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Removal of Accidental Degeneracy

Christopher M. Pierce

Supervised by
L. Ramdas Ram-Mohan

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Abstract

The energy degeneracies of charge carriers in cubic GaAs/GaAlAs quantum dots are analyzed and contrasted with the degeneracies of solutions to the infinite potential well problem. Accurate energy eigenvalues for realistic systems are computed by the finite element method and group theoretic arguments are applied to explain the removal of degeneracies only present in the infinite well case.

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1 Introduction

While the rules of quantum mechanics produce good testable results, many problems in its scope do not admit analytical solutions. In order to get around this, physicists and engineers often turn to solving an approximate form of their problems. Although the solutions to these approximate systems may mimic the solution of the exact system in a certain sense, the solutions often possess a fundamentally different structure. It is only through careful theoretical considerations and the use of robust techniques for the development of approximate solutions that accurate results may be derived.

Considered in this article is the case of the eigenenergies of charge carriers in cubic GaAs/GaAlAs quantum dots. The system, in the envelope function approximation, is modeled by a particle in the finite well potential

$$V = \begin{cases} 0 & 0 \leq x \leq L \text{ and } 0 \leq y \leq L \text{ and } 0 \leq z \leq L \\ V_0 & \text{Otherwise} \end{cases}. \tag{1}$$

The eigenergies of these charge carriers are governed by the solutions of the Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi. \tag{2}$$

There are, however, no analytical solutions for our problem.

Instead, one may turn to an approximate version of the system by taking $V_0 \to \infty$. The infinite potential well is a system familiar to anyone who has studied quantum mechanics at an undergraduate level and has well known analytical solutions.[1] To review, the eigenenergies of a particle in the infinite potential well are

$$E_{\alpha\beta\gamma} = \frac{\hbar^2\pi^2}{2mL^2}(\alpha^2 + \beta^2 + \gamma^2), \tag{3}$$

for the positive integers α, β, γ. In the position space representation, their associated eigenfunctions are

$$\psi_{\alpha\beta\gamma} = \sqrt{\frac{8}{L}} \sin\left(\frac{x\pi\alpha}{L}\right) \sin\left(\frac{y\pi\beta}{L}\right) \sin\left(\frac{z\pi\gamma}{L}\right). \tag{4}$$

It is well known that the eigenstates of the infinite potential well are highly degenerate. Any two sets of three integers whose squares sum to the same value will correspond to two different states with the same energy in the

Degeneracy Level	Example
1	{(1,1,1)}
3	{(1,2,2), (2,1,2), (2,2,1)}
6	{(1,2,3), (3,1,2), (2,3,1), (2,1,3), (3,2,1), (1,3,2)}

Table 1: Infinite Potential Well Degeneracies Due to Interchange of Quantum Numbers

problem. One way to visualize the solution space of the problem is as a three dimensional lattice where each point on the lattice of points in the positive octant is an eigenstate. The energy associated with each state is then just the square of its distance from the origin and sets of degenerate eigenstates are just those at the same distance from the origin. A representation of this is shown in Figure 1.

Symmetries in the Hamiltonian are one reason for the degeneracies found in the solutions of the infinite potential well. However, there are also degeneracies due to the fact that the energies of states are simply related to the quantum numbers describing that state. Three types of degeneracy from the interchange of quantum numbers are listed in Table 1. However, there are even more degeneracies from Pythagorean triplets such as

$$7^2 + 24^2 = 15^2 + 20^2,$$

or examples containing the product of three squares such as

$$3^2 + 3^2 + 3^2 = 5^2 + 1^2 + 1^2.$$

This leads to the existence of a much greater number of degenerate states than expected from the symmetries of the problem. These extra degeneracies are known as accidental degeneracies.

It has previously been shown that these accidental degeneracies are removed in the transition to the finite case in two dimensions.[2] Therefore, it is expected that solutions to the finite well problem in three dimensions will not have the same degeneracy structure as the infinite well case. On the other hand, the problem still has a highly symmetric Hamiltonian which should induce certain degeneracies into the set of solutions. Our goal, therefore is to study the degeneracies of the solutions to the infinite potential well in realistic circumstances. These results will then be contrasted with the known degeneracies of the infinite potential well.

2 Methodology

Two methods were used to explore the degeneracies of solutions to the finite potential well problem. The first was by using numerical techniques to develop highly accurate approximate solutions for the first few eigenstates. The development and ubiquity of high speed computers has led to the increased usage of numerical techniques by physicists and have put problems such as ours within the reach of certain algorithms. Degeneracy was also studied by using group theory to investigate the solutions to the infinite well problem. By distinguishing the so-called accidental degeneracies from those caused by symmetries in the problem's Hamiltonian, one can predict what the degeneracy structure of solutions to the finite case will look like.

2.1 Numerical Techniques

The Finite Element Method (FEM) was used to generate high quality approximate solutions to the Schrodinger equation. Partial differential equations are actually unable to be solved directly with the FEM as it solves a variational problem instead. Schrodinger's equation, however, may be reformulated to work with the FEM. Consider the action defined by

$$S = \int_{\Omega} \mathrm{d}\boldsymbol{r}^3 \left[\frac{\hbar^2}{2m} \nabla\psi^* \cdot \nabla\psi + \psi^*(V - E)\psi \right]. \tag{5}$$

Setting its variation to zero, denoted as

$$\delta S = 0, \tag{6}$$

leads to the Schrodinger equation.

The domain is now split into may small regions which are called elements. Solutions on each domain may be represented as a linear combination of basis functions

$$u = \sum_i A_i u_i. \tag{7}$$

By directly performing the integration in Equation 5 the action on any given element may be expressed as a bilinear form as

$$S_{\text{local}} = \sum_{i,j} \left[\psi_i^* A_{ij} \psi_j + \psi_i^* B_{ij} \psi_j \right], \tag{8}$$

where A_{ij} and B_{ij} are matrices.

Globally, the action is also bilinear and the A and B matrices are formed by overlaying each of the local matrices, being careful to consider continuity over the elements. Minimization of the action is now as simple as setting the various derivatives of the bilinear form to zero. This turns our entire problem into the generalized eigenvalue problem

$$A\boldsymbol{\psi} = EB\boldsymbol{\psi}. \tag{9}$$

Solutions may be readily acquired through a number of numerical solver packages.

No software of the quality needed for the project existed at the time of this writing. The author wrote a library for the development of FEM software as well as several pieces of software for developing the results of this MQP. The library which now measures over 25,000 lines of c++ code implements new algorithms for handling the integration, interpolation and mesh handling requirements of efficient FEM software.

One significant problem that was encountered early in the project was that the amount of computation required to achieve solutions of a reasonable accuracy exceeded the capabilities of even the fastest computers available. Displayed in Figure 2 is a representation of the computational complexity of the two problems used in the FEM: matrix generation and eigensolving. It was necessary to turn to parallel computing to get data in a sensible amount of time. Matrix generation was not difficult to parallelize as it involves a loop over each element in the mesh. This may be divided amongst the processors performing the calculation and each may perform its work and collect the results together at the end.

Eigensolving was a more difficult issue and is an area of active research. However, there already existed a suitable solver package available under an open source license. The package SLEPc was used and, as indicated in Figure 3 showed near ideal speedup under sufficient constraints.[3]

With a toolkit now assembled to retrieve accurate approximate solutions to the Schrodinger equation in three dimensions, it was time to validate the software. The solutions to the infinite potential well formed an excellent test as the energies and eigenfunctions are known analytically and could be compared to the approximate results from the solver. Trials were run using progressively finer and finer meshes and using linear basis functions. This is, for historical reasons, known as h-refinement. Energies for different states

were collected and a relative error computed by comparing them with the analytical values for the energies of their respective states. These were then plotted against the number of degrees of freedom in the problem. The result is shown in Figure 4.

It was now time to generate solutions to the finite potential well problem. A mesh was constructed to contain the well and a region twice the width of the well on either side. This allowed sufficient space for the eigenfunctions to die off before encountering the boundary. The mesh was constrained to prevent elements from crossing the barrier into the well. That is, the elements near the barrier were configured such that their faces lay against the surface without penetrating.

The trials shown in Figure 4 provided a lower bound for the size of the mesh in order provide a given accuracy. From that point, trials were run with progressively finer and finer meshes. A sense of the tolerance of the results could be gained by looking at the differences between approximate energy values between two successive trials. This was continued until an estimated relative error of 10^{-5} was achieved.

2.2 Group Theory

The infinite potential well and the finite potential well both possess a highly symmetric Hamiltonian. In the case of the infinite potential well, however, its separable potential gives rise to a much larger number of degeneracies than in the case of the finite well. Group theory allows us to categorize the degenerate states of the infinite case into classes of functions that are related by symmetry transformations. The cubic wells have O_h symmetry which itself has 10 conjugacy classes. Any function on the cube, such as our wavefunction, may be split into components that transform as the various conjugacy classes and irreducible representations by a projection operator.[4] The dimension of each representation will then give an indication of the degeneracy that that component possesses.

3 Results

The states that were looked at in this project were the $(1, 1, 3)$, $(1, 3, 1)$, and $(3, 1, 1)$ states of the infinite potential well. Applying the above group theory methodology to the state showed that these states are actually linear com-

Finite Well (meV)	Infinite Well (meV)
31.271	42.409
62.349	84.819
62.354	84.819
62.355	84.819
...	...
113.568	155.501
113.655	155.501
113.658	155.501

Table 2: Eigenenergies of the Infinite and Finite Potential Wells

binations of functions that transform as the irreducible representations A_{1g} and E_g. Therefore, theory predicts that in the absence of greater symmetry, the states will exist as a singlet and two doublets.

The numerical results provided by the finite element method are shown in Table 2. A width of 200 Å, effective mass of $0.0665m_e$ inside the well and $0.0858m_e$ outside the well, and barrier height of 276.0 meV was used in the trial. Wavefunctions were plotted as well by considering surfaces of constant value for the returned solutions. These are shown in Figures 5, 6, and 7. It can be clearly seen that the three fold degeneracy of the $(1, 1, 3)$, $(1, 3, 1)$, and $(3, 1, 1)$ states of the infinite potential well have now been broken into a singlet and doublet state. This is exactly as theory predicts.

4 Conclusion

Our results indicate a fundamental difference in the structure of the solutions to the infinite and finite potential wells. Approximations to our model of charge carriers in cubic GaAs/GaAlAs quantum dots such as that given by the infinite potential well give theorists an incorrect picture of the system. In this case, a biased understanding of the degeneracies of solutions.

Instead, one must use a variety of methods for the development of robust approximate solutions. Discussed here was the Finite Element Method which was shown to produce highly accurate solutions in three dimensions for problems that have no analytical solution. Frameworks such as the FEM are extremely important to our understanding of nature as they produce testable predictions for otherwise unworkable theories. Going forward, the

lessons learned from this case will help prevent misunderstanding of systems in the study of physics.

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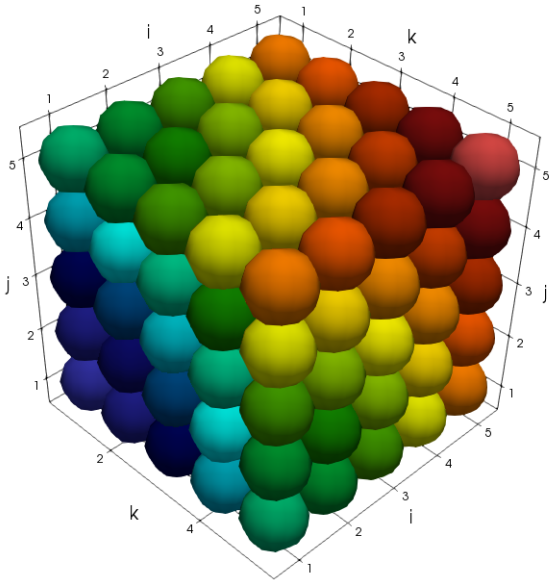
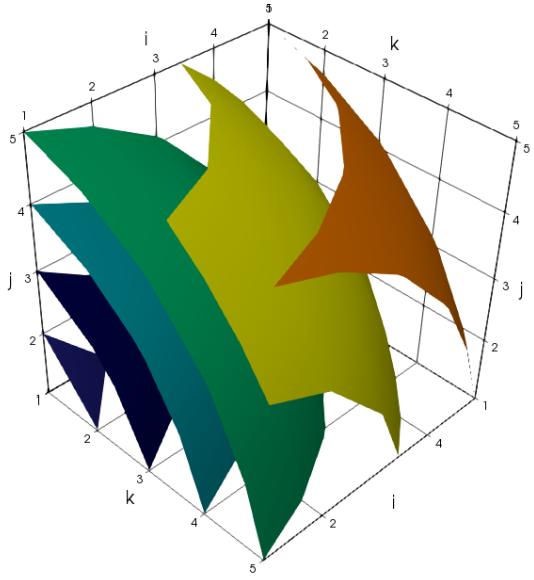


(a) Three Dimensional Lattice of Eigenstates



(b) Surfaces of Constant Energy

Figure 1: Degeneracy of States in Infinite Potential Well

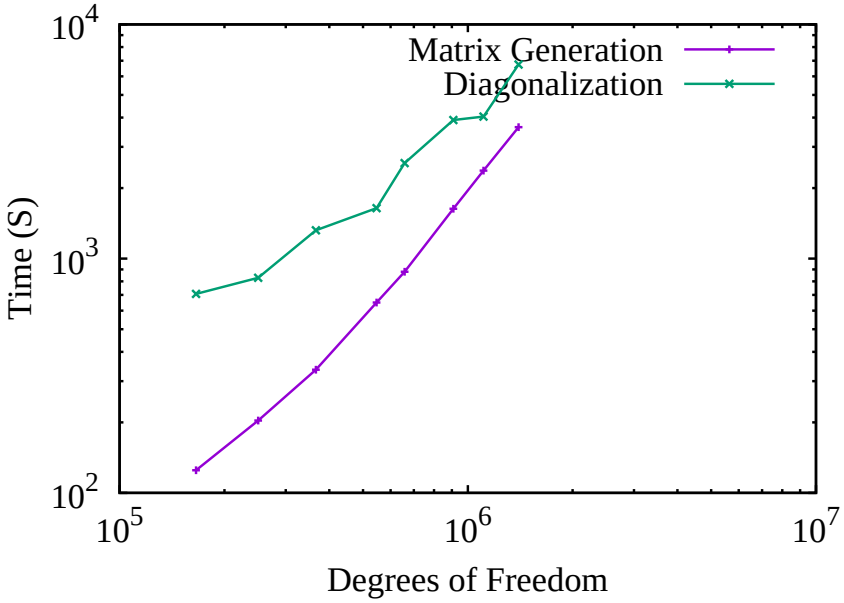


Figure 2: Time Complexity of Problems in FEM

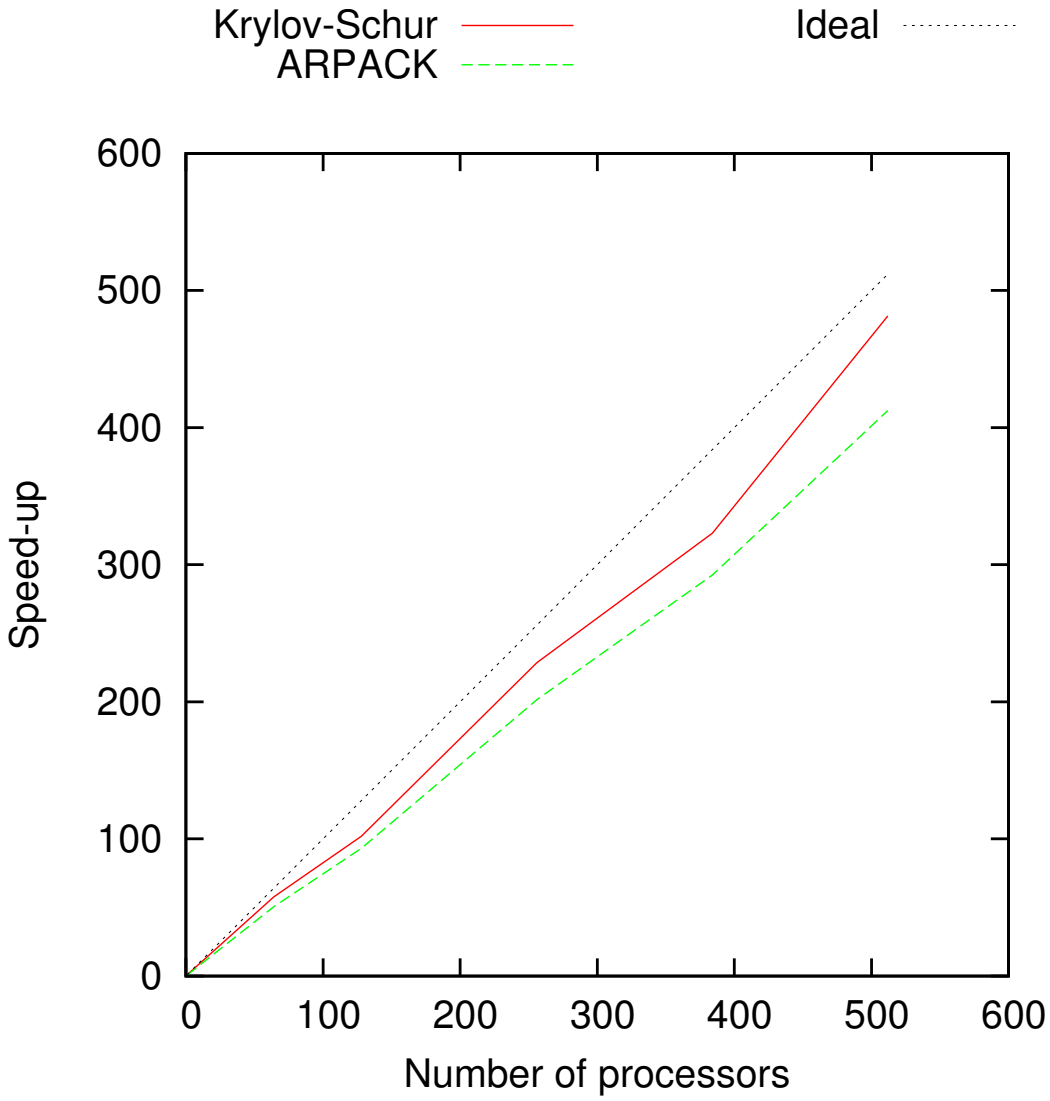


Figure 3: Eigensolver Speedup

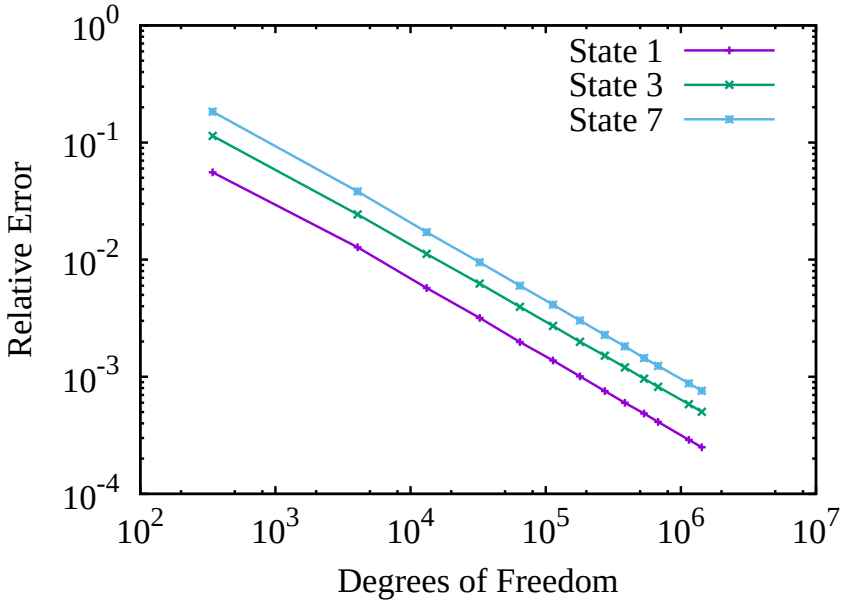


Figure 4: h-convergence of Solution to Infinite Potential Well Problem

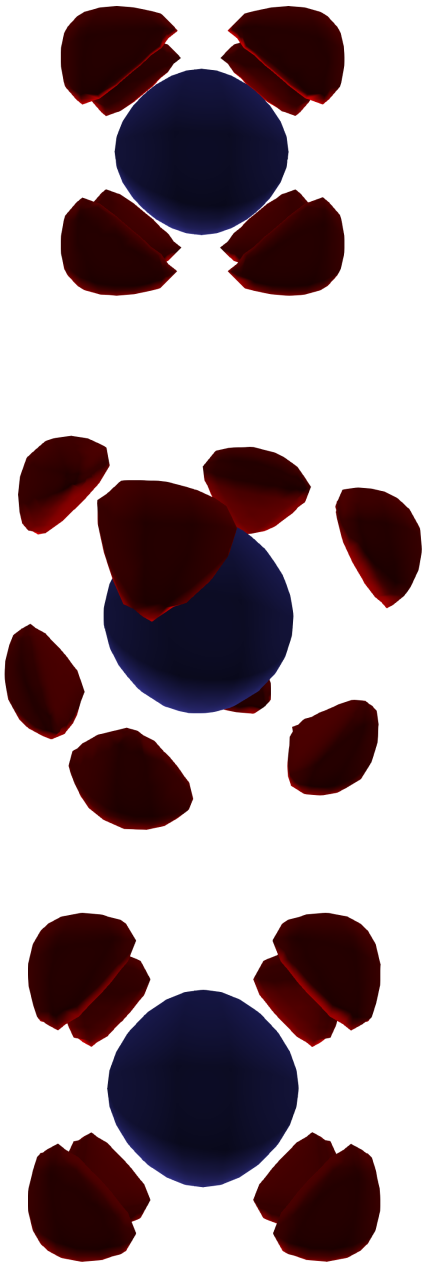


Figure 5: Singlet Eigenstate of Finite Potential Well

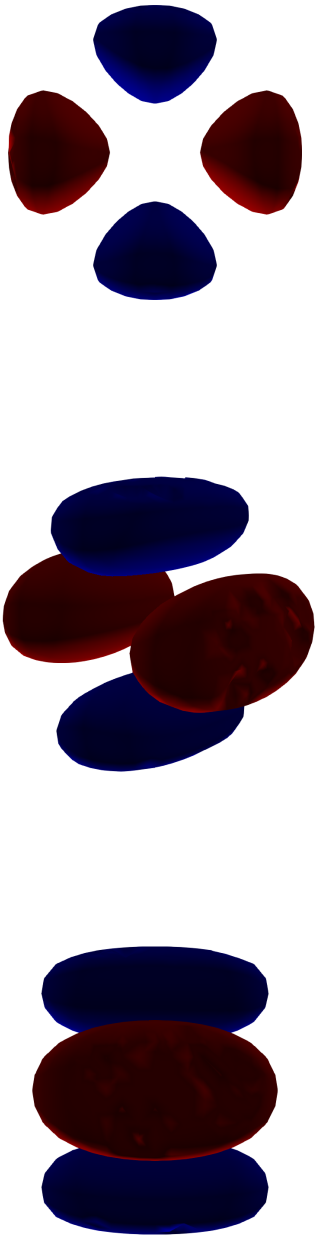


Figure 6: Doublet Eigenstate of Finite Potential Well

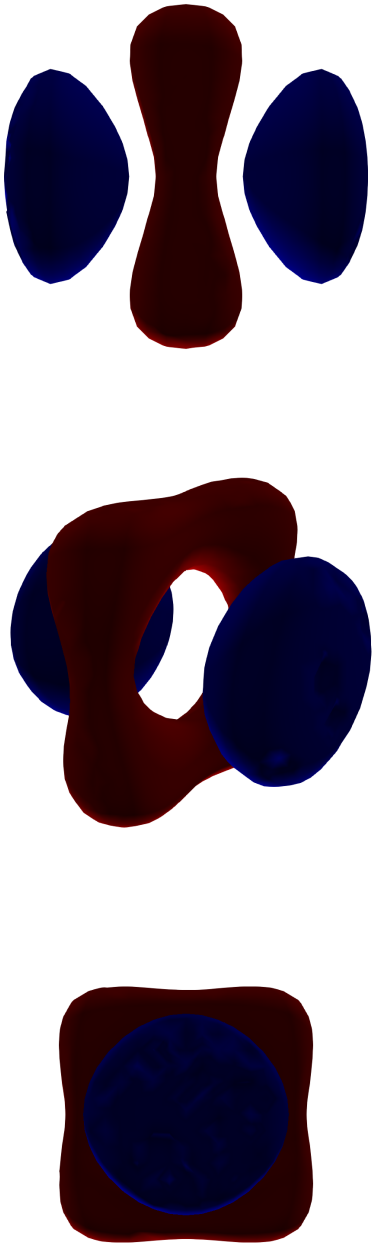


Figure 7: Doublet Eigenstate of Finite Potential Well