Quantum Tunneling via Finite Element

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1 Introduction

In this paper, we examine tunnelling solutions to the fundamental equation in quantum mechanics: the Schrödinger equation for a single particle.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \tag{1}$$

Here $\Psi = \Psi(\mathbf{x})$ is the wave function describing a quantum mechanical particle, t is time, $V = V(\mathbf{x}, t)$ is the potential with which the particle interacts. The constant m is the mass of the particle, and $\hbar$ is Planck's constant divided by 2π [1].

We consider the following scenario. A single particle is confined to an infinitely long cylinder. This may be approximated as a two dimensional problem, applying symmetry along the length of the cylinder. We suppose the cylinder corresponds to a potential well, posing a potential barrier at the boundary of the cylinder to the rest of $\mathbb{R}^2$.

We suppose further there is a second cylinder in the vincinity of the first and parallel to it, with its own potential well. We ask the question: what is the probability the particle will tunnel from the first cylinder to the second? The situation can be summarized in figure 1.

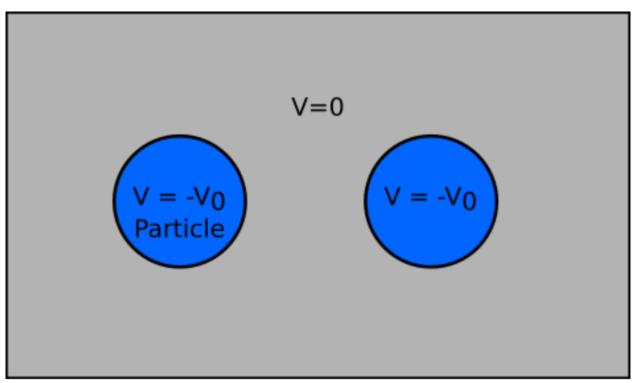

Figure 1: Two cylindrical potential wells

To solve this problem using finite elements, first we must compute the weak form, then construct the finite dimensional representation. Finally, an initial condition must be specified. Then solving the problem is the same as evolving the system forward in time.

To introduce notation, let Ω_0 denote the first cylinder and Ω_1 denote the second (the one without the particle initially). We suppose the radius of each is R and the distance between their centers is $L > 2R$.

1.1 Nondimensionalization

Nondimensionalizing the problem is essential since $\hbar \approx 10^{-34} J \cdot s$ in S.I. units. Let the spacial scaling be R, the radius of each of the cylinders. This induces a time scaling of $\dfrac{2mR^2}{\hbar}$. Finally there is an energy scaling of V_0. To summarize, if $\tilde{\mathbf{x}}, \tilde{t}, \tilde{V}$ all have units, then

$$\tilde{\mathbf{x}} = R\mathbf{x}, \quad \tilde{t} = \frac{2mR^2}{\hbar}t, \quad \tilde{V}(\tilde{\mathbf{x}}) = V_0 V(\mathbf{x}). \tag{2}$$

Let $\nu = \dfrac{2mR^2V_0}{\hbar^2}$. The nondimensionalized problem then reads

$$i\frac{\partial \Psi}{\partial t} = -\nabla^2\Psi + \nu V(\mathbf{x})\Psi. \tag{3}$$

Here, the form of $V(\mathbf{x})$ is

$$V(\mathbf{x}) = \begin{cases} -1 & \mathbf{x} \in \Omega_0 \cup \Omega_1 \\ 0 & \text{otherwise} \end{cases}. \tag{4}$$

1.2 Boundary Conditions

Since we are considering the problem defined on all of $\mathbb{R}^2$, the required boundary conditions are vanishing at infinity. That is

$$\lim_{|\mathbf{x}|\to\infty} \Psi(\mathbf{x}, t) = 0, \quad \lim_{|\mathbf{x}|\to\infty} |\nabla\Psi(\mathbf{x}, t)| = \mathbf{0} \tag{5}$$

This corresponds with the physical situation that the probability of finding the particle infinitely far away from either of the cylinders is zero.

1.3 Initial Conditions

Since the Schrödinger equation is only a first order equation in time, only $\Psi(\mathbf{x}, 0)$ needs to be specified. For this, we consider the initial condition corresponding to a particle in its lowest energy state, confined to the first cylinder. In this situation, only Ω_0 is present, and the potential reads

$$V^{(0)}(\mathbf{x}) = \begin{cases} -1 & \mathbf{x} \in \Omega_0 \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

For a quantum particle, its energy states are determined from the spatial component of its equation after separation of variables. Letting $\Psi(\mathbf{x}, t) = \psi(\mathbf{x})T(t)$, then this reads

$$i\frac{T'}{T} = \frac{-\nabla^2\psi + \nu V^{(0)}\psi}{\psi} = \epsilon.$$

Here ϵ, the eigenvalue, corresponds to the energy level of the quantum state [1]. Disregarding the time component, the initial condition for the above problem solves

$$-\nabla^2\Psi(\mathbf{x}, 0) + \nu V^{(0)}\Psi(\mathbf{x}, 0) = \epsilon\Psi(\mathbf{x}, 0). \tag{7}$$

Furthermore, this holds for the smallest possible value of ϵ.

2 Constructing the Weak Formulation

To construct the weak formulation of the nondimensionalized Schrödinger equation, consider a test function $\phi(\mathbf{x})$ which is sufficiently smooth (this will be clarified later). Integrating against the Schrödinger equation gives

$$i\left\langle \phi, \frac{\partial \Psi}{\partial t} \right\rangle_{L^2} = \langle \nabla\phi, \nabla\Psi \rangle_{L^2} + \nu \langle \phi, V\Psi \rangle_{L^2} .$$

Where each integral is on all of $\mathbb{R}^2$. Importantly, the quantity $\Psi^*\Psi$ represents a probability density function (pdf) for the particle. As a result, since the probability the particle exists somewhere in $\mathbb{R}^2$ is 1, $\Psi \in L^2(\mathbb{R}^2) \times C^1(\mathbb{R}_+)$. Applying the same approach to the initial condition: $\Psi_0(\mathbf{x}) := \Psi(\mathbf{x}, 0)$ gives

$$\langle \nabla\phi, \nabla\Psi_0 \rangle_{L^2} + \nu \left\langle \phi, V^{(0)}\Psi_0 \right\rangle_{L^2} = \epsilon \langle \phi, \Psi_0 \rangle .$$

For the weak form to exist, $\Psi \in H^1(\mathbb{R}^2) \times C^1(\mathbb{R}_+)$. However there is more to it than this. In quantum mechanics, the operator

$$\hat{\mathbf{p}} = -i\hbar\nabla$$

corresponds to the momentum of a particle; and the pdf for the momentum is represented by $\Psi^* \cdot \hat{\mathbf{p}}(\Psi)$ [1]. Consequentially, requiring the momentum be well defined everywhere necessitates $\Psi \in C^1(\mathbb{R}^2) \times C^1(\mathbb{R}_+)$. To ensure this, we must therefore require $\Psi \in H^2(\mathbb{R}^2) \times C^1(\mathbb{R}_+)$. Therefore we can now construct the weak form of the problem

$$i\left\langle \phi, \frac{\partial \Psi}{\partial t} \right\rangle_{L^2(\mathbb{R}^2)} = \langle \nabla\phi, \nabla\Psi \rangle_{L^2(\mathbb{R}^2)} + \nu \langle \phi, V\Psi \rangle_{L^2(\mathbb{R}^2)} \tag{8}$$

$$\langle \nabla\phi, \nabla\Psi_0 \rangle_{L^2(\mathbb{R}^2)} + \nu \left\langle \phi, V^{(0)}\Psi_0 \right\rangle_{L^2(\mathbb{R}^2)} = \epsilon_{\min} \langle \phi, \Psi_0 \rangle_{L^2(\mathbb{R}^2)} , \quad \forall \phi \in H_0^2(\mathbb{R}^2) \tag{9}$$

3 Finite Dimensional Approximation

To build a finite dimensional version for our problem to apply finite elements, first we make the following approximation. Let $\Omega \subset \mathbb{R}^2$ be bounded with $\Omega_0, \Omega_1 \subset \Omega$ and with

$$\max\{\mathrm{diam}(\Omega_0), \mathrm{diam}(\Omega_1)\} \ll \mathrm{diam}(\Omega).$$

We will then approximation the solution Ψ and its initial condition, Ψ_0 on Ω, by applying the boundary condition

$$\Psi_{(0)}\big|_{\partial\Omega} = 0.$$

Next let $\mathcal{T}$ be a triangulation for Ω, and on this triangulation we **TOOD: specify finite element in form** (K, P, N). Let V be the finite dimensional restriction of H_0^2 onto this triangulation, and let $\{\phi_\ell\}_{\ell=0}^{M}$ be a basis for V.

Suppose that

$$\Psi_0(\mathbf{x}) = \sum_{\ell=0}^{M} \alpha_\ell^{(0)} \phi_\ell(\mathbf{x}), \quad \Psi(\mathbf{x}, t) = \sum_{\ell=0}^{M} \alpha_\ell(t)\phi_\ell(\mathbf{x}), \quad \alpha_\ell(0) = \alpha_\ell^{(0)}.$$

The variational form of the problem then becomes:

$$i \sum_{k=0}^{M} \langle \phi_\ell \phi_k \rangle_{L^2(\Omega)} \alpha_k' = \sum_{k=0}^{M} \langle \nabla\phi_\ell, \nabla\phi_k \rangle_{L^2(\Omega)} \alpha_k + \nu \langle \phi_\ell, V\phi_k \rangle_{L^2(\Omega)} \alpha_k \tag{10}$$

$$\sum_{k=0}^{M} \langle \nabla\phi_\ell, \nabla\phi_k \rangle_{L^2(\Omega)} \alpha_k^{(0)} + \nu \left\langle \phi_\ell, V^{(0)}\phi_k \right\rangle_{L^2(\Omega)} \alpha_k = \epsilon_{\min} \langle \phi_\ell, \phi_k \rangle_{L^2(\Omega)} \alpha_k \tag{11}$$

Finally, let

$$M_{ij} = \langle \phi_i, \phi_j \rangle_{L^2(\Omega)}, \quad S_{ij} = \langle \nabla\phi_i, \nabla\phi_j \rangle_{L^2(\Omega)}, \quad V_{ij} = \langle \phi_i, V\phi_j \rangle_{L^2(\Omega)}.$$

Similarly for $V_{ij}^{(0)}$. The problem then reads in matrix form

$$iM\alpha' = S\alpha + \nu V\alpha \tag{12}$$

$$S\alpha^{(0)} + \nu V^{(0)}\alpha^{(0)} = \epsilon_{\min} M\alpha^{(0)} \tag{13}$$

The problem is now a set of coupled ODEs. Furthermore, the initial condition $\alpha^{(0)}$ satisfies the modified eigenvalue problem

$$(S + \nu V^{(0)})\alpha^{(0)} = \epsilon_{\min} M\alpha^{(0)}.$$

References

[1] D. J. Griffiths, *Introduction to Quantum Mechanics*, Pearson Education, Inc., New Jersey, 2005.