + \alpha\psi = 0$ (saw this before!)

Solution: $\psi(y) = A\cos\sqrt{\alpha}\,y + B\sin\sqrt{\alpha}\,y$ (Check: Ex)

$\sim A[1 + O(y^2)] + B[\sqrt{\alpha}\,y + O(y^3)]$ (expand sin/cos for small argument)

$\sim A + B'y + O(y^2) + \cdots$

$\sim$ a series in $y$

Putting Step 2 and Step 3 together

General Solution to Eq.(1) is of the form:

$$\boxed{\begin{aligned} &\psi(y) = H(y)\,e^{-\frac{1}{2}y^2} \quad (3) \\ &\text{where } H(y) \to A + By + O(y^2) \text{ as } y \to 0 \\ &\text{and } H(y) \to y^m \text{ as } y \to \pm\infty \end{aligned}}$$

<u>Step 4</u> : Problem becomes that of solving $H(y)$ in Eq.(3)

<u>What is the equation that $H(y)$ satisfies?</u>

Subst. (3) $\psi = H(y)\, e^{-\frac{1}{2}y^2}$ into $\frac{d^2\psi}{dy^2} + (\alpha - y^2)\psi = 0$ (2)

gives

$$\boxed{\frac{d^2H(y)}{dy^2} - 2y\,\frac{dH(y)}{dy} + (\alpha-1)H(y) = 0} \quad (4)$$

Check: Ex

$$\underbrace{\text{Solving TISE}}_{\substack{\text{Solving for}\\ \psi(x) \leftrightarrow E}} \Rightarrow \underbrace{\text{Solving Eq.(2)}}_{\substack{\text{Solving for}\\ \psi(y) \leftrightarrow \alpha}} \Rightarrow \underbrace{\text{Solving Eq.(4)}}_{\substack{\text{Solving for}\\ H(y) \leftrightarrow \alpha}}$$

Key Point: $\psi(x)$ or $\psi(y)$ must be well-behaved.

## Step 5 : Solve Eq.(4) using method of Series Solution

Write $H(y) = \sum_{n=0}^{\infty} a_n y^n$ (5) (Try $\underbrace{\text{a series}}$ solution) [whether it works or not, will see]

need to find coefficients $a_n$

Meaning: $\sum_{n=0}^{\infty}$

Substituting Eq.(5) into Eq.(4) (Ex.) shows that the coefficients are related by

$$\boxed{\frac{a_{n+2}}{a_n} = \frac{2n+1-\alpha}{(n+1)(n+2)}} \quad (6) \quad \text{Recursive Relation}$$

- Meaning: If $a_0$ is fixed, can get $a_2, a_4, \cdots$ by Eq.(6)
  If $a_1$ is fixed, can get $a_3, a_5, \cdots$ by Eq.(6)

Reason: $H(y)$ is governed by Eq.(4), which is in turn TISE for oscillator.

Step 6: Test behavior of $H(y)$ against some known behavior

- Consider $n\to\infty$ limit: $$\frac{a_{n+2}}{a_n} \to \frac{2n}{n^2} \to \frac{2}{n} \qquad (7)$$

- Is it behavior OK? No! It is bad because this is of the same behavior of the coefficients in $e^{+y^2}$.

Check: $$e^{+y^2} = \sum_{n=0}^{\infty} \frac{y^{2n}}{n!} = \sum_{p=0,2,4,\ldots}^{\infty} \frac{y^p}{\left(\frac{p}{2}\right)!} = \cdots + \underbrace{\frac{1}{\left(\frac{p}{2}\right)!}}_{a'_p} y^p + \underbrace{\frac{1}{\left(\frac{p+2}{2}\right)!}}_{a'_{p+2}} y^{p+2} + \cdots$$

$$\frac{a'_{p+2}}{a'_p} = \frac{1}{\left(\frac{p+2}{2}\right)!}\cdot\left(\frac{p}{2}\right)! = \frac{1}{\left(\frac{p}{2}\right)} = \frac{2}{p} \quad \text{same as (7)}$$

∴ For $H(y) = \sum_{n=0}^{\infty} a_n y^n$ satisfying Eq.(4) [TISE], it is of the same behavior as $e^{+y^2}$ $\boxed{\text{if}}$ (recall $n\to\infty$) $H(y)$ is really a series with $n\to\infty$ terms.

But this is <u>bad!</u> $\because$ $\psi(y) = H(y)\, e^{-\frac{1}{2}y^2} \sim e^{+y^2} e^{-\frac{1}{2}y^2} \sim \underline{e^{+\frac{y^2}{2}}}$

as $\underbrace{y \to \pm\infty, \quad \psi(y) \to \infty}_{\text{Unacceptable behavior!}}$ (diverges as $y \to \pm\infty$)

We must find a way <u>to avoid this problem</u>.

<u>What is the way out?</u>

Up to now, we have $H(y) = (a_0 + a_2 y^2 + a_4 y^4 + \cdots) + (a_1 y + a_3 y^3 + a_5 y^5 + \cdots)$

$$= a_0 \underbrace{(1 + \tilde{a}_2 y^2 + \tilde{a}_4 y^4 + \cdots)}_{u_1(y) \text{ (Even)}} + a_1 \underbrace{(y + \tilde{a}_3 y^3 + \tilde{a}_5 y^5 + \cdots)}_{u_2(y) \text{ (Odd)}}$$

- Problem arises if $u_1$ and $u_2$ have infinite number of terms
- If $u_1(y)$ OR $u_2(y)$ only has <u>FINITE NUMBER</u> of <u>TERMS</u>, then we can avoid the problem, i.e. we want <u>polynomials</u> (not infinite series)

∴ We want to <u>terminate</u> the series. How?

Inspect $$\frac{a_{n+2}}{a_n} = \frac{2n+1-\alpha}{(n+1)(n+2)} \quad (6) \qquad n = 0, 1, 2, \cdots$$

Somehow, if $a_{n+2} = 0$, then $a_{n+4}, a_{n+6}, \cdots = 0$

$\Rightarrow$ either $u_1(y)$ OR $u_2(y)$ terminates (becomes a polynomial)

This termination occurs when

$$2n+1-\alpha = 0 \Rightarrow \alpha = \frac{E}{\left(\frac{1}{2}\hbar\omega_0\right)} = 2n+1 \qquad (n = 0, 1, 2, \cdots)$$

$\Rightarrow$ Energy Eigenvalues (allowed energies) are

$$\boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega_0 = \frac{1}{2}\hbar\omega_0 + n\hbar\omega_0 \quad , n = 0, 1, 2, \cdots}$$

• Again, it is B.C. (well-behaved $\psi$) that selects allowed energies.

Energy Eigenfunctions: $\psi_n \sim H(y)\, e^{-\frac{1}{2}y^2}$ $\quad E_n = (n+\frac{1}{2})\hbar\omega_0$

$$H(y) = a_0 \underbrace{u_1(y)}_{\text{even powers of } y} + a_1 \underbrace{u_2(y)}_{\text{odd powers of } y}$$

| <u>$n$ is even</u> | <u>$n$ is odd</u> |
|---|---|
| $a_0 \underbrace{u_1(y)}_{\text{polynomial (OK)}} + a_1 \underbrace{u_2(y)}_{\text{infinite series (bad)}}$ | $a_0 \underbrace{u_1(y)}_{\text{infinite series (bad)}} + a_1 \underbrace{u_2(y)}_{\text{polynomial (OK)}}$ |
| Pick $a_1 = 0$ $\Rightarrow$ kill odd part $\Rightarrow$ OK | Pick $a_0 = 0$ $\Rightarrow$ kill even part $\Rightarrow$ OK |
| $H_n(y)$ is an <u>even function</u> of $y$ (hence $x$) and the highest power term in polynomial is $y^n$ | $H_n(y)$ is an <u>odd function</u> of $y$ (hence $x$) and the highest power term in polynomial is $y^n$ |
| $\left.\begin{matrix} H_0, & H_2, & H_4, & H_6 \cdots \\ \psi_0, & \psi_2, & \psi_4, & \psi_6 \cdots \end{matrix}\right\}$ even functions | $\left.\begin{matrix} H_1, & H_3, & H_5, \cdots \\ \psi_1, & \psi_3, & \psi_5, \cdots \end{matrix}\right\}$ odd functions |

$$\therefore \quad \boxed{\psi_n(y) = A_n \, H_n(y) \, e^{-\frac{1}{2}y^2}} \qquad y = \sqrt{\frac{m\omega_0}{\hbar}}\, x$$

($A_n$:) normalization constant (depends on $n$)

$H_n(y) \equiv$ Hermite Polynomial of order $n$

<u>By convention</u>, take $a_n$ = Highest coefficient in $H_n(y) = 2^n$

(then $a_{n-2}, a_{n-4}, \cdots$ by recursive relation)

$H_0 = 1$, $H_1(y) = 2y$, $H_2(y) = 4y^2 - 2$, $H_3(y) = 8y^3 - 12y$, $H_4(y) = 16y^4 - 48y^2 + 12$

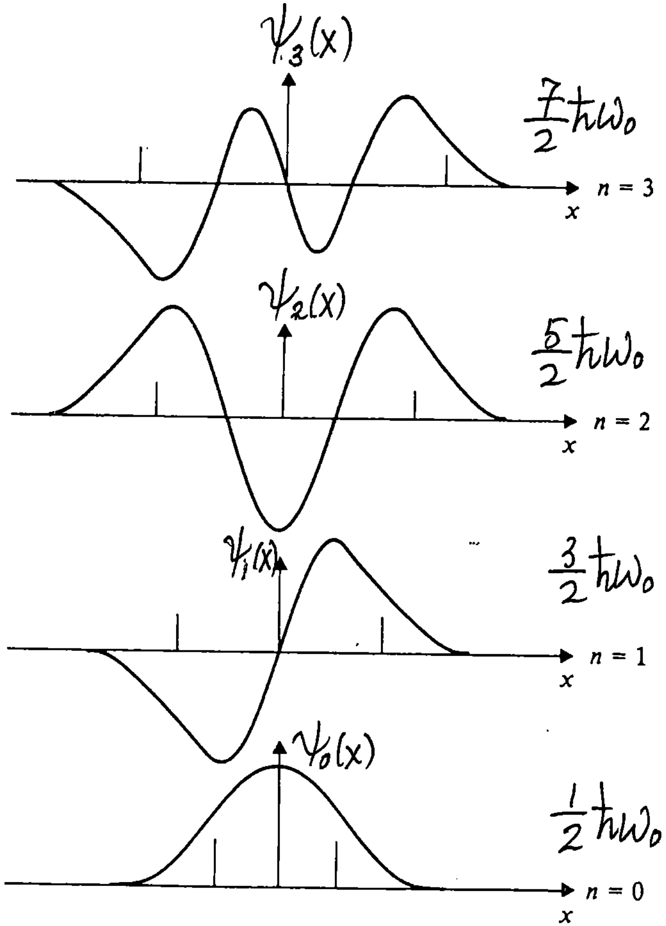
$\cdots$

Normalized $\psi_n$ for eigenenergy $E_n$ is

$$\psi_n = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) \, e^{-\frac{1}{2}y^2}, \text{ where } y = \sqrt{\frac{m\omega_0}{\hbar}}\, x \qquad (8)$$

with $E_n = (n + \frac{1}{2})\hbar\omega_0$, $n = 0, 1, 2, \cdots$

# Explicit form of a few $\psi_n(x)$'s (Just for fun)
## (From Eq. (8))




$$\psi_3(x) = \left(\frac{1}{9\pi}\right)^{1/4}\left(\frac{m\omega_0}{\hbar}\right)^{3/4}\left[\left(\frac{2m\omega_0}{\hbar}\right)x^3 - 3x\right] e^{-\frac{m\omega_0}{2\hbar}x^2}$$

$$\psi_2(x) = \left(\frac{m\omega_0}{4\pi\hbar}\right)^{1/4}\left[2\,\frac{m\omega_0}{\hbar}x^2 - 1\right] e^{-\frac{m\omega_0}{2\hbar}x^2}$$

$$\psi_1(x) = \left(\frac{4}{\pi}\right)^{1/4}\left(\frac{m\omega_0}{\hbar}\right)^{3/4} x\, e^{-\frac{m\omega_0}{2\hbar}x^2}$$

$$\psi_0(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{\frac{-m\omega_0 x^2}{2\hbar}}$$ (Gaussian function)

# Optional: 1-page Summary on the Maths Solving QM oscillator

## Solution of Schrödinger's Equation for the Harmonic Oscillator

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\psi(x) = E\psi(x)}$$

1D time-independent Schrödinger Equation (to solve for E and $\psi(x)$)

$\downarrow$ $U(x) = \frac{1}{2}m\omega_0^2 x^2$ (harmonic oscillator)

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega_0^2 x^2\right)\psi = 0}$$

The equation to be solved

$\downarrow$ $y = \sqrt{\frac{m\omega_0}{\hbar}}\,x$ ; $\alpha = \frac{E}{\frac{1}{2}\hbar\omega_0}$

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

The Schrödinger equation in dimensionless form [Mathematically, it is the Weber's differential equation when $\alpha$ is replaced by $2n+1$] (Weber 1842-1913)

$\downarrow$ $\psi(y) = e^{-\frac{1}{2}y^2}H(y)$

$$\boxed{\frac{d^2H(y)}{dy^2} - 2y\frac{dH(y)}{dy} + (\alpha-1)H(y) = 0}$$

Equation for $H(y)$ and $\alpha$.
Solve by use of the power series method

$\downarrow$ Series solution + condition for acceptable wavefunction
$\Rightarrow \alpha = 1 + 2n$

$$\boxed{\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} + 2nH = 0}$$

This is the Hermite differential equation with solutions $H_n$, the Hermite polynomials. (Hermite 1822-1902)

$\downarrow$

$$\boxed{H_n(y) = \sum_{j=0}^{N}\frac{(-1)^j\, n!\,(2y)^{n-2j}}{j!\,(n-2j)!}}$$

Hermite polynomial of degree $n$. $N = \begin{cases}\frac{n}{2} & \text{even } n\\ \frac{n-1}{2} & \text{odd } n\end{cases}$

$\downarrow$

$E_n = (n+\frac{1}{2})\hbar\omega_0$ energy eigenvalues $(n = 0, 1, 2, \ldots)$

$\psi_n = A_n H_n(y)\, e^{-\frac{1}{2}y^2}$, $y = \sqrt{\frac{m\omega_0}{\hbar}}\,x$, $A_n = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}$ (normalization constant)

(normalised energy eigenfunctions)

Remark: This is for the mathematically inclined students. The magical thing is that the equations (Weber and Hermite) were studied by mathematicians prior to QM was established. Schrödinger did this problem in his 1926 paper.

Hui

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