Comparison of Bound and Free Particles

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

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

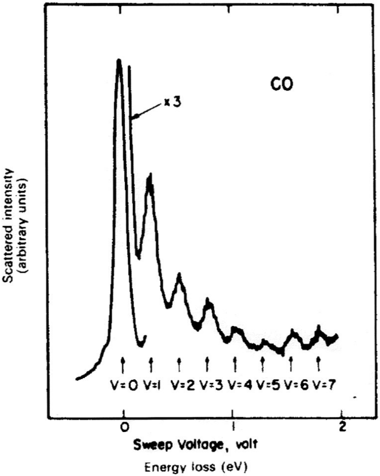
Time Dependence

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

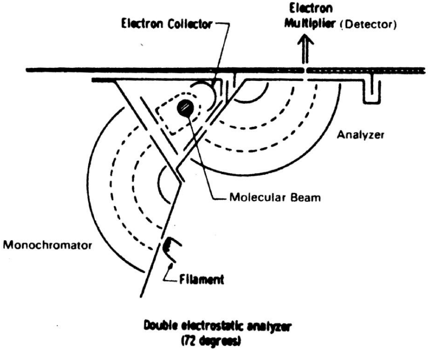
The Configurations of Carbon Monoxide

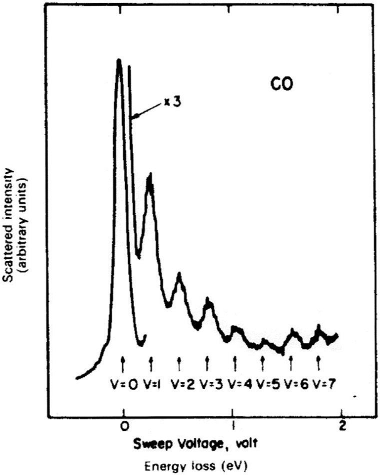
The excited states of the diatomic molecule carbon monoxide (CO) can be observed by crossing a beam of electrons with another beam of carbon monoxide. The energy spectrum of the scattered electrons is displayed here.

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?



The Experiment





The Infinite Rectangular Well Potential

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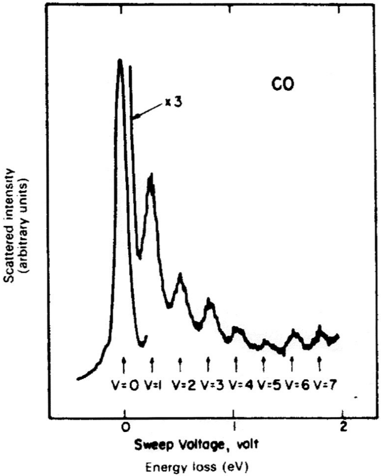
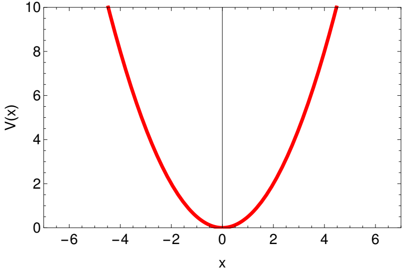


The Harmonic Oscillator Potential



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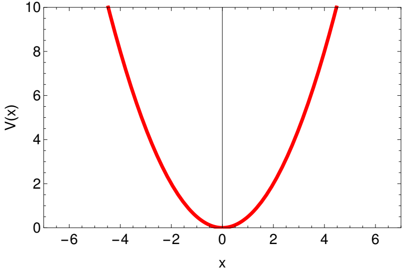
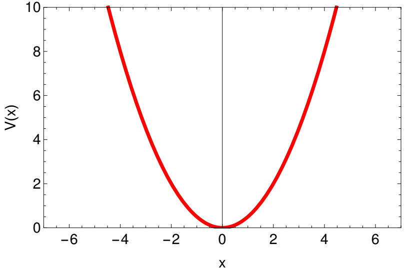


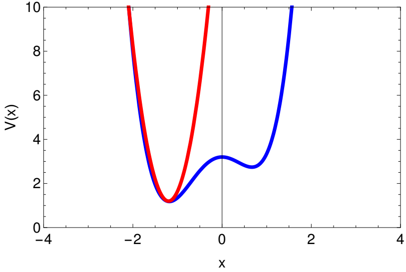
$$\vec{F} = -\kappa x \hat{i}$$

$$V = \frac{1}{2}\kappa x^2$$

$$E = \frac{p^2}{2m} + \frac{1}{2}\kappa x^2$$

The Harmonic Oscillator Potential





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The Postulates

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

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

Solving the Quantum Harmonic Oscillator

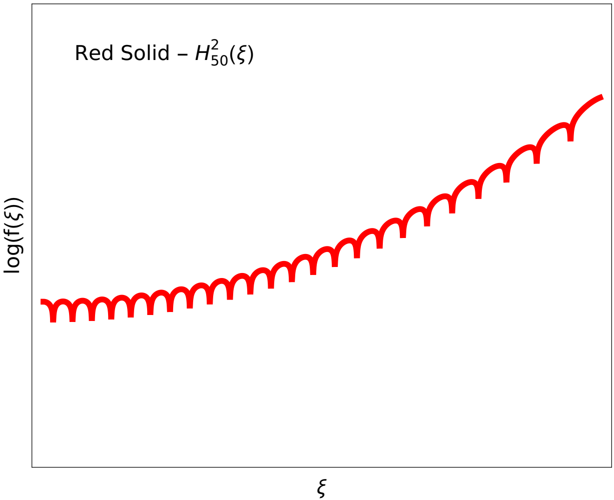
1. Potential energy: $\frac{\kappa x^2}{2}$
2. Hermite's equation:

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

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

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

The Harmonic Oscillator Disaster 1



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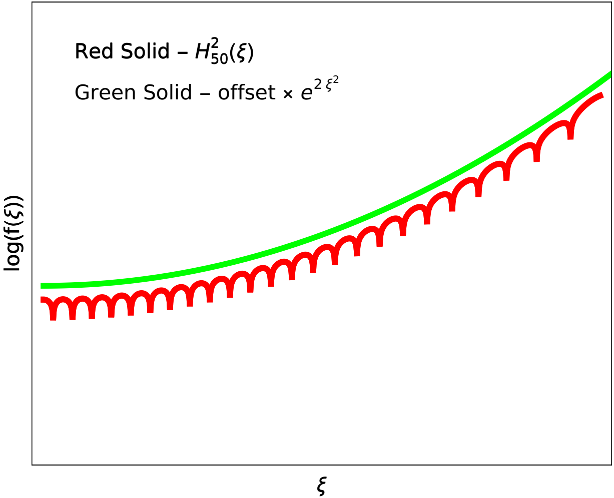
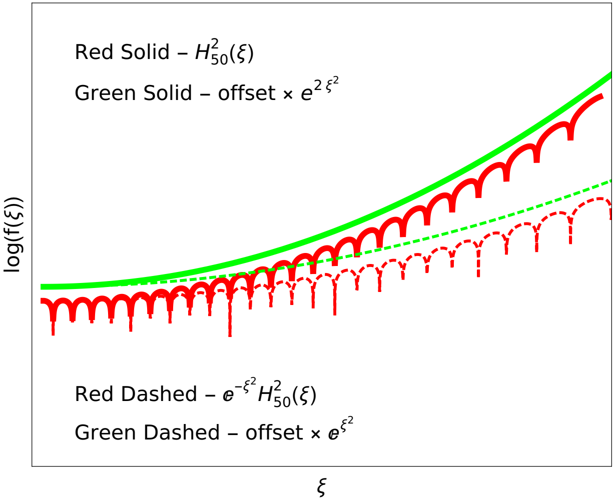
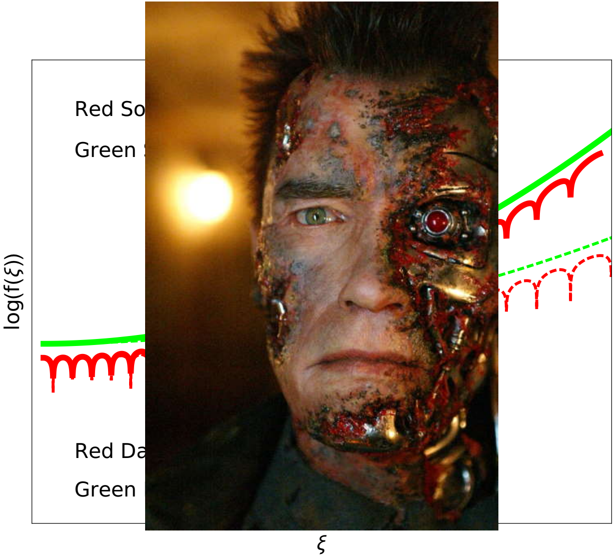


The Harmonic Oscillator Disaster 2



The Harmonic Oscillator Disaster 2



The Hermite Polynomials

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

$$|\phi_n\rangle = A_n e^{-\xi^2/2} H_n(\xi)$$

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

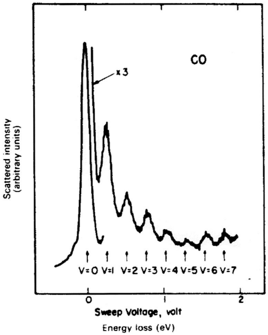
$$A_n = \left(2^n n! \sqrt{\pi}\right)^{-1/2}$$

$$\xi = \beta x$$

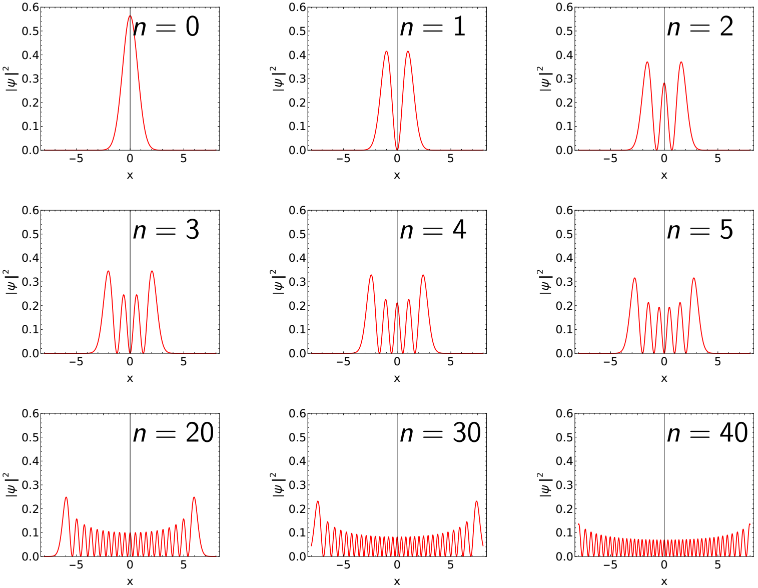
$$\beta^2 = \frac{m\omega_0}{\hbar} \qquad \alpha = \frac{2mE}{\hbar^2}$$

$$\omega_0 = \sqrt{\frac{\kappa}{m}}$$

$$a_{n+2} = -\frac{\frac{\alpha}{\beta^2} - 1 - 2n}{(n+1)(n+2)}$$



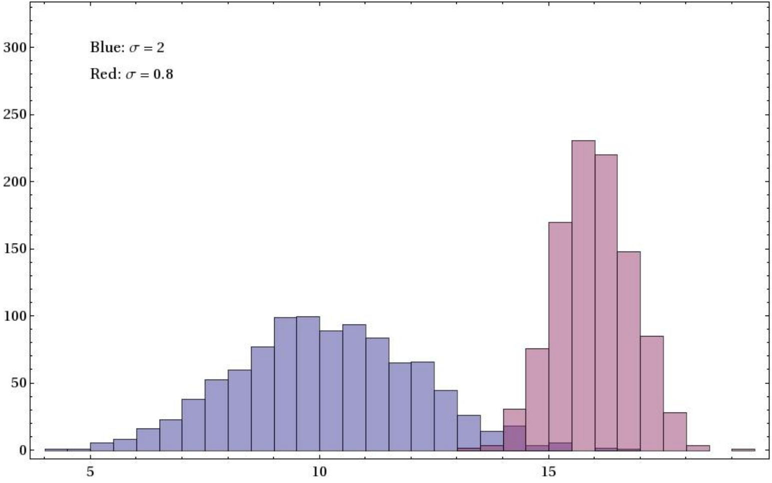
The Harmonic Oscillator Well Potential



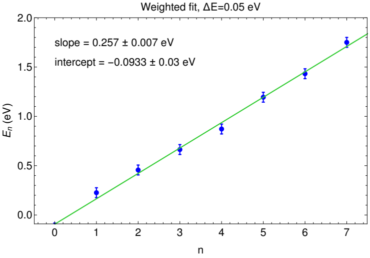
Quantum Weirdness

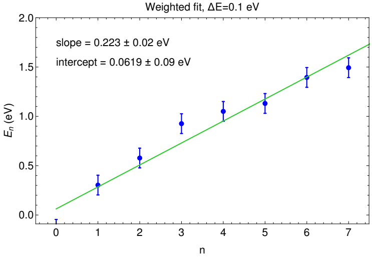
- QM is unreal - objects do not have an existence independent of a measurement.
- QM is non-local - different components of a single wave function can communicate instantaneously (at superluminal speeds).
- The Measurement Problem - What happens in a measurement? The wave function 'collapses' from a delocalized object that is unreal (see #1) into a 'real' (independent of observation) object that obeys naive realism.
- What is waving?
- Why are there two forms of time evolution - the Collapse in response to a measurement and the usual time development methods.
- Bell's inequalities - there are measurable differences between naive realism and QM. Experimental tests by Aspect in 1980's.
- Macroscopic scenarios - Schroedingers cat, effect of decoherence.
- The Wavefunction Collapse Problem - What happens physically? Can we see it at intermediate stages (yes)? What are Everett multi-worlds?

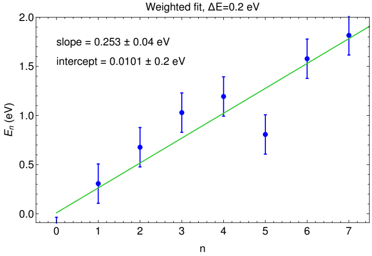
Is It Constant? The CO Spectrum Homework



Effect of Data Uncertainty On Fit







Effect of Data Uncertainty on Modeling