Chapter 8

Though he mispronounced it, physicist Ed Sullivan spoke of a simple harmonic oscillator of large magnitude every week when he introduced his "... really big SHO[1]."

The Simple Harmonic Oscillator

The simple harmonic oscillator is an important problem. Small oscillations in a smooth potential are modelled well by the SHO. If your studies include solid state physics you will encounter phonons, and the description of multiple coupled phonons relies on multiple simple harmonic oscillators. The quantum mechanical description of electromagnetic fields in free space uses multiple coupled photons modelled by simple harmonic oscillators. Further, the simple harmonic oscillator is an introduction to ladder operators, a and $a^\dagger$, which are the predecessors of the creation and annihilation operators. The SHO is an important problem.

The Picture and the Basic Mathematics

The functional form and graph of a simple harmonic oscillator from classical mechanics are

$$V(x) = \frac{1}{2}kx^2.$$

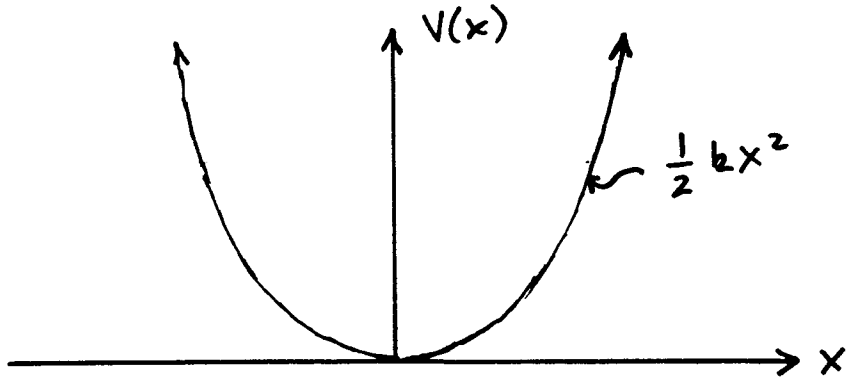

Figure 8 – 1. Simple Harmonic Oscillator.

The graph is a parabola. Given any smooth potential well, any relative minimum in a potential energy curve can be approximated by a simple harmonic oscillator model if the energy is small. Any of the relative minima in figure 8–2 can be modelled by the SHO if the energy of the particle

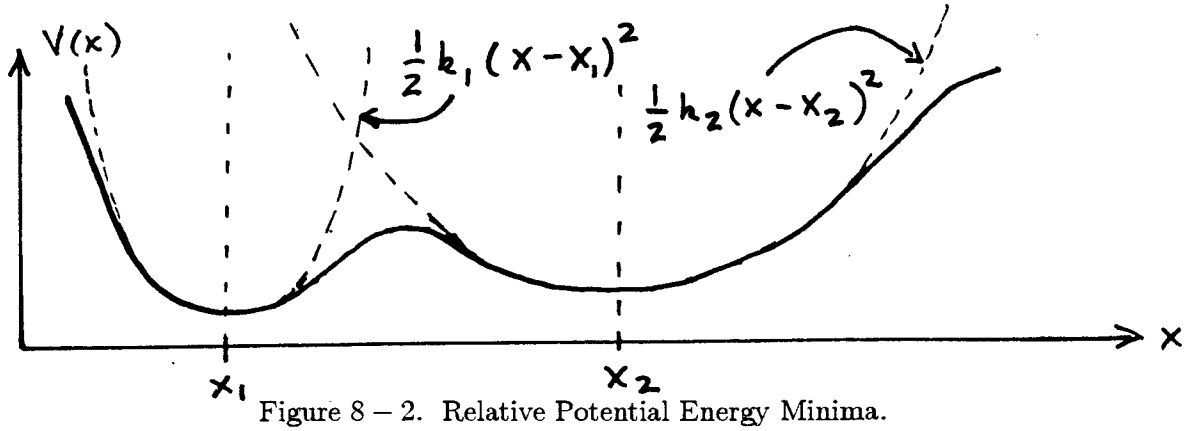

Figure 8 – 2. Relative Potential Energy Minima.

[1] Author *Title* (Publisher, Location, Year), page.

$$= \hbar\omega \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 5/2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 7/2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 9/2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \qquad (8-20)$$

Some words of caution before we proceed. Equations (8–18), (8–19), and (8–20) are in the energy basis for the simple harmonic oscillator. They are in the energy basis. They are not the matrix representations of every problem, just the SHO. Notice the constants in front of each matrix. Some authors will provide the matrix with constants implied. Realize the constants are necessary for both normalization and dimensional consistency.

An Improved Picture

The quantum mechanical simple harmonic oscillator has much in common with the one dimensional particle in a box. Both are infinite potential wells. As we drew energy levels for the particle in a box, we also draw them for the SHO. The effect is to update figure 8–1. The energy

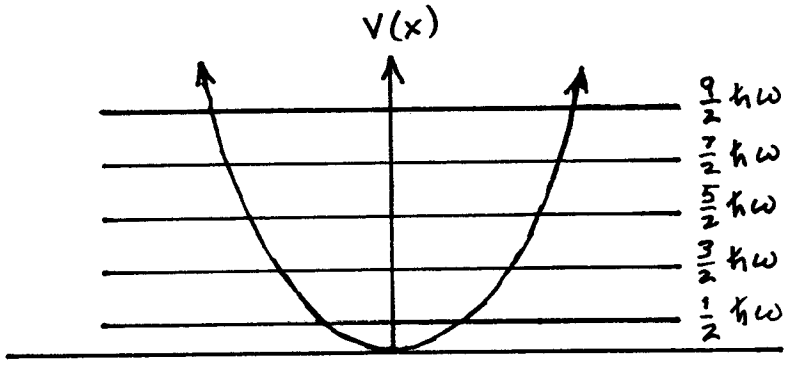

Figure 8 – 3. SHO Potential Energy Function and Energy Levels.

levels are given by equation (8–16),

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

Notice that unlike the infinite square well energies, where separation between adjacent levels increases as the quantum number increases, the separation between *all* adjacent energies in the SHO is always $\hbar\omega$.

We also graphed the eigenfunctions as functions of position for the infinite square well. We will do that for the SHO, but we need to get the wave functions. From analogy to the infinite square well, we can form a qualitative picture of what they must be. There is one significant difference. The potential walls of the particle in a box go from zero to infinity at a point, they are "hard" walls which are inpenetrable. The potential walls of the SHO have a finite slope at every point, they are not inpenetrable. This type of a potential wall is known as a "soft" wall. The meaning of this difference is that while the eigenfunctions must be zero outside a hard wall, they can and will have non–zero value outside a soft wall. The SHO eigenfunctions will have non–zero values outside the potential well.

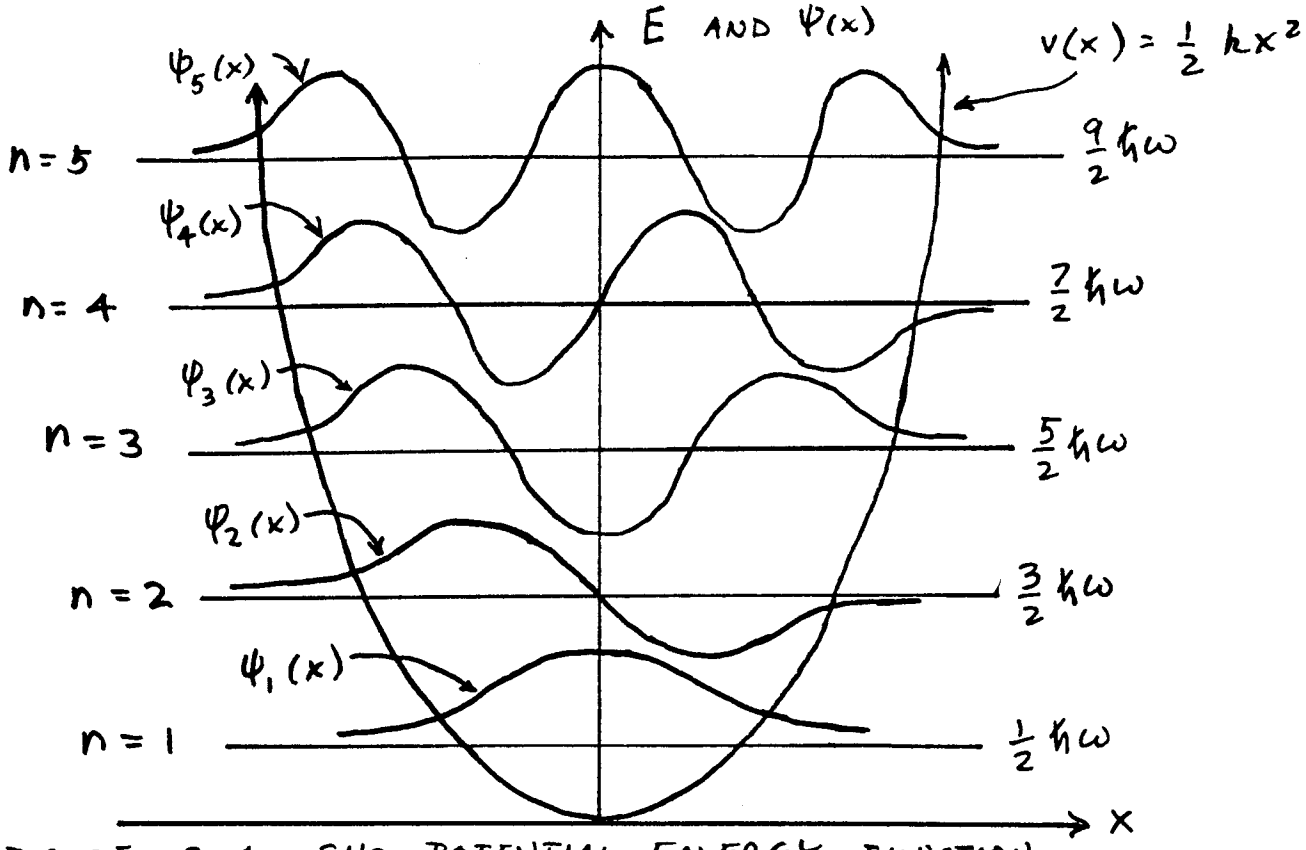

FIGURE 8-4. SHO POTENTIAL ENERGY FUNCTION, ENERGY LEVELS, AND EIGENFUNCTIONS.

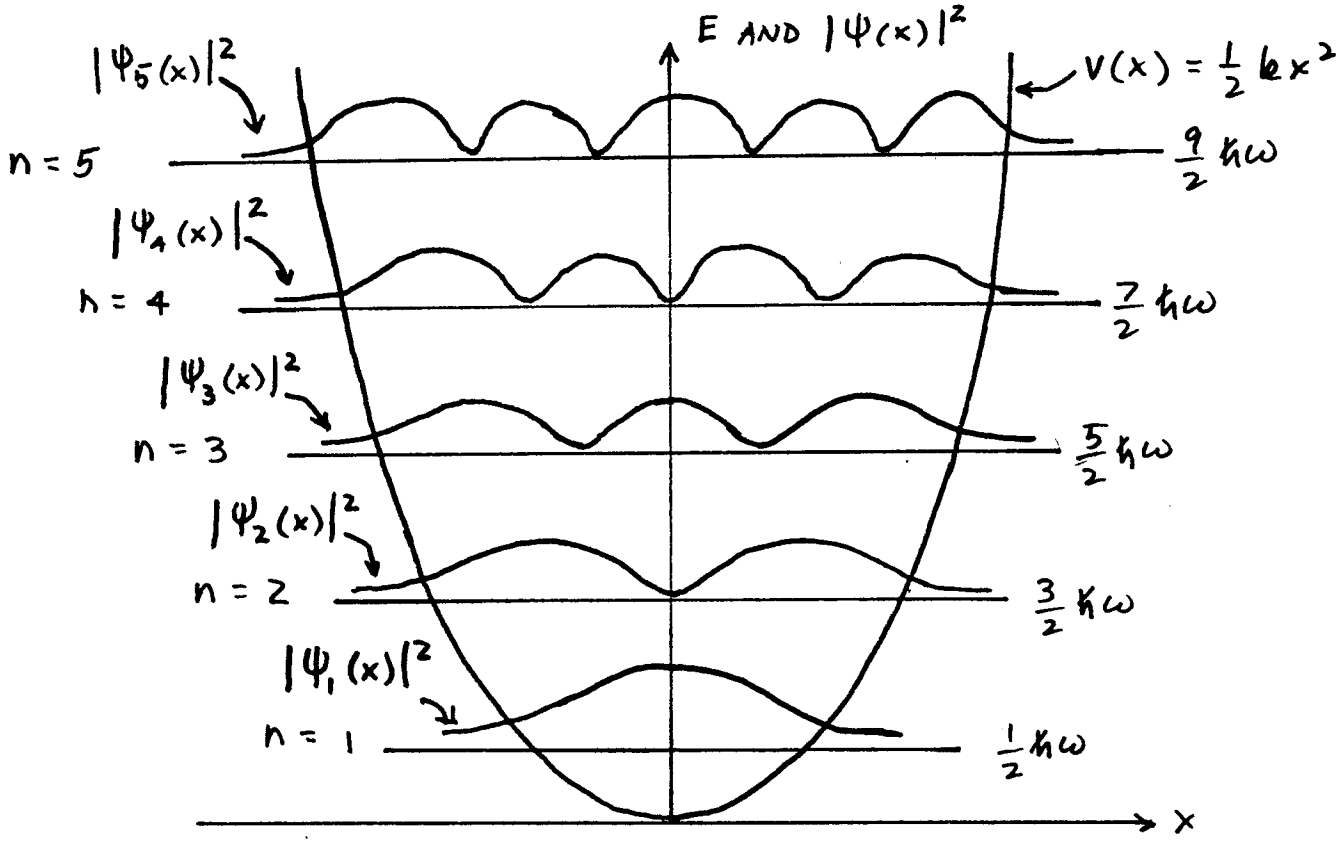

FIGURE 8-5. SHO POTENTIAL ENERGY FUNCTION, ENERGY LEVELS, AND PROBABILITY DENSITIES.

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where the a_n are constants which provide the relative contributions of each eigenfunction. As before, if we assume the general wave function is normalized, $\Psi(x) = 1$, the relative magnitudes of the a_n are fixed. But limited only by the constraint of normalization, the a_n can be any

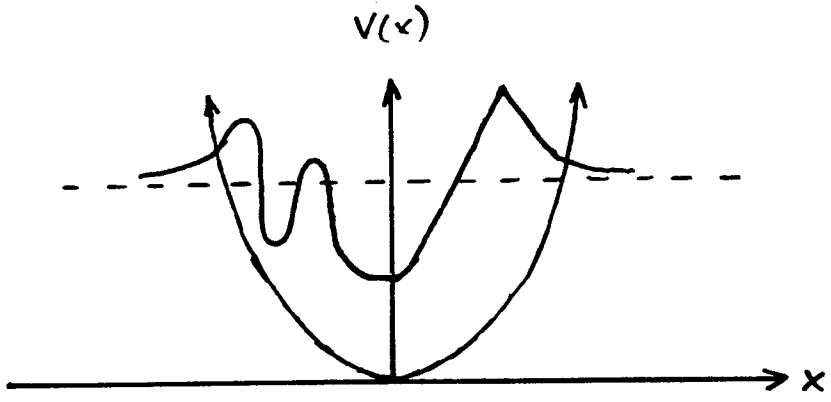

Figure 8 – 6. A General State Vector is the Superposition of Eigenstates.

values, meaning $\Psi(x)$ can have any shape, per figure 8–6. Also as before, the SHO has orthogonal eigenfunctions, so the a_n are unique.

We explicitly illustrated the concept of decomposing a general wave function into a linear combination of eigenfunctions in position space for an infinite square well potential in examples 7–5 through 7–7. In energy space, the linear combination of a general wave function may be written

$$|\Psi> = a_0|0> + a_1|1> + a_2|2> + a_3|3> + \cdots = \sum_{n=0}^{\infty} a_n|n> . \qquad (8-30)$$

This section will use the linear combination of equation (8–30) to illustrate the use of vector and matrix methods, Dirac notation, and the ladder operators in the energy basis. The vectors and matrices of this realistic system are infinite dimensional, so are a generalization of the finite dimensional objects used in earlier chapters. We start with a simple linear combination of two eigenstates,

$$|\Psi> = A\Big[\, 2\,|0> + 5\,|2> \,\Big], \qquad (8-31)$$

which is equation (8–30) for $a_0 = 2, a_2 = 5$, and all other $a_n = 0$. A is a normalization constant. Said another way, our example state vector is the superposition of two times of the ground state plus five times the second excited state.

Example 8–17: Normalize the wave function of equation (8–31).

To calculate the normalization constant, we will apply the normalization condition, $< \Psi \,|\, \Psi > = 1$, in two different ways: (1) using row and column vectors, and (2) using Dirac notation.

Using row and column vectors, we must calculate

$$(2,\ 0,\ 5,\ 0,\ 0, \cdots)^*\, A^*\, A \begin{pmatrix} 2 \\ 0 \\ 5 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = 1$$