

The radial wave function of 2D and 3D quantum harmonic oscillator

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Abstract. One dimensional quantum harmonic oscillator is well studied in elementary textbooks of quantum mechanics. The wave function of one-dimensional oscillator harmonic can be written in term of Hermite polynomial. Due to the symmetry of the spring energy, the wave functions of two-dimensional and three-dimensional harmonic oscillators can be written as products of the one-dimensional case. Because of that, the wave functions of two- and three-dimensional cases are focused on cartesian coordinates. In this article, we utilize polar and spherical coordinates to describe the wave function of two- and three-dimensional harmonic oscillators, respectively. The radial part of the wave functions can be written in term of associated Laguerre polynomials.

Keywords: *associated Laguerre polynomials, quantum harmonic oscillator, radial wave function, two dimension quantum harmonic oscillator, three dimension quantum harmonic oscillator.*

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INTRODUCTION

In elementary textbooks of quantum mechanics, one dimensional quantum harmonic oscillator is well studied using a potential energy analogous to classical harmonic oscillator

$$V(x) = \frac{1}{2}M\omega^2x^2. \quad (1)$$

Here M is mass of the particle, ω is the characteristic radial frequency. The eigen wave function of the Schrödinger equation $(p^2/(2m) + V(x))\psi = i\hbar\dot{\psi}$ can be written in term of Hermite polynomials H_n [1]

$$\psi_{1d} = e^{-\frac{i}{\hbar}E_n t} \sqrt{\frac{\alpha}{2^n n! \sqrt{\pi}}} e^{-\frac{1}{2}\alpha^2 x^2} H_n(\alpha x). \quad (2)$$

Here $\alpha = \sqrt{M\omega/\hbar}$, and $E_n = (n + \frac{1}{2})\hbar\omega$ is the quantized energy.

However, the potential is a central potential $V(\vec{r}) = \frac{1}{2}m\omega^2r^2$ and therefore the eigen wave functions should be able to be written as a product of radial and angular wave functions [2]. The angular wave functions of two- and three-dimensional potentials with central symmetry are well-described using sinusoidal and spherical harmonics

functions, respectively [3]. However, studies of higher dimension quantum oscillators elude the discussion of radial wave function [4]–[8].

It may be due to the additive property of the norm of \vec{r} . Because of that, the generalization of the potential energy into two and three dimensions is straightforward

$$V(\vec{r}) = \begin{cases} \frac{1}{2}M\omega^2(x^2 + y^2), & \text{for 2d,} \\ \frac{1}{2}M\omega^2(x^2 + y^2 + z^2), & \text{for 3d.} \end{cases} \quad (3)$$

Because of this symmetry, the wave functions of two- and three-dimensional cases are focused on cartesian coordinates

$$\begin{cases} \psi_{2d} = e^{-i(n_x+n_y+1)\omega t} \left(\frac{\alpha}{2^n n! \sqrt{\pi}}\right) e^{-\frac{1}{2}\alpha^2(x^2+y^2)} H_{n_x}(\alpha x) H_{n_y}(\alpha y), \\ \psi_{3d} = e^{-i(n_x+n_y+n_z+\frac{3}{2})\omega t} \left(\frac{\alpha}{2^n n! \sqrt{\pi}}\right)^{\frac{3}{2}} e^{-\frac{1}{2}\alpha^2(x^2+y^2+z^2)} H_{n_x}(\alpha x) H_{n_y}(\alpha y) H_{n_z}(\alpha z). \end{cases} \quad (4)$$

Coefficient of time-dependent exponential indicates that the energy eigenvalues also have the additive properties.

$$E_n = \begin{cases} \hbar\omega(n_x + n_y + 1), & \text{for 2d,} \\ \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right), & \text{for 3d.} \end{cases} \quad (5)$$

In this article, we utilize polar and spherical coordinates to describe the wave function of two- and three-dimensional harmonic oscillators, respectively. The understanding of radial wave function should provide better insight on the mathematical physics of basic quantum mechanics.

VARIABLES SEPARATIONS OF SCHRÖDINGER EQUATION

Schrodinger equation of quantum particle under the influence of central potential energy

$$\left(-\frac{\hbar^2}{2M}\nabla^2 + \frac{1}{2}m\omega^2 r^2\right)\psi(\vec{r}, t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t), \quad (6)$$

can be rewritten using variable separation with energy's eigen values E

$$\frac{1}{u(\vec{r})}\left(-\frac{\hbar^2}{2M}\nabla^2 + \frac{1}{2}m\omega^2 r^2\right)u(\vec{r}) = E = \frac{i\hbar}{T(t)}\frac{\partial T(t)}{\partial t}, \quad (7)$$

to arrive at the time-independent wave function $u(\vec{r})$ and space-independent $T(t)$. One can show that straight-forwardly shows that

$$T(t) = e^{-\frac{1}{\hbar}Et}. \quad (8)$$

The Laplacian ∇^2 in polar (r, θ) and spherical (r, θ, ϕ) coordinates is

$$\nabla^2 = \begin{cases} \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}, & \text{for 2d,} \\ \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), & \text{for 3d.} \end{cases} \quad (9)$$

In the following subsections the time-independent wave function is further separated into radial and angular wave functions. In particular, the radial wave equation can be written as associated Laguerre differential equation [9]

$$\left(x \frac{d^2}{dx^2} + (v + 1 - x) \frac{d}{dx} + \lambda\right) L_\lambda^v(x), \quad (10)$$

where $L_\lambda^v(x)$ is the associated Laguerre polynomial [10]. For non-integer v , L_λ^v is also called generalized Laguerre function [11].

Two-dimensional quantum harmonic oscillator in polar coordinate

Substituting $u(\vec{r}) = R(r)\Theta(\theta)$

$$\frac{1}{R(r)} \left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \frac{1}{r^2} \left[\frac{1}{\Theta(\theta)} \frac{d^2\Theta(\theta)}{d\theta^2} \right] \right) R(r) = E \quad (11)$$

we can arrive at the equation for radial $R(r)$ and angular wave function $\Theta(\theta)$

$$\frac{1}{R(r)} \left(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{l^2}{r^2} \right) R(r) = E, \quad (12a)$$

$$\frac{1}{\Theta(\theta)} \frac{d^2\Theta(\theta)}{d\theta^2} = -l^2. \quad (12b)$$

The solution of Eq. (12b)

$$\Theta(\theta) = \frac{1}{\sqrt{2\pi}} e^{il\theta}. \quad (13)$$

Setting $R(r) = r^l e^{-\frac{1}{2}\alpha^2 r^2} f(\alpha^2 r^2)$, substitution Eq. (12a) can be written in similar form to Eq. (10)

$$\left(u \frac{d^2}{du^2} + (l + 1 - u) \frac{d}{du} + \frac{E}{2\hbar\omega} - \frac{(l + 1)}{2} \right) f(u), \quad (14)$$

Therefore

$$R(r) \propto r^l e^{-\frac{1}{2}\alpha^2 r^2} L_n^l(\alpha^2 r^2), \quad (15)$$

and the quantization of eigen energy is similar to Eq. (5)

$$E_v = \hbar\omega(2n + l + 1). \quad (16)$$

Three-dimensional quantum harmonic oscillator in spherical coordinate

Substituting $u(\vec{r}) = R(r)\Theta(\theta)\Phi(\phi)$

$$\frac{1}{R(r)} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \right) R(r) = E \quad (17)$$

we can arrive at the equation for radial $R(r)$ and angular wave function $\Theta(\theta)$

$$\frac{1}{R(r)} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\hbar l(l + 1)}{r^2} \right) R(r) = E, \quad (18a)$$

$$\frac{1}{\Theta(\theta)} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) - \frac{m^2}{\sin^2\theta} \right) \Theta(\theta) = -l(l + 1), \quad (18b)$$

$$\frac{1}{\Phi(\phi)} \frac{d^2\Phi(\phi)}{d\phi^2} = -m^2. \quad (18c)$$

The solution of Eq. (17b) and (17c) is the spherical harmonics function [12], [13]

$$\Theta(\theta)\Phi(\phi) = Y_{lm}(\theta, \phi). \quad (19)$$

Setting $R(r) = r^l e^{-\frac{1}{2}\alpha^2 r^2} g(\alpha^2 r^2)$, substitution Eq. (12a) can be written in similar form to Eq. (10)

$$\left(u \frac{d^2}{du^2} + \left(l + \frac{3}{2} - u \right) \frac{d}{du} + \frac{E}{2\hbar\omega} - \frac{(l + 3/2)}{2} \right) g(u), \quad (20)$$

Therefore

$$R(r) \propto r^l e^{-\frac{1}{2}\alpha^2 r^2} L_n^{l+\frac{1}{2}}(\alpha^2 r^2), \quad (21)$$

and the quantization of eigen energy is similar to Eq. (5)

$$E_v = \hbar\omega \left(2n + l + \frac{3}{2} \right). \quad (22)$$

RADIAL AND ANGULAR WAVE FUNCTIONS

Eq. (51) and (21) show that the radial wave functions can be written in term of associated Laguerre polynomials. The normalization factors that satisfy

$$1 = \begin{cases} \int_0^\infty [R(r)]^2 r dr, & \text{for 2d,} \\ \int_0^\infty [R(r)]^2 r^2 dr, & \text{for 3d,} \end{cases} \quad (23)$$

can be found using the orthogonality of associated Laguerre polynomials

$$\int_0^\infty x^k e^{-x} L_v^k(x) L_w^k(x) dx = \frac{\Gamma(v+k+1)}{v!} \delta_{vw} \quad (24)$$

Such that

$$R(\vec{r}) = \begin{cases} \sqrt{\frac{n! 2(a)^{2l+2}}{(n+l)!}} r^l e^{-\frac{1}{2}\alpha^2 r^2} L_n^l(\alpha^2 r^2), & \text{for 2d,} \\ \sqrt{\frac{n! 2(a)^{2l+3}}{\Gamma(n+l+\frac{3}{2})}} r^l e^{-\frac{1}{2}\alpha^2 r^2} L_n^{l+\frac{1}{2}}(\alpha^2 r^2) & \text{for 3d.} \end{cases} \quad (23)$$

Here $\Gamma(x)$ is the Gamma function.

Concerning the angular wave function Eqs. (12b) and (18b-c) can be associated with the eigen equations of the angular momentum in two and three dimensions, respectively [14]. Eq. (12b) is equivalent with the eigen equation

$$\vec{L}_{2d}\Theta(\theta) = \hbar l\Theta(\theta) \quad (24)$$

of the two-dimensional angular momentum

$$\vec{L}_{2d} = -i\hbar \frac{\partial}{\partial \theta}. \quad (25)$$

Meanwhile, Eq. (18b) is equivalent with the eigen equations

$$L_{3d}^2 Y_{lm}(\theta, \phi) = \hbar^2 l(l+1) Y_{lm}(\theta, \phi) \quad (26)$$

$$\hat{z} \cdot \vec{L}_{3d} Y_{lm}(\theta, \phi) = \hbar m Y_{lm}(\theta, \phi)$$

of the three-dimensional angular momentum

$$\vec{L}_{3d} = -i\hbar \left[\hat{x} \left(-\sin \phi \frac{\partial}{\partial \theta} - \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right) + \hat{y} \left(\cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right) + \hat{z} \frac{\partial}{\partial \phi} \right]. \quad (27)$$

Finally, the full time-space dependent eigen wave function is

$$\psi = \begin{cases} \sqrt{\frac{n! (a)^{2l+2}}{\pi(n+l)!}} r^l e^{-\frac{1}{2}\alpha^2 r^2} L_n^l(\alpha^2 r^2) e^{il\theta} e^{-i(2n+l+1)\omega t}, & \text{for 2d,} \\ \sqrt{\frac{n! 2(a)^{2l+3}}{\Gamma(n+l+\frac{3}{2})}} r^l e^{-\frac{1}{2}\alpha^2 r^2} L_{\nu}^{l+\frac{1}{2}}(\alpha^2 r^2) Y_{lm}(\theta, \phi) e^{-i(2n+l+\frac{3}{2})\omega t}, & \text{for 3d.} \end{cases} \quad (28)$$

CONCLUSION

Two- and three-dimensional quantum oscillator harmonics is discussed in terms of radial and angular eigen wave functions. The angular wave functions are well-described using sinusoidal and spherical harmonics functions, respectively. Using appropriate ansatz, it is shown that the radial wave function is proportional to $r^l e^{-\frac{1}{2}\alpha^2 r^2} L_n^k(\alpha^2 r^2)$, where l is related to the eigenvalues of angular momentum operators and L_n^k is generalized/associated Laguerre polynomials.

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