School of Artificial Intelligence

Amrita Vishwa Vidyapeetham, Delhi NCR

Project Report

Quantum Mechanics of Gravitational Potential Wells: Analytical and Numerical Solutions to the One-Dimensional Time-Independent Schrödinger Equation with $V(x) = \frac{\alpha}{x}$

23PHY114 Computational Mechanics 2

23MAT112 Mathematics for Intelligent Systems 2

Semester: II

Academic Year: 2024 – 2025 [Even]

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2024 - 25

CERTIFICATE

This is to certify that the report entitled **Quantum Mechanics of Gravitational Potential Wells: Analytical and Numerical Solutions to the One-Dimensional Time-Independent Schrödinger Equation** with $V(x) = \frac{\alpha}{x}$ submitted by **Anagha Manoj** (24105),**Gowripriya R.** (24113),**Parkhi Mahajan** (24126) & **Tanvi Bhardwaj** (24136) to the Amrita Vishwa Vidyapeetham, Faridabad in partial fulfillment of the B.Tech. degree in Artificial Intelligence and Data Science is a bonafide record of the seminar work carried out by him under our guidance and supervision. This report in any form has not been submitted to any other University or Institute for any purpose.

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DECLARATION

We hereby declare that the project report **Quantum Mechanics of Gravitational Potential Wells: Analytical and Numerical Solutions to the One-Dimensional Time-Independent Schrödinger Equation** with $V(x) = \frac{\alpha}{x}$, submitted for partial fulfillment of the requirements for the award of the degree of Bachelor of Technology of the School of AI, Amrita Vishwa Vidyapeetham, Faridabad, India is a bonafide work done by us under supervision of Dr.Mrittunjoy Guha Majumdar and Dr.Rakesh Kumar .

This submission represents our ideas in our own words and where ideas or words of others have been included, we have adequately and accurately cited and referenced the original sources.

We also declare that we have adhered to ethics of academic honesty and integrity and have not misrepresented or fabricated any data or idea or fact or source in my submission. We understand that any violation of the above will be a cause for disciplinary action by the institute and/or the University and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been obtained. This report has not been previously formed the basis for the award of any degree, diploma or similar title of any other University.

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09-06-2025

Abstract

This project explores the quantum mechanical behavior of a particle under the influence of a gravitational potential $V(x) = \frac{\alpha}{x}$ in one dimension. We derive the dimensionless form of the time-independent Schrödinger equation and solve it leading to energy quantization and Laguerre polynomial-based wavefunctions. The project incorporates advanced linear algebra techniques, optimization methods (e.g., using MATLAB's 'fmincon'), statistical analysis of expectation values, and conditional probability models.

Acknowledgement

We take this opportunity to express our deepest sense of gratitude and sincere thanks to everyone who helped us to complete this work successfully. We express our sincere thanks to **Prof. Kamal Bijlani**, Dean of school of AI, Amrita Vishwa Vidyapeetham, Faridabad, for providing us with all the necessary facilities and support. We would like to place on record our sincere gratitude to our project guides **Dr.Mrittunjoy Guha Majumdar** and **Dr.Rakesh Kumar** , School of AI, Amrita Vishwa Vidyapeetham, Faridabad for their continuous guidance, mentorship, and encouragement throughout the course of this work. Without their support and cooperation, this work would not have been completed.Finally, we thank our family, and friends who contributed to the successful fulfillment of this seminar work.

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$\hbar$	Reduced Planck's constant
m	Mass of the particle
$\psi(x)$	Wavefunction as a function of position
$V(x)$	Potential energy as a function of position
E	Total energy of the particle
k	Wave number, defined as $k^2 = \frac{2mE}{\hbar^2}$
A, B, C, D	Constants of integration from general solutions
L	Width of the infinite potential well
n	Quantum number ($n = 1, 2, 3, \ldots$)
α	Constant in the inverse potential $\frac{\alpha}{x}$
$F(x)$	Force acting on the particle
v	Velocity of the particle
T	Kinetic energy
Ω	Unit of resistance
ϵ	Epsilon
λ	Wavelength
δ	Delta
π	Pi
$\int$	Integral

Chapter 1

Objectives of the Project

- To obtain solutions to the one- dimensional time-independent Schrödinger equation for the gravitational potential $V = \frac{\alpha}{x}$.
- To derive the corresponding normalized wavefunction and their discrete energy levels.
- To analyze the impact of boundary conditions, with a focus on hard-wall confinement.
- To perform optimization based on the results found
- To relate the findings to practical applications.

Chapter 2

Literature Survey

Quantum mechanics has long been applied to investigate bound states in various potential fields. Our work builds upon and extends several foundational studies and methods from the literature, as outlined below:

- Quantum Bound States in Inverse Potentials

  Quantum systems involving inverse potentials such as $V(x) = -\frac{1}{x}$ are known for producing discrete bound states with energy quantization. Such systems, resembling hydrogen-like atoms, exhibit singularities that significantly affect wavefunction behavior near the origin. The standard solutions involve special functions and boundary condition analysis. This foundational understanding provides the basis for solving our gravitational potential well problem. [1]

- Dimensional Analysis and Non-dimensionalization:

  Transforming physical equations into non-dimensional forms is essential for generalizing solutions across systems with different scales. In quantum mechanics, non-dimensionalization simplifies the Schrödinger equation, enabling easier numerical computation and deeper theoretical insights. In our study, this technique was crucial to eliminate constants like $\hbar$ and m, leading to a simplified dimensionless differential equation. [2]

- Associated Laguerre Polynomial Solutions: Laguerre and associated Laguerre polynomials frequently appear in the solutions of radial and singular potential problems in quantum mechanics, particularly in hydrogen-like systems. These

polynomials arise naturally through transformation of the Schrödinger equation into the confluent hypergeometric form. In our project, they are used to derive normalized, physically meaningful wavefunctions for the gravitational potential. [3]

- Gravitational Analogues to Quantum Systems: Theoretical studies have explored the analogy between gravitational and electrostatic forces in quantum mechanics. The concept of gravitationally bound "Bohr-like" systems introduces new challenges due to the vastly different strength of gravitational interactions. Our project adopts this analogy to construct a quantum system where the gravitational potential is modeled using $V(x) = \frac{\alpha}{x}$, and explores the implications for bound states. [4]

- Optimization of Quantum States:

  Recent advancements in computational physics have incorporated optimization techniques to refine solutions of quantum systems. Using tools such as MATLAB's fmincon, researchers can minimize spatial variance, energy, or other functionals to obtain optimal wavefunctions. In our work, optimization was applied to construct superpositions of wavefunctions with minimal spatial spread, providing improved understanding of quantum confinement. [5]

- Ultracold Neutrons in Earth's Gravitational Potential: Ultracold neutrons (UCNs) are particles possessing extremely low kinetic energies, typically in the picoelectronvolt (peV) range, which makes them susceptible to confinement by Earth's gravitational field [6]. These low-velocity neutrons are governed by quantum mechanics and can be experimentally manipulated to observe gravitational quantum effects.

  The gravitational potential generated by Earth acts as a natural quantum well, enabling the formation of discrete energy levels for UCNs. This real-world manifestation of quantum bound states under gravity offers strong experimental support for theoretical models that study gravitational potentials of the form $V(x) = \frac{\alpha}{x}$.

  UCNs have been utilized in several cutting-edge experiments, including:

- **Gravity Resonance Spectroscopy (GRS):** Determining the resonant frequencies of UCNs trapped in gravitational potentials to investigate gravitational quantization [6].
- **Quantum States of Neutrons:** Probing how UCNs behave in confined gravitational environments and interact with reflecting surfaces.
- **Fundamental Physics:** Testing the weak equivalence principle and exploring deviations from the Standard Model through precision neutron experiments.
- **Thermodynamics of Quantum Neutron Gas:** Studying how gravitational confinement influences the thermodynamic behavior of ultracold neutron ensembles [7].

These experimental insights validate the feasibility of gravitationally bound quantum states and motivate the use of idealized models in this project to analyze the Schrödinger equation under inverse gravitational potentials.

Chapter 3

Introduction To Quantum Mechanics

Quantum mechanics describes the behavior of particles at atomic and subatomic scales. It departs from classical mechanics by introducing wavefunctions, quantization of energy levels, and probabilistic interpretations of particle properties.

3.1 General Case: Particle in an Infinite Square Well (V (x) = 0 in $0 < x < L$) Derivation of Time-Independent Schrödinger Equation for V (x) = 0

The time-independent Schrödinger equation in one dimension is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)\} \tag{3.1}$$

where:

- $\hbar$ is the reduced Planck's constant,
- m is the mass of the particle,
- $\psi(x)$ is the wavefunction,
- $V(x)$ is the potential energy as a function of position,
- E is the total energy of the particle.

Substituting $V(x) = 0$: For a particle confined in a region where $V(x) = 0$, such as inside an infinite potential well, the equation reduces to:

$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{3.2}$$

Rewriting the above expression, we bring all terms to one side:

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \tag{3.3}$$

We now define $k^2 = \frac{2mE}{\hbar^2}$, simplifying the equation to:

$$\frac{d^2\psi}{dx^2} + k^2\psi(x) = 0 \tag{3.4}$$

On Solving the Differential Equation: The above second-order linear differential equation has the general solution:

$$\psi(x) = A \cdot \sin(kx) + B \cdot \cos(kx)$$

where A and B are constants determined using boundary conditions.

On Applying Boundary Conditions: We examine two typical scenarios:

- **Free Particle (no boundaries, $-\infty < x < \infty$)**
  - In this case, any values of A and B are valid.
  - Alternatively, the solution may be expressed using complex exponentials: $\psi(x) = C \cdot e^{ikx} + D \cdot e^{-ikx}$
  - The energy spectrum is continuous with $E > 0$
- **Infinite Potential Well ($0 < x < L$, $V = \infty$ outside)**
  - Boundary conditions are: $\psi(0) = 0$ and $\psi(L) = 0$
  - Applying $\psi(0) = 0 \Rightarrow B = 0$
  - Applying $\psi(L) = 0 \Rightarrow \sin(kL) = 0 \Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}$

Hence, the wavefunction simplifies to:

$$\psi_n(x) = A \cdot \sin\left(\frac{n\pi x}{L}\right) \tag{3.5}$$

On Normalizing the Wavefunction: To ensure the wavefunction represents a valid probability distribution, we require:

$$\int_0^L |\psi_n(x)|^2 dx = 1$$

Substituting $\psi_n(x) = A \cdot \sin\left(\frac{n\pi x}{L}\right)$, we get:

$$\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = A^2 \cdot \frac{L}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

Thus, the normalized wavefunction becomes:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{n\pi x}{L}\right) \tag{3.6}$$

Energy Quantization:

Substituting the value of $k = \frac{n\pi}{L}$ into the expression for E, we obtain the quantized energy levels:

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \cdot \left(\frac{n\pi}{L}\right)^2 = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{3.7}$$

Here, $n = 1, 2, 3, \ldots$ represents the quantum number. The energy spectrum is discrete and increases quadratically with n.

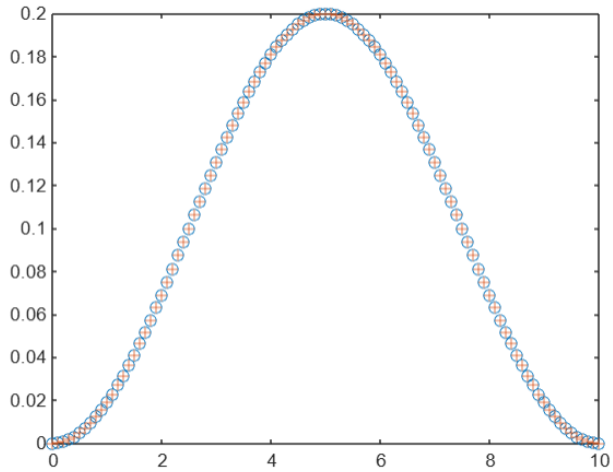

Figure 3.1: Plot of the normalized wavefunction $\psi_n(x)$ for a particle in an infinite potential well of width $L = 10$.

3.2 Our Specific System: $V(x) = \frac{\alpha}{x}$

The potential studied here resembles an attractive gravitational field in one dimension.Unlike polynomial or linear potentials, the inverse form leads to modified boundary conditions and non-trivial wavefunctions.

Motivation: Integrating Quantum Mechanics with Gravity

The integration of quantum mechanics with gravitational systems serves as a theoretical framework to probe the behavior of matter under conditions where both quantum and gravitational effects are non-negligible. In this context, quantum mechanics enables us to:

- Define gravitationally bound wavefunctions $\psi_n(r)$ that describe the spatial distribution of a quantum particle under a gravitational potential.
- Derive quantized energy levels within a gravitational potential well, in contrast to the continuous energy spectrum predicted by classical mechanics.
- Normalize wavefunctions to satisfy the probabilistic interpretation of quantum theory, ensuring that the total probability of finding the particle in the defined region is unity.

- Predict the probabilistic position distribution of particles influenced by gravity, thereby highlighting phenomena such as quantum uncertainty and delocalization—effects not captured by classical Newtonian physics.

Although gravitational forces are extremely weak at quantum scales (e.g., between a particle and Jupiter), such scenarios offer a simplified and idealized model—a theoretical test bed—for understanding the nature of quantum states under gravitational influence.

This approach allows us to pose and reflect on foundational questions such as:

"What would a quantum gravity system look like in the non-relativistic regime?"

Such studies help bridge the gap between quantum mechanics and gravitational physics, contributing to the broader quest for a unified theory that consistently explains nature at all scales.

Chapter 4

Classical Description of Specific Physical System

4.1 Classical Description of the System with $V(x) = \frac{\alpha}{x}$

In classical mechanics, the motion of a particle of mass m under a potential energy function $V(x)$ is governed by Newton's second law. For this system, the potential energy is given by:

$$V(x) = \frac{\alpha}{x}$$

where α is a constant determining the strength and nature of the interaction. This potential is defined for $x > 0$ and becomes singular as $x \to 0$.

1. Force Acting on the Particle

The force $F(x)$ is obtained from the negative gradient of the potential:

$$F(x) = -\frac{dV}{dx} = -\frac{d}{dx}\left(\frac{\alpha}{x}\right) = \frac{\alpha}{x^2}$$

For $\alpha > 0$, this is a repulsive force pushing the particle away from the origin.

2. Total Mechanical Energy

The total energy E of the particle is given by:

$$E = T + V(x) = \frac{1}{2}mv^2 + \frac{\alpha}{x}$$

where T is the kinetic energy of the particle.

3. Classically Allowed Region

A particle can only exist where its kinetic energy is non-negative, i.e.,

$$E \geq V(x) \Rightarrow \frac{1}{2}mv^2 \geq 0 \Rightarrow E \geq \frac{\alpha}{x}$$

This gives the classically allowed region:

$$x \geq \frac{\alpha}{E}$$

Hence, the particle is confined to the region $x \in \left[\frac{\alpha}{E}, \infty\right)$ and cannot approach the origin.

4. Nature of Motion

- As the particle moves closer to $x = \frac{\alpha}{E}$, its velocity decreases due to increasing potential energy.
- As it moves away (i.e., $x \to \infty$), the potential energy decreases and kinetic energy increases.

5. Potential Energy Plot

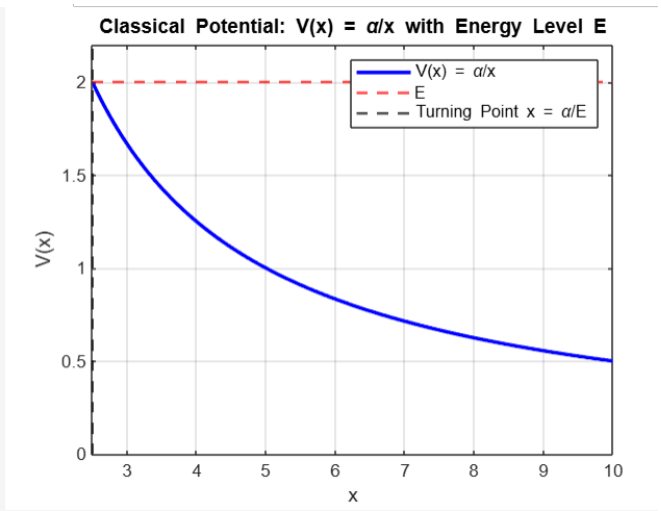

Figure 4.1: Classical potential energy function $V(x) = \frac{\alpha}{x}$, showing the singularity at $x = 0$ and the classically allowed region for a particle with energy E. The vertical line indicates the classical turning point at $x = \frac{\alpha}{E}$.

Chapter 5

Quantum Realization

Introduction

The Schrödinger's time-independent equation is a cornerstone of quantum mechanics, traditionally applied to microscopic particles. In our project, we extend this framework to a gravitational system, where the potential energy is defined as:

$$V(x) = \frac{\alpha}{x}, \quad \text{with } \alpha = -GMm$$

The Potential

The potential used is:

$$V(x) = \frac{\alpha}{x}, \quad \text{where } \alpha = -GMm$$

$$G = 6.6743 \times 10^{-11}\ \text{m}^3\text{kg}^{-1}\text{s}^{-2}, \quad M = 1.898 \times 10^{27}\ \text{kg}, \quad m = 1.48 \times 10^{23}\ \text{kg}$$

Calculation

We consider the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

With $V(x) = \frac{\alpha}{x}$, the equation becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{\alpha}{x}\psi = E\psi$$

Behavior near the origin ($x \to 0$)

As $x \to 0$, the potential grows, increasing the wave function significantly. Assume:

$$\psi(x) = x^p$$

Behavior at infinity ($x \to \infty$)

As $x \to \infty$, $V(x) \to 0$, the equation approximates:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

So:

$$\psi(x) \sim e^{-\beta x}$$

Combining both behaviors:

$$\psi(x) = x^p e^{-\beta x}$$

Now we find the second derivative of $\psi(x)$ and substitute into the Schrödinger equation. Comparing coefficients, we find allowed values of $n = 0, 1$ and solve for β.

However, using physical constants, we observe:

$$\text{Magnitude of } \alpha \sim 10^{39}, \quad \hbar^2 \sim 10^{-68}$$

This results in extreme decay, rendering the wave function physically meaningless due to scale mismatch.

Dimensionless Form

To address this, we redefine variables using:

$$\xi = \frac{x}{a}$$

Let wave function be:

$$\psi(x) = \phi(\xi)$$

Rewrite Schrödinger's Equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{\alpha}{x}\psi = E\psi \qquad \left[\mu = \frac{m_1 m_2}{m_1 + m_2}\right] \tag{5.1}$$

Let

$$\xi = \frac{x}{a}$$

Substituting into Schrödinger's equation:

$$-\frac{\hbar^2}{2\mu a^2}\frac{d^2\phi}{d\xi^2} + \frac{\alpha}{a\xi}\phi = E\phi \tag{5.2}$$

Multiply both sides by $\frac{2\mu a^2}{\hbar^2}$:

$$-\frac{d^2\phi}{d\xi^2} + \left(\frac{2\mu a\alpha}{\hbar^2}\cdot\frac{1}{\xi}\right)\phi = \left(\frac{2\mu a^2 E}{\hbar^2}\right)\phi \tag{5.3}$$

Let:

$$\lambda = \frac{2\mu a\alpha}{\hbar^2} = -1 \rightarrow \textit{choosen for mathematical simplification}$$

$$\gamma = \frac{2\mu a^2 E}{\hbar^2}$$

$$\left[a = \frac{\hbar^2}{2\mu\alpha}\right] \rightarrow \textit{this makes equation dimensionless}$$

$$-\frac{d^2\phi}{d\xi^2} + \frac{\lambda}{\xi}\phi = \gamma\epsilon \tag{5.4}$$

Trial function prediction using ansatz

As $\xi \to \infty$:

$$-\frac{d^2\phi}{ds^2} \approx \gamma\epsilon$$

For bound states, $\epsilon < 0$. Let:

$$\kappa = \sqrt{-\epsilon} > 0, \quad \phi(\xi) \sim e^{-\kappa\xi}$$

As $\xi \to 0$:

$$-\frac{d^2\phi}{d\xi^2} - \frac{1}{\xi}\phi \approx 0$$

$$\phi(\xi) = \xi^t$$

$$\phi'(\xi) = s\xi^{s-1}, \quad \phi''(\xi) = s(s-1)\xi^{s-2}$$

Substitute into the equation:

$$-s(s-1)\xi^{s-2} - \frac{1}{\xi}\xi^s = 0$$

$$\Rightarrow -\left[s(s-1)\xi^{s-2} + \xi^{s-1}\right] = 0$$

$$\xi^{s-2}[s[s-1] - \xi] = 0$$

$$\xi = 0, 1$$

Case 1: $\phi(\xi) \sim \xi$

Then:

$$|\phi(\xi)|^2 \sim \xi^2 \quad \Rightarrow \quad \int_\epsilon^L \xi^2 \, d\xi = \left[\frac{\xi^3}{3}\right]_\epsilon^L$$

$$|\phi(\xi)|^2 = \frac{L^3 - \epsilon^3}{3}$$

This is finite for any $\epsilon > 0$.

Case 2: $\phi(\xi) \sim 1$

Then:

$$|\phi(\xi)|^2 \sim 1 \quad \Rightarrow \quad \int_\epsilon^L 1 \, d\xi = L - \epsilon$$

This is also finite for $\epsilon > 0$, but

$$V(\xi)\phi(\xi) = -\frac{1}{\xi} \cdot \phi(\xi) \sim -\frac{1}{\xi}$$

$$\Rightarrow -\int_{\epsilon}^{L} \frac{1}{\xi}\, d\xi = \frac{1}{\xi} - \frac{1}{L}$$

This blows up as $\epsilon \to 0$.

$$\langle V \rangle \approx \infty, |\phi(\xi)|^2 = finite$$

Therefore, un-physical. Hence, rejected.

We assign a trial solution:

$$\phi(\xi) = \xi e^{-\xi} F(\xi)$$

So:

$$\frac{d^2\phi}{d\xi^2} + \left(\frac{2}{\xi} - 2\right)\frac{dF}{d\xi} + \left(E + \frac{\alpha}{a\xi}\right)F = 0$$

We assign a trial solution to ensure normalizability, $F(\xi)$ must be a polynomial, reducing the equation to a "confluent hypergeometric equation", and subsequently to "associated Laguerre polynomials". This introduces a quantization condition.

Compute derivatives:

$$\phi'(\xi) = e^{-K\xi}\left[(F + \xi\frac{dF}{d\xi}\right) - K\xi F]$$

$$\phi''(\xi) = e^{-K\xi}\left[\frac{2dF}{d\xi} - 2KF + \xi\frac{d^2F}{d\xi} - 2K\xi\frac{d^2F}{d\xi^2} + K^2\xi\right]$$

Plug into original equation:

$$\xi\frac{d^2F}{d\xi^2} + (2 - 2K\xi)\frac{dF}{d\xi} + \Big[(\gamma - K^2)\xi + 2K - 1\Big]F = 0$$

Quantization & Laguerre Polynomial Solution

For wavefunction $\phi(\xi)$ to be normalizable, $F(\xi)$ must be finite.

$$\Rightarrow F(\xi) \to \text{polynomial} \quad \checkmark, \quad \text{infinite series} \quad \times$$

1. Our equation:

$$\xi \frac{d^2F}{d\xi^2} + (2 - 2K\xi)\frac{dF}{d\xi} + \Big[(\gamma - K^2)\xi + 2K - 1\Big]F = 0$$

2. Target form:

$$z\frac{d^2y}{dz^2} + (k + 1 - z)\frac{dy}{dz} + ny = 0$$

Substitute:

$$z = 2K\xi \quad \Rightarrow \quad \xi = \frac{z}{2K}, \quad \frac{d}{d\xi} = \frac{dz}{d\xi} \cdot \frac{d}{dz} = 2K\frac{d}{dz}$$

$$F(\xi) = F(z)$$

$$\frac{dF}{d\xi} = \frac{dF}{dz} \cdot \frac{dz}{d\xi} = 2K\frac{dF}{dz}$$

$$\frac{d^2F}{d\xi^2} = \frac{d}{d\xi}\left(2K\frac{dF}{dz}\right) = 2K\frac{d}{d\xi}\left(\frac{dF}{dz}\right)$$

$$\frac{d}{d\xi}\left(\frac{dF}{dz}\right) = \frac{d^2F}{dz^2} \cdot \frac{dz}{d\xi} = \frac{d^2F}{dz^2} \cdot 2K$$

$$\Rightarrow \frac{d^2F}{d\xi^2} = (2K)^2\frac{d^2F}{dz^2}$$

Substitution into the equation:

$$\frac{z}{2K}(2K)^2\frac{d^2F}{dz^2} + (2 - z)2K\frac{dF}{dz} + \left[\frac{(\gamma - K^2)z}{2K} + 2K - 1\right]F = 0$$

Dividing by: $2K$:

$$z\frac{d^2F}{dz^2} + (2-z)\frac{dF}{dz} + \left[\frac{(\gamma - K^2)z}{4K^2} + \frac{2K-1}{2K}\right]F = 0$$

Match to laguerre's equation:

$$z\frac{d^2F}{dz^2} + (2-z)\frac{dF}{dz} + \left[\frac{(\gamma - K^2)z}{4K^2} + \frac{(2K-1)}{2K}\right]F = 0$$

$$z\frac{d^2y}{dx^2} + (K+1-z)\frac{dy}{dx} + ny = 0$$

Coefficient of second order differential equation $\rightarrow$ same.

Coefficient of first order differential equation $\rightarrow k + 1 - z = 2 - z \Rightarrow k = 1$

$\left(\frac{\gamma - K^2}{4K^2}\right)z + \frac{2K-1}{2K} = n$ this term is positive, so cannot be negative

Unwanted term:

$$\left(\frac{\gamma - K^2}{4K^2}\right)zF$$

To match Laguerre's equation:

$$\frac{\gamma - K^2}{4K^2} = 0 \Rightarrow \gamma = K^2$$

$$1 - \frac{1}{2K} = n \Rightarrow \frac{1}{2K} = 1 - n \Rightarrow K = \frac{1}{2(1-n)}$$

This means we have negative values of n if $n < 1$, which makes no physical sense.

$$K > 0 \Rightarrow 1 - n > 0 \Rightarrow n < 1 \quad \rightarrow \text{Unphysical}$$

To get something that makes sense:

Our equation:

$$z\frac{d^2F}{dz^2} + (2-z)\frac{dF}{dz} + \left(\frac{1}{2K} - 1\right)F = 0$$

Confluent hypergeometric equation:

$$z\frac{d^2F^2}{dz^2} + (k+1-z)\frac{dF}{dz} - F = 0$$

$$\text{where } O = 2, \quad n = 1 - \frac{1}{2K}$$

The confluent hypergeometric f^n becomes a polynomial of degree n only if:

$$\frac{1}{2K} - 1 = -n$$

$$K = \frac{1}{2(n+1)}, [\gamma = \frac{1}{4(n+1)^2}]$$

Conventionally, ground state $\Rightarrow n = 1$, so:

$$K = \frac{1}{2n}, \quad \gamma = \frac{1}{4n^2}, \quad n = 1, 2, 3, \ldots$$

Final Wavefunction

The solution has the form:

$$F(z) = L_{n-1}^{(1)}(z) \cdot z \qquad \text{(Laguerre Polynomial)}$$

where

$$k = \frac{1}{2n}, \qquad \left[\gamma = \frac{1}{4n^2}\right]$$

Now the full wavefunction is given by:

$$\phi(\xi) = \xi e^{\kappa\xi} F(\xi) = \xi e^{\kappa\xi} L_{n-1}^{(1)}(2.\kappa.\xi)$$

Change of variables:

$$\xi = \frac{x}{a}, \qquad a = \frac{\hbar^2}{2\mu|\alpha|}$$

Substituting back:

$$\phi\left(\frac{x}{a}\right) = \frac{x}{a} \cdot e^{-\frac{x}{2na}} \cdot L_{n-1}^{(1)}\left(\frac{\alpha x}{na}\right)$$

$$\psi_n(x) = \frac{1}{a}\, x\, e^{-\frac{x}{2na}} \cdot L_{n-1}^{(1)}\left(\frac{x}{na}\right)$$

$$n = 1, 2, 3, \ldots \quad , \quad a = \frac{\hbar^2}{2\mu|\alpha|}$$

Normalization

Change of variables:

$$v = \frac{x}{na} \quad \Rightarrow \quad x = vna, \quad dx = na\,dv$$

Limits:

$$x = 0 \Rightarrow v = 0, \qquad x = L \Rightarrow v = \frac{L}{na}$$

$$A_n^2 \int_0^{\frac{L}{na}} \left(\frac{v.n.a}{a}\right)^2 e^v \left[L_{n-1}^{(1)}(v)\right]^2 na.dv = 1$$

$$A_n^2\, n^3 a \int_0^{\frac{L}{na}} v^2 e^{-v} \left[L_{n-1}^{(1)}(v)\right]^2 dv = 1$$

$$A_n = \left(n^3 a \int_0^{\frac{L}{na}} v^2 e^{-v} \left[L_{n-1}^{(1)}(v)^2\right] dv\right)^{\frac{-1}{2}}$$

$$\psi_n(x) = \left(n^3 a \int_0^{\frac{L}{na}} v^2 e^{-v} \left[L_{n-1}^{(1)}(v)^2\right] dv\right)^{-1/2} \cdot \frac{x}{a}\, e^{-\frac{x}{2na}} \cdot L_{n-1}^{(1)}\left(\frac{x}{na}\right)$$

To solve the integral, we use the known orthogonality identity:

$$\int_0^\infty z^\alpha e^{-z} L_n^{(\alpha)}(z) L_m^{(\alpha)}(z)\, dz = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{nm}$$

If the limits of the wavefunction were from [0,∞)

$$\int_0^\infty z^2 e^{-z} \left[L_n^{(1)}(z)\right]^2 dz = 2n(n+1)$$

$$I(n, L, a) = 2n(n+1) - \int_{L/(na)}^\infty v^2 e^{-v} \left[L_{n-1}^{(1)}(v)^2\right] dv$$

where,

$$\int_{L/(na)}^{\infty} v^2 e^{-v} \left[L_{n-1}^{(1)}(v)^2 \right] dv = R(n, L, a)$$

$$I(n, L, a) = \int_{0}^{L/(na)} v^2 e^{-v} \left[L_{n-1}^{(1)}(v)^2 \right] dv$$

$$I(n, L, a) = 2n(n+1) - R(n, L, a)$$

$$\psi_n(x) = \left[n^3 a \left(2n(n+1) - R(n, L, a) \right) \right]^{-\frac{1}{2}} \cdot \frac{x}{a} \cdot e^{-\frac{x}{2na}} \cdot L_{n-1}^{(1)} \left(\frac{x}{na} \right)$$

Therefore, the final wavefunction is:

$$\psi_n(x) = a^{-\frac{3}{2}} \cdot \left(n^3 \cdot I(n, L, a) \right)^{-\frac{1}{2}} \cdot x \cdot e^{-\frac{x}{2na}} \cdot L_{n-1}^{(1)} \left(\frac{x}{na} \right)$$

where, n = *quantum number* (1, 2, 3,...)

$$a = \frac{\hbar^2}{2\mu|\alpha|}, \quad \alpha = -GMm, \quad \mu = Mm/M + m$$

Energy

$$-\frac{d^2\phi}{d\xi^2} + \frac{n}{\xi}\phi = \gamma\phi$$

$$\xi = \frac{x}{a}, \quad \gamma = \frac{2\mu a^2 E}{\hbar^2}, \quad a = \frac{\hbar^2}{2\mu|\alpha|}$$

$$\phi(\xi) = \frac{x}{a}$$

To ensure normalizability, we require F(z) to be a polynomial, which is possible only when:

$$\kappa = \frac{1}{2n} \quad \Rightarrow \quad \gamma_n = \frac{1}{4n^2}$$

$$\frac{2\mu a^2 E_n}{\hbar^2} = \frac{1}{4n^2} \quad \Rightarrow \quad E_n = \frac{1}{8n^2} \cdot \frac{\hbar^2}{\mu a^2}$$

$$a = \frac{\hbar^2}{2\mu\alpha} \quad \Rightarrow \quad E_n = \frac{1}{2n^2} \cdot \frac{\mu\alpha^2}{\hbar^2}$$

Chapter 6

Simulation and Analysis Results

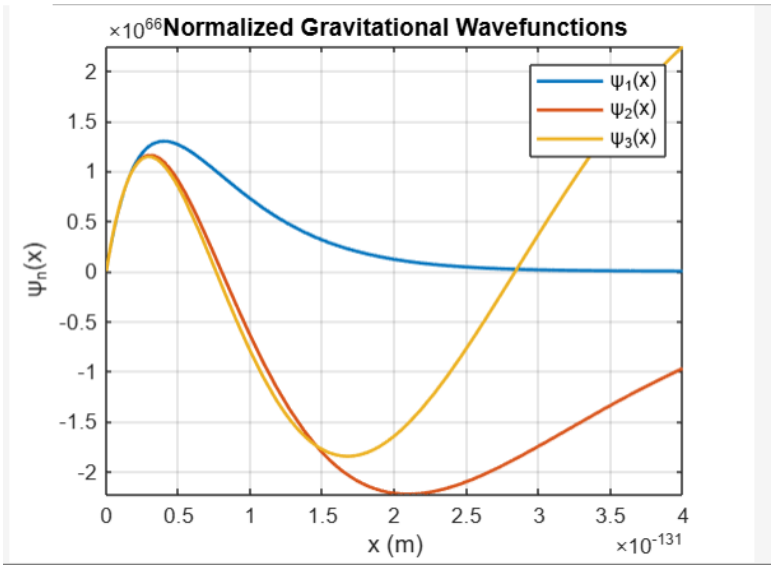

Figure 6.1: Normalized Gravitational Wavefunction

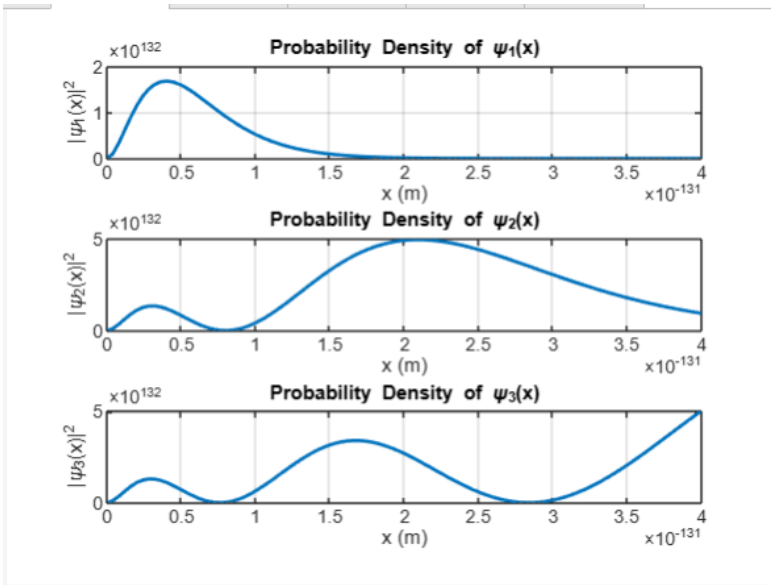

Figure 6.2: Probability Density Graphs for $\psi(x) = 1\&2\&3$

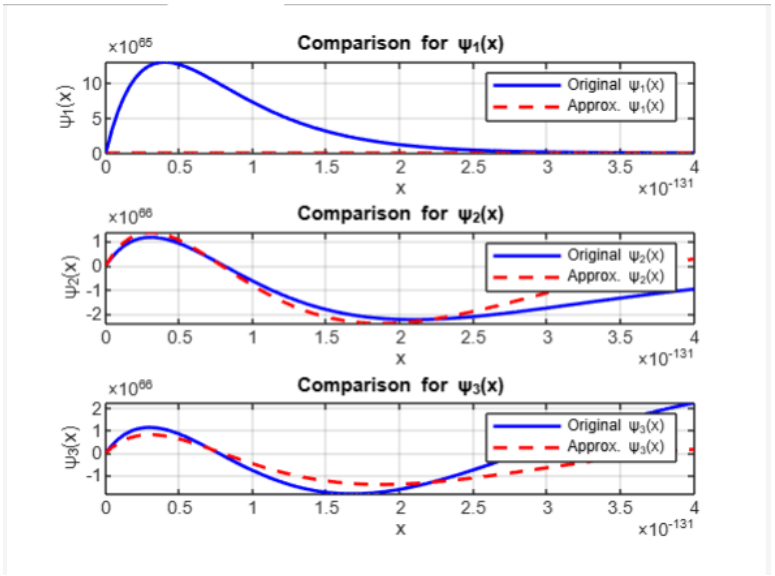

Figure 6.3: Comparison of wavefunctions

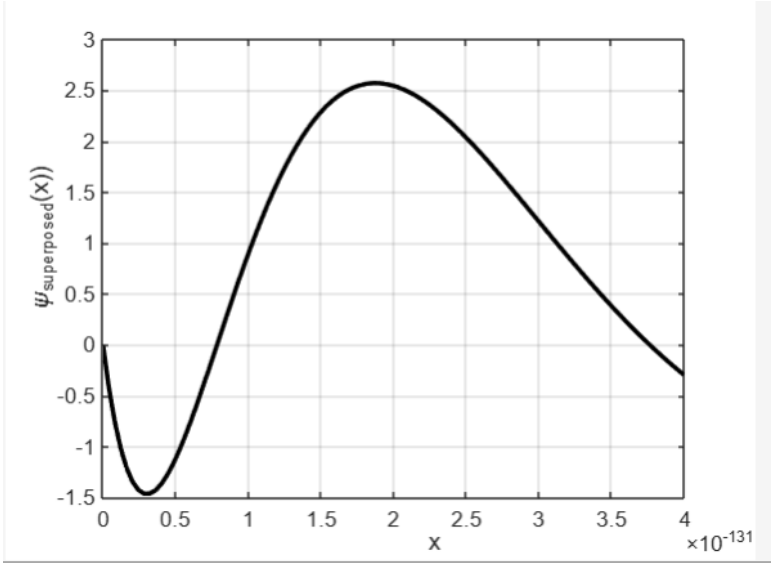

Figure 6.4: Superposed Wavefunction

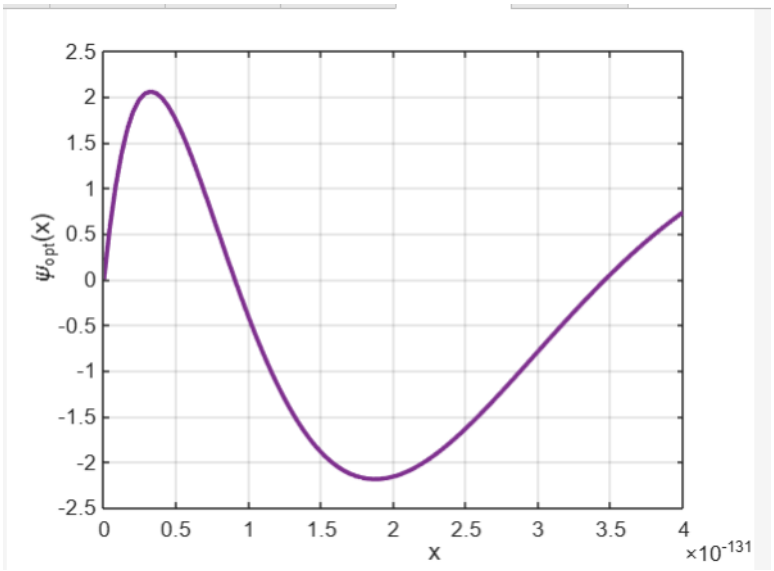

Figure 6.5: Optimized Wavefunction

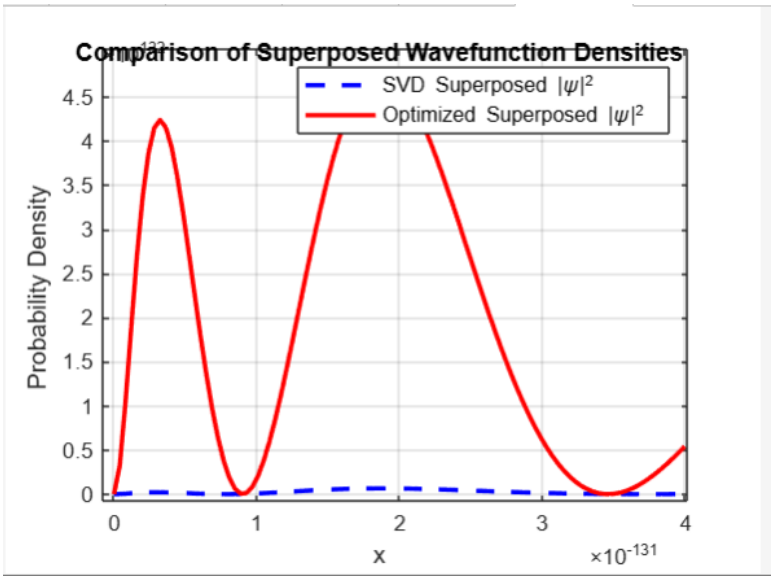

Figure 6.6: Comparison for superposed wavefunction densities

```
Weights (α_n) for dominant mode (from U(:, 1)):
    0.0000
   -0.8580
   -0.5136


Weights αₙ (contribution of each ψₙ to ϕ(x)):
α_1 = 68881625416515711953097410725557440810198928743304426309445222 4.0000
α_2 = -14573920843417686381769113603841367386197546263892130692842420961280.0000
α_3 = -87240592545984549908450297163103673067286237645313297904139040194 56.0000
 Iter  Func-count            Fval   Feasibility   Step Length       Norm of   First-order
                                                                       step    optimality
    0           4   7.095416e-263     2.220e-16     1.000e+00     0.000e+00    4.324e-263

Initial point is a local minimum that satisfies the constraints.

Optimization completed because at the initial point, the objective function is non-decreasing
in feasible directions to within the value of the optimality tolerance, and
constraints are satisfied to within the value of the constraint tolerance.

<stopping criteria details>

Optimized weights αₙ (minimizing spatial variance):
    0.5774
    0.5774
    0.5774
```

Chapter 7

Interpretations, Insights and Discussions

- Singular Nature of the Gravitational Potential: The inverse gravitational potential $V(x) = \frac{\alpha}{x}$ exhibits a singularity at $x = 0$, leading to unique mathematical challenges not seen in standard harmonic or square well potentials. Quantum mechanically, this necessitates specific boundary conditions and careful consideration of the behavior of the wavefunction near the origin.

- Wavefunction Behavior and Normalization: The wavefunction exhibits sharp decay at large x and divergence at small x unless carefully controlled. By expressing the wavefunction in the form $\psi(x) = xe^{-x/2na}L_{n-1}^{(1)}\left(\frac{x}{na}\right)$, we ensured normalizability using associated Laguerre polynomials, thereby obtaining physically valid bound states.

- Energy Quantization: A key insight from the dimensionless Schrödinger equation is the quantization of energy levels:

$$E_n = \frac{\mu\alpha^2}{2n^2\hbar^2}$$

  This mirrors the quantization in hydrogenic systems, reaffirming that even gravitational potentials yield discrete energy spectra when bound state conditions are met.

- Numerical Accuracy via MATLAB: Symbolic and numerical solutions using MATLAB validated the analytical form of the wavefunctions and energy levels. The simulation plots for $n = 1, 2, 3$ showed consistency with theoretical predictions and emphasized the decaying nature and orthogonality of higher-order wavefunctions.

- Optimization through Superposition: Using techniques such as Singular Value Decomposition (SVD) and optimization via fmincon, we successfully minimized spatial variance of the wavefunction by superposing the first three bound states. This demonstrates a practical method for localizing quantum states using numerical tools.

Chapter 8

Conclusion and Future Scope

This project successfully explored the *quantum behavior of a particle in a one-dimensional gravitational potential of the form* $V(x) = \frac{\alpha}{x}$. The system was treated analytically and numerically using both classical and modern computational techniques. Key conclusions include:

- Laguerre polynomials naturally arise as solutions to the dimensionless Schrödinger equation.
- The system exhibits discrete energy levels analogous to the hydrogen atom, despite the gravitational origin of the potential.
- Numerical simulations and MATLAB-based visualization confirmed the behavior and properties of the wavefunctions.
- Optimization techniques were effectively used to construct superposed states with reduced spatial variance.

Future Scope:

- Extending the model to three-dimensional gravitational wells or relativistic corrections.
- Incorporating time-dependent potentials to study quantum dynamics under gravitational fields.
- Applying similar analytical techniques to black hole analog systems or quantum cosmology.

Chapter 9

Contributions of Individual Group Members

Anagha Manoj: Dimensionless conversion, final editing of report writing and ppt.

Gowripriya R.: Solving for the time dependent Schrodinger equation, solved for the wave function before non dimensionalizing, idea for dimensionless equation, ppt writing.

Parkhi Mahajan: Solved for v=0 case, derived analytical solutions for the dimensionalized and non-dimensionalized system, normalization, implementing MATLAB solutions and visualization, ppt and report editing.

Tanvi Bhardwaj: Solving for the time independent Schrodingers equation, solved for the wave function before non dimensionalization, idea for dimensionless equation, report writing.

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Chapter 10

Appendix

Matrix Formulation of Wavefunctions

What is it?

A symbolic diagonal matrix T containing the gravitational quantum wavefunctions $\psi_1(x)$, $\psi_2(x)$, $\psi_3(x)$ for $n = 1, 2, 3$.

How is it implemented?

- Each wavefunction is derived symbolically.
- The matrix is defined as: $T = \text{diag}(\psi_1, \psi_2, \psi_3)$.
- Each $\psi_n(x)$ is multiplied by its normalization constant $C_n = \frac{1}{\sqrt{\int |\psi_n(x)|^2 dx}}$.

Why is it done?

- Encodes energy eigenstates in a structured matrix form.
- Enables linear algebraic operations like SVD and linear combinations.
- Connects quantum mechanical solutions to matrix-based formulations.

Sampling and SVD of $\psi_n(x)$

What is it?

Numerical evaluation of $\psi_1(x)$, $\psi_2(x)$, and $\psi_3(x)$ at 100 spatial points, followed by Singular Value Decomposition (SVD) for analysis and compression.

How is it implemented?

- Evaluate each $\psi_n(x)$ on $x = \texttt{linspace}(0, a, 100)$.
- Form a 3×100 matrix Ψ of sampled wavefunctions.
- Apply SVD:

$$[U, S, V] = \texttt{svd}(\Psi)$$

- The rows of V represent the weight vectors α_n.

Why is it done?

- Reduces data dimensionality.
- Highlights dominant wavefunction combinations.
- Prepares for building physical superpositions.

Quantum Superposition from SVD

What is it?

A linear combination of wavefunctions $\psi_1(x)$, $\psi_2(x)$, and $\psi_3(x)$ using weights α_n from SVD.

How is it implemented?

- Take the dominant weight vector: $\boldsymbol{\alpha} = V(1, :)$.
- Compute the combined wavefunction:

$$\psi_{\text{superposed}}(x) = \alpha_1\psi_1(x) + \alpha_2\psi_2(x) + \alpha_3\psi_3(x)$$

- Normalize $\psi_{\text{superposed}}(x)$ over $[0, a]$.

Why is it done?

- Generates physically realizable superpositions.
- Models a single quantum state composed from eigenstates.
- Prepares ground for optimization and confinement analysis.

Optimization of Superposition

What is it?

Optimization of the coefficients α_1, α_2, and α_3 to form a superposition with minimal spatial spread (variance).

How is it implemented?

- Define the total wavefunction: $\psi_{\text{total}}(x) = \sum \alpha_n\psi_n(x)$.
- Calculate variance:

$$\text{Var} = \langle x^2 \rangle - \langle x \rangle^2$$

- Use `fmincon()` in MATLAB to minimize Var with constraint: $\sum \alpha_n^2 = 1$.

Why is it done?

- Produces a more localized quantum state.
- Demonstrates quantum control through optimization.
- Provides insight into efficient quantum confinement.

Summary Table

Step	**What**	**How (In Code)**	**Why (Purpose)**
Matrix Formulation	Store ψ_n in diagonal matrix	`diag(`ψ_1`, `ψ_2`, `ψ_3`)`	Structured representation of eigenstates
Normalization	Normalize each ψ_n	Multiply by $1/\sqrt{\int \lvert\psi_n\rvert^2 dx}$	Ensure valid probability interpretation
Sampling	Discretize wavefunctions	`linspace`, `subs`	Prepare for matrix operations and SVD
SVD	Decompose wavefunction matrix	$[U, S, V] =$ `svd`(Ψ)	Find dominant directions for superposition
Superposition	Combine ψ_n using weights	$\sum \alpha_n \psi_n(x)$	Construct new valid wavefunctions
Optimization	Minimize variance	`fmincon()` on $\langle x^2 \rangle - \langle x \rangle^2$	Localize wavefunction for physical relevance

MATLAB Code for Gravitational Bound States

```
1
2  clc; close all; clear;
3
4  %% Step 1: Constants
5  hbar = 1.054571817e-34;     % Reduced Planck constant [J s]
6  G = 6.67430e-11;            % Gravitational constant [m^3/kg s^2]
7  m1 = 1.898e27;              % Mass of Jupiter [kg]
8  m2 = 1.4819e23;             % Mass of Ganymede [kg]
9
10 mu = (m1 * m2) / (m1 + m2);         % Reduced mass [kg]
11 alpha = G * m1 * m2;                % |-alpha| = G * m1 * m2
12 a_val = hbar^2 / (2 * mu * alpha);  % Bohr-like gravitational radius
       [m]
13
14 fprintf('Gravitational Bohr radius a = %.3e meters\n\n', a_val);
15
16 %% Step 2: Symbolic definitions
17 syms x a v real
18 assume([a > 0, v > 0])  % Prevent negative radii
19
20 psi = sym('psi', [3,1]);       % Unnormalized  _n (x)
21 I_expr = sym('I', [3,1]);      % I(n, L = a, a)
22
23 for n = 1:3
24     Ln = laguerreL(n-1, 1, v);  % Associated Laguerre polynomial
25     R = int(v^2 * exp(-v) * Ln^2, v, 1/n, Inf);  % L = a     L/(na)
           = 1/n
26     I_expr(n) = simplify(2*n*(n+1) - R);
27
28     vsub = x / (n*a);  % Substitution for normalized variable
29     prefactor = a^(-3/2) * (n^3 * I_expr(n))^(-1/2);
30     psi(n) = simplify(prefactor * (x/a) * exp(-x/(2*n*a)) *
           laguerreL(n-1, 1, vsub));
31 end
32
```

```
T = diag(subs(psi, a, a_val));  % Diagonal matrix with unnormalized
        (x)

%% Step 3: Substitute a = a_val and normalize      (x) over [0, a]
C = sym('C', [3,1]);          % Normalization constants
psi_norm = sym('psi_norm', [3,1]);

for n = 1:3
    psi_sub = simplify(subs(psi(n), a, a_val));
    C(n) = vpa(1 / sqrt(int(psi_sub^2, x, 0, a_val)));  % Compute
        and store C_n
    psi_norm(n) = simplify(C(n) * psi_sub);             % Normalize
        the wavefunction
end

%% Step 4: Display results
fprintf('\nDiagonal matrix T (unnormalized      (x)):\n');
pretty(vpa(T, 4))

fprintf('\nNormalization constants C_n (with L = a):\n');
for n = 1:3
    fprintf('C_%d = %.4e\n', n, C(n));
end

fprintf('\nNormalized wavefunctions      (x):\n');
digits(4);
for n = 1:3
    fprintf(' _ %d(x) =\n', n);
    pretty(vpa(psi_norm(n)));
end

%% Step 5: Plot
% Wave function vs x
figure;
fplot(matlabFunction(psi_norm(1)), [0, 20*a_val], 'LineWidth', 1.5)
hold on
fplot(matlabFunction(psi_norm(2)), [0, 20*a_val], 'LineWidth', 1.5)
fplot(matlabFunction(psi_norm(3)), [0, 20*a_val], 'LineWidth', 1.5)
```

```
68
69 legend(' _1 (x)', ' _2 (x)', ' _3 (x)')
70 xlabel('x (m)')
71 ylabel(' _n (x)')
72 title('Normalized Gravitational Wavefunctions')
73 grid on;
74
75 % Probability density vs x
76 % Discretize x
77 x_vals = linspace(0, 20*a_val, 100);      % 100 spatial points
78
79 figure;
80 for n = 1:3
81     % Convert symbolic      (x) to numeric function
82     f_psi = matlabFunction(psi_norm(n), 'Vars', x);
83
84     % Evaluate on x_vals
85     psi_n_vals = f_psi(x_vals);
86
87     % Compute probability density
88     prob_density = abs(psi_n_vals).^2;
89
90     % Plot
91     subplot(3,1,n);
92     plot(x_vals, prob_density, 'LineWidth', 1.5);
93     xlabel('x (m)');
94     ylabel(['|\psi_', num2str(n), '(x)|^2']);
95     title(['Probability Density of \psi_', num2str(n), '(x)']);
96     grid on;
97 end
98
99 %% Step 6: Data Reduction using SVD
100 num_x = length(x_vals);
101 psi_vals = zeros(3, num_x);               % Matrix to hold      (x)
    samples
102
103 % Evaluate each normalized wavefunction numerically
104 for n = 1:3
```

```
    f = matlabFunction(psi_norm(n), 'Vars', x);  % Convert symbolic
        to numeric
    psi_vals(n, :) = f(x_vals);                  % Store sampled
        values
end

% Apply SVD
[U, S, V] = svd(psi_vals, 'econ');   % 'econ' is efficient for non-
    square

% Extract dominant mode (rank-1 approximation)
rank1 = S(1, 1) * U(:, 1) * V(:, 1)';   % 3 1  * 1 100      3 100
    approx matrix

% Visualize weights (U(:,1))     tells how much      ,      ,
    contribute
disp('Weights ( _n ) for dominant mode (from U(:, 1)):');
disp(U(:, 1));

% Compare original vs approximated      (x)
figure;
for n = 1:3
    subplot(3,1,n)
    plot(x_vals, psi_vals(n,:), 'b-', 'LineWidth', 1.5); hold on;
    plot(x_vals, rank1(n,:), 'r--', 'LineWidth', 1.5);
    legend(sprintf('Original  _ %d(x)', n), sprintf('Approx.  _ %d(x
        )', n));
    xlabel('x'); ylabel(sprintf(' _ %d(x)', n));
    title(sprintf('Comparison for  _ %d(x)', n));
    grid on;
end

%% Step 7: Visualize dominant mode   (x) and weight       for each


% Extract dominant spatial pattern
phi = V(:,1);              % 100 1      shape of dominant shared
    pattern   (x)
```

```
phi = phi / max(abs(phi)); % Normalize for easier viewing

% Extract weights       =  s       u  (n)
alpha = S(1,1) * U(:,1);   % 3 1  vector of contributions to   (x)

% Display       values
fprintf('\nWeights       (contribution of each       to   (x)):\n');
for n = 1:3
    fprintf(' _ %d = %.4f\n', n, alpha(n));
end

% Superpose      (x) using the extracted       values
psi_superposed = alpha(1)*psi_vals(1,:) + alpha(2)*psi_vals(2,:) +
    alpha(3)*psi_vals(3,:);

% Normalize the superposed wavefunction
norm_super = trapz(x_vals, abs(psi_superposed).^2);
psi_superposed = psi_superposed / sqrt(norm_super);

% Plot it
figure;

plot(x_vals, psi_superposed, 'k-', 'LineWidth', 2);
xlabel('x'); ylabel('\psi_{superposed}(x)');
title('Superposed Wavefunction');
grid on;

%% Step 8: Optimization     Find       minimizing variance of
    superposed   (x)

% Initial guess
alpha0 = ones(3,1)/sqrt(3); % normalized initial guess

% Objective function handle
obj_fun = @(alpha) calcVariance(alpha, psi_vals, x_vals);

% Nonlinear equality constraint (unit norm)
nonlcon = @(alpha) deal([], sum(alpha.^2) - 1);
```

```
171
172 % Optimization options
173 opts = optimoptions('fmincon','Display','iter','Algorithm','sqp');
174
175 % Run optimization
176 [alpha_opt, var_min] = fmincon(obj_fun, alpha0, [], [], [], [], [],
    [], nonlcon, opts);
177
178 fprintf('\nOptimized weights       (minimizing spatial variance):\n'
    );
179 disp(alpha_opt);
180
181 % Plot optimized superposed wavefunction
182 psi_opt = alpha_opt' * psi_vals;
183
184 figure;
185 plot(x_vals, psi_opt, 'Color', [0.4940, 0.1840, 0.5560], 'LineWidth'
    , 2);
186 xlabel('x'); ylabel('\psi_{opt}(x)');
187 title('Optimized Superposed Wavefunction (Min Variance)');
188 grid on;
189
190 % Plot probability density before and after optimiztion
191 figure;
192 psi_opt_density = abs(psi_opt).^2;
193 plot(x_vals, abs(psi_superposed).^2, 'b--', 'LineWidth', 2); hold on
    ;
194 plot(x_vals, psi_opt_density, 'r-', 'LineWidth', 2);
195 xlabel('x');
196 ylabel('Probability Density');
197 legend('SVD Superposed |\psi|^2', 'Optimized Superposed |\psi|^2');
198 title('Comparison of Superposed Wavefunction Densities');
199 grid on;
200
201 {subroutine}
202 function var_val = calcVariance(cf, psi_vals, x_vals)
203     % Ensure cost fn (cf) is a column vector
204     cf = cf(:);
```

```
205
206     % Superpose wavefunction
207     psi_superposed = cf' * psi_vals;  % 1 N
208
209     % Normalize
210     psi_superposed = psi_superposed / max(abs(psi_superposed));
211
212     % Probability density (square of amplitude)
213     prob_density = psi_superposed.^2;
214
215     % Normalize probability density to sum=1 for discrete approx
216     prob_density = prob_density / sum(prob_density);
217
218     % Expected position E[x]
219     expected_x = sum(prob_density .* x_vals);
220
221     % Expected  x   E[ x  ]
222     expected_x2 = sum(prob_density .* (x_vals.^2));
223
224     % Variance = E[ x  ] - (E[x])
225     var_val = expected_x2 - expected_x^2;
226 end
```

Listing 10.1: Normalized wavefunctions psi_n(x) for gravitational potential