

# Quantum Harmonic Oscillators in One and Two Dimensions

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**Abstract.** The Schrödinger equation is a significant achievement on the development of quantum mechanics. By solving the Schrödinger equation, the fundamental behaviors and properties of a microscopic particle can be found in one- to three-dimensions. The article focuses on the derivations of quantum harmonic oscillators in one dimension by solving second order-differential equation. The wave functions, probability densities under different energy levels are presented. The results can be used to estimate different forms of continuous potential experienced by an oscillator. By calculating the uncertainty relation of the oscillator under one specific excited state, the general relation  $\sigma_x \sigma_p = \hbar(n + 1/2)$  can be confirmed. Based on the output, by splitting the variables, the two-dimensional harmonic oscillator can also be derived. The degenerate energy levels are presented as  $m + n + 1$ . Numerical simulations are made to visualize those results and suggests the relation of energy levels and number of maxima of the probability densities.

**Keywords:** Quantum mechanics; Harmonic oscillator; Schrödinger equation; Wave function.

## 1. Introduction

Quantum mechanics is a vital branch in physics which tells the nature of particles exists as waves at microscopic scale. The behavior of a particle can be expressed as a wave function which can be obtained by solving Schrödinger equation. However, the equations are usually trivial or even unsolvable since the potential energy experienced is very complex. To solve the corresponding differential equation, a solution is made by approximating it into series of strict solutions. One of the famous and well-used strict solution is the infinite potential wells. A method to make approximations is the Runge-Kutta methods. The main idea of it is replacing Taylor's expansions into linear combinations of function values on the curve to find the coefficients of them. The advantage of the method is that the difficulties of calculating higher derivatives are avoided. One numerical method is used which is called Nemerov method. It is used to solve a special case of second-order differential equation in which the first-order term does not exist. These methods are applied in many cases such as the hydrogen-like atom [1].

Quantum harmonic oscillator is settled with a quadratic relation between potential energy and displacement. It is also a well-discussed strict solution and one of the most important but simple models in quantum mechanics. Since any arbitrary smooth potential can be modified by transformations into sets of harmonic ones [2]. Comparing with the infinite potential wells, combinations of parabolas are more efficient to approximate a smooth potential. The physical model of one-dimensional harmonic oscillator can be described a mass point  $m$  vibrating back and forth about an equilibrium position. In classical mechanics, the problem can be easily solved by the differential equation that had already been worked out, i.e.,  $F = m\ddot{x} = -kx$  where the solution is given by  $x = A\sin(\omega t + \phi)$  with the angular frequency is expressed as  $\omega = \sqrt{k/m}$ . By doing simple calculus, the expression for potential energy is expressed as  $V = m\omega^2 x^2/2$ . The article will mainly talk about the derivations of energy levels, wave function, probability density, uncertainty relation of harmonic oscillators in one- and two-dimension by calculus respectively. Brief discussions are made on some other properties of harmonic oscillators with some intuitive understandings on the difference of quantum and classical observations.

## 2. Quantum Harmonic Oscillator in One Dimension

### 2.1. Analytic Derivations

The only condition which satisfies in both classical and quantum scale is the potential energy. Therefore, the possible energies of mass point in which it could conserve in this vibrating system, the possibilities of observations at certain position, can be found by solving time-independent Schrödinger's equation in one dimension. It has a general form, where the potential energy  $V$  is the same as classical version. However, the differential equation still seems to be complex. Even though the dimension of wavefunction in Hilbert space is unlimited, it still brings inconvenience when solving the equation, such as products of the functions, which can be seen in next few steps.

Therefore, the original Schrödinger equation should be made simpler by nondimensionalization. Firstly, divide the equation on both sides by  $-\frac{\hbar^2}{2m}$ , it is found that

$$\frac{d^2}{dx^2}\psi - \frac{m^2\omega^2}{\hbar^2}x^2\psi = -\frac{2mE}{\hbar^2}\psi. \quad (1)$$

The dimension on each side is  $L^{-2}[\psi]$ , and at the same time  $\left[\frac{m\omega}{\hbar}\right] = L^{-2}$ . If one sets  $q = \sqrt{\frac{m\omega}{\hbar}}x = \alpha x$ , where  $[q] = 1$  and divides the equation Eq. (1) by  $\frac{m\omega}{\hbar}$  on both sides, the dimension will be only relative to the wavefunction which can still be non-dimensional by setting it to be a function of  $q$  [3]. So,

$$\frac{d^2}{dq^2}\psi(q) + (\lambda - q^2)\psi(q) = 0. \quad (2)$$

A classical boundary condition to solve the differential equation is when  $q$  approaches to infinity the wavefunction tends to zero, since it is not expected to have a particle which is possible to be observed from far distance, so  $\lim_{\pm q \rightarrow \infty} \psi(q) = 0$ . At the same time,  $\lambda$  can also be ignored since  $q$  is increasing quadratically, therefore  $\frac{d^2}{dq^2}\psi(q) - q^2\psi(q) \sim 0$ . The function that only suit both condition is expressed as  $\lim_{\pm q \rightarrow \infty} \psi(q) = Ae^{-\frac{q^2}{2}}$  where  $A$  is a constant. Certainly, a constant  $A$  cannot help suit the reduced Eq. (2), it is usually thought to be another function of  $q$  which the article assume it is  $u(q)$ , a product of functions made the equation solvable and mostly do not break the boundary condition. Therefore  $\psi(q) = u \cdot e^{-\frac{q^2}{2}} = u \cdot v$ . Yet if the wavefunction is still a function of  $x$ , wave function will be much more complex, since the dimension of index should be 0, and the dimension of wavefunction should be  $L^{-1/2}$ . To make the sum of probabilities dimensionless, the expression for  $u$  will be largely limited, that is why the equation should be made dimensionless.

After substituting the wave function into Eq. (2), it is found that  $u$  satisfies the following second-order differential equation

$$u''(q) - 2qu'(q) + (\lambda - 1)u = 0. \quad (3)$$

Even though a second-order differential equations are usually unsolvable, fortunately, but unaware for whether it was firstly intended to solve the harmonic oscillator, the Hermite polynomials fit equation (2) perfectly [4]. It is often expressed as  $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$ , where

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0 \quad (4)$$

With  $n = 1, 2, 3 \dots$ . By trivial calculations, the functions of individual values of 'n' can be obtained, as illustrated in Table 1.

To conclude, the energy level of the harmonic oscillator is

$$E = \frac{1}{2} \hbar \omega (2n + 1) \tag{5}$$

And the corresponding unnormalized wave function is

$$\psi(q) = uv = H_n(q) e^{-\frac{q^2}{2}}. \tag{6}$$

**Table 1.** The first few examples of Hermite polynomials.

n	$H_n$	n	
0	1	1	$2x$
2	$4x^2 - 2$	3	$8x^3 - 12x$
4	$16x^4 - 48x^2 + 12$	5	$32x^5 - 160x^3 + 120x$

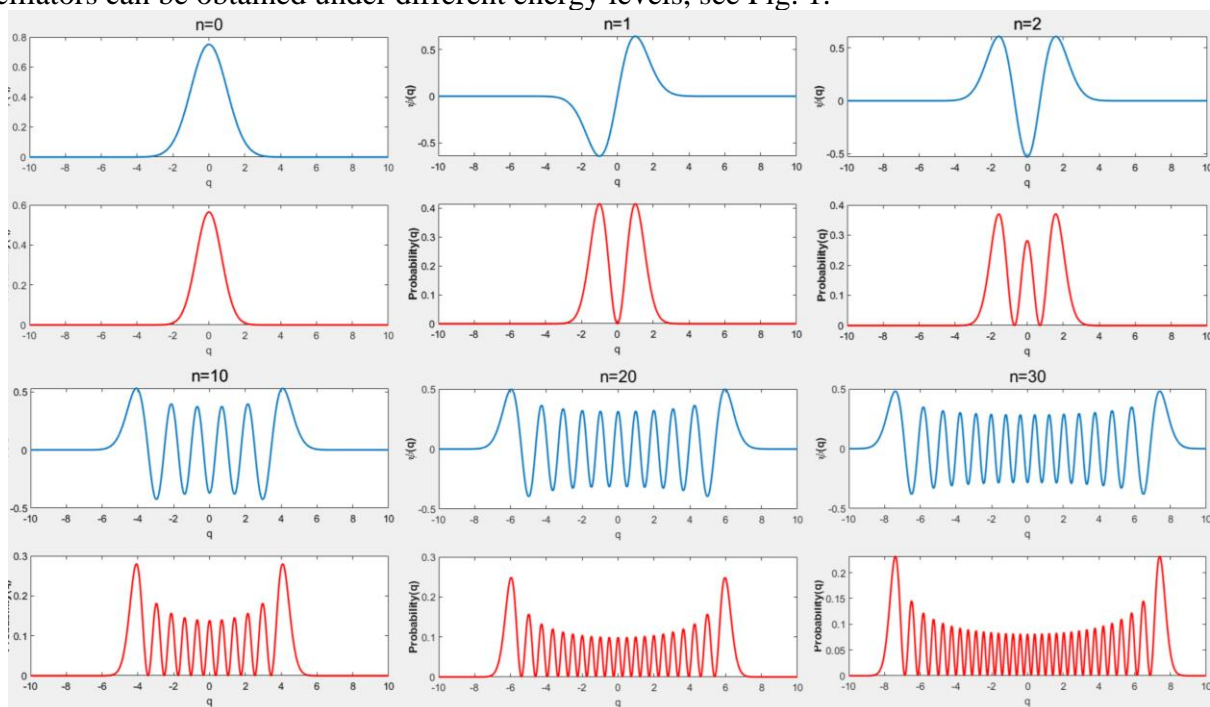
The normalization is to make the inner product of the wavefunction and the integrand probability over the space equals to 1. Since the solution have already transform ‘x’s into ‘q’s, the modules square of the wavefunction can be integrated by the dimensionless coordinate, the normalizing constant can be determined by a known conclusion which is used for showing the polynomials are orthogonal [4]

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = n! 2^n \sqrt{\pi} \delta_{mn}. \tag{7}$$

For the inner product of the same wavefunction,  $m = n$ , so it is a non-zero value and it satisfies the identity  $1 = \langle \psi | \psi \rangle = \int_{-\infty}^{\infty} \frac{\|N\|^2}{\alpha} H_n^2(q) e^{-q^2} dq = \frac{\|N\|^2}{\alpha} n! 2^n \sqrt{\pi}$ , with  $N = \sqrt{\frac{\alpha}{n! 2^n \sqrt{\pi}}}$ . The complete wavefunction is then expressed as

$$\psi(x) = \sqrt{\frac{\alpha}{n! 2^n \sqrt{\pi}}} H_n(\alpha x) e^{-\frac{1}{2} \alpha^2 x^2}. \tag{8}$$

By solving equations with MATLAB, the wavefunctions and probability densities of a harmonic oscillators can be obtained under different energy levels, see Fig. 1.



**Fig. 1** 1-D oscillators at different energy levels

The numerical simulations directly suggest that as the energy levels increase, the possibility density of the oscillator spreads out from equilibrium positions. It can be compared with taking pictures of a classical pendulum between the same time interval, the displacement where the pendulum is moving the lowest is where it is more likely to be captured at.

### 2.2. Heisenberg Uncertainty

In this part, the article will specifically calculate the uncertainty of harmonic oscillators in one-dimension. It is not complex since the function of potential energy is even and the distribution is symmetric. The uncertainty relation is expressed as

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}, \tag{9}$$

Where  $\sigma$  is the standard deviation. The uncertainty relation of harmonic oscillator in ground state is  $\sigma_x \sigma_p = \frac{\hbar}{2}$ . However, if the oscillator is in excited state, the uncertainty may increase. The article will calculate the uncertainty when  $n = 1$ , where the corresponding wave function is given by  $\psi(x) = \frac{\sqrt{2\alpha}}{\sqrt{\pi}} \alpha x e^{-\frac{1}{2}\alpha^2 x^2}$ . The expression for expectation of position  $x$  is expressed as

$$\langle x \rangle = \langle \psi | x \psi \rangle = \int_{-\infty}^{\infty} x \psi^2 dx = c \int_{-\infty}^{\infty} x^3 e^{-\alpha^2 x^2} dx = 0. \tag{10}$$

Where  $c$  is a constant. The function is odd and symmetric, so the area under the curve is expected to be 0. It is also intuitively correct since the distribution with respect to position is even and centered at  $x = 0$ . Turning to the mean of momentum, it is a bit complex but can still be cancelled easily

$$\langle p \rangle = \langle \psi | \hat{p} \psi \rangle = c \left[ \int_{-\infty}^{\infty} x e^{-\alpha^2 x^2} dx - \int_{-\infty}^{\infty} x^3 e^{-\alpha^2 x^2} dx \right] = 0. \tag{11}$$

The remaining two function is still odd, so the value should also be zero, as the motion of harmonic oscillator is expected to be symmetric. The symmetry properties of Hermite polynomials confirms this intuition [5]. As for the expectation of  $x^2$ , one specific known conclusion of Gaussian integral is needed to be introduced  $\int_0^{\infty} x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \dots (2n-1)}{2^{2n+1} a^n} \left(\frac{\pi}{a}\right)^{\frac{1}{2}}$ . In this situation, the expectation of  $x^2$  is expressed as

$$\langle x^2 \rangle = \langle \psi | x^2 \psi \rangle = \frac{2\alpha^3}{\sqrt{\pi}} \int_{-\infty}^{\infty} x^4 e^{-\alpha^2 x^2} dx = \frac{3}{2} \frac{\hbar}{m\omega} \tag{12}$$

Where the relation  $\sqrt{\frac{m\omega}{\hbar}} = \alpha$  is used. The expectation of momentum squared can be easily determined using energy relation of classical harmonic oscillator, but in statistical formulation. The relation is always true in all energy levels  $E = \frac{\langle p^2 \rangle}{2m} + \frac{1}{2} m\omega^2 \langle x^2 \rangle$ . An intuitive explanation for this is that since the variance of the observables is negligible in classical scale, the expectation value can be regard as a determined value. Then the relation can be easily deduced.

$$\langle p^2 \rangle = \frac{3}{2} m\hbar\omega \tag{13}$$

In light of the above equations, it is found that

$$\sigma_x \sigma_p = \sqrt{\langle x^2 \rangle} \sqrt{\langle p^2 \rangle} = \frac{3}{2} \hbar \geq \frac{\hbar}{2}. \tag{14}$$

According to the analytical derivations, the uncertainty relation of harmonic oscillator increases as the energy level increases. The theoretical relation respect to energy level is  $\sigma_x\sigma_p = \hbar\left(n + \frac{1}{2}\right)$  [6]. The calculations confirm one specific case of that.

Harmonic oscillators along one axis have properties of parity since the function of potential energy is even, which means the wave functions are space inversion invariance. To be specified, when energy level is an even number, the wave function is unchanged, which indicates to even parity. When it is odd, the wave function is reversed which indicates odd parity. A general expression can be found by using of a unitary operator [7].

### 3. Two-dimensional Quantum Harmonic Oscillator

#### 3.1. Exact Solution

Generally, a two-dimensional harmonic oscillator is similar to a particle in a gravitational field, except for its potential energies are directly proportional to the distance squared from the equilibrium position. The Schrödinger equation for this model in an  $x$  and  $y$  plane can be expressed as

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi + \frac{1}{2}m\omega(x^2 + y^2)\psi = E\psi. \quad (15)$$

By making the same nondimensionalization process, the wave function can be easily obtained with non-dimensional 'x' and 'y':

$$\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right)\psi(x, y) + (\lambda - x^2 - y^2)\psi(x, y) = 0. \quad (16)$$

There are two ways to solve the equation, one is by applying it into polar coordinates, while the other is by separating the variables since a one-component situation has been already obtained.

Since the model is perfectly symmetric in two components, it can be firstly assumed that  $\psi(x, y) = \phi(x)\phi(y)$  where  $\phi$  are two axes which are just the same as Eq. (8). At the same time, energy levels differed in different axes. Assuming the coordinates are already non-dimensional the wave function can be easily obtained as [8]

$$\psi(x, y) = N_x N_y H_n(x) H_m(y) e^{-\frac{1}{2}(x^2+y^2)} \quad (17)$$

Where  $n$  and  $m$  are different energy levels in  $x$  and  $y$  coordinates,  $N_x, N_y$  are normalization constants as in one dimensional situation which also differ in energy levels.  $H$  are Hermite polynomials in different coordinates.

The assumption can be related to the build-up of wavefunction in an infinite potential well from 1-3 dimension. By taking partial derivatives with respect to one component of the function, the part of the function that dominated by the other component can be regarded as coefficients or constants, which can be then cancelled out.

As for the value of  $\lambda$ , by splitting  $\lambda = \lambda_x + \lambda_y$ , the equation can be more obvious in the final identification that is quite equivalent in 1D situations from Eq. (17),

$$u''(x) - 2xu'(x) + (\lambda_x - 1)u(x) + u''(y) - 2yu'(y) + (\lambda_y - 1)u(y) = 0. \quad (18)$$

One obvious but promising solution for  $\lambda$  is

$$\lambda = \lambda_x + \lambda_y = (2n + 1) + (2m + 1) \quad (19)$$

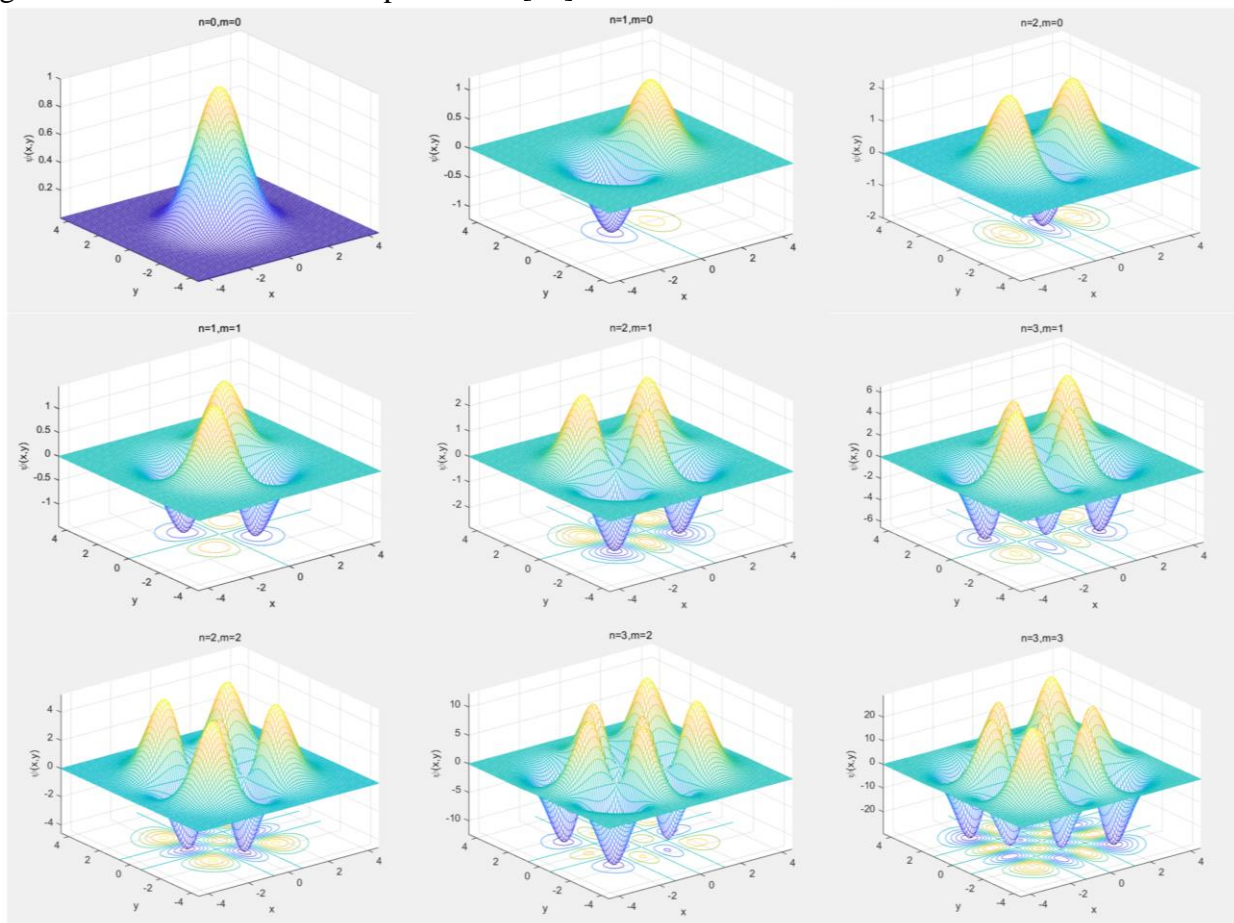
Where  $n$  and  $m$  are the individual energy level, the energy of the oscillator can also be performed as a summation of the 'component' of the total energy:

$$E = E_x + E_y = \frac{1}{2}\hbar\omega(2n + 1) + \frac{1}{2}\hbar\omega(2m + 1) = \hbar\omega(n + m + 1). \quad (20)$$

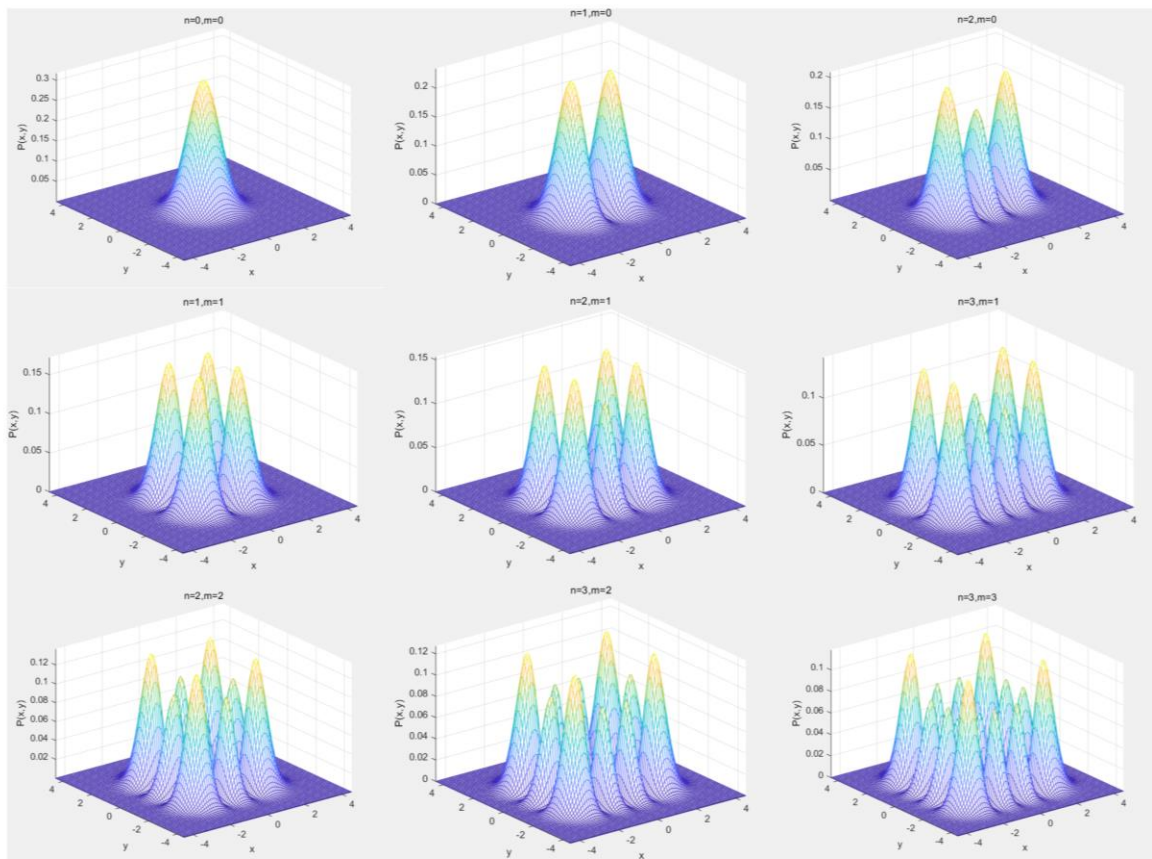
The degenerate energy levels in quantum mechanics are used to simplify two or more different states of an oscillator into one energy level if they have the same amount of energy. It is more often to be used on generalizing the electron orbits and the main shells of an atom in chemistry. For instance, the quantum state of a two-dimensional quantum expressed as  $(m, n)$  has the same degenerate energy level as  $(n, m)$  or  $(m + 1, n - 1)$ , which can be directly confirm by Eq. (20). The eigen energy directly shows that the degenerate energy level is just a simple linear superposition which is expressed as  $n + m + 1$  [9].

### 3.2. Numerical Simulations

From Eq. (17), by using MATLAB, the wavefunctions and probabilities of a two-dimensional harmonic oscillator in dimensionless  $x$  and  $y$  plane can be obtained as graphs under different energy levels in different components, albeit the values are not normalized, see Fig. 2 and Fig. 3. The number of probability maxima under degenerate energy levels is  $(n + 1)(m + 1)$ , and these figures confirm this theoretical prediction [10].



**Fig. 2** wave functions of 2D harmonic oscillator under energy level  $(n, m)$



**Fig. 3** probability densities of 2D harmonic oscillators

#### 4. Conclusion

By using analytical derivations, the fundamental properties of harmonic oscillator in one dimension can be found. The research derived the basic wave function by non-dimensionalizing the Schrödinger equation firstly. The eigen energy of it is  $\hbar\omega(n + 1)/2$ . From ground state to an increase of energy level by one unit, the value of principle relation increases by one amount of  $\hbar$ . A general expression can be roughly suggested as  $\sigma_x\sigma_p = \hbar(n + 1/2)$ , which is the theoretical conclusion. The oscillator in one dimension is in parity considering that the potential is even. By splitting the variables, the two-dimensional harmonic oscillator can also be derived. The eigenenergy of it is the sum of two eigenenergy of one-dimensional case, which is expressed as  $\hbar\omega(n + m + 1)$ . The degenerate energy levels are presented as  $m + n + 1$ . The wave functions can be used in any arbitrary smooth potential by using different methods of approximations. The solutions can then be made on the differential equations that seems unsolvable. However, the subsequent calculations are needed to be verified by perturbation theory. Numerical simulations are made on these two situations. According to them, a more intuitive distributions are obtained which is sufficient to develop applications on that. It is also concluded that the oscillator is more possible to be observed on the area surrounding the equilibrium position.

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