Advanced Quantum Mechanics Lab

Plotting Landau Levels

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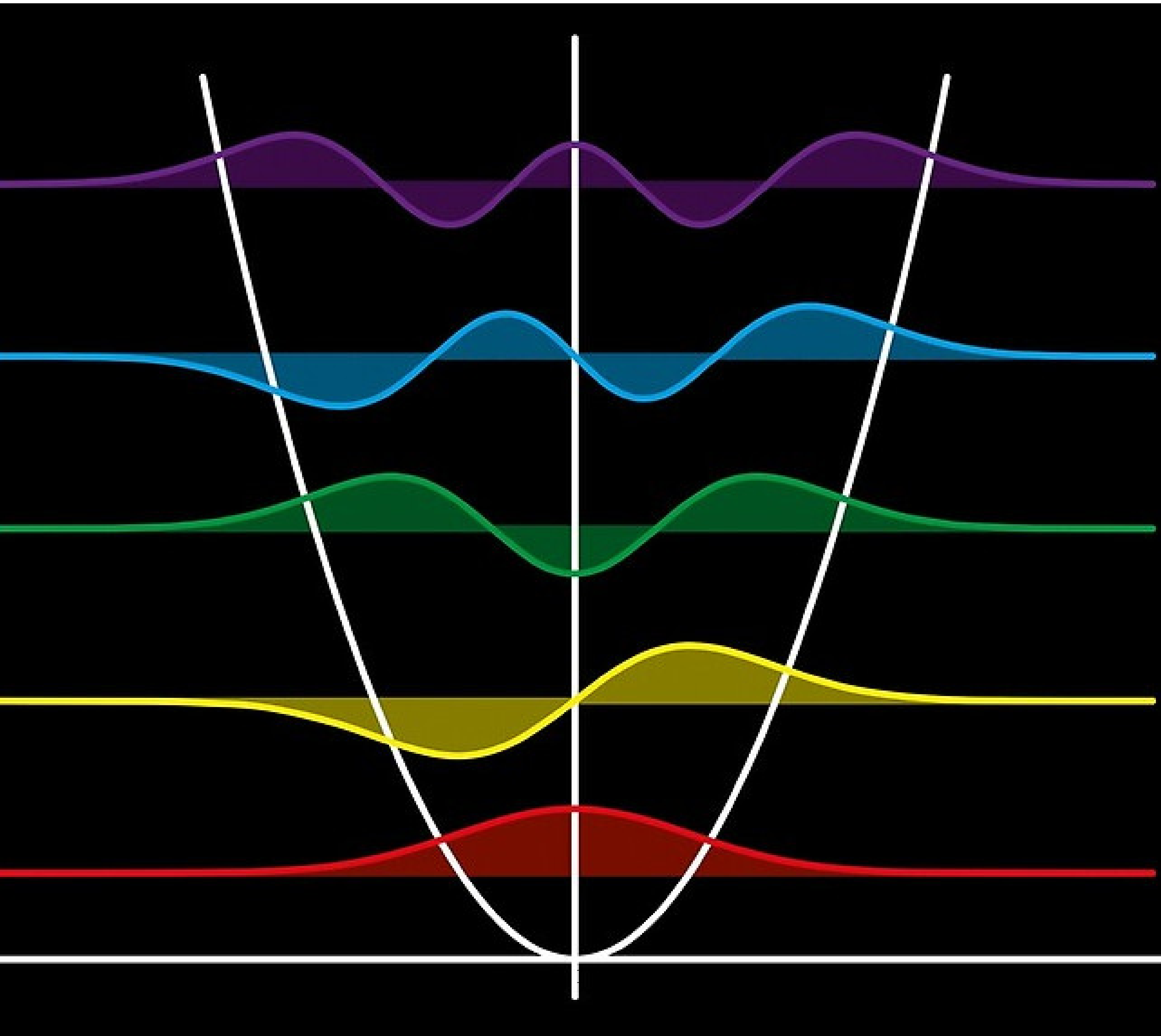
Engineering Physics



Contents

1. Objectives

The aim of this experiment is to numerically calculate the wave function and probability density of a Landau state and study the convergence with classical mechanics at high Landau level indices.

2. Overview and Theory

2.1 Theoretical basis

Classically, when an electron enters a constant or stationary magnetic field, it is pulled into a circular orbit such that the magnetic field is directed normal to the plane of the orbit. The motion arises from the Lorentz force acting on the electron, which is given by:

$$\vec{F} = -e\left(\vec{v} \times \vec{B}\right) \tag{2.1}$$

The constant angular frequency of the orbital motion is called the cyclotron orbit, and it is given by:

$$\omega_c = \left|\frac{eB}{m}\right| \tag{2.2}$$

The radius of the orbit is:

$$R_C = \frac{v}{\omega_C} = \frac{\sqrt{2mE}}{eB}, \tag{2.3}$$

where v is the constant magnitude of the velocity, and E is the kinetic energy.

Here, we want to examine the quantisation of these orbits. The simplest algebra is in the Landau gauge where there is only one component of the vector potential:

$$\vec{A} = (0, Bx, 0) \tag{2.4}$$

Thus, in the absence of any external potential, other than the vector potential giving rise to the magnetic field, the stationary Schrödinger equation can be written as:

$$\left\{\frac{1}{2m}\left[-\hbar^2\frac{\partial^2}{\partial x^2} + \left(-i\hbar\frac{\partial}{\partial y} + eBx\right)^2\right]\right\}\psi(r) = E\psi(r) \tag{2.5}$$

Expanding the inner bracket:

$$\left[-\frac{1}{2m}\nabla^2 - \frac{ie\hbar Bx}{m} + \left(-i\hbar\frac{\partial}{\partial y} + eBx\right)^2\right]\psi(r) = E\psi(r) \tag{2.6}$$

The vector potential does not depend on y, which suggests that the wave function should be a product of a plane wave depending on y and another kind of function that depends on x:

$$\psi(x)e^{iky} \tag{2.7}$$

Substituting this in the Schrödinger equation, we obtain:

$$\left[-\frac{1}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega_c^2\left(x+\frac{\hbar k}{eB}\right)^2\right]\psi(x)=E\psi(x), \tag{2.8}$$

where k is the y component of the electron momentum. This expression we have obtained is very close to Schrödinger's equation for a one-dimensional quantum harmonic oscillator, with $\omega=\omega_c$ and a small displacement in the x coordinate, of magnitude $x_0=\frac{\hbar k}{eB}$. From this equation, we obtain the so called **Landau Levels**, defined as:

$$\hbar\omega_c\left(\frac{1}{2}+n\right) \tag{2.9}$$

The wave function in this case is just the wave function of the harmonic oscillator shifted by x_0:

$$\psi_n(x)=\frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega_c}{\hbar\pi}\right)^{1/4}e^{-m\omega_c(x-x_0)^2/2\hbar}H_n\left(\sqrt{\frac{m\omega_c}{\hbar}}(x-x_0)\right), \tag{2.10}$$

where n is the Landau Level index $n=1,2,3,...$, and H_n are the Hermite polynomials.

The characteristic length of this problem, called the magnetic length, is defined as:

$$l_B=\sqrt{\frac{\hbar}{m\omega_c}}=\sqrt{\frac{\hbar}{eB}} \tag{2.11}$$

2.2 Numerical calculation of Landau levels

In order to compute the Landau levels with a computer program, we will use the following recursive formula:

$$\psi_n(\xi)=\sqrt{\frac{2}{n}}\left(\xi\psi_{n-1}(\xi)-\sqrt{\frac{n-1}{2}}\psi_{n-2}(\xi)\right), \tag{2.12}$$

where:

$$\xi=\left(\frac{m\omega_c}{\hbar}\right)x \tag{2.13}$$

Note that here we neglect the x_0 offset, as it is very small. Knowing the expression for the first two landau levels, we can find all the rest:

$$\psi_0(x)=\left(\frac{m\omega_c}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega_c}{2\hbar}x^2\right) \tag{2.14}$$

$$\psi_0(x)=\sqrt{2\pi}\left(\frac{m\omega_c}{\pi\hbar}\right)^{3/4}x\exp\left(-\frac{m\omega_c}{2\hbar}x^2\right) \tag{2.15}$$

The code implementing this method can be found in this GitHub repository.

3. Results

The results obtained for the Landau levels $n=18$, $n=50$ and $n=100$ are shown in the following figures:

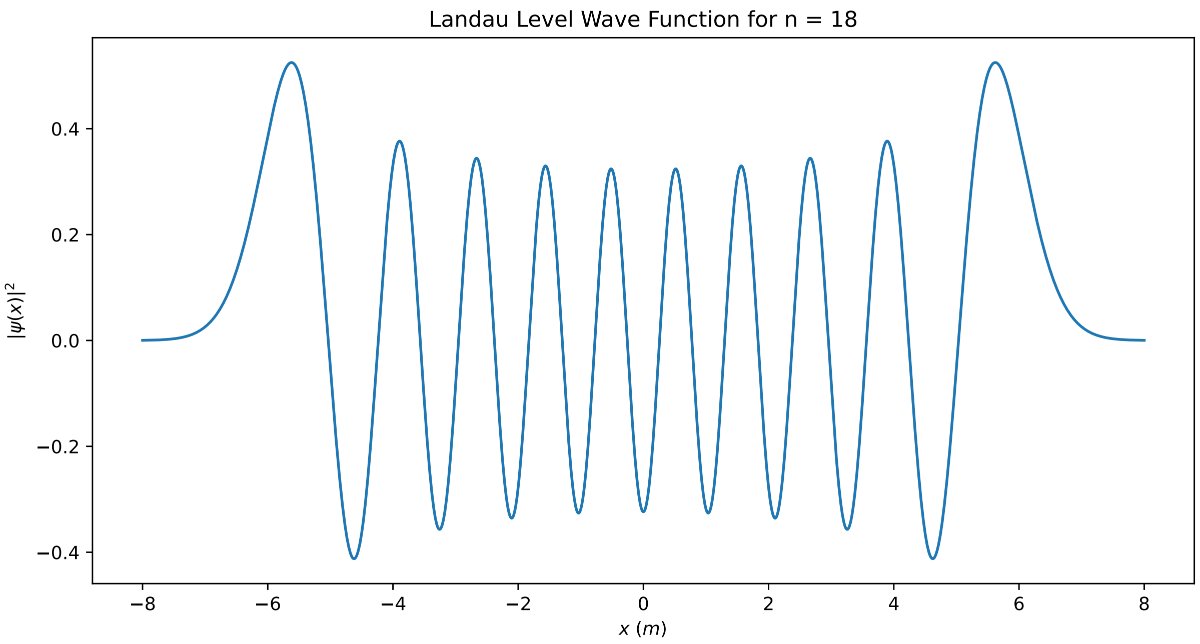


Figure 1: Wave function for the 18-th Landau level.

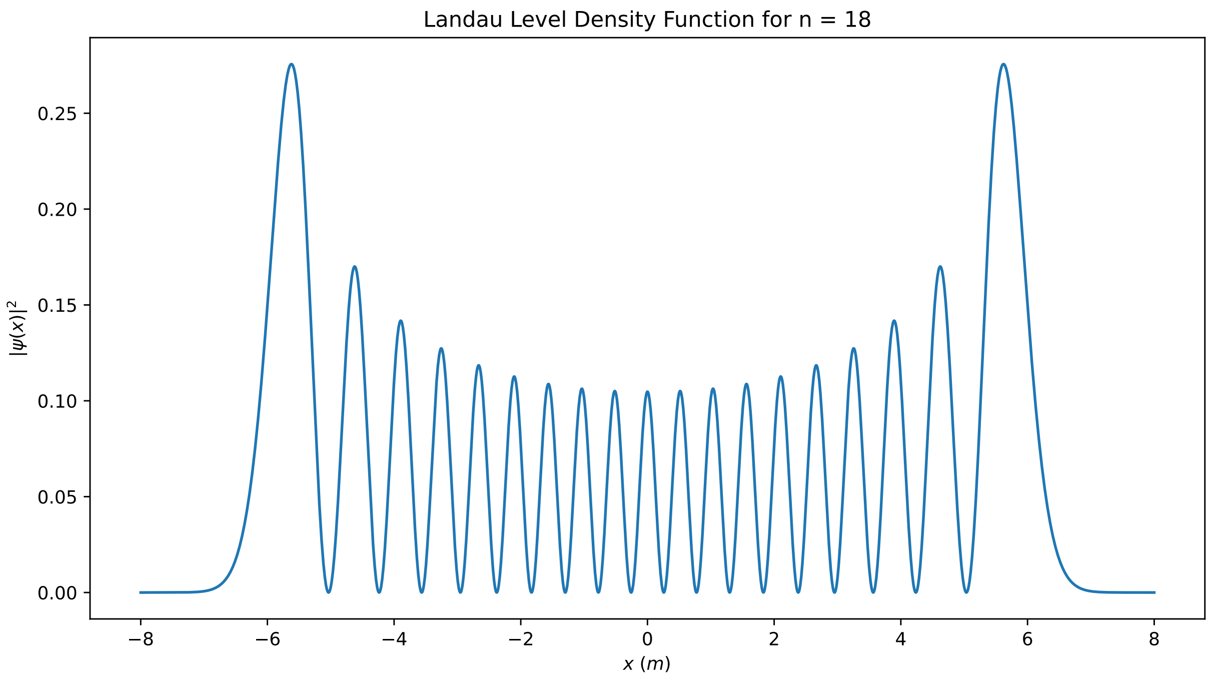


Figure 2: Density function for the 18-th Landau level.

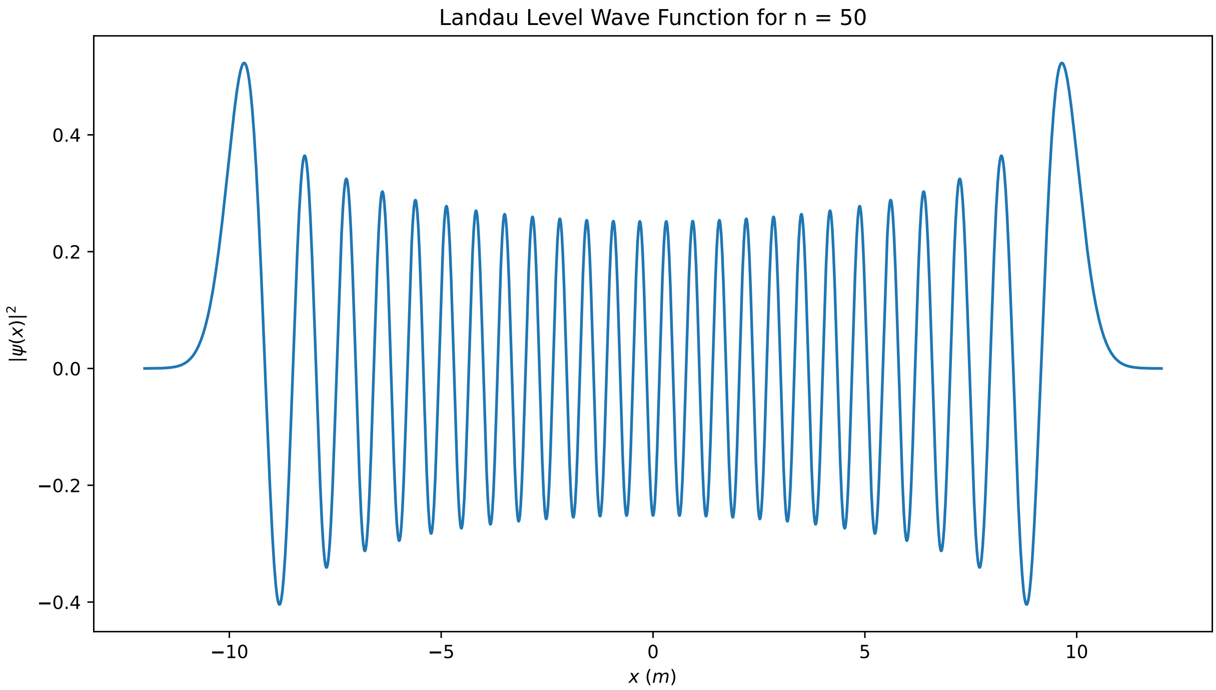


Figure 3: Wave function for the 50-th Landau level.

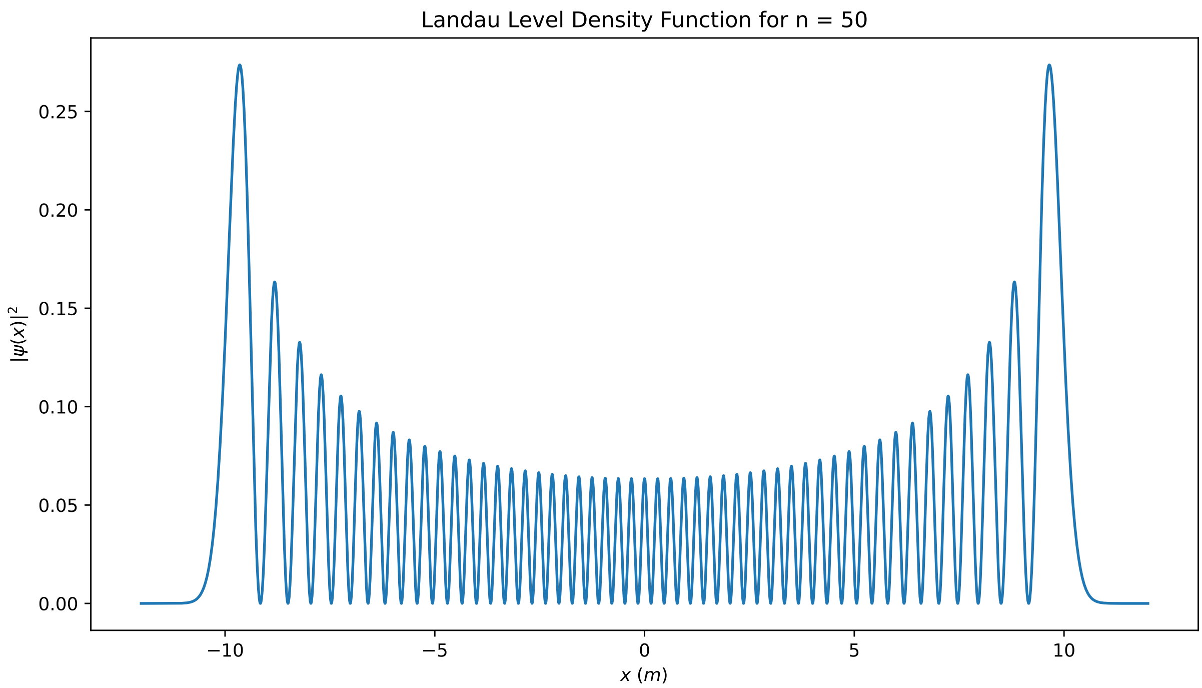


Figure 4: Density function for the 50-th Landau level.

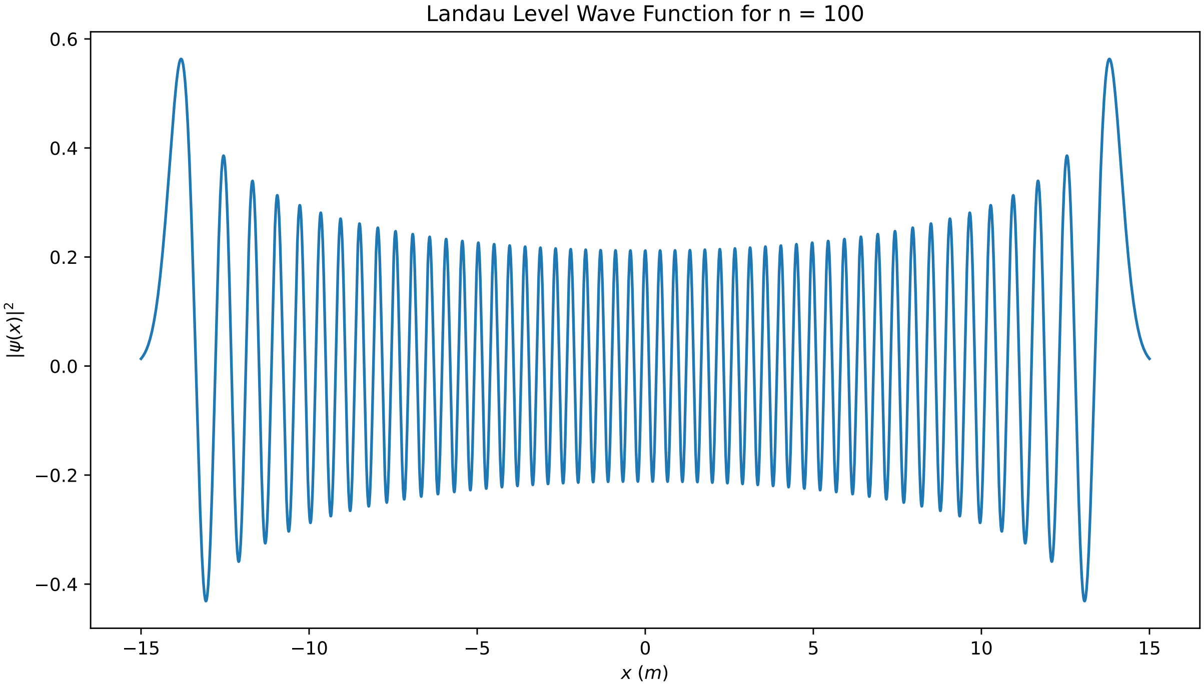


Figure 5: Wave function for the 100-th Landau level.

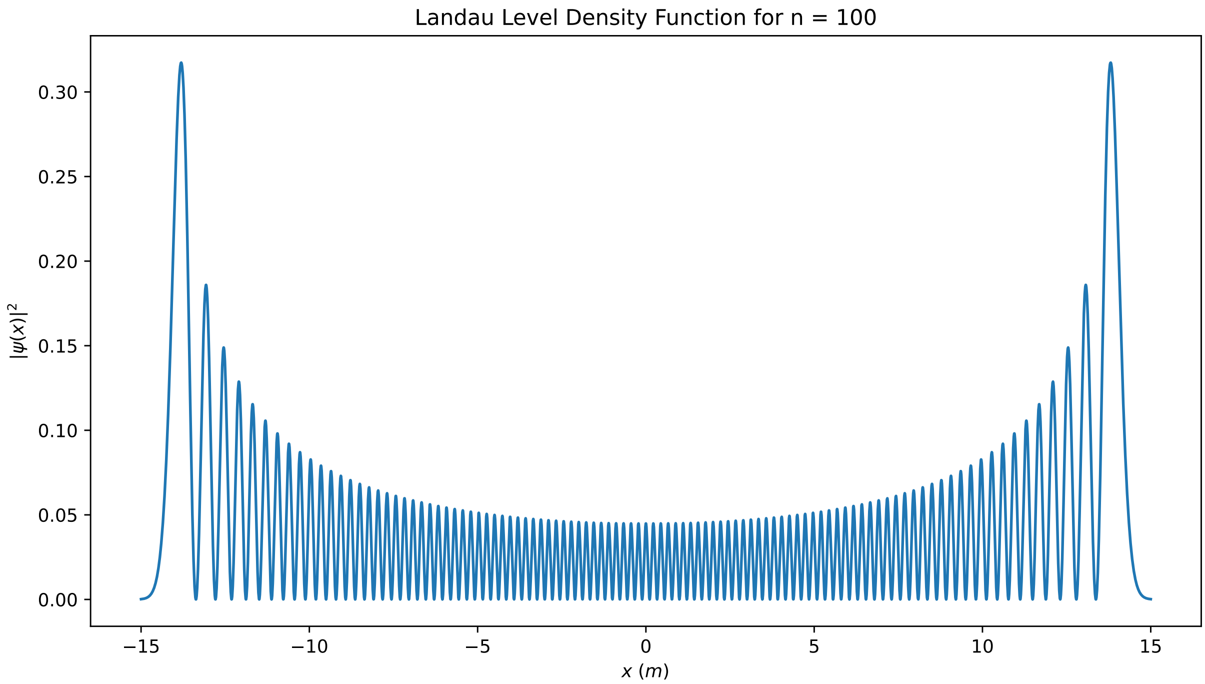


Figure 6: Density function for the 100-th Landau level.

4. Discussion

It is interesting to check that as $n \to \infty$, things get closer and closer to the classical state of things. The classical probability distribution of finding the particle between any given location x and $x + dx$ can be calculated because the motion is completely defined. For instance, assuming that the particle is initially at A with zero velocity, we have that $x(t) = A\cos\omega_c t$, with $A = \sqrt{2E/m}$. It is evident that, at time t, the probability of finding the particle at $x(t)$ is one; and the probability of finding it anywhere else is zero. This can be expressed using probability distributions by using the δ-function[1]:

$$p(x,t) = \delta(x - A\cos\omega_c t) \tag{4.1}$$

To calculate the probability of finding the particle at x at any time, we need to average $p(x,t)$ over time. We can do this over half a period, due to the periodic nature of the motion, so we find:

$$p(x) = \frac{\omega}{\pi}\int_0^{\pi/\omega} \delta(x - A\cos\omega_c t)dt = \frac{1}{\pi}\frac{1}{\sqrt{A^2 - x^2}} \tag{4.2}$$

Intuitively, what this means is that the probability is minimum where the velocity is largest, which is at the centre of the potential region. As the speed is larger there, the particle remains in that position less time, and thus the probability of finding the particle there is lower. On the other hand, the probability is largest at the extremes of the potential region, for the same reason (there are the points of minimum velocity).

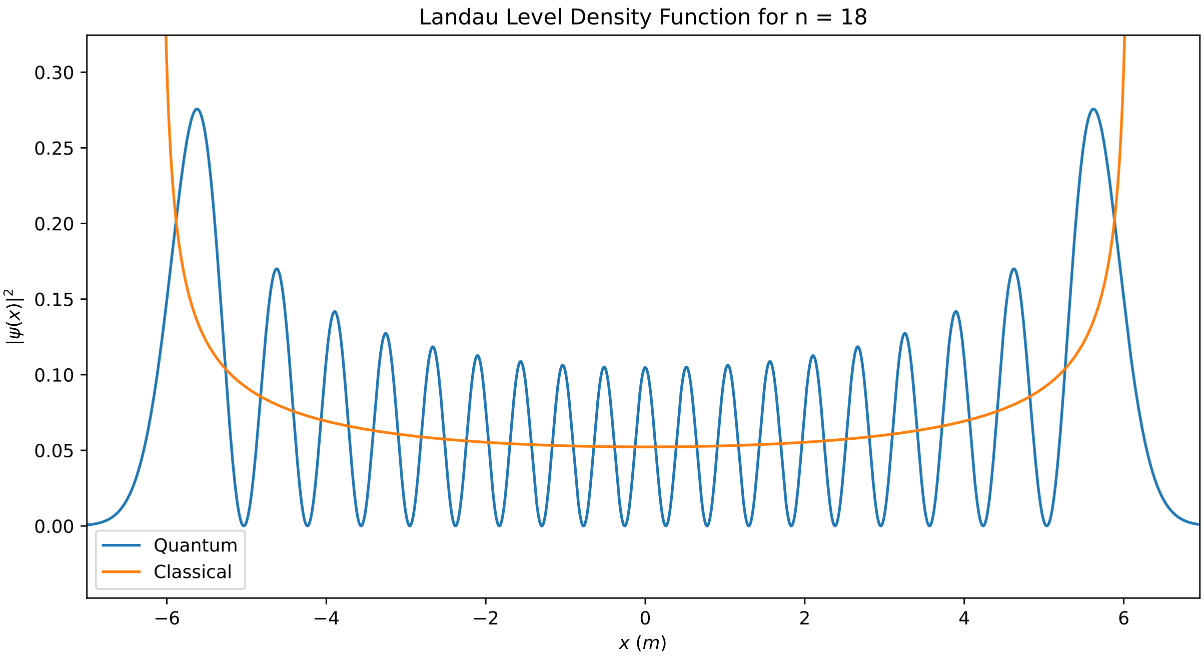


Figure 7: Quantum and classical density function for the 18-th Landau level.

[1] Remember that $\delta(x - x_0)$ is zero everywhere except at $x = x_0$. It also satisfies $\int_{-\infty}^{\infty} \delta(x - x_0)f(x)dx = f(x_0)$.

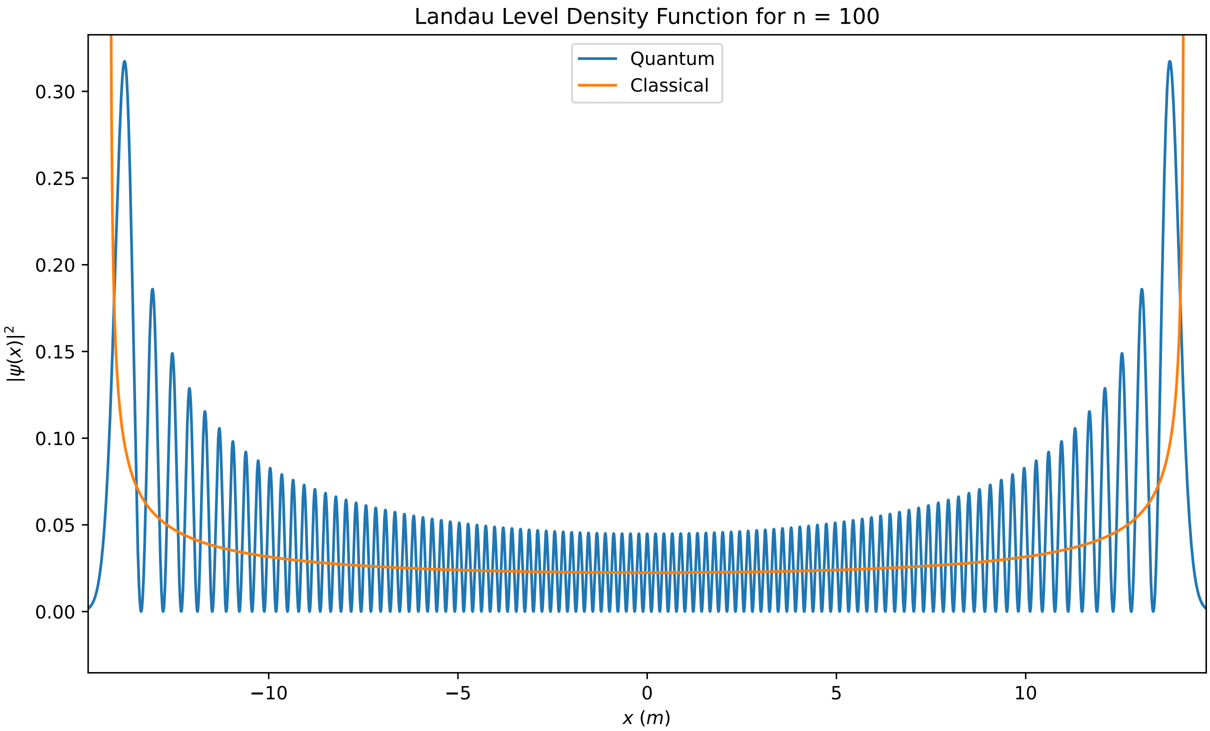


Figure 8: Quantum and classical density function for the 100-th Landau level.

If we take the expression in **Equation 4.2** and plot it over the density function for the $n = 18$ and the $n = 100$ Landau levels, we obtain the plots in **Figure 7** and **Figure 8**. Note the similarity between the classical and the quantum density functions, which is clearer the larger the n.

5. Conclusion

In this simulation experiment, we have been able to calculate the wave functions and the density functions for the $n = 18, 50, 100$ Landau levels. Furthermore, by computing the classical density function for the quantum oscillator, we have been able to verify Bohr's correspondence principle, which states that, for large quantum numbers, the laws of quantum physics must give identical results to the laws of classical physics.