ENERGY STATES OF A GAUSSIAN WAVEPACKET IN A HARMONIC OSCILLATOR

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May 5th, 2011

1 Introduction

An expression is derived for the probability of an arbitrary energy state of a Gaussian wavepacket confined to a harmonic oscillator. This study is inspired from an earlier work on 'Energy states of a Gaussian wavepacket in a infinite square well' by David Etlinger. We will use the same approach to solve this problem. My goal is to determine analytically the first three Fourier constants associated with the first three energies and the probability of finding the particle in these first few states. Finally, I will show a graph of the probability that the system be in the nth energy state, p_n vs n to show the least and most probable energies.

2 The Initial Model

In the initial model that inspired me to look at a harmonic oscillator, we had a Gaussian wave packet to describe a particle moving in a infinite square well. The wavefunction as well as with all the wavefunctions, must obey the Schrodinger equation.

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

where V(x) is the potential of the infinite square well. At t = 0, a Gaussian wave function of the form

$$\Psi(x,0) = N\exp\left[-\frac{(x-x_0)^2}{2\alpha^2}\right]\exp\left[\frac{ipx}{\hbar}\right] \tag{2}$$

is initially centered at $x = x_0$. The momentum of the particle is given by $p = k\hbar$ and $\psi(x) = \Psi(x,0)$, the parameter α is the width of the Gaussian wave function and N is the normalization constant. For our convenience, we assume that k is positive although it can be modified to obtain a negative momentum. Before we can calculate an expression for the energy probabilities, we need to solve for the normalization constant.

Assume the wave is centered at $x_0 = \frac{L}{2}$ where L is the fixed length of the potential well. It can be rewritten as

$$\psi(x) = \Psi(x,0)$$

$$= Nexp\left[-\frac{(x-\frac{L}{2})^2}{2\alpha^2}\right]exp\left[ik(x-\frac{L}{2})\right]exp\left[ik\frac{L}{2}\right]$$

such that $k = \frac{p}{\hbar}$.

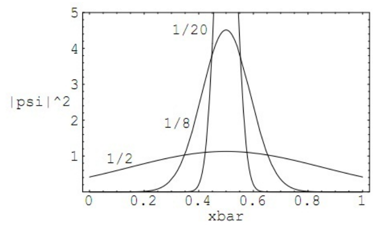

Figure 1
Plot of the probability density as a function of x for Gaussian wavepackets with α = 1/2, 1/8 and 1/20.

Figure 1: Different Gaussian wave functions in infinite square well

The values of x, α, and k are meaningful only in relation to this fixed value. The wavefunction was rewritten in terms of three dimensionless variables $\bar{x} = \frac{x}{L}$, $\bar{\alpha} = \frac{\alpha}{L}$, $\bar{k} = kL$. Therefore the wave equation can be rewritten as $\Psi(\bar{x}) = Nexp\left[-\frac{(\bar{x}-\frac{1}{2})^2}{2\bar{\alpha}^2}\right] exp\left[i\bar{k}\left(\bar{x}-\frac{1}{2}\right)\right] exp\left[\frac{i\bar{k}}{2}\right]$ where the well now extends from $\bar{x} = 0$ to $\bar{x} = 1$. Figure 1 shows the probability distribution, $|\psi(\overline{x})|^2$for several values of $\overline{\alpha}$. Wider packets have larger values of $\overline{\alpha}$. The energy and momentum in a square well due to boundary condition: $k_n = \frac{n\pi}{L}$, $E_n = \frac{\hbar^2}{2m}k^2$. In the dimensionless notation, the momentum $\bar{k_n} = n\pi$. Therefore in order to approximate the energy probabilities, we solve for the normalization constant. Set up the following integral and solve for N.

$$\int_0^1 |\Psi(x,0)|^2 \, dx = 1$$

$$\int_0^{+1} Nexp\left[\frac{(x-x_0)^2}{2\alpha^2}\right] exp\left[\frac{ipx}{\hbar}\right] dx = 1.$$

Since we can't analytically evaluate this integral, we need to change the bounds from -∞ to + ∞ giving us a value of $N = \frac{1}{\sqrt{\alpha\sqrt{\pi}}}$. Since the integral was done from - ∞ to + ∞, there is a small contribution of the wavefunction outside of the potential well that we consider and show under what conditions it can be tolerated. Let E_{norm} be the size of the error. We know

$$\int_0^1 |\psi(\overline{x})|^2 \, dx = \int_{-\infty}^{+\infty} |\psi(\overline{x})|^2 \, dx - \int_{-\infty}^{0} |\psi(\overline{x})|^2 \, dx - \int_{1}^{+\infty} |\psi(\overline{x})|^2 \, dx$$

$$\int_0^1 |\psi(\overline{x})|^2 \, dx = 2 * \int_{1}^{+\infty} |\psi(\overline{x})|^2 \, dx.$$

Let $z = 2\overline{x} - 1$ and can only have values between -1 and 1 and $z \geq 1$

$$E_{norm} = \int_1^{\infty} exp\left[\frac{-z^2}{4\overline{\alpha}}\right] dz$$

. To get the upper bound of the error, we can rewrite the equation as

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

The upper bound is much small than 1.

For a square well potential, one for which V(x) between two infinite potential walls at $x = 0$ and $x = L$ (written as $\overline{x} = 0$) and $\overline{x} = 1$, the wavefunction of the nth energy eigenstate is

$$\Psi_n(\overline{x}, t) = exp\left[-\frac{iE_nt}{\hbar}\sqrt{2}sin(n\pi\overline{x})\right] = exp\left[-\frac{iE_nt}{\hbar}\psi_n(\overline{x})\right]$$

The most general solution to Schrodinger's equation is an infinite sum of the stationary states.

$$\Psi(\overline{x}, t) = \sum c_n exp\left[-\frac{iE_nt}{\hbar}\right] \psi_n\overline{x}.$$

Each term in the sum corresponds to a specific particle energy E_n. A particle whose wavefunction is given by the sum of stationary states will have a probability of being found in the nth energy state given by $p_n = \left|c_n^2\right|$ Therefore we need to find the coefficients of c_n to predict the range of energies that will be

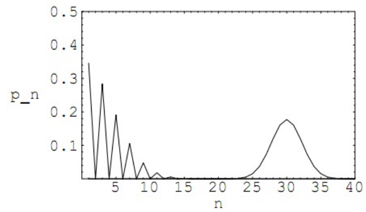

Figure 3
The probability of finding the Gaussian packet in energy state n vs n for: ($\bar{k}$ = 0, k_a = 20) and ($\bar{k}$ = 30π, k_a = 10).

Figure 2: Probability of finding the gaussian packet in nth energy state vs n

present when $\Psi(\overline{x}, 0)$ is given by the Gaussian function.

$$c_n = \int_0^1 \psi_m * \Psi_n d\overline{x}$$

We stumble upon the same problem as when we were finding the normallization constant because of the bounds of the integral. Therefore we calculate the coefficients with the limits going from - ∞ to + ∞ and approximate the error due to the wave packet in the outside walls from 0 to 1. After making substitution and evaluating the integrals, we get a value of

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

Figure 3 shows the probability of finsing the Gaussian packet in energy state n vs n.

3 My Model

We will use the same Gaussian wave packet in the initial model to describe a particle moving in a Harmonic Oscillator with potential $V(x) = \frac{1}{2}m^2\omega^2x^2$. Figure 3 shows the behavior of the gaussian wave packet with NO momentum

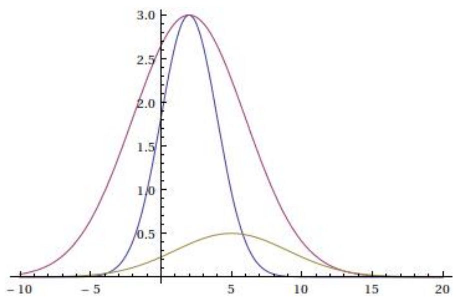

Figure 3: Gaussian wave function with different widths and centers

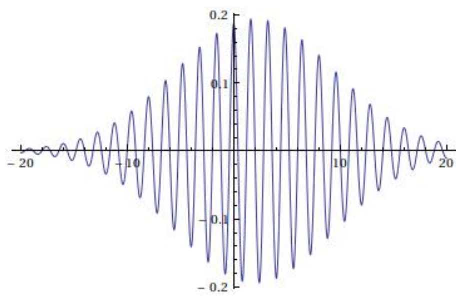

Figure 4: Gaussian wave function with momentum added

added centered at different locations and with different widths.

Figure 4 shows the behavior of this packet with a momentum added.

This wavefunction must also satisfy the Schrodinger equation as shown in (1) above. In the same way to find the energy states in a harmonic oscillator, we need to first find the normalization constant N before finding the expression for the energy probabilities. The probability density $|\Psi(x,t)|^2$ for finding the particle at a point x at t = 0, must be equal to 1. This time, our integral goes from $-\infty$ to $+\infty$ according to the following $\int_{-\infty}^{+\infty} Nexp\left[\frac{(x-x_0)^2}{2\alpha^2}\right] exp\left[\frac{ipx}{\hbar}\right] dx$. We can easily solve this integral by using the Gaussian integral. We found N to have a value of $\frac{1}{\sqrt{\alpha\sqrt{\pi}}}$.

The total energy (kinetic plus potential) is called the Hamiltonian. $H(x,p) =$

$\frac{p^2}{2m} + V(x)$ such that $V(x) = \frac{1}{2}m^2\omega^2x^2$ or $\langle E \rangle = \frac{1}{2}k\left\langle x^2 \right\rangle + \frac{\left\langle p^2 \right\rangle}{2m}$. To find the expected value of the energy, we need to calculate the expectation value of x, x^2, p and p^2 using equation (2) above for the equation of Ψ. The expected value of the position is given by

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \left|\Psi(x,0)\right|^2 dx$$

$$\left\langle x^2 \right\rangle = \int_{-\infty}^{+\infty} x \left|\Psi(x,0)\right|^2 dx$$

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi * \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,0) dx$$

$$\left\langle p^2 \right\rangle = \int_{-\infty}^{+\infty} \Psi * \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \Psi(x,0) dx$$

After calculations, we find

$$\langle x \rangle = x_0,$$

$$\left\langle x^2 \right\rangle = \frac{\alpha^2}{2} + (x_0)^2,$$

$$\langle p \rangle = p,$$

$$\left\langle p^2 \right\rangle = p^2 + \frac{\hbar^2}{2\alpha^2}$$

$$\sigma_x^2 = \left\langle x^2 \right\rangle - \langle x \rangle^2 = \frac{\alpha^2}{2} + x_0^2 - x_0^2 = \frac{\alpha^2}{2}$$

$$\sigma_p^2 = \left\langle p^2 \right\rangle - \langle p \rangle^2 = p^2 + \frac{\hbar^2}{2\alpha^2} - p^2 = \frac{\hbar^2}{2\alpha^2}$$

$$\sigma_x \sigma_p = \frac{\alpha}{\sqrt{2}} . \frac{\hbar}{\sqrt{2}\alpha} = \frac{\hbar}{2}$$

We verified the Heisenberg uncertainty principle since $\sigma_x \sigma_p \geq \frac{\hbar}{2}$. Since the gaussian is centered at $x = x_0$ and $\langle x \rangle = \int_{-\infty}^{+\infty} x \left|\Psi(x,0)\right|^2 dx = x_0$, the particle will most likely be found at x_0 where $P(x) = \left|\psi(x)\right|^2$ is largest. The expectation value of the momentum is equal to the momentum term of the Gaussian wave function.

Now we can write energy in terms of its expected value for the ground state.

$$\langle E \rangle = \frac{1}{2}k\left\langle x^2 \right\rangle + \frac{\left\langle p^2 \right\rangle}{2m}$$

$$\langle E \rangle = \frac{1}{2}k\left(\frac{\alpha^2}{2} + x_0^2\right) + \frac{1}{2m}\left(p^2 + \frac{\hbar^2}{2\alpha^2}\right)$$

We found the minimum energy by taking the derivative of $\langle E \rangle$ with respect to α because the wave function will shrink or spread out with respect to the parameter α. Setting

$$\frac{d\langle E \rangle}{d\alpha} = 0 \Leftrightarrow \frac{1}{2}k\alpha - \frac{\hbar^2}{2m}\left(\frac{1}{\alpha^3}\right) = 0$$

We get $\alpha^2 = \frac{\hbar}{m\omega}$, therefore $\alpha = \sqrt{\frac{\hbar}{m\omega}}$. We plug this value of α to get the minimum energy to get $\langle E \rangle_{min}$ and use $k = m\omega^2$.

$$\langle E \rangle_{min} = \frac{1}{2}kx_0^2 + \frac{p^2}{2m} + \frac{3}{4}\hbar\omega.$$

Therefore the minimum energy depends on the localization of the center of the wave function and the momentum added to it. If the wave packet is centered at $x_0 = 0$ and $p = 0$, then the kinetic energy expression as well as the momentum term would all go to zero and we are only left with $\langle E \rangle_{min} = \frac{3}{4}\hbar\omega$ which corresponds to half of the energy of the harmonic oscillator in the first excited state, n = 1 .

4 Calculation of Energy probabilities

For a harmonic oscillator with potential $V(x) = \frac{1}{2}m\omega^2x^2$, the wavefunction of the nth energy eigenstate is

$$\Psi_n(x,t) = \psi_n(x)exp\left[-\frac{iE_nt}{\hbar}\right]$$

The general solution is a linear combination of separable solutions. The time dependent Schrodinger equation as seen in (1) has the property that any linear combination of solutions is itself a solution. Once we have found the separable solutions, then we can immediately construct a much more general solution of the form

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)exp\left[-\frac{iE_nt}{\hbar}\right]. \tag{3}$$

The infinite set of solutions ($\psi_1(x), \psi_2(x), \psi_3(x)...$) each solution with its own associated energy $(E_1, E_2...)$. A particle whose wavefunction is given by the sum in equation (3) will have a probability of being found in the nth energy state given by

$$p_n = \left|c_n^2\right|.$$

Our job is to find the value for c_n. First we notice that the functions

$$\psi(x)_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^nn!}}H_n(\xi)e^{-\xi^2/2}$$

such that $\xi = \sqrt{\frac{m\omega}{\hbar}}x$ are orthogonal, so $\int_0^1 \psi_m^*\psi ndx = \delta_{mn}$, where δ_{mn} is the kronecker delta defined as:

$$\delta_{mn} = 0$$

if m $\neq$ n ;

$$\delta_{mn} = 1$$

if m = n. Now we consider the general solution to the Schrodinger equation at time t = 0: $\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$. When we multiply both sides of this equation by ψ_m and integrate , the kronecker delta will cause all the terms to cancel except for the case where m = n.

$$\int_{-\infty}^{\infty} \psi_m^* \Psi(x,0) dx = \sum_{n=1}^{\infty} c_n \int_{-\infty}^{\infty} \psi_m(x)\psi_n(x) = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_n.$$

Now we calculate the values of the c_n's to predict the range of energies that will be present when the gaussian wave packet is introduced in the harmonic oscillator system.

We can calculate the first few coefficients c_0, c_1 and c_2 to determine the different energy states.We will use approximation techniques or computer software (mathematica) to compute graph the value of all these coefficients. To find c_0, set up the following integral $c_0 = \int_{\infty}^{-\infty} \psi_0 \Psi(x,0) dx$. We have $H_0 = 1$, therefore $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$ and $\Psi(x,0) = Nexp\left[\frac{(x-x_0)^2}{2\alpha^2}\right] exp\left(\frac{ipx}{\hbar}\right)$.

$$c_0 = \int_{-\infty}^{\infty} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} * Nexp\left[\frac{(x-x_0)^2}{2\alpha^2}\right] exp\left(\frac{ipx}{\hbar}\right) dx.$$

Regrouping the terms of the same exponent and completing the squares, we obtain a new equation of the form $\int_{-\infty}^{\infty} a\ e^{-bx^2+cx+f}\ dx = a\ \sqrt{\frac{\pi}{b}}\ e^{\frac{c^2}{4b}+f}$ such that $b = \left(\frac{m\omega}{2\hbar}\right)$ $c^2 = \frac{p^2}{\hbar^2} + \frac{x_0^2}{(\alpha^2)^2}$ and $f = -\frac{x_0^2}{2\alpha^2}$. As a result, we have

$$c_0 = (m\omega\hbar)^{1/4} * \frac{2\alpha}{m\omega\alpha^2} * e^{\frac{1}{2}\left(\frac{\hbar\alpha^2}{m\omega\alpha^2}\right)\left[\left(\frac{x_0^2}{\alpha^2}\right)^2 - \frac{p^2}{2\alpha^2}\right] - \frac{x_0^2}{2\alpha^2}}.$$

Case for c_1, $H_1(\xi) = 2\xi$

$c_1 = \int_{-\infty}^{\infty} \psi_1 \ \Psi(x,0)dx.$

$$\psi_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} * 2\sqrt{\frac{m\omega}{\hbar}} x e^{-\frac{m\omega}{2\hbar}x^2}$$

We regroup the terms with the same coefficients and do the completing squares as we did for c_0. This time, use the following $ax^2 + bx + c = a(x-h)^2 + k$ where $h = -\frac{b}{2a}$ and $k = c - \frac{b^2}{4a}$.

$$c_1 = \int_{\infty}^{-\infty} \psi_1 \Psi(x,0)dx.$$

$$c_1 = \int_{\infty}^{-\infty} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} * 2\sqrt{\frac{m\omega}{\hbar}} x e^{-\frac{m\omega}{2\hbar}x^2} N exp\left[\frac{(x-x_0)^2}{2\alpha^2}\right] exp\left(\frac{ipx}{\hbar}\right) dx.$$

$$k = \frac{1}{2}\left(\frac{\hbar\alpha^2}{m\omega\alpha^2}\right)\left[\left(\frac{x_0^2}{\alpha^2}\right)^2 - \frac{p^2}{2\alpha^2}\right] - \frac{x_0^2}{2\alpha^2}$$

$$h = \frac{ip\alpha^2 + \hbar x_0}{\hbar + m\omega\alpha^2}$$

We know that $\int_{-\infty}^{\infty} x e^{a(x-h)^2} dx = \frac{\sqrt{\pi}h}{\sqrt{-a}}$ and

$$a = -\left(\frac{m\omega\alpha^2 + \hbar}{2\hbar\alpha^2}\right)$$

Our value of c_1 yields to

$$c_1 = 2\frac{(m\omega)^{3/4}}{\hbar^{1/4}} * \frac{\sqrt{\alpha}}{\hbar + m\omega\alpha^2}(ip\alpha^2 + \hbar x_0)e^k$$

or

$$c_1 = 2\frac{(m\omega)^{3/4}}{\hbar^{1/4}} * \frac{\sqrt{\alpha}}{\hbar + m\omega\alpha^2}(ip\alpha^2 + \hbar x_0)e^{\frac{1}{2}\left(\frac{\hbar\alpha^2}{m\omega\alpha^2}\right)\left[\left(\frac{x_0^2}{\alpha^2}\right)^2 - \frac{p^2}{2\alpha^2}\right] - \frac{x_0^2}{2\alpha^2}}$$

We calculate c_2 by using

$$c_2 = \int_{-\infty}^{\infty} \psi_2(x) * \Psi(x,0) dx$$

We rewrite this long integral as $\int_{-\infty}^{\infty} x^2 e^{a(x-h)^2} dx = \frac{\sqrt{\pi}(1-2ah^2)}{2(-a^{3/2})}$ and $H_2 = 4(\xi)^2 - 2$Therefore,

$$c_2 = \left(\frac{m\omega}{\hbar}\right)^{5/4} \sqrt{\frac{2}{\pi\alpha}} \left[\frac{1}{2}\sqrt{\pi} \left(\frac{2\hbar\alpha^2}{m\omega\alpha^2}\right)^{3/2} + \frac{(p\alpha^2)^2 + (\hbar x_0^2)}{(\hbar + m\omega\alpha^2)^2 \left(\sqrt{\frac{2\hbar\alpha^2}{m\omega\alpha^2+\hbar}}\right)} \right] e^k - \frac{1}{\sqrt{2}} c_0$$

Then, the probability of the particle being found in the ground energy, first excited and 2nd excited states are respectively given by

$$p_0 = |c_0|^2$$

$$p_1 = |c_1|^2$$

$$p_2 = |c_2|^2$$

For coefficients greater or equal to 3, we need to do some approximations (WKB approximation) to generalize the coefficients of the stationary states and express all the terms in terms of n. Ffigure 5 shows the coefficients c_n vs n. In this case, we have $x_0 = 5$, $\alpha = 1$, $p = 5$, $m = 1$ and $\omega = 1$ so the expected value of the energy using this value is 25.5. Figure 5 shows We notice that the highest coefficient in figure 5 corresponds to the expected value of the energy. Figure 6 represents the probability of finding the Gaussian packet in the nth energy state p_n vs n.

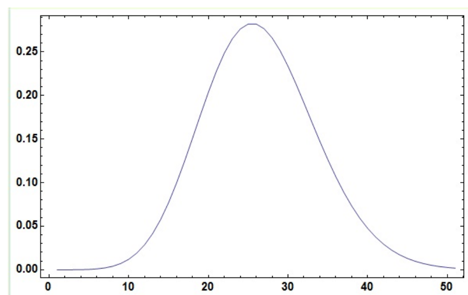

Figure 5: Coefficient c_n vs n

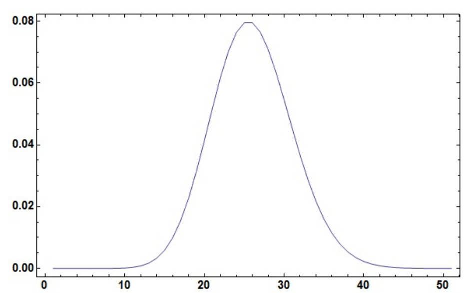

Figure 6: probability of finding Gaussian wave function in nth energy state vs n ($p_n = \left|c_n^2\right|$ vs n)

Therefore the most probable state of energy is most likely to happen at n = 25.5 as we can see from the graph, which corresponds to the expected value of the energy for specific values of $x_0, \alpha, \hbar, \omega$. We also notice that the bigger the width is, the more spread out the shape of the probability of the nth energy will be and the smaller it is, the smaller the probability would be.

5 Conclusion

We begin with a Gaussian wave function in a harmonic oscillator of potential $Vx = \frac{1}{2}m\omega^2 x^2$. The goal of the analysis was to predict the likely energies for the system and relating it to the energy of the harmonic oscillator. We started by normalizing our wavefunction. Then we used the theory of orthogonal function and the superposition principle to show how to express any wavefunction as an infinite sum and calculate the coefficients of the terms of that sum. In this paper, we can only calculate the first three coefficients analytically and therefore the the probability of finding the particle in the ground and the first two excited states. The absolute square of a particular coefficient gives the probability of the corresponding energy level. A graph with these probabilities vs n was also included in the paper. Another study needs to be done with the WKB Approximation for higher values of n to generalize the Fourier coefficients c_n in terms of n.

6 References

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