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 particle is confined to a well in $\mathbb{R}^2$. It passes by a ring-shaped well which is connected to a second well leaving the system (see figure 1). Such a situation is the problem of interest in characterizing quantum ring resonators **TODO: citation**.

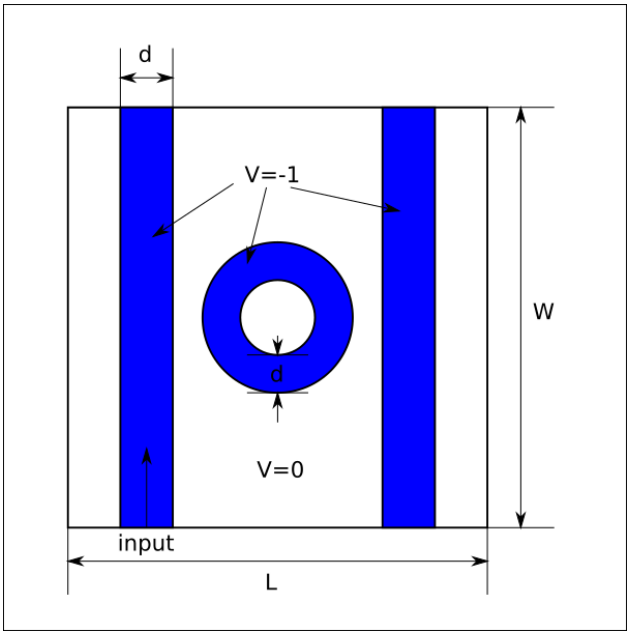

Figure 1: Sketch of Ring resonator. The domain excluding the shaded regions is Ω_0. The two shaded rectangles are Ω_1 and Ω_2 from left to right. Finally the center ring is Ω_3. The entire domain is $\Omega = \Omega_0 \cup \Omega_1 \cup \Omega_2 \cup \Omega_3$.

We will solve this problem using finite elements, and using the Python library FEniCS, which will take care of the heavy lifiting in constructing the finite element representation, as well as solving the resulting linear algebra system.

Let Ω_0 be the region without color, a rectangle of width W and length L, excluding the colored regions. The two long rectangles, in order from left to right are Ω_1 and Ω_2 respectively. Finally, the ring in the center is Ω_3.

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 d, the width of each of the long potential wells. This induces a time scaling of $\frac{2md^2}{\hbar}$. Finally there is an energy scaling of V_0, which characterizes the strength of the potential. To summarize, if $\tilde{\mathbf{x}}, \tilde{t}, \tilde{V}$ all have units, then

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

Let $\nu = \frac{2md^2 V_0}{\hbar^2}$. 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

$$V(\mathbf{x}) = \begin{cases} -1 & \mathbf{x} \in \Omega_1 \cup \Omega_2 \cup \Omega_3 \\ 0 & \mathbf{x} \in \Omega_0 \end{cases}. \tag{4}$$

1.2 Boundary and Initial Conditions

An input is specified on the lower portion of the left-most shaded rectangle. This will be denoted by the region Γ_{in}. All other boundaries of Ω which are also boundaries of Ω_i for $i = 1, 2$ will be denoted Γ_{out}. Finally, the rest of the boundary will be denonted Γ_D.

On Γ_{in}, there is a specified Dirichlet boundary condition: $f(\mathbf{x}, t)$, and on Γ_D the Dirichlet condition is zero. Lastly, on Γ_{out} we specify an outflow boundary condition. In quantum mechanics, the momentum operator, in this dimensionless system: $\hat{\mathbf{p}} = -\frac{i\hbar}{d}\nabla$. The outflow condition relates $\partial_t \psi$ with the momentum. All together the boundary conditions are

$$\text{Boundary Conditions} = \begin{cases} \Psi(\mathbf{x}, t) = 0 & \mathbf{x} \in \Gamma_D \\ \Psi(\mathbf{x}, t) = f(\mathbf{x}, t) & \mathbf{x} \in \Gamma_{\text{in}} \\ \dfrac{\partial \Psi}{\partial t} = -2i\dfrac{\partial \Psi}{\partial n} & \mathbf{x} \in \Gamma_{\text{out}} \end{cases} \tag{5}$$

Where $f(\mathbf{x}, t)$ is a prespecified function.

Finally for simplicity, we take an initial condition of an empty system: i.e.

$$\Psi(\mathbf{x}, 0) = 0.$$

2 Constructing the Weak Formulation

Since FEniCS will be doign the heavy lifting for the matrix construction and equation solving, the weak formulation will be optimized to fit this framework. FEniCS is designed around elliptic-like problems, so the problem will be discretized in time first, then each update will be computed by solving an elliptic problem.

The time discretization applied to the Schrödinger equation gives

$$i\frac{\Psi^{n+1}(\mathbf{x}) - \Psi^n(\mathbf{x})}{\Delta t} = \frac{1}{2}\left[-\nabla^2\Psi^{n+1} - \nabla^2\Psi^n + \nu V\Psi^{n+1} + \nu V\Psi^n\right].$$

Where $t^n = n\Delta t$ and $\Psi^n(\mathbf{x}) = \Psi(\mathbf{x}, t^n)$. Crank-Nicolson can be shown to be second order in time.

Rearranging this above expression gives

$$i\Psi^{n+1} + \frac{\Delta t}{2}\nabla^2\Psi^{n+1} - \frac{\nu\Delta t}{2}V\Psi^{n+1} = i\Psi^n - \frac{\Delta t}{2}\nabla^2\Psi^n + \frac{\nu\Delta t}{2}V\Psi^n.$$

At each time step, we can assume Ψ^n is known, with $\Psi^0 \equiv 0$ by the initial condition. Therefore this is now an elliptic problem for the $n+1$'st time step.

Next, for a quantum mechanical problem: the wavefunction must be continuously differentiable, which ensures that position and momentum are well defined everywhere. To guarentee this in $\mathbb{R}^2$ we require $\Psi \in H^4(\Omega)$.

To build the weak form, let

$$\mathcal{V} = \{u \in H^4(\Omega) : u|_{\Gamma_D \cup \Gamma_{\text{in}}} = 0\}.$$

This will be our test function space. Let $\Phi \in \mathcal{V}$. Then the weak formulation comes from 3 terms:

$$\int_\Omega \Phi\Psi\, dx, \quad \int_\Omega \Phi\nabla^2\Psi\, dx, \quad \int_\Omega \Phi V\Psi\, dx.$$

Here we are considering the real and imaginary components of Ψ separately. In sticking with the quantum mechanical theme, I will be using bra-ket notation. That is Ψ will be known as $|\Psi\rangle$. The bar and angle denote that Ψ is an element of the Hilbert space $\mathcal{V}$. Next I will denote the linear functional:

$$\langle\Phi|\cdot = \int_\Omega \Phi\cdot\, dx.$$

That is $\langle\Phi|$ is the linear functional built by the L^2 inner product with $|\Phi\rangle$. Finally an inner product with an operator $\mathcal{O}$ will be denoted:

$$\langle\Phi|\,\mathcal{O}\,|\Psi\rangle = \int_\Omega \Phi\mathcal{O}(\Psi)\, dx.$$

The first and second components of the variational form are not interesting. Instead what is interesting is the middle term.

$$\begin{aligned}\int_\Omega \Phi\nabla^2\Psi\, dx &= \langle\Phi|\,\nabla^2\,|\Psi\rangle \\ &= \int_{\partial\Omega} \Phi\frac{\partial\Psi}{\partial n}\, d\sigma - \int_\Omega \nabla\Phi\cdot\nabla\Psi\, dx. \\ &= \int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi}{\partial n}\, d\sigma - \langle\nabla\Phi|\nabla\Phi\rangle\end{aligned}$$

Due to the boundary condition on Γ_{out}, we know

$$\frac{\partial\Psi}{\partial t} = i\frac{\partial\Psi}{\partial n}.$$

Using the Crank-Nicolson time discretization on the boundary changes this to

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \frac{i}{2}\left(\frac{\partial\Psi^{n+1}}{\partial n} + \frac{\partial\Psi^n}{\partial n}\right).$$

Therefore

$$\int_{\Gamma_{\text{out}}} \Phi\Psi^{n+1}\,d\sigma - \frac{i\Delta t}{2}\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n+1}}{\partial n}\,d\sigma = \int_{\Gamma_{\text{out}}} \Phi\Psi^{n}\,d\sigma + \frac{i\Delta t}{2}\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n}}{\partial n}\,d\sigma.$$

Giving

$$\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n+1}}{\partial n}\,d\sigma = \frac{2i}{\Delta t}\left(-\int_{\Gamma_{\text{out}}} \Phi\Psi^{n+1}\,d\sigma + \int_{\Gamma_{\text{out}}} \Phi\Psi^{n}\,d\sigma + \frac{i\Delta t}{2}\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n}}{\partial n}\,d\sigma\right).$$

Therefore the weak form of the PDE reads

$$\begin{aligned} i\left\langle\Phi\middle|\Psi^{n+1}\right\rangle - \frac{\Delta t}{2}\left\langle\nabla\Phi\middle|\nabla\Psi^{n+1}\right\rangle - \frac{\nu\Delta t}{2}\left\langle\Phi\middle|V\middle|\Psi^{n+1}\right\rangle - i\int_{\Gamma_{\text{out}}}\Phi\Psi^{n+1}\,d\sigma = \\ i\left\langle\Phi|\Psi^{n}\right\rangle + \frac{\Delta t}{2}\left\langle\nabla\Phi|\nabla\Psi^{n}\right\rangle + \frac{\nu\Delta t}{2}\left\langle\Phi\middle|V\middle|\Psi^{n}\right\rangle - i\int_{\Gamma_{\text{out}}}\Phi\Psi^{n}\,d\sigma \end{aligned} \tag{6}$$

FEniCS uses UFL - unified form assembly language, which is able to take a (nearly verbatim mathematically formatted) variational form, and convert this into a matrix system and solve automatically. The only adjustment that needs to be made is to the boundary integrals. To enforce the integration take place only on Γ_{out}, we use

$$\int_{\Gamma_{\text{out}}} \Phi\Psi\,d\sigma = \int_{\partial\Omega} \Phi\mathbb{1}(\mathbf{x}\in\Gamma_{\text{out}})\Psi\,d\sigma.$$

3 Finite Dimensional Approximation

Since FEniCS cannot handle complex numbers, we are considering the real and imaginary components of Ψ separately. To that end, thus far all variational terms are between real functions. Next, we suppose

$$\Psi = \Psi_R + i\Psi_I.$$

Where $\Psi_{R,I}$ are real functions corresponding to the real and imaginary components of Ψ respectively. Let $H^1(\Omega)$ be the function space considered (Note however that the potential needs to only live in L^2). Let ψ_ℓ be the ℓ'th basis function in the finite dimensional approximation of H^1, which is build on top of a mesh built in FEniCS. FEM demands

$$\Psi = \sum_\ell \lambda_\ell(t)\phi_\ell, \quad \lambda_\ell : \mathbb{R}^+ \to \mathbb{C}.$$

Here λ_ℓ are the (complex) scalings of the basis functions. This takes care of the fact that Ψ is complex.

Now the bra-ket notation can really shine. In the ket $|\Psi\rangle$, Ψ is just a dummy indicator. So it can be anything we want. To that end, let

$$\langle k|\ell\rangle = \int_\Omega \psi_k\psi_\ell\,dx, \quad \langle D,k|D,\ell\rangle = \int_\Omega \nabla\psi_k\cdot\nabla\psi_\ell\,dx.$$

And so on... This means the mass, stiffness and potential matrices are indexed by

$$M_{k\ell} = \langle k|\ell\rangle, \quad S_{k\ell} = \langle D,k|D,\ell\rangle, \quad V_{k\ell} = \langle k|V|\ell\rangle = \int_\Omega \psi_k V\psi_\ell\,dx.$$

We also denote a boundary operator:

$$B_{k\ell} = \int_{\Gamma_{\text{out}}} \psi_k\psi_\ell\,d\sigma.$$

Then the finite dimensional variational form reads

$$\begin{aligned} \sum_\ell\left(i\langle k|\ell\rangle - \frac{\Delta t}{2}\langle D,k|D,\ell\rangle - \frac{\nu\Delta t}{2}\langle k|V|\ell\rangle - iB_{k\ell}\right)\lambda_\ell^{n+1} = \\ \sum_\ell\left(i\langle k|\ell\rangle + \frac{\Delta t}{2}\langle D,k|D,\ell\rangle + \frac{\nu\Delta t}{2}\langle k|V|\ell\rangle - iB_{k\ell}\right)\lambda_\ell^{n} \end{aligned} \tag{7}$$

Finally the boundary conditions. All remaining boundary conditions are Dirichlet. Let I_D correspond to the indices of coordinates on Γ_D and I_{in} those on Γ_{in}. These indices can be extracted in the above matrices, and assigned in λ^{n+1} after solving. The remaining indices: I_{free} are the free indices which need to be solved to determine the appropriate values.

References

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