MATH 131P WINTER 2024 FINAL PROJECT

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Solving the Three-Dimensional Infinite Potential Well

1. Introduction

The goal of this text is to use the knowledge regarding the Generalized Fourier Series, the method of Separation of Variables, Sturm-Liouville Problems, and the Heat Equation in Cartesian coordinates to find a general solution for the infinite potential well in three dimensions. This problem is one of the extremes regarding the "quantum tunneling" that can occur for any non-infinite potential well. This entails a particle, usually an electron, overcoming an energy boundary greater than what it would classically be able to overcome.

This phenomenon causes leakage current and is one of the biggest obstacles to improving modern circuitry since producing too small components may render them useless due to electrons passing through regions that should isolate the circuit. Then, understanding solutions to the infinite potential well can help study this phenomenon as a whole and provide a framework for the approximation of the wave functions of particles in a large but finite potential well.

After applying the aforementioned techniques, it was found that the solution to the three-dimensional infinite potential well is analogous to that of the three-dimensional heat equation, though with added care of the constants and imaginary components involved.

2. Orthogonality and Generalized Fourier Series

Before diving into PDEs, it's important to review the theoretical background needed to solve them, in particular when it comes to orthogonality and producing general solutions.

Definition 2.1. (Dot Product & Orthogonality) For complex-valued functions $f(x)$ & $g(x)$, the dot product on the interval $[a, b]$ is defined as:

$$\langle f, g\rangle = \int_a^b f(x)\overline{g(x)}dx$$

$f(x)$ & $g(x)$ are said to be **orthogonal** on the interval $[a, b]$ if:

$$\langle f, g\rangle = \int_a^b f(x)\overline{g(x)}dx = 0$$

Definition 2.2. (Orthogonal Set) A set of functions S is said to be **orthogonal** if all its functions are **pairwise orthogonal**.

Theorem 2.3. ***(Generalized Fourier Series)*** *If S is a complete set of orthogonal functions in a class of functions A, any f in A can be written as a linear combination of f_n in S:*

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

Any coefficient c_k can be calculated by applying the dot product with the respective f_k and using the orthogonality of the f_n's:

$$\langle f, f_k \rangle = \sum_{n=1}^{\infty} c_n \langle f_n, f_k \rangle = c_k \langle f_k, f_k \rangle$$

$$c_k = \frac{\langle f, f_k \rangle}{\langle f_k, f_k \rangle}$$

*These coefficients c_n are called **Fourier Coefficients** and the associated series is called **Generalized Fourier Series**:*

$$f(x) = \sum_{n=1}^{\infty} \frac{\langle f, f_n \rangle}{\langle f_n, f_n \rangle} f_n(x)$$

3. Sturm-Liouville Theory

Sturm-Liouville Theory is what provides the rigorous framework that guarantees the functions found as solutions to ordinary differential equations are orthogonal eigenfunctions, thus permitting the application of the Fourier formulas discussed in the previous section. For the scope of this text, there isn't a need to discuss singularity in the context of Sturm-Liouville theory, so the following theorems and definitions will refer exclusively to when the regularity conditions of Definition 3.1 are met.

Definition 3.1. (Regular Sturm-Liouville Problem) A regular Sturm-Liouville problem on a **finite** interval [a,b] is a boundary value problem for known $p(x)$, $q(x)$, and $w(x)$, unknown $y(x)$, and parameter λ:

$$(p(x)y')' + (q(x) + \lambda w(x))y = 0 \quad , \quad a < x < b$$

with boundary conditions of the form:

$$\begin{cases} c_1 y(a) + c_2 y'(a) = 0 \\ d_1 y(b) + d_2 y'(b) = 0 \end{cases}$$

Where we need c_1 and/or c_2 nonzero, d_1 or d_2 nonzero, as well as the conditions:

(1) $p(x)$, $w(x) > 0$

(2) $p(x)$, $p'(x)$, $q(x)$, & $w(x)$ are continuous on $[a, b]$

Theorem 3.2. ***(Regular Sturm-Liouville Theorem)*** *For a regular Sturm-Liouville problem with eigenvalues λ as in Definition 3,1, the following statements are always valid:*

- *All eigenvalues are such that $\lambda_n \in \mathbb{R}$ and:*

$$\lambda_1 < \lambda_2 < \lambda_3 < \cdots < +\infty$$

- *All eigenvalues have a corresponding one-dimensional eigenspace.*
- *Eigenfunctions $y_n(x)$ are orthogonal with respect to the weight function $w(x)$.*

Theorem 3.3. ***(Eigenfunction Expansion)*** *For a weight function $w(x)$, and eigenfunctions y_n of a regular Sturm-Liouville problem on $[a, b]$, any piecewise smooth function f can be expressed as:*

$$f(x) = \sum_{n=1}^{\infty} \frac{\langle f, y_n \rangle_w}{\langle y_n, y_n \rangle_w} y_n(x)$$

4. Separation of Variables

Separation of variables is a relatively simple method of solving partial differential equations in which the solution u is assumed to be a product of functions of only one variable. While it only works under some rather restrictive conditions, this method is sufficient to solve the **regular** Sturm-Liouville problems discussed before.

Theorem 4.1. ***(Separation of Variables)*** *Let $u_n(t, x, y)$ be the orthogonal functions that solve a particular PDE. Then, assume $u_n(t, x, y) = T_n(t)X_n(x)Y_n(y)$ and apply Theorem 2.3 to get that the general solution $u(t, x, y)$ to the PDE can be written as:*

$$u(t, x, y) = \sum_{n=1}^{\infty} A_n T_n(t) X_n(x) Y_n(y)$$

This method can be used whenever the separated ODEs can be written as Sturm-Liouville problems, as that guarantees orthogonal functions $u_n(t, x, y)$ can be found. These conditions mean that Separation of Variables can be used to solve linear, homogeneous PDEs with linear, homogeneous boundary conditions, meaning that, for $x \in [0, \ell_1]$ and $y \in [0, \ell_2]$:

$$\begin{cases} a_1 \frac{\partial u}{\partial x}(t, 0, y) + a_2 u(t, 0, y) = 0 \\ b_1 \frac{\partial u}{\partial x}(t, \ell_1, y) + b_2 u(t, \ell_1, y) = 0 \\ c_1 \frac{\partial u}{\partial y}(t, x, 0) + c_2 u(t, x, 0) = 0 \\ d_1 \frac{\partial u}{\partial y}(t, x, \ell_2) + d_2 u(t, x, \ell_2) = 0 \end{cases}$$

The reason the method of Separation of Variables works is that plugging the assumption $u_n(t, x, y) = T_n(t)X_n(x)Y_n(y)$ into a PDE yields terms dependent on different variables on opposing sides of an equality, meaning they must both be constant.

Example 4.2. The partial differential equation defined as:

$$\frac{\partial u}{\partial t}(t,x) = c^2 \frac{\partial^2 u}{\partial x^2}(t,x)$$

is the one-dimensional heat equation. Applying Separation of Variables gives $u_n(t,x) = T(t)X(x)$ which, plugging into the PDE yields:

$$T''(t)X(x) = c^2 X''(x)T(t)$$

Since $T(t) = 0$ or $X(x) = 0$ imply $u(t,x) = 0$, which is the trivial solution, consider nonzero $T(t)$ and $X(x)$. Then, dividing both sides by $T(t)X(x)$:

$$\frac{T''}{T}(t) = c^2 \frac{X''}{X}(x)$$

Now note that $\frac{T''}{T}(t)$ only depends on t and $c^2\frac{X''}{X}(x)$ only depends on x. In search of a contradiction, assume $\frac{T''}{T}(t)$ is not a constant. Then there exists at least two values of t, call them t_1 and t_2 for which

$$\frac{T''}{T}(t_1) \neq \frac{T''}{T}(t_2)$$

However, $c^2\frac{X''}{X}(x)$ can't have changed since x didn't change. Therefore, $\frac{T''}{T}(t)$ is constant, and an analogous reasoning provides $c^2\frac{X''}{X}(x)$ is also constant.

Though this is just an example, such reasoning can always be applied to separable partial differential equations with varying degrees of difficulty. The constants each side of the equality must equal are called the **Separation Constants**, and finding them is an important step in solving a separable PDE.

5. Heat Equation and Time-Dependent Schrödinger's Equation

As the name suggests, the Heat Equation is the equation that models how heat flows in a given system. It is a partial differential equation, so the tools discussed in previous sections can provide its solutions.

Definition 5.1. (Heat Equation) The heat equation is a partial differential equation that, as the name indicates, describes heat transfer in materials. In Cartesian coordinates it is defined as:

$$\frac{\partial u}{\partial t}(t,x,y,z) = c^2\left(\frac{\partial^2 u}{\partial x^2}(t,x,y,z) + \frac{\partial^2 u}{\partial y^2}(t,x,y,z) + \frac{\partial^2 u}{\partial z^2}(t,x,y,z)\right)$$

Theorem 5.2. ***(Solution to the Heat Equation)*** *The general solution to the heat equation on a parallelepiped* $[0,\ell_1]\times[0,\ell_2]\times[0,\ell_3]$ *with vanishing Dirichlet Boundary Conditions and initial conditions:*

$$u(t,0,y,z) = u(t,\ell_1,y,z) = u(t,x,0,z) = u(t,x,\ell_2,z) = u(t,x,y,0) = u(t,x,y,\ell_3) = 0$$

$$u(0,x,y,z)=f(x,y,z) \qquad \frac{\partial u}{\partial t}(0,x,y,z)=g(x,y,z)$$

is

$$u(t,x,y,z)=\sum_{n_1=1}^{\infty}\sum_{n_2=1}^{\infty}\sum_{n_3=1}^{\infty}A_{n_1,n_2,n_3}e^{\lambda ct}\sin\left(\frac{n_1\pi}{\ell_1}x\right)\sin\left(\frac{n_2\pi}{\ell_2}y\right)\sin\left(\frac{n_3\pi}{\ell_3}z\right)$$

for coefficients A_{n_1,n_2,n_3} *and* B_{n_1,n_2,n_3}*:*

$$A_{n_1,n_2,n_3}=\frac{8}{\ell_1\ell_2\ell_3}\int_0^{\ell_1}\int_0^{\ell_2}\int_0^{\ell_3}f(x,y,z)\sin\left(\frac{n_1\pi}{\ell_1}x\right)\sin\left(\frac{n_2\pi}{\ell_2}y\right)\sin\left(\frac{n_3\pi}{\ell_3}z\right)dzdydx$$

where $\lambda=-\left(\frac{n_1^2}{\ell_1^2}+\frac{n_2^2}{\ell_2^2}+\frac{n_3^2}{\ell_3^2}\right)\pi^2$.

Definition 5.3. (Schrödinger's Equation) For a wave function ψ [1, p.574, 575], given scalar potential $V(x,y,z)$, constant $\hbar$, and mass μ, Schrödinger's Equation is a PDE of the form:

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2\mu}\nabla^2\psi+V(x,y,z)\psi$$

Note that while technically a wave equation, Schrödinger's Equation can often be treated similarly to a heat equation due to its first-order time derivative. The imaginary number i that appears makes it so the time-dependent term oscillates just as it would in a wave equation, so solving it as a heat equation is not a problem. Another important observation is that Schrödinger's Equation is generally a **singular** Sturm-Liouville problem due to unboundedness, but there are situations in which some boundaries can be enforced, such as the infinite potential well.

6. Solution to Three-Dimensional Infinite Potential Well

The infinite potential well is one of the simplest regimes to analyze Schrödinger's equation since it gets rid of the problems with singularity. Generalizing it to three dimensions can be a bit tricky, but using the solution to the Heat Equation provides a good guess of the structure of the general solution.

Theorem 6.1. ***(Solution to Three-Dimensional Infinite Potential Well)*** *The general solution to Schrödinger's Equation with piecewise potential function:*

$$V(x,y,z)=\begin{cases}0 & \text{if} \quad x,y,z\in[0,\ell_1]\times[0,\ell_2]\times[0,\ell_3]\\ \infty & \text{else}\end{cases}$$

boundary and initial conditions:

$$\begin{cases}\psi(t,x,y,z)=0 & \text{if} \quad x,y,z\notin[0,\ell_1]\times[0,\ell_2]\times[0,\ell_3]\\ \psi(0,x,y,z)=u(x,y,z) & \end{cases}$$

is the zero function everywhere except when $x, y, z \in [0, \ell_1] \times [0, \ell_2] \times [0, \ell_3]$*, where it is:*

$$\psi(t, x, y, z) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{k=1}^{\infty} A_{n,m,k} e^{-\frac{\pi^2\hbar^2}{2\mu}\left(\frac{n^2}{\ell_1^2}+\frac{m^2}{\ell_2^2}+\frac{k^2}{\ell_3^2}\right)ct} \sin\left(\frac{n\pi}{\ell_1}x\right)\sin\left(\frac{m\pi}{\ell_2}y\right)\sin\left(\frac{k\pi}{\ell_3}z\right)$$

for coefficients:

$$A_{n,m,k} = \frac{8}{\ell_1\ell_2\ell_3}\int_0^{\ell_1}\int_0^{\ell_2}\int_0^{\ell_3} u(x, y, z)\sin\left(\frac{n\pi}{\ell_1}x\right)\sin\left(\frac{m\pi}{\ell_2}y\right)\sin\left(\frac{k\pi}{\ell_3}z\right) dzdydx$$

Proof. First, note that the solution only considers the piece $[0, \ell_1] \times [0, \ell_2] \times [0, \ell_3]$ in which $V(x, y, z)$ is finite. This makes it so the method of Separation of Variables can be applied. Then, let $\psi(t, x, y, z) = T(t)X(x)Y(y)Z(z)$. Inserting this into the PDE yields:

$$i\hbar(T'XYZ) = -\frac{\hbar^2}{2\mu}T(X''YZ + XY''Z + XYZ'')$$
$$i\hbar\frac{T'}{T} = -\frac{\hbar^2}{2\mu}\left(\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}\right)$$

solving first for $T(t)$, let $i\hbar\frac{T'}{T} = \alpha$ for a constant alpha. Then:

$$i\hbar\frac{T'}{T} = \alpha$$
$$T' = -\frac{i}{\hbar}\alpha T$$
$$T(t) = C_1 e^{-i\alpha t/\hbar}$$

where C_1 is a constant. Note that this solution is general, meaning it works for any potential function $V(x, y, z)$. Moving on to the spatial variables, their solutions are analogous, so solving for one solves for all.

Let $-\frac{\hbar^2}{2\mu}\frac{X''}{X} = \beta_x$, $-\frac{\hbar^2}{2\mu}\frac{Y''}{Y} = \beta_y$, and $-\frac{\hbar^2}{2\mu}\frac{Z''}{Z} = \beta_z$. Solving the ODE over x:

$$-\frac{\hbar^2}{2\mu}\frac{X''}{X} = \beta_x$$
$$X'' + \frac{2\mu}{\hbar^2}\beta_x X = 0$$

for eigenvalues λ, this ODE can be solved as follows:

$$\lambda^2 + \frac{2\mu}{\hbar^2}\beta_x = 0$$
$$\lambda = \pm\sqrt{-\frac{2\mu}{\hbar^2}\beta_x}$$

the solution then depends on β_x which can be found by applying the boundary conditions. $X(x)$ is continuous and, for $x \notin [0, \ell_1]$, $X(x) = 0$. Then, $X(0) = 0 = X(\ell_1$, otherwise there would be a discontinuity at the boundary. Because of this, it turns out that there are no non-trivial solutions when $\beta_x \le 0$ because $g(x) = c_1 \sinh\left(\sqrt{\frac{-2\mu\beta_x}{\hbar}}x\right) + c_2 \cosh\left(\sqrt{\frac{-2\mu\beta_x}{\hbar}}x\right)$ and $h(x) = ax + b$ only have more than one zero when they're identically the zero function. Then, the only case left is $\beta_x > 0$:

$$X(x) = A_1 \sin\left(\sqrt{\frac{2\mu\beta_x}{\hbar}}x\right) + A_2 \cos\left(\sqrt{\frac{2\mu\beta_x}{\hbar}}x\right)$$

$$X(0) = 0 = A_2$$

$$X(\ell_1) = 0 = A_1 \sin\left(\sqrt{\frac{2\mu\beta_x}{\hbar}}\ell_1\right)$$

$$\sqrt{\frac{2\mu\beta_x}{\hbar}}\ell_1 = n\pi$$

$$\beta_x = \frac{n^2\pi^2\hbar^2}{2\mu\ell_1^2}$$

this yields the general solution for $X(x)$, $Y(y)$, and $Z(z)$:

$$X(x) = A_1 \sin\left(\frac{n\pi}{\ell_1}x\right) \quad Y(y) = B_1 \sin\left(\frac{m\pi}{\ell_2}y\right) \quad Z(z) = C_1 \sin\left(\frac{k\pi}{\ell_3}z\right)$$

since the initial equality must hold, the following relationship arises:

$$\alpha = \beta_x + \beta_y + \beta_z = \frac{n^2\pi^2\hbar^2}{2\mu\ell_1^2} + \frac{m^2\pi^2\hbar^2}{2\mu\ell_2^2} + \frac{k^2\pi^2\hbar^2}{2\mu\ell_3^2} = \frac{\pi^2\hbar^2}{2\mu}\left(\frac{n^2}{\ell_1^2} + \frac{m^2}{\ell_2^2} + \frac{k^2}{\ell_3^2}\right)$$

putting all of it together then gives, for $x, y, z \in [0, \ell_1] \times [0, \ell_2] \times [0, \ell_3]$:

$$\psi(t, x, y, z) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{k=1}^{\infty} A_{n,m,k} e^{-\frac{\pi^2\hbar^2}{2\mu}\left(\frac{n^2}{\ell_1^2} + \frac{m^2}{\ell_2^2} + \frac{k^2}{\ell_3^2}\right)ct} \sin\left(\frac{n\pi}{\ell_1}x\right) \sin\left(\frac{m\pi}{\ell_2}y\right) \sin\left(\frac{k\pi}{\ell_3}z\right)$$

using Theorem 2.3 together with the initial condition gives $A_{n,m,k}$:

$$\psi(0, x, y, z) = u(x, y, z) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{k=1}^{\infty} A_{n,m,k} \sin\left(\frac{n\pi}{\ell_1}x\right) \sin\left(\frac{m\pi}{\ell_2}y\right) \sin\left(\frac{k\pi}{\ell_3}z\right)$$

$$A_{n,m,k} = \frac{8}{\ell_1\ell_2\ell_3}\int_0^{\ell_1}\int_0^{\ell_2}\int_0^{\ell_3} u(x, y, z) \sin\left(\frac{n\pi}{\ell_1}x\right) \sin\left(\frac{m\pi}{\ell_2}y\right) \sin\left(\frac{k\pi}{\ell_3}z\right) dzdydx$$

$\square$

Note: While this solution is only valid for these specific conditions, one can find solutions to Schrödinger's Equation for numerous other potential functions. This is because the ODEs about the spatial coordinates can be written as a Sturm-Liouville problem. Since the time-dependent term is independent of $V(x, y, z)$, let $\psi(t, x, y, z) = T(t)u(x, y, z)$, so:

$$\frac{-\hbar^2}{2\mu}\nabla^2 u + V(x, y, z)u = \alpha u$$

For the separation constant $\alpha = \frac{\pi^2\hbar^2}{2\mu}\left(\frac{n^2}{\ell_1^2} + \frac{m^2}{\ell_2^2} + \frac{k^2}{\ell_3^2}\right)$. Then, whenever $V(x,y,z) = \chi(x) + \gamma(y) + \zeta(z)$ for arbitrary continuous functions $\chi(x)$, $\gamma(y)$, and $\zeta(z)$, this can PDE can be separated into the three Sturm-Liouville problems:

$$\begin{cases} X'' + (\frac{-2\mu}{\hbar^2}\chi(x) + \frac{2\mu}{\hbar^2}\alpha)X = 0 \\ Y'' + (\frac{-2\mu}{\hbar^2}\gamma(y) + \frac{2\mu}{\hbar^2}\alpha)Y = 0 \\ Z'' + (\frac{-2\mu}{\hbar^2}\zeta(z) + \frac{2\mu}{\hbar^2}\alpha)Z = 0 \end{cases}$$

7. Conclusion

Using some of the methods and theorems discussed during the course, notably the Generalized Fourier Series, Sturm-Liouville Theory, Separation of Variables, and the Heat Equation, one can solve Schrödinger's equation in numerous situations and get a good qualitative understanding of various others. The simplest conditions are those of the discussed infinite potential well in which the solution closely resembles that of a Heat Equation.

Further study of change of variables, Hermite Polynomials, and other concepts/techniques concerning partial differential equations are crucial to allow someone to solve Schrödinger's Equation under more complex conditions such as is necessary for advanced studies on quantum physics.

References

[1] N. H. Asmar. *Partial Differential Equations with Fourier Series and Boundary Value Problems.* 3rd ed. Dover Publications, 2017.