Energy States of a Gaussian Wavepacket in the Infinite Square Well

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Abstract

An explicit expression is derived for the probability of an arbitrary energy state of a Gaussian wavepacket confined to a square well. Approximations are made to do so; the error introduced is bounded.

1 Introduction

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

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.

2 Model

In this paper we will use a Gaussian wave packet to describe a particle moving in a one-dimensional square well. Our wave function, like all wave functions, must obey Schrödinger's equation [1]:

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

We will start at $t = 0$ with a Gaussian wave function of the form:

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

which is initially centered in the well, and will then evolve in time according to equation (1).

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

$$\psi(x) \equiv \Psi(x,0) = N \exp\left[-\frac{(x-L/2)^2}{2\alpha^2}\right] e^{ik(x-L/2)} e^{ikL/2}, \qquad (3)$$

where we've begun to use the particle's wave number $k \equiv p/\hbar$ in place of momentum p and $\psi(x) \equiv \Psi(x,0)$, both for notational simplicity. Throughout this paper, we assume for convenience that k is positive; it is easy to modify our calculations for a negative momentum. The parameter α governs the "size" of the Gaussian. It is roughly the width at 1/2-height. The factor N is the normalization constant; it is discussed more fully in section 3.

The model we are using implicitly considers L to be the fixed length of the potential well. The values of x, α and k are meaningful only in relation to this fixed value. To make this more clear, and to simplify later calculations, we rewrite our wave function in terms of three dimensionless variables:

$$\overline{x} \equiv x/L \qquad \overline{\alpha} \equiv \alpha/L \qquad \overline{k} \equiv kL \qquad (4)$$

This gives us

$$\psi(\overline{x}) = N \exp\left[\frac{-(\overline{x}-1/2)^2}{2\overline{\alpha}^2}\right] e^{i\overline{k}(\overline{x}-1/2)} e^{i\overline{k}/2}, \qquad (5)$$

and the well now extends from $\overline{x}=0$ to $\overline{x}=1$. For several values of $\overline{\alpha}$, Figure 1 shows the probability distribution $|\psi(\overline{x})|^2$, which we will refer to as the "packet". Wider packets have larger values of $\overline{\alpha}$. The probability of finding the particle in an infinitesimal interval $d\overline{x}$ is given by $|\psi(\overline{x})|^2\, d\overline{x}$. Note that the momentum term does not affect the packet graph.

Of course, energy and momentum are quantized in a square well:

$$k_n = \frac{n\pi}{L}, \qquad \text{and} \qquad E_n = \frac{\hbar^2}{2m} k_n^2,$$

and in our dimensionless notation the momentum is:

$$\overline{k}_n = n\pi$$

The primary challenge that we will consider is to obtain a simple predictive understanding of the probability distribution of energies that are possible for the particle. That is, we want to be able to predict reliably, by reference only to the two packet parameters $\overline{k}$ and $\overline{\alpha}$, what are the most probable particle energies. The answer is not likely to be simply $E = k^2\hbar^2/2m$ because of the Heisenberg Uncertainty Principle: the spatial confinement of the Gaussian function roughly within the range $|\overline{x}-1/2| \leq \overline{\alpha}$ implies the presence of "uncertainty momenta" because of the confinement, independent of the value of $\overline{k}$.

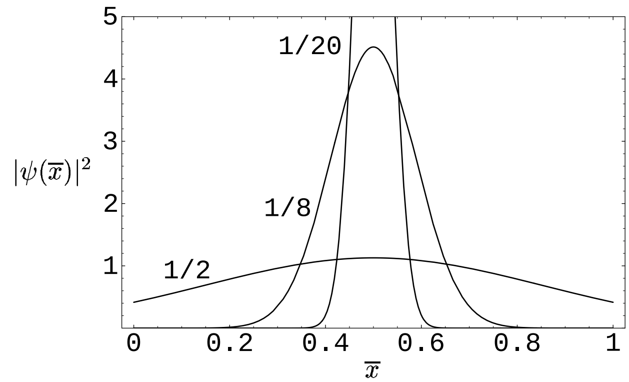

Figure 1: $|\psi\left(\overline{x}\right)|^2$ for $\overline{\alpha} = 1/2, 1/8, 1/20$.

That role of $\overline{\alpha}$ deserves further discussion. It does not simply control the width of the packet. Rather, it serves as a kind of "wave-particle selector." The larger the value of $\overline{\alpha}$, the less spatially localized the packet is, and the more it behaves like a wave. Consequently, higher values of $\overline{\alpha}$ imply (by the Uncertainty Principle) that the packet will have a smaller variance (i.e., less energy variability). This discussion will be made quantitative when we derive an expression for the energy probabilities.

As we mentioned, any Gaussian wave function has non-zero value outside the walls of the square well. This will lead to approximations in obtaining our energy estimates, and thus to the need to establish careful 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. We will show that this is not difficult to do. 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 our errors.

3 Normalization and Error Bounding

As stated, the factor N is the normalization constant. To solve for it, we use the fact that the sum of the probabilities for all locations is 1: $\int_0^1 |\psi(\overline{x})|^2 d\overline{x} = 1$. After we eliminate the factors with absolute magnitude equal to unity (recall $|e^{i\phi}| = 1$, for any real ϕ), this simplifies to

$$N^2 \int_0^1 \exp\left[-\left(\overline{x} - 1/2\right)^2 / \overline{\alpha}^2\right] \, d\overline{x} = 1. \tag{6}$$

With these limits of integration, this integral cannot be carried out analytically, but we can evaluate

$$N^2 \int_{-\infty}^{\infty} \exp\left[-\left(\overline{x}-1/2\right)^2/\overline{\alpha}^2\right]\, d\overline{x}.$$

However, in this integral the contribution of the wavefunction outside of the potential well is physically incorrect, because of the infinite height of the potential wall, and should be discarded. Instead of discarding it, we will include it but show carefully under what conditions the error introduced is so small that it can be tolerated. The form of the bound we will establish for the error will tell us under what parameter conditions the model is physically reliable.

We begin by separating the integral into two parts. The first part is our approximation; the second part is what we will bound to establish the maximum error. Note that the following equivalences are valid for our wave packet, but not necessarily for all wave functions.

$$\begin{aligned}\int_0^1 |\psi(\overline{x})|^2\, d\overline{x} &\equiv \int_{-\infty}^{\infty} |\psi(\overline{x})|^2\, d\overline{x} - \int_{-\infty}^{0} |\psi(\overline{x})|^2\, d\overline{x} - \int_{1}^{\infty} |\psi(\overline{x})|^2\, d\overline{x} \\ &\equiv \int_{-\infty}^{\infty} |\psi(\overline{x})|^2\, d\overline{x} - 2\int_{1}^{\infty} |\psi(\overline{x})|^2\, d\overline{x} \\ &\equiv \int_{-\infty}^{\infty} |\psi(\overline{x})|^2\, d\overline{x} - \mathbf{E}_{norm}. \end{aligned} \tag{7}$$

The first of these integrals is fairly standard; looking up the result [4] gives $N^2\left[\overline{\alpha}\sqrt{\pi}\right] = 1$, or

$$N = 1/\sqrt{\overline{\alpha}\sqrt{\pi}}. \tag{8}$$

To bound the error (the second term in eqn. (7)), we first make two cosmetic changes of variables: $y \equiv \overline{x} - 1/2$ and then $z \equiv 2y$. We obtain:

$$\mathbf{E}_{norm} = 2\int_1^{\infty} \exp\left[-\left(\overline{x}-1/2\right)^2/\overline{\alpha}^2\right]\, d\overline{x} \rightarrow \int_1^{\infty} \exp\left[-z^2/4\overline{\alpha}^2\right]\, dz \tag{9}$$

Now note that $z \geq 1$ over the entire range of integration, so $z^2 \geq z$. We can therefore use the following inequality to bound the error:

$$\begin{aligned}\mathbf{E}_{norm} &= \int_1^{\infty} \exp\left[-z^2/4\overline{\alpha}^2\right]\, dz \\ &\leq \int_1^{\infty} \exp\left[-z/4\overline{\alpha}^2\right]\, dz \\ &= 4\overline{\alpha}^2 e^{-1/4\overline{\alpha}^2} \end{aligned} \tag{10}$$

Figure 2 shows the error as a function of $\overline{\alpha}$. We know that the normalization integral must equal 1. Therefore, we will want to confine our attention to the

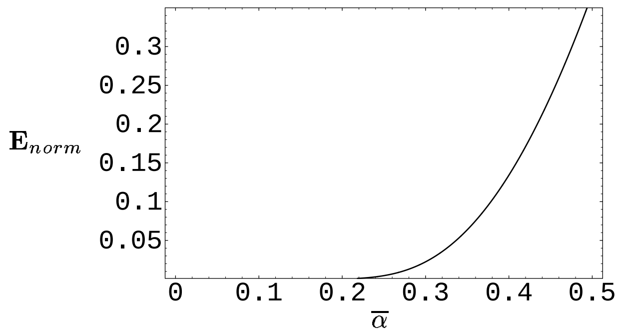

Figure 2: Error bound for normalization constant

range of values of $\overline{\alpha}$ where $\mathbf{E}_{norm} \ll 1$. For the sake of concreteness, we will assume from now on that $\overline{\alpha} \leq 1/8$, or $\mathbf{E}_{norm} \leq 7.03 \times 10^{-9}$ (this might seem needlessly small, but it will keep later error bounds manageable). See fig. 1 for a picture of the packet with $\overline{\alpha} = 1/8$.

4 Background Details

We are almost ready to derive an explicit expression for the energy probabilities, but first we review some background information in the general case. Let $\Psi(x,t)$ be the wavefunction of a particle confined to one dimension, and let $U(x)$ be the potential energy function. Then Ψ must be a solution to Schrödinger's equation (1). For a "square well" potential, one for which $U = 0$ between two infinite potential walls at $x = 0$ and $x = L$ (which we write as $\overline{x} = 0$ and $\overline{x} = 1$), the wavefunction of the nth energy eigenstate can be expressed as

$$\begin{aligned} \Psi_n(\overline{x},t) &= e^{-iE_n t/\hbar}\sqrt{2}\sin\left(n\pi\overline{x}\right) \\ &= e^{-iE_n t/\hbar}\psi_n(\overline{x}). \end{aligned} \tag{11}$$

The superposition principle states that any linear superposition of valid wavefunctions is a valid wavefunction. The most general solution to Schrödinger's equation is therefore an infinite sum of stationary states:

$$\begin{aligned} \Psi\left(\overline{x},t\right) &= \sum_{n=1}^{\infty} c_n \Psi_n\left(\overline{x},t\right) \\ &= \sum_n c_n e^{-iE_n t/\hbar}\psi_n(\overline{x}), \end{aligned} \tag{12}$$

each term in the sum corresponding to a specific particle energy E_n.

A particle defined by the sum in eqn. (12) will have a probability of being found in the nth energy state given by $p_n = |c_n|^2$. Our main goal is the ability to calculate the values of the c_n's in order to predict the range of energies that will be present, when $\Psi(\overline{x}, 0)$ is given by the Gaussian function in eqn. (5).

To solve for c_n, first note that the functions $\psi_n(\overline{x}) = \sqrt{2}\sin(n\pi\overline{x})$ are orthogonal. Precisely, this means that

$$\int_0^1 \psi_m^*(\overline{x})\psi_n(\overline{x})\, d\overline{x} = \delta_{mn}, \tag{13}$$

where δ_{mn} is called the Kronecker delta and is defined as

$$\delta_{mn} = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases} \tag{14}$$

and where $\psi_m^*(\overline{x})$ denotes the complex conjugate.

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

$$\Psi(\overline{x}, 0) = \sum_{n=1}^{\infty} c_n \psi_n(\overline{x}). \tag{15}$$

Note that the time exponential has dropped out. Now multiply both sides of this equation by $\psi_m^*(\overline{x})$ and integrate. Since $\psi_m^*(\overline{x}) = \psi_m(\overline{x})$, the Kronecker delta will cause all the terms to cancel except for the case $n = m$ [2]:

$$\begin{aligned} \int_0^1 \psi_m^*(\overline{x})\Psi(\overline{x}, 0)\, d\overline{x} &= \sum_{n=1}^{\infty} c_n \int_0^1 \psi_m^*(\overline{x})\psi_n(\overline{x})\, d\overline{x} \\ &= \sum_{n=1}^{\infty} c_n \delta_{mn} \\ &= c_m, \end{aligned} \tag{16}$$

and this is the expression we will need to evaluate.

5 Solving for Energy Probabilities

Now we are prepared to solve for c_n in the case of our Gaussian wave packet. The integral is challenging because we can't evaluate it exactly, and approximations will be needed. First, note that we will be integrating from $\overline{x} = -\infty$ to ∞, not 0 to 1. As with the normalization constant, the integral can only be done if we integrate over all the reals, and we find an expression similar to eqn. (7):

$$\int_0^1 \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x} \equiv \int_{-\infty}^{\infty} \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x} - \int_{-\infty}^{0} \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x} - \int_1^{\infty} \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x}$$

$$\equiv \int_{-\infty}^{\infty} \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x} - 2\int_1^{\infty} \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x}$$

$$\equiv \int_{-\infty}^{\infty} \psi(\overline{x})\psi_n(\overline{x})\,d\overline{x} - \mathbf{E}_{tot} \tag{17}$$

Using the first integral as our approximation, we again make the cosmetic substitution $y \equiv \overline{x} - 1/2$. Using the expression from eqn. (16) and the packet from eqn. (5), we find

$$c_n = \Delta \int_{-\infty}^{\infty} e^{-y^2/2\overline{\alpha}^2} e^{i\overline{k}y} \sin\left[n\pi(y+1/2)\right] dy, \tag{18}$$

where Δ stands for the constant factors: $\Delta \equiv \sqrt{2/(\overline{\alpha}\sqrt{\pi})}e^{i\overline{k}/2}$. Note that, using the dimensionless y, $\psi_n(y) = \sqrt{2}\sin\left[n\pi\,(y+1/2)\right]$.

Now we use Euler's Theorem ($2i\sin\phi = e^{i\phi} - e^{-i\phi}$) to replace the sin term with two exponentials, and then combine like powers:

$$c_n = \left\{ \frac{\Delta}{2i} \int_{-\infty}^{\infty} e^{-y^2/2\overline{\alpha}^2} e^{i\overline{k}y} e^{in\pi(y+1/2)}\, dy \right\} - \{n \to -n\}, \tag{19}$$

where the notation $\{n \to -n\}$ means to rewrite the term written explicitly, replacing all n's with negative n's. This leads to

$$c_n = \left\{ \frac{\Delta}{2i} e^{in\pi/2} \int_{-\infty}^{\infty} e^{-y^2/2\overline{\alpha}^2} e^{iy(\overline{k}+n\pi)} dy \right\} - \{n \to -n\}. \tag{20}$$

This integral can be looked up, although usually in a trigonometric form [4]:

$$\int_{-\infty}^{\infty} e^{-au^2} \cos bu\, du = \int_{-\infty}^{\infty} e^{-au^2} e^{ibu}\, du = \sqrt{\frac{\pi}{a}} e^{-b^2/4a}. \tag{21}$$

To see why the transformation holds, use Euler's Theorem again: $e^{i\theta} = \cos\theta + i\sin\theta$, and note that sin is odd, so that $\int e^{-au^2} i \sin bu\, du$ converges due to the exponential, but is 0 due to the sin term. Using this formula and rearranging, we get

$$c_n = (\sqrt{2\pi}/2) i \Delta \overline{\alpha} e^{in\pi/2} \times \left\{ e^{-in\pi} e^{-\overline{\alpha}^2(n\pi-\overline{k})^2/2} - e^{-\overline{\alpha}^2(n\pi+\overline{k})^2/2} \right\}. \tag{22}$$

Noting that $e^{-in\pi} = (-1)^n$, we can rewrite this as:

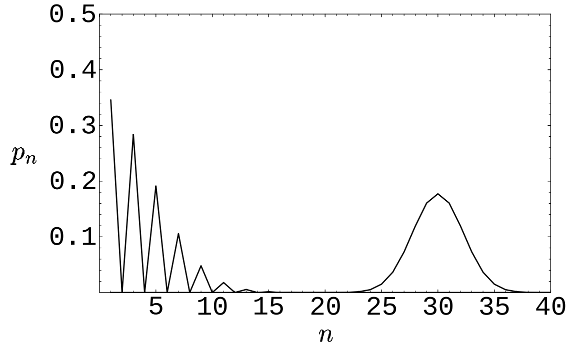

Figure 3: p_n vs. n for $\overline{k} = 0$, $k_\alpha = 20$ and $\overline{k} = 30\pi$, $k_\alpha = 10$

$$\begin{aligned} c_n &= i\sqrt{\overline{\alpha}\sqrt{\pi}}e^{i\overline{k}/2}e^{in\pi/2} \\ &\times \left\{(-1)^n e^{-\overline{\alpha}^2(n\pi-\overline{k})^2/2} - e^{-\overline{\alpha}^2(n\pi+\overline{k})^2/2}\right\}. \end{aligned} \tag{23}$$

From this we can directly obtain

$$p_n = |c_n|^2 = \overline{\alpha}\sqrt{\pi} \cdot \left\{(-1)^n e^{-\overline{\alpha}^2(n\pi-\overline{k})^2/2} - e^{-\overline{\alpha}^2(n\pi+\overline{k})^2/2}\right\}^2. \tag{24}$$

In anticipation of our analysis, we now define

$$k_\alpha \equiv 1/\overline{\alpha}. \tag{25}$$

This cosmetic change will make the interpretation of our results slightly easier. By convention, we use $\overline{\alpha}$ when discussing the original packet and k_α when discussing the energy distributions. We now have

$$p_n = \frac{\sqrt{\pi}}{k_\alpha} \cdot \left\{(-1)^n e^{-(n\pi-\overline{k})^2/2k_\alpha^2} - e^{-(n\pi+\overline{k})^2/2k_\alpha^2}\right\}^2. \tag{26}$$

Figure 3 shows p_n as a function of n for two different sets of parameters: one with $\overline{k} = 0$ and a relatively large value of k_α, and one for $\overline{k} = 30\pi$ and small k_α. The graph is jagged because p_n is only defined on the integers, but we have interpolated a continuous curve to add visual clarity. Also, note that when $\overline{k} = 0$, p_n is exactly 0 for even n.

6 Analysis of Results

The expressions we have derived for c_n and p_n are accurate, but a reasonable approximation will allow us to write them in a much simpler form. We start by examining the ratio of the two exponentials in eqn. (23):

$$\begin{aligned} \text{ratio} &= \exp\left[-(n\pi+\overline{k})^2/2k_\alpha^2\right] / \exp\left[-(n\pi-\overline{k})^2/2k_\alpha^2\right] \\ &= e^{-2\overline{k}n\pi/k_\alpha^2} \end{aligned} \tag{27}$$

The top exponential will quickly become negligible compared to the bottom, provided $\overline{k}$ is sufficiently large compared to k_α^2, which we have kept large (because $\overline{\alpha}^2$ is small) to manage the error. For example, if $k_\alpha = 10$ and $\overline{k} = 10\pi$, then at $n = 1$ we have ratio $= e^{-\pi^2/5} \approx .139$. Larger values of n will only decrease this ratio, with the exponential form ensuring that the ratio rapidly approaches zero. We therefore impose an additional constraint on our parameters: from now on, we assume that $\overline{k} \gtrsim k_\alpha^2/\pi$, with the effect that we can ignore the top exponential (we say approximately greater because it is convenient to choose $\overline{k}$ an integral multiple of π, as we show in this section). This allows us to rewrite our results in a much simpler form:

$$c_n \approx (-1)^n i\sqrt{\sqrt{\pi}/k_\alpha}\, e^{i\overline{k}/2} e^{in\pi/2} e^{-(n\pi-\overline{k})^2/2k_\alpha^2} \tag{28}$$

and

$$p_n \approx \frac{\sqrt{\pi}}{k_\alpha} e^{-(n\pi-\overline{k})^2/k_\alpha^2}. \tag{29}$$

This is a Gaussian distribution, as is made obvious by our k_α notation. This packet is in some sense the complement to the Gaussian packet we began with. It is centered at $n\pi = \overline{k}$ or $n = \overline{k}/\pi$, and its width is controlled by k_α (note the lack of the 1/2-factor in the exponent). The effect of requiring a large $\overline{k}$ is now clear: it ensures that the probability distribution is essentially Gaussian, and that we can reasonably call one energy level the "primary" energy level. By the Uncertainty Principle, as the position wavepacket becomes narrower, the range of possible energies becomes broader, and conversely. This is confirmed by the form of these two packets and the inverse relation between $\overline{\alpha}$ and k_α. We can conclude that the range of likely energy levels for the particle is roughly

$$n = \overline{k}/\pi \pm k_\alpha/4 \qquad n \in \mathbb{N}. \tag{30}$$

This is exactly what we set out to do. Given only the momentum and width of the original packet, we have a simple equation that fully describes the energy distribution within the well. The only remaining task is to manage the error.

7 Error

We have obtained our primary goal—an explicit formula which gives the probability of an energy state as a function of the packet's initial momentum and width. We must now bound the error in our formula, given in eqn. (17). This is very easy to do—in fact, we can use almost the same bound we used for the normalization constant! This results from a very simple pair of inequalities:

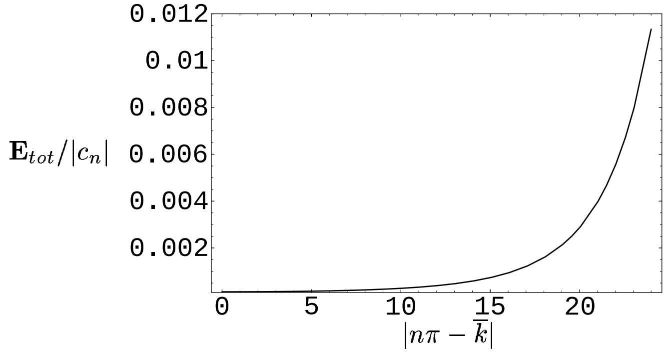

Figure 4: $\mathbf{E}_{tot}/|c_n|$ for $\overline{\alpha} = 1/8$

$$\begin{aligned}
\mathbf{E}_{tot} &= 2\int_1^\infty \psi(\overline{x})\psi_n(\overline{x})\, d\overline{x} \\
&= 2\sqrt{2}\int_1^\infty \psi(\overline{x})\sin(n\pi\overline{x})\, d\overline{x} \\
&\leq 2\sqrt{2}\int_1^\infty \psi(\overline{x})\, d\overline{x} \\
&\leq 2\sqrt{2}\int_1^\infty |\psi(\overline{x})|\, d\overline{x} \\
&= 2\sqrt{2}\int_1^\infty \exp\left[-(\overline{x}-1/2)^2/2\overline{\alpha}^2\right]\, d\overline{x}, \qquad (31)
\end{aligned}$$

which, aside from a few constant factors, is the same as the expression bounded in section 3. Using identical logic, we obtain:

$$\mathbf{E}_{tot} \leq 8\sqrt{2}\overline{\alpha}^2 e^{-1/8\overline{\alpha}^2}. \qquad (32)$$

Unlike section 3, the exact value of the original integral is unknown. However, we can look at the ratio of error to approximation. Taking the absolute value of c_n (we are only interested in the magnitude of the error),

$$\frac{\mathbf{E}_{tot}}{|c_n|} \leq \frac{8\sqrt{2\overline{\alpha}^3}}{\sqrt[4]{\pi}} e^{-1/8\overline{\alpha}^2} e^{\overline{\alpha}^2(n\pi-\overline{k})^2/2}. \qquad (33)$$

Using this expression, the error can be made less than any desired percentage of the approximation, by choosing a small enough value of $\overline{\alpha}$. Figure 4 shows this in the case $\overline{\alpha} = 1/8$, plotted as a function of the distance $|n\pi - \overline{k}|$. It is clear that the error is tolerable over the important range of values. In this case, for $|n\pi - \overline{k}| = 24$ (i.e., at $n = \overline{k}/\pi \pm 3k_\alpha$), the percent error is 1.13%. The exponential dependence on $\overline{\alpha}$ means that only a slight decrease in $\overline{\alpha}$ is needed to drastically reduce this.

8 Summary

We began with a Gaussian wavefunction, eqn. (5), in an infinite square well. The goal of our analysis was to predict the likely energies for the system. Our first task was to normalize the wavefunction. In doing so, we made approximations and exhibited a careful bound, eqn. (10), on the error introduced. 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, eqn. (16). 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, and the error was also bounded. Finally, we imposed the additional condition that $\overline{k}$ be large enough so that we could approximate our expression for p_n as another Gaussian. This allowed us to derive a very simple expression for the most likely energy levels of the system. The case where $\overline{k}$ is small can be examined by the reader.

References

[1] Ohanian, Hans C. *Modern Physics.* Second ed. New Jersey: Prentice Hall, 1995.

[2] Griffiths, David J. *Introduction to Quantum Mechanics.* New Jersey: Prentice Hall, 1995.

[3] Q-H. Park and J.H. Eberly, Phys. Rev. Lett. **85**, 4195 (2000).

[4] Spiegel, Murray R. *Mathematical Handbook.* New York: McGraw-Hill, 1968.