Particle in a Box

The potential

$$V = 0 \qquad 0 < x < a$$
$$= \infty \qquad otherwise$$

Eigenfunctions and eigenvalues

$$|\phi_n\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$$

Superposition

$$|\psi\rangle = \sum_{n=1}^{\infty} b_n |\phi_n\rangle \qquad \langle \phi_m | \phi_n \rangle = \delta_{m,n}$$

Getting the coefficients

$$b_n = \langle \phi_n | \psi \rangle \qquad P_n = |b_n|^2$$

Time Dependence

$$\Psi(x,t) = \sum_{n=1}^{\infty} b_n |\phi_n(x)\rangle e^{-i\omega_n t}$$

Free Particle

The potential

$$V = 0$$

Eigenfunctions and eigenvalues

$$|\phi(k)\rangle = \frac{1}{\sqrt{2\pi}} e^{\pm ikx} \qquad E = \frac{\hbar^2 k^2}{2m}$$

Superposition

$$|\psi\rangle = \int_{-\infty}^{\infty} b(k)\phi(k) dk$$
$$\langle \phi(k') | \phi(k) \rangle = \delta(k - k')$$

Getting the coefficients

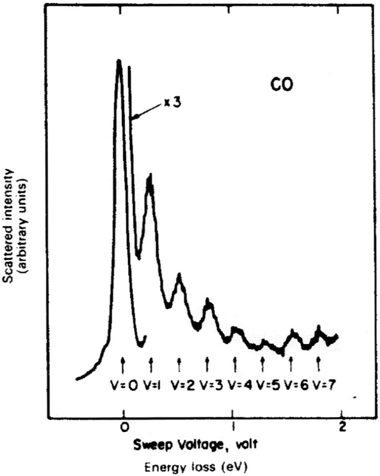
$$b(k) = \langle \phi(k) | \psi \rangle \qquad P_n = |b(k)|^2$$

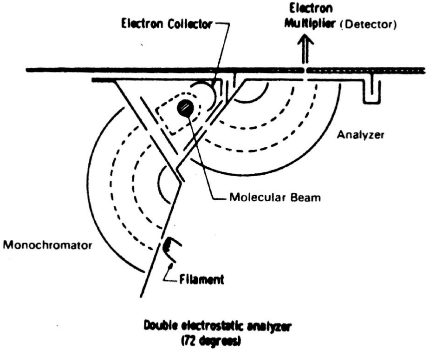
Time Dependence

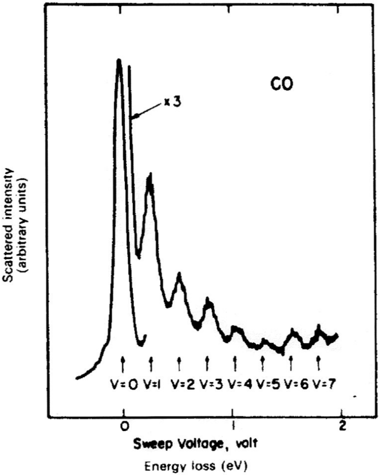
$$\Psi(x,t) = \int_{-\infty}^{\infty} b(k)\phi_k(x) e^{-i\omega(k)t} dk$$

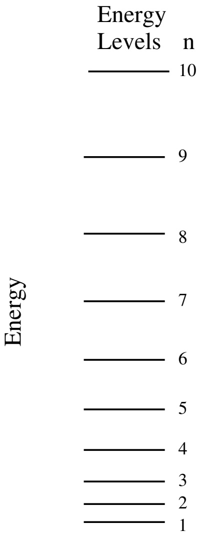
The excited states of the diatomic molecule carbon monoxide (CO) can be observed by crossing a beam of electrons with another beam of carbon monoxide. The energy spectrum of the scattered electrons is displayed here.

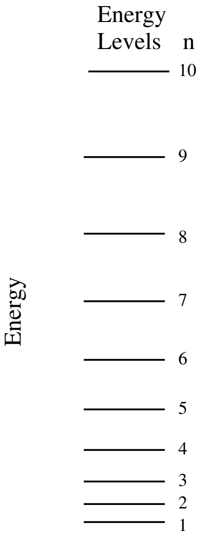
1. What is the simplest potential we used for a bound system?
2. What is the energy spectrum predicted for that potential? Does it fit here?
3. Find the eigenfunctions and eigenvalues of the harmonic oscillator. Does the energy spectrum reproduce the data?




Electron Collector
Electron Multiplier (Detector)
Analyzer
Molecular Beam
Monochromator
Filament
Double electrostatic analyzer (72 degrees)


CO
x 3
Scattered intensity (arbitrary units)
V=0 V=1 V=2 V=3 V=4 V=5 V=6 V=7
0
1
2
Sweep Voltage, volt
Energy loss (eV)

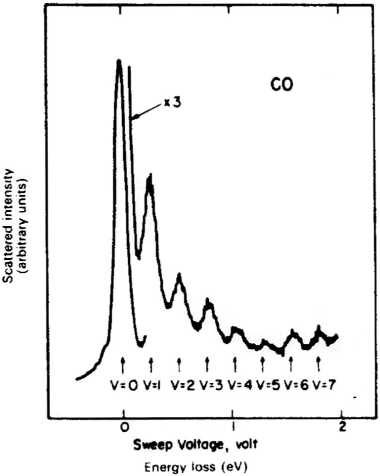

Energy
Levels
n
10
9
8
7
6
5
4
3
2
1
Energy

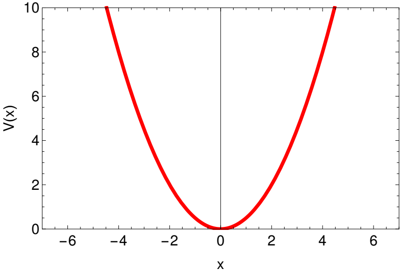


$$E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$$

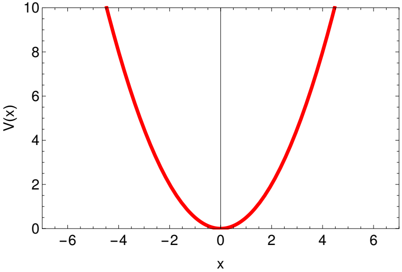
The excited states of the diatomic molecule carbon monoxide (CO) can be observed by crossing a beam of electrons with another beam of carbon monoxide. The energy spectrum of the scattered electrons is displayed here.

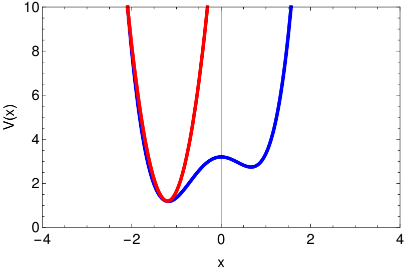
1. What is the simplest potential we used for a bound system?
2. What is the energy spectrum predicted for that potential? Does it fit here?
3. Find the eigenfunctions and eigenvalues of the harmonic oscillator. Does the energy spectrum reproduce the data?




10
8
6
4
2
0
V(x)
−6
−4
−2
0
2
4
6
x

The Harmonic Oscillator Potential





1. Each physical, measurable quantity, A, has a corresponding operator, $\hat{A}$, that satisfies the eigenvalue equation $\hat{A}\,\phi = a\phi$ and measuring that quantity yields the eigenvalues of $\hat{A}$.
2. Measurement of the observable A leaves the system in a state that is an eigenfunction of $\hat{A}$.
3. The state of a system is represented by a wave function Ψ which is continuous, differentiable and contains all the information about it.
    - The average value of any observable A is determined by $\langle A \rangle = \int_{all\ space} \Psi^* \hat{A}\, \Psi d\vec{r}$.
    - The 'intensity' is proportional to $|\Psi|^2$.
4. The time development of the wave function is determined by

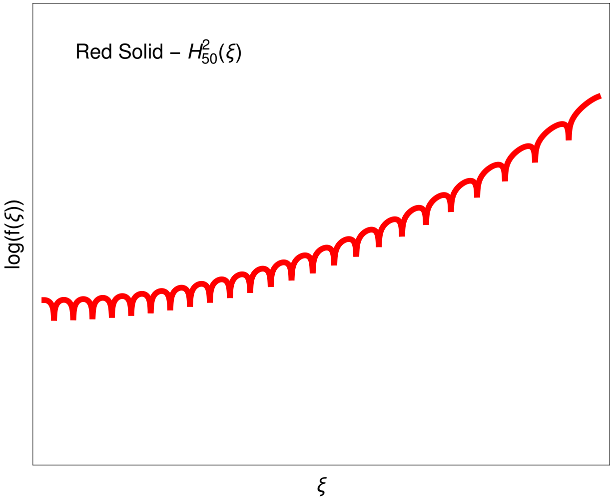
$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2\mu}\nabla^2 \Psi(\vec{r},t) + V(\vec{r})\Psi(\vec{r},t) \qquad \mu \equiv \text{reduced mass.}$$

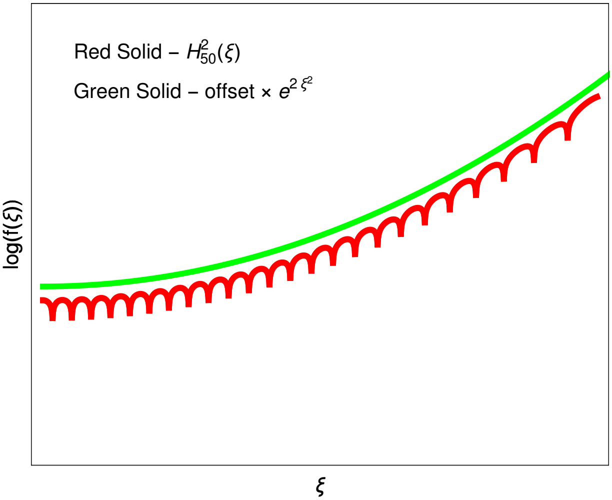
1. Potential energy: $\frac{\kappa x^2}{2}$
2. Hermite's equation:

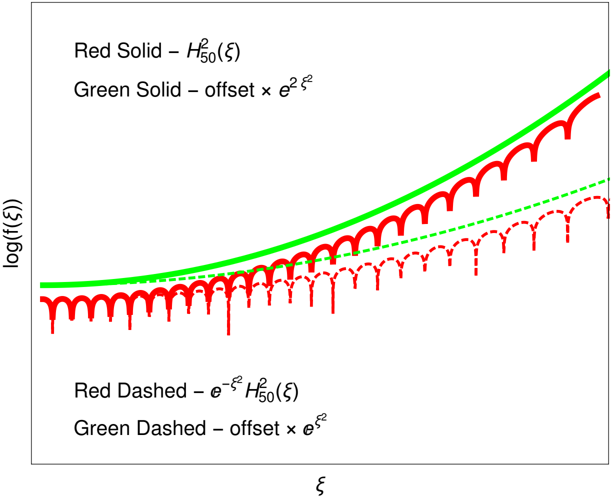
$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + \left(\frac{\alpha}{\beta^2} - 1\right)H = 0$$

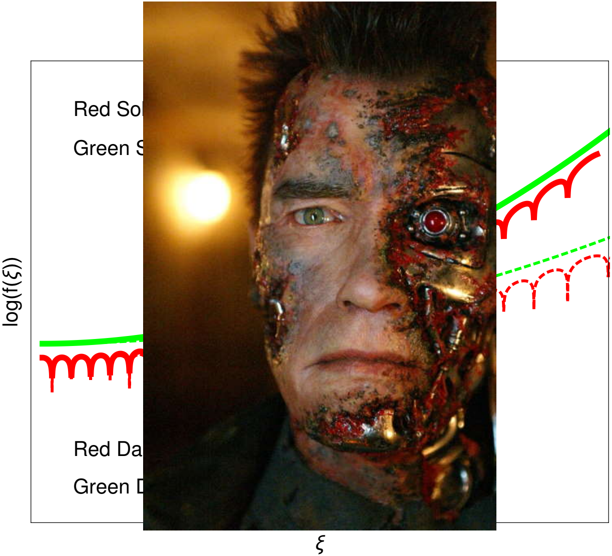
3. Second-order, linear, ordinary, homegeneous differential equation
    1. second-order: has a second derivative in it.
    2. linear: only derivatives to the first power.
    3. ordinary: one independent variable.
    4. homogeneous: equal to zero.
4. Method of Frobenius (19th century German mathematician)
    1. Used to generate an infinite series solution.
    2. Applies to equations of the form

$$u'' + \frac{p(z)}{z}u' + \frac{q(z)}{z^2}u = 0$$


Red Solid – $H^2_{50}(\xi)$
log(f(ξ))
ξ


Red Solid – $H_{50}^2(\xi)$
Green Solid – offset × $e^{2\xi^2}$
log(f(ξ))
ξ

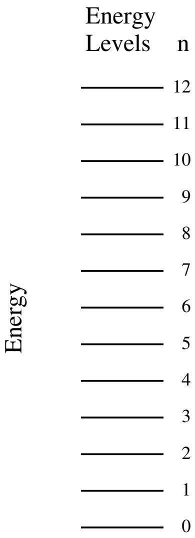

Red Solid – $H_{50}^2(\xi)$
Green Solid – offset × $e^{2\xi^2}$
Red Dashed – $e^{-\xi^2}H_{50}^2(\xi)$
Green Dashed – offset × e^{ξ^2}
log(f(ξ))
ξ


Red Sol
Green S
Red Da
Green D
log(f(ξ))
ξ

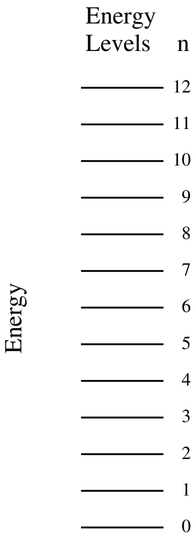
The Hermite Polynomials

$$
\begin{aligned}
H_0(\xi) &= \frac{1}{\sqrt{\sqrt{\pi}}} \\
H_1(\xi) &= \frac{1}{\sqrt{2\sqrt{\pi}}} 2\xi \\
H_2(\xi) &= \frac{1}{\sqrt{8\sqrt{\pi}}} (4\xi^2 - 2) \\
H_3(\xi) &= \frac{1}{\sqrt{48\sqrt{\pi}}} (8\xi^3 - 12\xi) \\
H_4(\xi) &= \frac{1}{\sqrt{384\sqrt{\pi}}} (16\xi^4 - 48\xi^2 + 12) \\
H_5(\xi) &= \frac{1}{\sqrt{3840\sqrt{\pi}}} (32\xi^5 - 160\xi^3 + 120\xi) \\
H_6(\xi) &= \frac{1}{\sqrt{46080\sqrt{\pi}}} (64\xi^6 - 480\xi^4 + 720\xi^2 - 120)
\end{aligned}
$$

The Harmonic Oscillator Well Potential

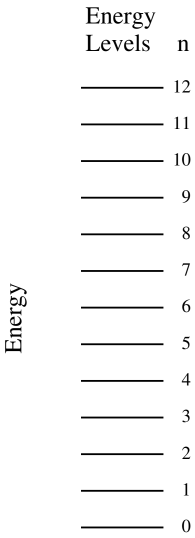


The Harmonic Oscillator Well Potential 17

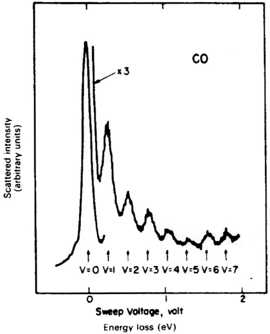


$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0$$

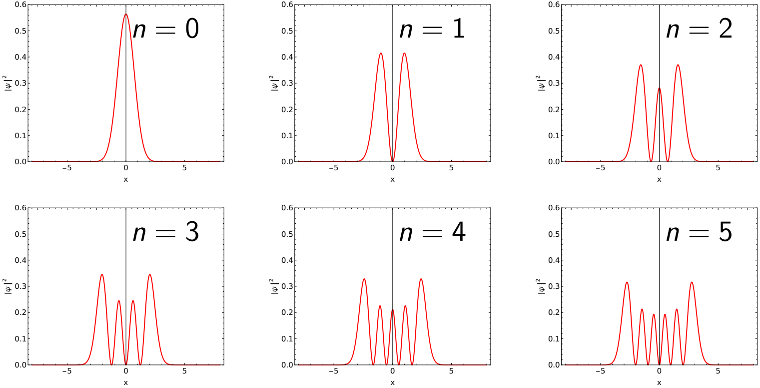
The Harmonic Oscillator Well Potential 18

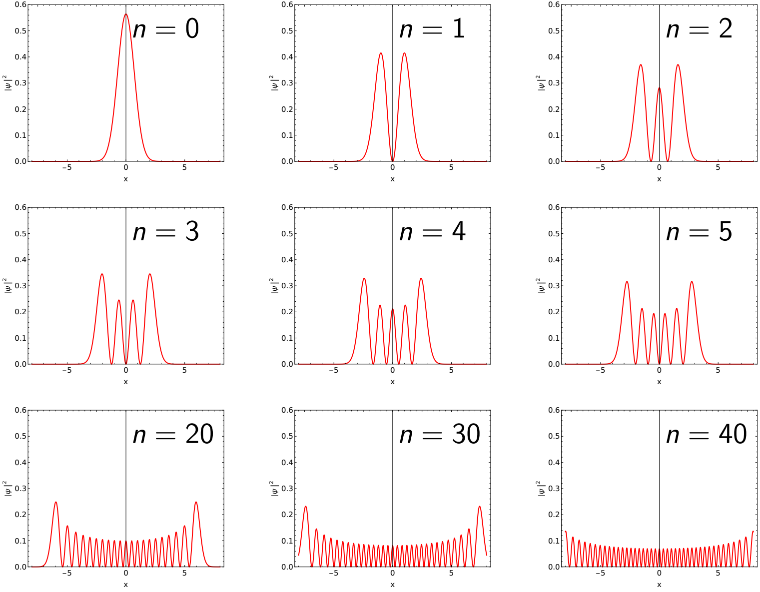


$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega_0$$

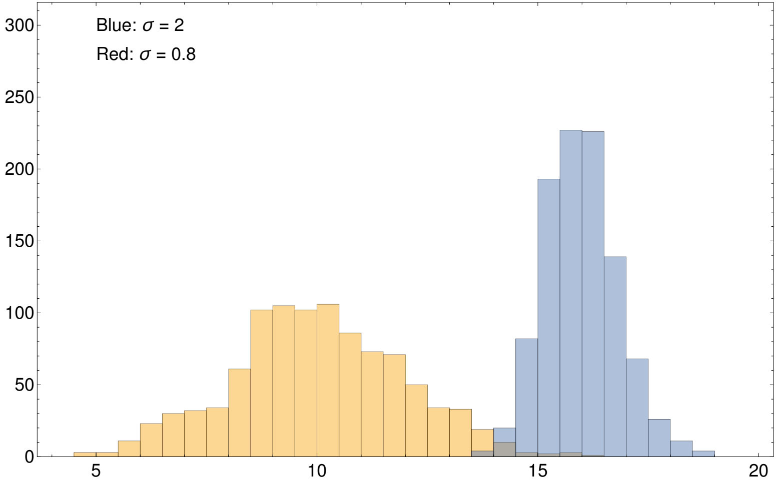


The Harmonic Oscillator Well Potential 19

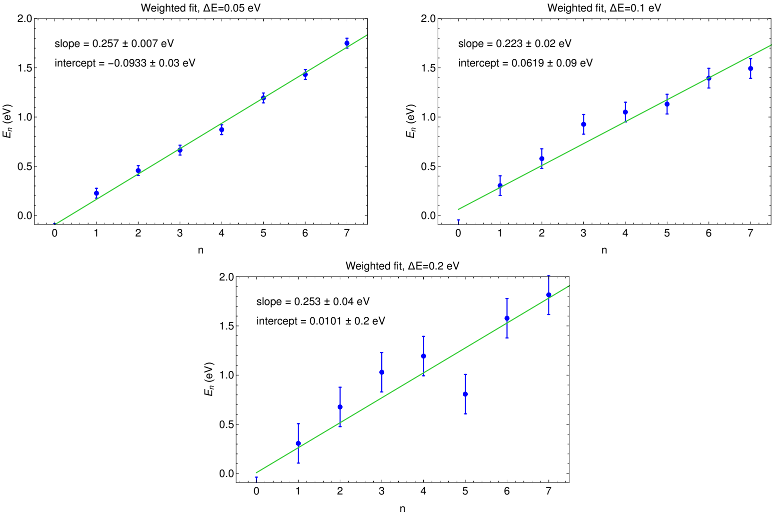




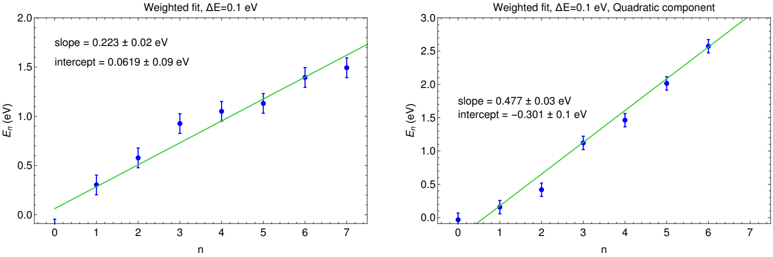
n = 0
n = 1
n = 2
n = 3
n = 4
n = 5
n = 20
n = 30
n = 40
$|\psi|^2$
x

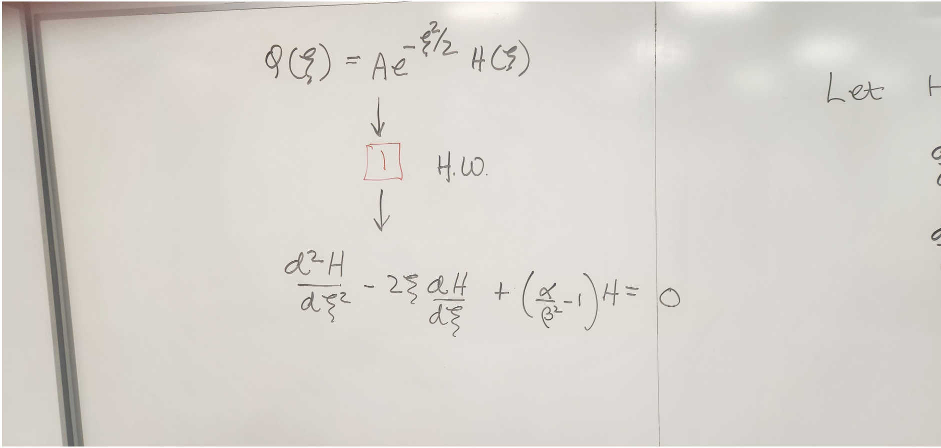

Blue: σ = 2
Red: σ = 0.8
300
250
200
150
100
50
0
5
10
15
20

Effect of Data Uncertainty On Fit

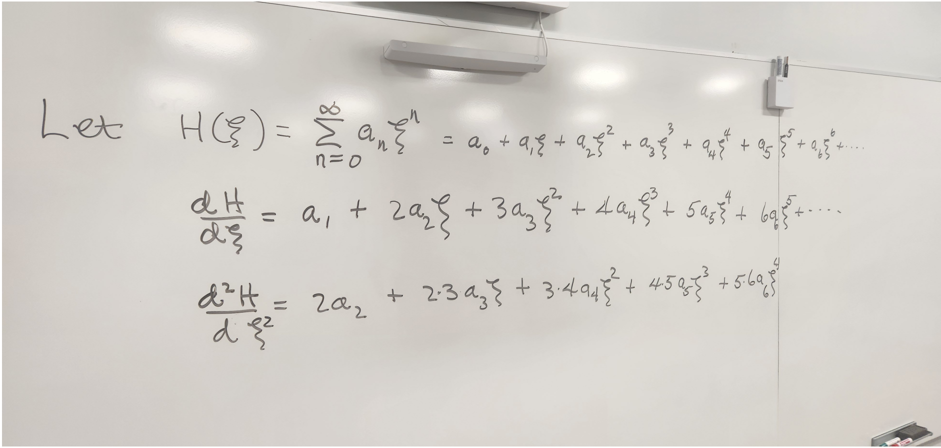


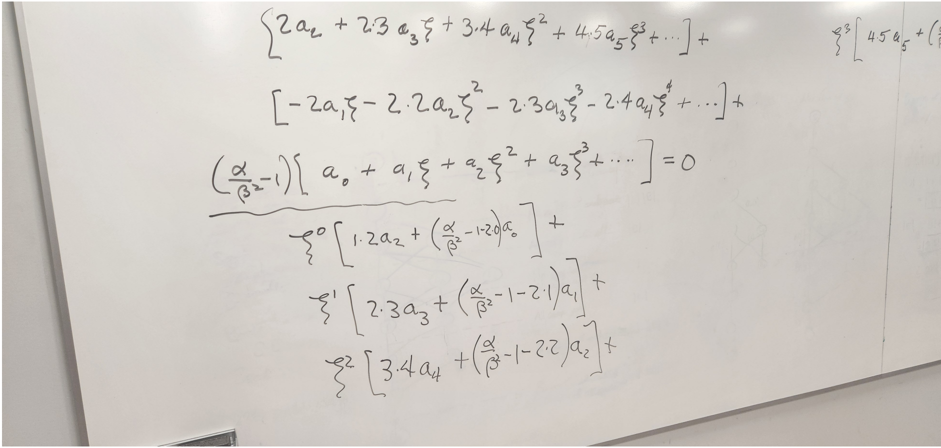
Effect of Data Uncertainty on Modeling




$\phi(\xi) = Ae^{-\xi^2/2} H(\xi)$
1
H.W.
$\frac{d^2H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + \left(\frac{\alpha}{\beta^2} - 1\right)H = 0$
Let

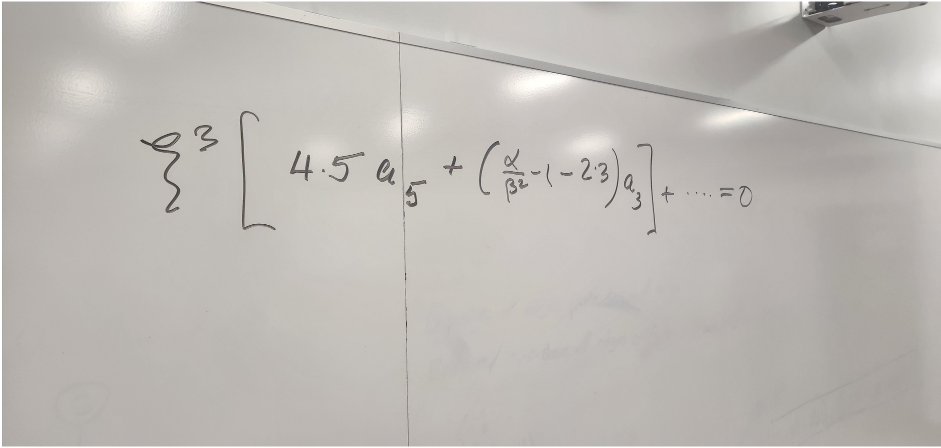
Board 2 25


Let $H(\xi) = \sum_{n=0}^{\infty} a_n \xi^n = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + a_5\xi^5 + a_6\xi^6 + \cdots$
$\frac{dH}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + 4a_4\xi^3 + 5a_5\xi^4 + 6a_6\xi^5 + \cdots$
$\frac{d^2H}{d\xi^2} = 2a_2 + 2\cdot3a_3\xi + 3\cdot4a_4\xi^2 + 4\cdot5a_5\xi^3 + 5\cdot6a_6\xi^4$


$\{2a_2 + 2\cdot3\, a_3\xi + 3\cdot4\, a_4\xi^2 + 4\cdot5\, a_5\xi^3 + \dots] +$
$\xi^3 [4\cdot5\, a_5 + ($
$[-2a_1\xi - 2\cdot2a_2\xi^2 - 2\cdot3a_3\xi^3 - 2\cdot4a_4\xi^4 + \dots] +$
$\left(\frac{\alpha}{\beta^2}-1\right)[a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \dots] = 0$
$\xi^0\left[1\cdot2a_2 + \left(\frac{\alpha}{\beta^2}-1-2\cdot0\right)a_0\right] +$
$\xi^1\left[2\cdot3a_3 + \left(\frac{\alpha}{\beta^2}-1-2\cdot1\right)a_1\right] +$
$\xi^2\left[3\cdot4a_4 + \left(\frac{\alpha}{\beta^2}-1-2\cdot2\right)a_2\right] +$

Board 4

27


$\xi^3 \left[4\cdot5\, a_5 + \left(\frac{\alpha}{\beta^2} - 1 - 2\cdot3 \right) a_3 \right] + \cdots = 0$