Hermite Polynomials
Quantum Harmonic Oscillator

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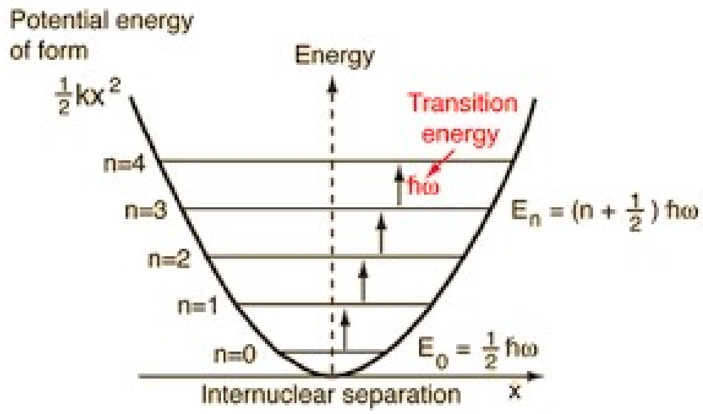
Overview

Last lectures:

- Legendre functions

$$(1-x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + \lambda P = 0$$

- Expansion in Legendre polynomials
- Associated Legendre polynomials
- Spherical harmonics



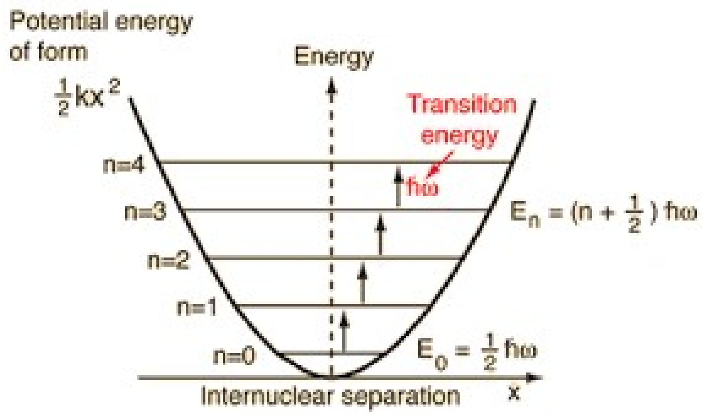
This lecture:

- Hermite Polynomials
- Quantum Harmonic Oscillators

Reading: Chapter 8 of lecture notes

Hermite Polynomials

One of the most important problems in **quantum mechanics** is the harmonic oscillator.



Write down and solve Schrodinger equ for this system

- another special case of **Sturm-Liouville** Eq …
- find solutions using the **Frobenius method**,
- leads to a family of functions called **Hermite polynomials.**

Overview

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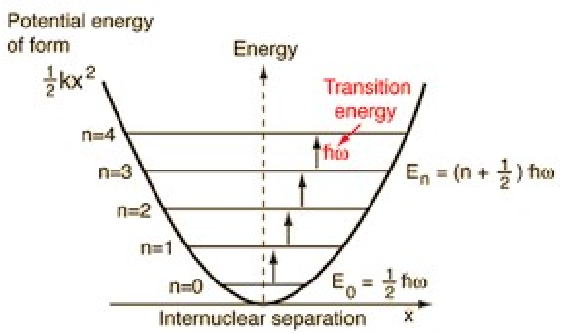
This lecture:

- Schrodinger Equation 1D Quantum Harmonic Oscillator
- Put in a Sturm-Liouville form: re-write in a new variable
- Solve this equation
- Gives Hermite's Equation
- Solve using Frobenuis Method
- Find recurrence relation
- Do the series solutions converge? Make converge



$$\boxed{\varepsilon = 2n + 1}$$

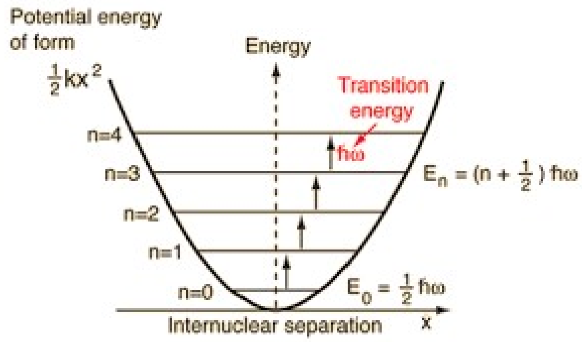
- Hermite Polynomials

$$\boxed{v'' - 2yv' + (\varepsilon - 1)v = 0}$$

- Orthogonality of Hermite Polynomials

Hermite Polynomials

Time-independent Schrodinger eq. (S.E) for a one-dimensional quantum harmonic oscillator:



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

units

$$\begin{aligned}
[x] &= \mathrm{m}\,, \\
[m] &= \mathrm{kg}\,, \\
[\hbar] &= \mathrm{J\,s} = \mathrm{kg\,m^2\,s^{-1}}\,, \\
[\omega] &= \mathrm{s^{-1}}\,.
\end{aligned}$$

construct a new dimensionless variable y of the form

$$y = x/a$$

Schrodinger Equation

The proportionality constant a should have units of metres.

need ħ

$$a = \frac{\sqrt{\hbar}\,(\mathrm{kg}^{1/2}\,\mathrm{m}\,\mathrm{s}^{-1/2})}{\sqrt{\omega}\,(\mathrm{s}^{-1/2})\,\sqrt{m}\,(\mathrm{kg}^{1/2})}\,.$$

Dimensionless parameter

$$y = \frac{x}{a} = \sqrt{\frac{\omega m}{\hbar}}\,x\,.$$

Rewrite the S.E. in this new variable.....

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

Rewrite the S.E. in this new variable:

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

Solution to S.E.: rewrite:

$$\psi(x)=u(y(x))\ .$$

Let

$$\varepsilon=\frac{2E}{\hbar\omega}$$

S.E. becomes a fn of y:

$$u''+(\varepsilon-y^2)u=0$$

Schrodinger Equation

S.E. in this new variable (y):

$$u'' + (\varepsilon - y^2)u = 0$$

Rearrange to have the form of the Sturm-Liouville equation:

$$u'' - y^2 u = -\varepsilon u$$

Equate terms:

$$\begin{aligned} p(y) &= 1\,, \\ q(y) &= -y^2\,, \\ w(y) &= 1\,. \end{aligned}$$

The wavefunction must be normalisable:

so need $u(y) \longrightarrow 0$ for $y \longrightarrow +/- \infty$,

which means the S.L. for this problem is self-adjoint

Solving the S.E.

S.E. in this new variable:

$$-u'' + y^2 u = \varepsilon u$$

- Is not singular in range $-\infty < y < \infty$:
  so can solve using series method
- Also solution = (exponential term) x (finite-order polynomial)

Behaviour for $y \to \pm\infty$, then $y^2 \gg \varepsilon$

S.E. becomes: $$u'' \approx y^2 u \ .$$

Try solution: $$u = e^{-y^2/2}$$

Solving the S.E.

S.E. becomes:

$$u'' \approx y^2 u\ .$$

Try solution:

$$u = e^{-y^2/2}$$

$$u' = \frac{-\cancel{2}y}{\cancel{2}} e^{-y^2/2}$$

$$u'' = -e^{-y^2/2} + y^2 e^{-y^2/2}$$

$$u'' = e^{-y^2/2}(y^2 - 1)$$

Gives

$$u'' = e^{-y^2/2}(y^2 - 1) \approx y^2 u$$ for y >> 1

So, try now solution:

$$\boxed{u(y) = e^{-y^2/2} v(y)}$$

Sub into S.E.

$$u'' + (\varepsilon - y^2)u = 0$$

$$u' = e^{-y^2/2}\left(\frac{-2y}{2}\right) v + e^{-y^2/2} v'$$

$$u'' = y^2 e^{-y^2/2} v + -e^{-y^2/2} v - y e^{-y^2/2} v' + e^{-y^2/2} v'' + -y e^{-y^2/2} v'$$

gives:

$$u'' + (\varepsilon - y^2)u = e^{-y^2/2}[v'' - 2yv' + (\varepsilon - 1)v] = 0$$

$$e^{-y^2/2}[v'' - 2yv' + (\varepsilon - 1)v]$$

Solving the S.E.

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Sub into S.E. gives:

$$u'' + (\varepsilon - y^2)u = e^{-y^2/2}\left[v'' - 2yv' + (\varepsilon - 1)v\right] = 0$$

Cancel exponentials:

$$\boxed{v'' - 2yv' + (\varepsilon - 1)v = 0}$$

Hermite's equation

$$\boxed{u(y) = e^{-y^2/2}v(y)}$$

B.C. u(y) $\longrightarrow$ 0 for y $\longrightarrow$ +/- ∞ :
means wavefunction is normalisable

Series solution for Hermite's equation

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$$\boxed{v'' - 2yv' + (\varepsilon - 1)v = 0}$$

Hermite's equation

y=o is an ordinary point,

so can find a solution in form of a power series

$$\boxed{v(y) = \sum_{n=0}^{\infty} a_n y^n}$$

Ingredients are:

$$yv' = \sum_{n=0}^{\infty} a_n n y^n \,,$$

Let m = n-2, so n=m+2

$$v'' = \sum_{n=0}^{\infty} a_n n(n-1) y^{n-2}$$

then relabel m=n

$$= \sum_{n=-2}^{\infty} a_{n+2}(n+2)(n+1) y^n$$

terms n=-2 and -1 are 0

Series solution for Hermite's equation

Substitute into Hermite's equation

$$\boxed{v'' - 2yv' + (\varepsilon - 1)v = 0}$$

gives:

$$\sum_{n=0}^{\infty} \left[a_{n+2}(n+2)(n+1) - 2a_n n + (\varepsilon - 1)a_n\right] y^n = 0 \,.$$

Set all coefficients of y_n = 0, gives **recurrence relation**

$$a_{n+2} = \frac{2n + 1 - \varepsilon}{(n+2)(n+1)} a_n \,.$$

Gives 2 series: an odd and even series

Full solution is the **sum** of the 2 series

When do the series converge?

Even series

$$\frac{a_{n+2}}{a_n} = \frac{2n+1-\varepsilon}{(n+2)(n+1)} .$$

For large n:

$$\frac{a_{n+2}}{a_n} \approx \frac{2}{n} .$$

Odd series, same ratio, also $\to 0$ for large n

So from the ratio test, both series converge

When do the series converge?

The boundary conditions, require that the function

$u(y) \to 0$ for $y \to \infty$

Since:

$$u = e^{-y^2/2} v$$

This means: $v(y)$ can not blow up at large y faster than $e^{-y^2/2}$

To investigate how the series solution for $v(y)$ behaves for large y, write e^{-y^2} as a Taylor series

$$e^{y^2} = 1 + y^2 + \frac{y^4}{2!} + \frac{y^6}{3!} + \cdots = \sum_{n=0,2,4,\ldots}^{\infty} \frac{y^n}{(n/2)!},$$

When do the series converge?

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$$e^{y^2} = 1 + y^2 + \frac{y^4}{2!} + \frac{y^6}{3!} + \cdots = \sum_{n=0,2,4,\ldots}^{\infty} \frac{y^n}{(n/2)!}\,,$$

$$= \sum_{n=0,2,4,\ldots}^{\infty} c_n y^n \quad \text{where} \quad c_n = [(n/2)!]^{-1}$$

Ratio of neighbouring co-efficients for large n:

$$\frac{C_{n+2}}{C_n} = \frac{1}{\left(\frac{n+2}{2}\right)!}\left(\frac{n}{2}\right)! \approx \frac{2}{n}$$

So for large y: the series behaves asymptotically like e^{+y^2}

So for $u = e^{-y^2/2} v \sim e^{+y^2/2}$ will diverge for large y, so can't satisfy the B.C that $u(y) \to 0$ for y→ ∞

When do the series converge?

So to make the series converge:

Only way to get $u(y) \to 0$ is if the series for $\mathrm{v}(y)$ **terminates** after a finite number of terms.

Look at the recurrence relation:

$$\frac{a_{n+2}}{a_n} = \frac{2n+1-\varepsilon}{(n+2)(n+1)} .$$

Need to **stop** the series at some point: so have $\boxed{\varepsilon = 2n+1}$

Then all terms with $n > \frac{\varepsilon - 1}{2} = 0$

and $\mathrm{v}(y)$ is a polynomial of order n.

☺

$u = e^{-y^2/2}v$ product of $e^{-y/2}$ and a polynomial->0 for y $\to \pm\infty$ and results in a square integrable u(y).

When do the series converge?

If convert ε back into energy:

$$\varepsilon = 2n + 1$$

$$\varepsilon = \frac{2E}{\hbar\omega}$$

$$\varepsilon = \frac{2E}{\hbar\omega} = 2n + 1$$

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

n= 0, 1, 2….

☺

As you are familiar with from Quantum Mechanics

Hermite polynomials

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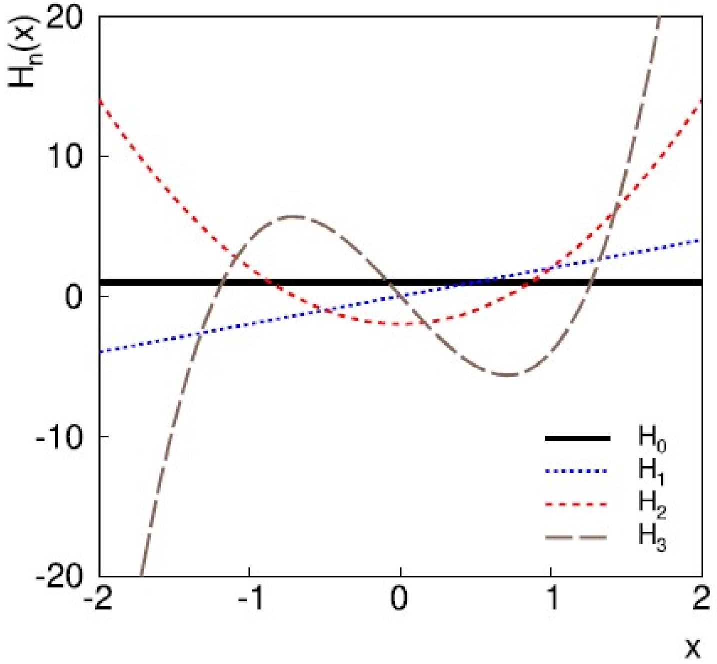
The solutions $v(y)$ are the **Hermite polynomials** of order (n)

They are defined choosing the constants: a_0, a_1 such that $H_0(y)=1$ and $H_1(y)=2y$



$$
\begin{aligned}
H_0(y) &= 1 \, , \\
H_1(y) &= 2y \, , \\
H_2(y) &= 4y^2 - 2 \, , \\
H_3(y) &= 8y^3 - 12y \, , \\
H_4(y) &= 16y^4 - 48y^2 + 12 \, , \\
H_5(y) &= 32y^5 - 160y^3 + 120y \, .
\end{aligned}
$$

Hermite Series

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series

$$v(y) = \sum_{n=0}^{\infty} a_n y^n$$

recurrance

$$a_{n+2} = \frac{2n+1-\varepsilon}{(n+2)(n+1)} a_n .$$

truncation

$$\varepsilon = 2n + 1$$

Work out the H_2 (n=2) series: so ε= 5

First even: let n=0: ε=5 $\quad a_2 = \frac{1-5}{(2)(1)} a_0 = \frac{-4}{2} a_0 = -2a_0$

Then: $\quad a_2 = -2a_0$

$$H_2(y) = a_0 y^0 + a_2 y^2 = a_0 - 2a_0 y^2$$

If $\quad a_0 = -2 \quad H_2(y) = 4y^2 - 2$ ☺

$$\begin{aligned} H_0(y) &= 1 , \\ H_1(y) &= 2y , \\ H_2(y) &= 4y^2 - 2 , \\ H_3(y) &= 8y^3 - 12y , \end{aligned}$$

Application of the recurrence relation

$$\frac{a_{n+2}}{a_n} = \frac{2n + 1 - \varepsilon}{(n + 2)(n + 1)} \; .$$

is equivalent to:

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}$$

The generalisation of Rodrigue's formula for Hermite polynomials

Orthogonality of Hermite Polynomials

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$$\boxed{v'' - 2yv' + (\varepsilon - 1)v = 0}$$

Hermite's equation

Hermite's equation does not seem to be in Sturm-Liouville form,

But x e^{-y^2}

Gives:

$$e^{-y^2}v'' - 2ye^{-y^2}v' + (\varepsilon - 1)e^{-y^2}v = 0$$

Rewrite as:

$$-\frac{d}{dy}\left[e^{-y^2}\frac{dv}{dy}\right] + e^{-y^2}v = \varepsilon e^{-y^2}v\ .$$

Compare with Sturm-Liouville::

$$\begin{aligned} p(y) &= e^{-y^2}\ , \\ q(y) &= -e^{-y^2}\ , \\ w(y) &= e^{-y^2}\ . \end{aligned}$$

$p(y) \to 0$ for $y \to \pm\infty$

So B.C in Lagrange identity is 0, so the corresponding operator is self-adjoint

Orthogonality of Hermite Polynomials

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$$\boxed{v'' - 2yv' + (\varepsilon - 1)v = 0}$$

Hermite's equation

Therefore the Hermite polynomials and the related u(y) have the usual properties as solutions to the SL equation

(real eigenvalues, orthogonality , completeness , etc)

For orthogonality:

$$\langle H_n, H_m \rangle = \int_{-\infty}^{\infty} H_n(y) H_m(y) e^{-y^2}\, dy = \sqrt{\pi} 2^n n! \delta_{nm}$$

Here the weight function in the inner product is:

$$w(y) = e^{-y^2}.$$

Wavefunction of a quantum harmonic oscillator

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From solving the D.E. find the solution is:

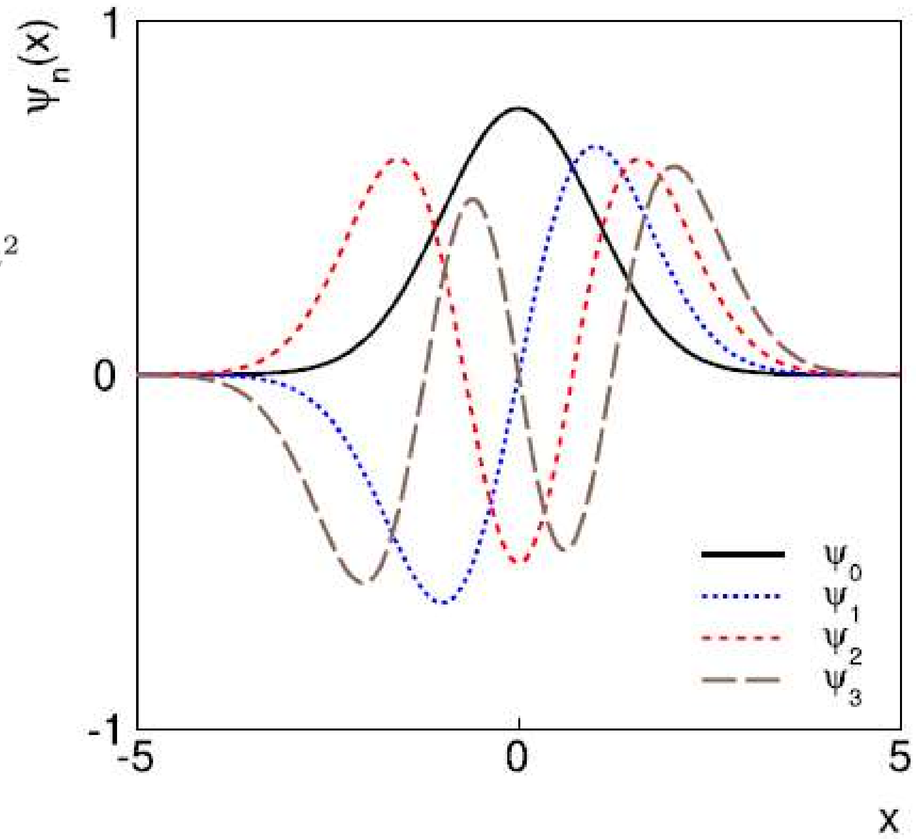
$$u(y) = e^{-y^2/2} v(y)$$

Convert this back into the wavefunction for the harmonic oscillator, using y = x/a.

The D.E. for u(y) was a special case of the **Sturm-Liouville** equation: so know:

Wavefunction of a quantum harmonic oscillator

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}(\pi a^2)^{1/4}} H_n(x/a) e^{-x^2/2a^2}$$



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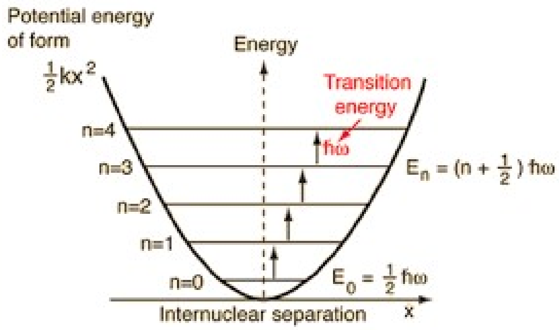
- Orthogonality of Hermite Polynomials



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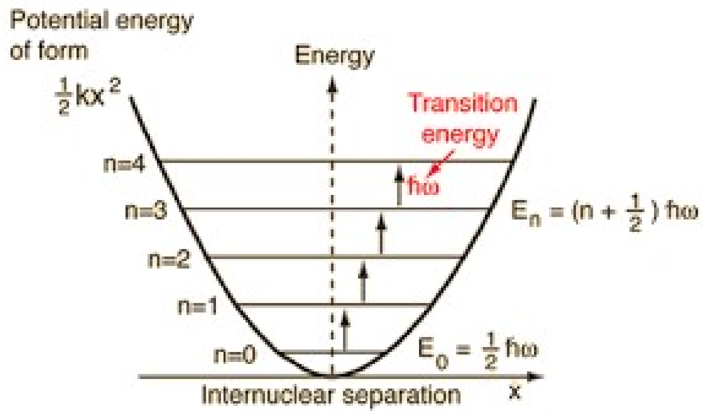

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