

## ENERGY STATES OF A GAUSSIAN WAVEPACKET IN AN INFINITE SQUARE WELL

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received April 20, 2001

### ABSTRACT

An explicit expression is derived for the probability of an arbitrary energy state of a Gaussian wavepacket confined to an infinite square well potential. Approximations are made to determine the normalization factor and the probability. An upper bound on the errors due to the approximations is determined.

### INTRODUCTION

Despite its simplicity and familiarity to most students of physics, the “square well” model of particle motion in quantum theory is still applicable in practice to new situations.<sup>1,2</sup> One of these arose recently in an explanation of spin flips in Bose-Einstein condensed atomic vapors confined in magnetic traps.<sup>3</sup>

One of the problems encountered in making simplified mathematical models of particle motion in confined spaces, such as traps, arises from the boundary conditions. For example, the infinite square well model requires a trapped particle to have a vanishing wave function outside the trap walls. However, the mathematical functions used to describe wave functions of particles moving in traps are frequently taken to be of Gaussian form, and the infinite wings of Gaussian functions are certainly non-zero outside the walls of the trap potential.

### The Model

We will use a Gaussian wave packet to describe a particle moving in a one-dimensional square well. The wavefunction, as with all wavefunctions, must obey Schrödinger’s equation:

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$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x) \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}, \quad (1)$$

where  $U(x)$  is the potential well. At  $t=0$ , a Gaussian wave function of the form:

$$\Psi(x,0) = N \exp\left[-\frac{\left(x - \frac{L}{2}\right)^2}{2\alpha^2}\right] \exp\left[\frac{ipx}{\hbar}\right], \quad (2)$$

is initially centered in the well, and evolves in time according to Equation 1.

The wavefunction can be rewritten entirely as a function of the distance from the center of the well:

$$\begin{aligned} \psi(x) &\equiv \Psi(x,0) \\ &= N \exp\left[-\frac{\left(x - \frac{L}{2}\right)^2}{2\alpha^2}\right] \exp\left[ik\left(x - \frac{L}{2}\right)\right] \exp\left[ik\frac{L}{2}\right], \end{aligned} \quad (3)$$

where for notational simplicity, the particle’s wave number  $k = p/\hbar$  is used in place of momentum  $p$ ,  $\psi(x) = \Psi(x,0)$ , the parameter  $\alpha$  governs the “size” of the Gaussian (roughly the width of the function at half-height), and  $N$  is the normalization constant. For convenience, we assume that  $k$  is positive (it is possible to modify our calculations for a negative momentum).

The model implicitly considers  $L$  to be the fixed length of the potential well. The values of  $x$ ,  $\alpha$ , and  $k$  are meaningful only in relation to this fixed value. To simplify later calculations, we rewrite the wavefunction in terms of three dimensionless variables:

$$\bar{x} \equiv \frac{x}{L} \quad \bar{\alpha} \equiv \frac{\alpha}{L} \quad \bar{k} \equiv kL. \quad (4)$$

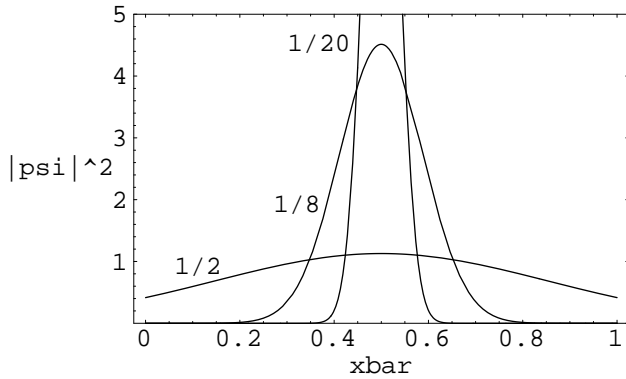


Figure 1

Plot of the probability density as a function of  $x$  for Gaussian wavepackets with  $\alpha = 1/2, 1/8$  and  $1/20$ .

This allows Equation 3 to be rewritten as:

$$\psi(\bar{x}) = N \exp\left[-\frac{(\bar{x} - \frac{1}{2})^2}{2\alpha^2}\right] \exp\left[ik\left(\bar{x} - \frac{1}{2}\right)\right] \exp\left[\frac{ik}{2}\right], \quad (5)$$

where the well now extends from  $\bar{x}=0$  to  $\bar{x}=1$ . Figure 1 shows the probability distribution,  $|\psi(\bar{x})|^2$ , for several values of  $\alpha$ . The shapes are the “packets”. Wider packets have larger values of  $\alpha$ . Note that the momentum term does not affect the packet shapes shown in Figure 1.

Energy and momentum are quantized in a traditional square well due to boundary conditions:

$$k_n = \frac{n\pi}{L}, \quad E_n = \frac{\hbar^2}{2m} k_n^2. \quad (6)$$

In the dimensionless notation, the momentum is:

$$\bar{k}_n = n\pi. \quad (7)$$

The primary challenge is to obtain a simple predictive understanding from the probability distribution of the energies that are possible for the particle. That is, to predict reliably, by reference only to the two packet parameters  $\bar{k}$  and  $\alpha$ , the most probable particle energies. The answer is not likely to be the result given in Equation 6 because of the Heisenberg Uncertainty Principle. The spatial confinement of the Gaussian function, roughly within the range  $|\bar{x} - 1/2| \leq \alpha$ , implies the presence of “uncertainty momenta” due to the confinement of the packet in the well, independent of the value of  $\bar{k}$ .

The role of  $\alpha$  deserves further discussion. It does not just control the width of the packet. Rather, it serves as a kind of “wave-particle selector”. The larger the value of  $\alpha$ , the less spatially localized the packet, and the more it behaves like a wave. Consequently, higher values of  $\alpha$  imply (due to the Uncertainty Principle) that the packet will have a smaller variance (i.e., less energy variability).

Any Gaussian wave function has non-zero value outside the walls of the square well. This leads to an approximation in obtaining our energy estimates, and thus, to the

need to establish bounds on the error introduced by the approximations. Gaussian wave packets are sometimes used in textbook discussions of particle behavior, but elementary texts don’t generally carry through either an estimate or a careful bound of the errors introduced.

Before we can actually calculate an expression for the energy probabilities, we need to solve for the normalization constant. In doing so, we will also do the bulk of the work required to bound the errors.

### Normalization and Error Bounding

The factor  $N$  in Equation 3 is the normalization constant. To solve for it, we use the fact that the sum of the probabilities for all locations is 1:

$$\int_0^1 \left| N \exp\left[-\frac{(\bar{x} - \frac{1}{2})^2}{2\alpha^2}\right] \exp\left[ik\left(\bar{x} - \frac{1}{2}\right)\right] \exp\left[\frac{ik}{2}\right] \right|^2 d\bar{x} = 1. \quad (8)$$

After we eliminate the factors with absolute magnitude equal to unity (recall that  $|e^{i\phi}| = 1$ , for any real  $\phi$ ), this simplifies to:

$$N^2 \int_0^1 \exp\left[-\frac{(\bar{x} - 1/2)^2}{\alpha^2}\right] d\bar{x} = 1. \quad (9)$$

With these limits of integration, the integral in Equation 9 cannot be carried out analytically. However, we can evaluate the integral if the limits are different:

$$N^2 \int_{-\infty}^{+\infty} \exp\left[-\frac{(\bar{x} - 1/2)^2}{\alpha^2}\right] d\bar{x} = 1. \quad (10)$$

The integral in Equation 10 can be found in most integral tables<sup>4</sup>, giving a value of  $N$ :

$$N = \frac{1}{\sqrt{\alpha} \sqrt{\pi}}. \quad (11)$$

Unfortunately, the integral in Equation 10 includes the contribution of the wavefunction outside of the potential well. Because of the infinite height of the potential wall, the contribution due to the wave function outside the potential well should be discarded. Instead of discarding it, we include it and show under what conditions the error introduced is so small that it can be tolerated. The bound that is established for the error tells under what parameter conditions the model is physically reliable.

To determine the bound of the error, the integral in Equation 9 is separated into two parts. The first part is the approximation; the second part is the error. We will find the upper bound for this integral:

$$\begin{aligned}
\int_0^1 |\Psi(\bar{x})|^2 d\bar{x} &\equiv \int_{-\infty}^{+\infty} |\Psi(\bar{x})|^2 d\bar{x} - \int_{-\infty}^0 |\Psi(\bar{x})|^2 d\bar{x} \\
&\quad - \int_1^{+\infty} |\Psi(\bar{x})|^2 d\bar{x} \\
&\equiv \int_{-\infty}^{+\infty} |\Psi(\bar{x})|^2 d\bar{x} - 2 \int_1^{+\infty} |\Psi(\bar{x})|^2 d\bar{x} \\
&\equiv \int_{-\infty}^{+\infty} |\Psi(\bar{x})|^2 d\bar{x} - E_{norm}, \quad (12)
\end{aligned}$$

where  $E_{norm}$  is the size of the error. The equivalences in Equation 12 are valid for our wave packet, but not necessarily for all wavefunctions.

From Equations 9 and 12:

$$E_{norm} = 2 \int_1^{\infty} |\Psi(\bar{x})|^2 d\bar{x} = \int_1^{\infty} \exp\left[-\frac{(\bar{x}-1/2)^2}{\alpha^2}\right] d\bar{x}. \quad (13)$$

To simplify the integral in Equation 12, we make the substitution,  $z = 2\bar{x} - 1$ :

$$E_{norm} = 2 \int_1^{\infty} \exp\left[-\frac{(\bar{x}-1/2)^2}{\alpha^2}\right] d\bar{x} = \int_1^{\infty} \exp\left[-\frac{z^2}{4\alpha^2}\right] dz. \quad (14)$$

Since  $z \geq 1$  over the entire range of integration,  $z^2 \geq z$ . Therefore, Equation 14 can be rewritten to give the upper bound of the error as:

$$E_{norm} \leq \int_1^{\infty} \exp\left[-\frac{z}{4\alpha^2}\right] dz = 4\alpha^2 \exp\left[-\frac{1}{4\alpha^2}\right]. \quad (15)$$

Figure 2 shows the upper bound of the error as a function of  $\alpha$ . The normalization integral, Equation 9, must equal 1. Therefore, we confine our attention to the range of values of  $\alpha$  where the upper bound of  $E_{norm} \ll 1$ . For the sake of concreteness, we will assume that  $\alpha < 1/8$ , or  $E_{norm} \leq 7 \times 10^{-9}$  (this might seem needlessly small, but it will keep later error bounds manageable). Figure 1 shows the packet for  $\alpha = 1/8$ .

### Calculation of Energy Probabilities

#### Background

For a "square well" potential, one for which  $U(x)$  between two infinite potential walls at  $x = 0$  and  $x = L$  (which we write as  $\bar{x} = 0$  and  $\bar{x} = 1$ , the wavefunction of the  $n^{\text{th}}$  energy eigenstate is:

$$\Psi_n(\bar{x}, t) = \exp\left[-\frac{iE_n t}{\hbar}\right] \sqrt{2} \sin(n\pi\bar{x}) = \exp\left[-\frac{iE_n t}{\hbar}\right] \Psi_n(\bar{x}). \quad (16)$$

The superposition principle states that any linear superposition of valid wave functions is also a valid wave function. The most general solution to Schrödinger's equation is an infinite sum of the stationary states:

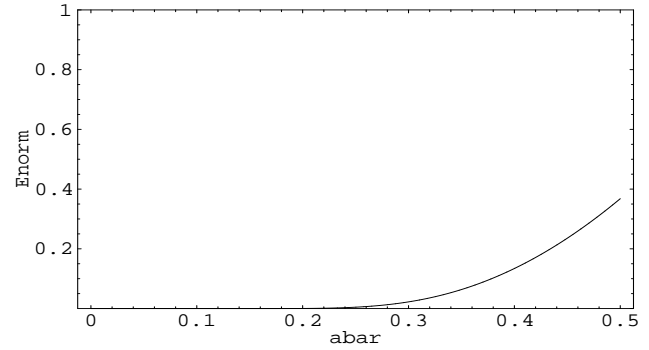


Figure 2

The size of the error in the normalization of the approximation to the Gaussian wave packet as a function of  $\alpha$ , the width of the packet.

$$\Psi(\bar{x}, t) = \sum_{n=1}^{\infty} c_n \Psi_n(\bar{x}, t) = \sum_{n=1}^{\infty} c_n \exp\left[-\frac{iE_n t}{\hbar}\right] \Psi_n(\bar{x}). \quad (17)$$

Each term in the sum corresponding to a specific particle energy  $E_n$ . A particle whose wavefunction is given by the sum in Equation 17 will have a probability of being found in the  $n^{\text{th}}$  energy state given by:

$$p_n = |c_n|^2. \quad (18)$$

To find values for  $c_n$ , note that the functions  $\Psi_n(\bar{x}) = \sqrt{2} \sin(n\pi\bar{x})$  are orthogonal, so:

$$\int_0^1 \Psi_m^*(\bar{x}) \Psi_n(\bar{x}) d\bar{x} = \delta_{nm}, \quad (19)$$

where  $\delta_{nm}$  is called the Kronecker delta and is defined as:

$$\delta_{mm} = 1 \quad m = n; \quad \delta_{mn} = 0 \quad m \neq n. \quad (20)$$

Now consider the general solution to the Schrödinger equation at time  $t=0$ :

$$\Psi(\bar{x}, 0) = \sum_{n=1}^{\infty} c_n \Psi_n(\bar{x}). \quad (21)$$

Note that the time exponential has dropped out. Now multiply both sides of this equation by  $\Psi_m^*(\bar{x})$  and integrate. The Kronecker delta will cause all the terms to cancel except for the case  $n = m$ :

$$\begin{aligned}
\int_0^1 \Psi_m^*(\bar{x}) \Psi(\bar{x}, 0) d\bar{x} &= \sum_{n=1}^{\infty} c_n \int_0^1 \Psi_m^*(\bar{x}) \Psi_n(\bar{x}) d\bar{x} \\
&= \sum_{n=1}^{\infty} c_n \delta_{nm} = c_m. \quad (22)
\end{aligned}$$

Now, we calculate the values of the  $c_n$ 's to predict the range of energies that will be present when  $\Psi(\bar{x}, 0)$  is given by the Gaussian function in Equation 5.

#### The Gaussian Packet

Now to solve for the  $c_n$ 's in the case of the Gaussian wave packet. The integral in Equation 22 is challenging because it cannot be evaluated exactly; approximate techniques will be needed to find the probability of finding the system in the  $n^{\text{th}}$  energy state. To find the  $c_n$ 's, we use a technique similar to that used to find the normalization constants. The first approximation is to assume that the limits of the

integral go from  $-\infty$  to  $+\infty$ , rather than from 0 to 1. Then we find the upper bound of the error for this approximation.

$$\begin{aligned} c_n &= \int_0^1 \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} \equiv \int_{-\infty}^{\infty} \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} \\ &\quad - \int_{-\infty}^0 \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} - \int_1^{\infty} \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} \\ &\equiv \int_{-\infty}^{\infty} \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} - 2 \int_1^{\infty} \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} \\ &\equiv \int_{-\infty}^{\infty} \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} - E_{tot}, \end{aligned} \quad (23)$$

where  $E_{tot}$  is the error in the approximation.

To find an analytic expression for the integral in the last part of Equation 23, we make the substitution  $y = \bar{x} - 1/2$  giving:

$$\psi_n(y) = \sqrt{2} \sin[n\pi(y + 1/2)]. \quad (24)$$

Using the expression from equation 5 for the Gaussian packet:

$$c_n = \Delta \int_{-\infty}^{\infty} \exp\left[-\frac{y^2}{2\alpha^2}\right] \exp[iky] \sin[n\pi(y + 1/2)] dy, \quad (25)$$

where  $\Delta$  is the constant factor:

$$\Delta = \sqrt{\frac{2}{\alpha\sqrt{\pi}}} \exp\left[\frac{ik}{2}\right]. \quad (26)$$

Using Euler's theorem to replace the sine term with two exponentials gives:

$$\begin{aligned} c_n &= \frac{\Delta}{2i} \int_{-\infty}^{\infty} \exp\left[-\frac{y^2}{2\alpha^2}\right] \exp[iky] \exp[in\pi(y + 1/2)] dy \\ &\quad - \frac{\Delta}{2i} \int_{-\infty}^{\infty} \exp\left[-\frac{y^2}{2\alpha^2}\right] \exp[iky] \exp[-in\pi(y + 1/2)] dy. \end{aligned} \quad (27)$$

Combining like powers of  $n$  gives:

$$\begin{aligned} c_n &= \frac{\Delta}{2i} \exp\left[\frac{in\pi}{2}\right] \int_{-\infty}^{\infty} \exp\left[-\frac{y^2}{2\alpha^2}\right] \exp[iy(k + n\pi)] dy \\ &\quad - \frac{\Delta}{2i} \exp\left[\frac{-in\pi}{2}\right] \int_{-\infty}^{\infty} \exp\left[-\frac{y^2}{2\alpha^2}\right] \exp[iy(k - n\pi)] dy. \end{aligned} \quad (28)$$

Equation 28 has an analytical solution that can be determined by using the general form found in many integral tables:<sup>4</sup>

$$\int_{-\infty}^{\infty} \exp(-au^2) \exp(ibu) du = \sqrt{\frac{\pi}{a}} \exp\left(-\frac{b^2}{4a}\right). \quad (29)$$

Using Equation 29 and rearranging some terms, the integrals in Equation 28 yield:

$$\begin{aligned} c_n &= \sqrt{\frac{\pi}{2}} i\Delta\alpha \exp\left(\frac{in\pi}{2}\right) \\ &\quad \times \left\{ \exp(-in\pi) \exp\left[-\frac{\alpha^2(n\pi - \bar{k})^2}{2}\right] - \exp\left[-\frac{\alpha^2(n\pi + \bar{k})^2}{2}\right] \right\}. \end{aligned} \quad (30)$$

Since  $\exp(in\pi) = (-1)^n$ , and using Equation 26, we can write Equation 30 as:

$$\begin{aligned} c_n &= i\sqrt{\alpha\sqrt{\pi}} \exp\left(\frac{ik}{2}\right) \exp\left(\frac{in\pi}{2}\right) \\ &\quad \times \left\{ (-1)^n \exp\left[-\frac{\alpha^2(n\pi - \bar{k})^2}{2}\right] - \exp\left[-\frac{\alpha^2(n\pi + \bar{k})^2}{2}\right] \right\}. \end{aligned} \quad (31)$$

The approximate value of the probability of finding Gaussian packet in the  $n^{\text{th}}$  energy state becomes:

$$\begin{aligned} p_n &= |c_n|^2 \\ &= \alpha\sqrt{\pi} \left\{ (-1)^n \exp\left[-\frac{\alpha^2(n\pi - \bar{k})^2}{2}\right] - \exp\left[-\frac{\alpha^2(n\pi + \bar{k})^2}{2}\right] \right\}^2. \end{aligned} \quad (32)$$

In anticipation of the analysis of the results, we define:

$$k_\alpha = \frac{1}{\alpha}. \quad (33)$$

This change will make the interpretation of the results slightly easier. By convention,  $\alpha$  is used when discussing the original packet and  $k_\alpha$  is used when discussing the energy distributions. Making the substitution in Equation 33 into Equation 32 gives:

$$p_n = \frac{\sqrt{\pi}}{k_\alpha} \left\{ (-1)^n \exp\left[-\frac{(n\pi - \bar{k})^2}{2k_\alpha^2}\right] - \exp\left[-\frac{(n\pi + \bar{k})^2}{2k_\alpha^2}\right] \right\}. \quad (34)$$

Figure 3 shows  $p_n$  as a function of  $n$  for two different sets of parameters: one with  $\bar{k} = 0$  and a relatively large value of  $k_\alpha$ ; and one for  $\bar{k} = 30\pi$  and small  $k_\alpha$ . Figure 3 is jagged because  $p_n$  is only defined for the integer values of  $n$ . We have interpolated a continuous curve to add visual clarity. When  $\bar{k} = 0$ ,  $p_n$  is exactly 0 for even values of  $n$ .

### Upper Bound of Error

We now find the upper bound to the error,  $E_{tot}$ , given in Equation 23. Using the same technique as done in the calculation of the upper bound to the error in the normalization constant,  $E_{norm}$ , (Equations 9 - 15). From Equation 23:

$$\begin{aligned}
 E_{tot} &= 2 \int_1^{\infty} \psi(\bar{x}) \psi_n(\bar{x}) d\bar{x} = 2\sqrt{2} \int_1^{\infty} \psi(\bar{x}) \sin(n\pi\bar{x}) d\bar{x} \\
 &\leq 2\sqrt{2} \int_1^{\infty} \psi(\bar{x}) d\bar{x} \leq 2\sqrt{2} \int_1^{\infty} |\psi(\bar{x})| d\bar{x} \\
 &\leq 2\sqrt{2} \int_1^{\infty} \exp\left[-\frac{(\bar{x} - 1/2)^2}{2\alpha^2}\right] d\bar{x}. \tag{35}
 \end{aligned}$$

Evaluating the integral in Equation 35 gives:

$$E_{tot} \leq 8\sqrt{2} \alpha^2 \exp\left[-\frac{1}{8\alpha^2}\right]. \tag{36}$$

To decide how large is upper bound is, we compare it to the absolute value of  $c_n$ , since we are only interested in the magnitude of the error:

$$\frac{E_{tot}}{|c_n|} \leq \frac{8\sqrt{2}\alpha^3}{\sqrt[4]{\pi}} \exp\left[-\frac{1}{8\alpha^2}\right] \exp\left[\frac{\alpha^2(n\pi - \bar{k})^2}{2}\right]. \tag{37}$$

Using Equation 37, the error can be made less than any desired percentage of the approximation, by choosing a small enough value of  $\alpha$ .

Figure 4 shows the upper bound of the error,  $E_{tot}$ , from Equation 36 for  $\alpha = 1/8$ , plotted as a function of the distance  $|n\pi - \bar{k}|$ .

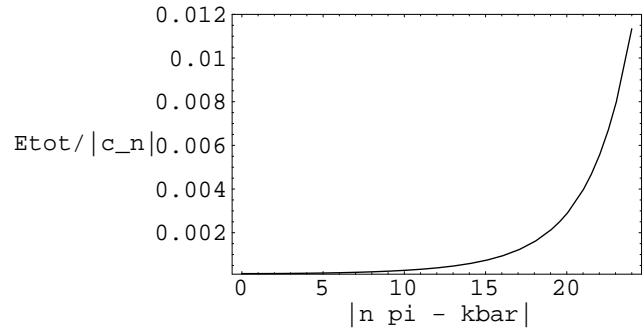


Figure 4

Ratio of the error in the coefficient to the size of the coefficient for the Gaussian wave packet as a function of  $|n\pi - \bar{k}|$  for  $\alpha = 1/8$ .

### Analysis of Results

The expressions we have derived for  $c_n$  (Equation 34) and  $p_n$  (Equation 36) can be written in a simpler form. The ratio of the two exponentials in Equation 34 is:

$$\text{ratio} = \frac{\exp\left[-\frac{\alpha^2(n\pi + \bar{k})^2}{2}\right]}{\exp\left[-\frac{\alpha^2(n\pi - \bar{k})^2}{2}\right]} = \exp\left[-\frac{2\bar{k}n\pi}{k_\alpha^2}\right]. \tag{38}$$

The numerator in Equation 38 will become negligible compared to the denominator, provided  $\bar{k}$  is sufficiently

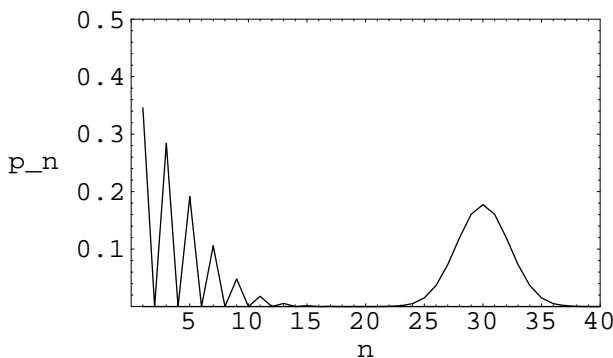


Figure 3

The probability of finding the Gaussian packet in energy state  $n$  vs  $n$  for: ( $\bar{k} = 0, k_a = 20$ ) and ( $\bar{k} = 30\pi, k_a = 10$ ).

large compared to  $k_\alpha^2$ . To keep the error bound small,  $k_\alpha^2$  is large because  $\alpha$  is a small number. For example, if  $k_a = 10$  and  $\bar{k} = 10\pi$ , then at  $n = 1$ , the ratio (in Equation 39)  $\approx 0.14$ . Larger values of  $n$  will only decrease this ratio, the exponential form ensuring that the ratio rapidly approaches zero. Therefore, if we impose an additional constraint on our parameters: that  $\bar{k} \geq k_\alpha^2/\pi$ , we can ignore the top exponential. This allows us to rewrite Equation 34 in a much simpler form:

$$c_n \approx (-1)^n i \sqrt{\frac{\sqrt{\pi}}{k_\alpha}} \exp\left(\frac{i\bar{k}}{2}\right) \exp\left(\frac{in\pi}{2}\right) \exp\left[-\frac{(n\pi - \bar{k})^2}{2k_\alpha^2}\right]. \tag{39}$$

Equation 36 can be approximated as:

$$p_n \approx \frac{\sqrt{\pi}}{k_\alpha} \exp\left[-\frac{(n\pi - \bar{k})^2}{k_\alpha^2}\right]. \tag{40}$$

Equation 40 is a Gaussian distribution, as is made obvious by our  $k_\alpha$  notation. This packet is in some sense the complement to the Gaussian packet with which began. It is centered at  $n = \bar{k}/\pi$ , and its width is controlled by  $k_\alpha$  (note the lack of the 1/2-factor in the exponent). The effect of requiring a large  $\bar{k}$  is now evident: it ensures that the probability distribution is essentially Gaussian, and that one energy level can be considered the “primary” energy level. By the Uncertainty Principle, as the position wavepacket becomes narrower, the range of possible energies becomes broader, and vice versa. This is confirmed by the form of these two packets and the inverse relation between  $\bar{k}$  and  $k_\alpha$ .

We can conclude that the range of likely energy levels for the particle is roughly:

$$n = \frac{\bar{k}}{\pi} \pm \frac{k_\alpha}{4}. \tag{41}$$

The upper bound for the error in the probability (see Figure 4) is tolerable in this range as well. For  $|n\pi - k| = 24$ , or  $n = k/\pi \pm 3k_\alpha$ , the error is 1.1%.

### Summary

We began with a Gaussian wave function, Equation 5, in an infinite square well potential. The goal of the analysis was to predict the likely energies for the system. The first task was to normalize the wavefunction. In doing so, we made approximations and exhibited an upper bound to the error in the normalization constant, Equation 15. This also established the range of parameters for which our model is physically meaningful.

We then used the theory of orthogonal functions and the superposition principle to show how to express any wavefunction as an infinite sum, and to calculate the coefficients of the terms of that sum, Equation 22. The absolute square of a particular coefficient gives the probability of the corresponding energy level. We then applied the general expression to our specific wavefunction. This again required approximations. The upper bound on the error in the approximation was once again determined.

Finally, we imposed the additional condition that  $k$  be large enough so that we could approximate our expression for the probability that the system be in the  $n^{\text{th}}$  energy state,  $p_n$ , as another Gaussian. This allowed us to derive a very simple expression for the most likely energy levels of the system, Equation 41.

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