Quantum particles in fractal external potential

GEP Deliverable 1: Context and scope of the project

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1 Context

1.1 Introduction

The investigation world is always closely related to computer science. It is very frequent to solve a problem by modelling it on a computer using a certain programming language, and then making simulations to get a solution.

The physics investigation field highly benefits of this problem-solving approaches, as we find plenty of equations with physical meaning without an exact solution. To fix this, we try to solve them by representing these equations in a discrete and finite way, so our computers can handle it, and then we write algorithms to get approximations of a real solution.

This is an interdisciplinary research project, with an important theoretical part that involves some physics knowledge and a practical part that covers the design and development of algorithms to simulate and solve physics systems.

1.2 Theoretical concepts

I will summarize some theoretical concepts that are necessary to understand the rest of this document, so the reader can fully comprehend the aim and objectives of this project.

1.2.1 Quantum mechanics

Quantum mechanics is the theory that describes the physical properties of Nature at the scale of atoms and subatomic particles. When it was first formulated during the early decades of the 20th century, it introduced some ground-breaking concepts such as energy quantization, the uncertainty of position and momentum of a particle and the wave-particle duality of matter.

In classical physics we have Newton's second law, which given a set of initial conditions it can make a mathematical prediction of what path a given physical system will take over time. Its quantum analogous would be the Schrödinger equation which instead requires a statistical interpretation.

1.2.2 Schrödinger equation

Quantum mechanics tells us how the particles behave over time. This description is done using the Schrödinger equation, which provides the time evolution of the wavefunction (Ψ) of particles. The wavefunction is a mathematical description of the quantum state of the system, and with it, you can obtain the distribution of probability of the measurements that you can do over this system.

The Schrödinger equation is a differential equation, and has the following form:

$$i\hbar \frac{\partial}{\partial t} \Psi\left(r,t\right) = \hat{H}\Psi\left(r,t\right) \tag{1}$$

Here we define the Hamiltonian operator $\hat{H}$, which is an operator corresponding to the total energy of that system, including both kinetic (T) and potential energy (V), and for a single particle it takes the form:

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\nabla^2 + V\left(\mathbf{r},t\right) \tag{2}$$

The kinetic energy in quantum mechanics is proportional to the Laplace operator ∇^2, which is the addition of the second partial derivatives of the wavefunction. The potential energy is a function of the position of the particle, similarly to the classical case.

We are interested in the stationary properties, so we take the time-independent version of the Schrödinger equation:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \tag{3}$$

When solving it, the set of energy eigenvalues that provides (also called energy spectrum) is the set of possible energies obtained when measuring the system's total energy. Here we are interested in finding the ground state of the system, which is its lowest energy state. Differently from the classical systems where the energy of a single particle at zero temperature is finite due to zero-point motion, this ground state energy is always present in the quantum system, even in absolute zero temperature conditions.

1.2.3 Bose–Einstein condensate and Gross–Pitaevskii equation

Bose–Einstein condensate [1] (BEC) is a state of matter which occurs when a gas of bosons is cooled down to nearly the absolute zero. Under such conditions, a macroscopic fraction of bosons occupy the ground state and the whole system can be described by the same wavefunction. Such a wavefunction satisfies the Gross–Pitaevskii equation, which describes the ground state of a quantum system of identical bosons.

1.2.4 Fractals

A fractal is a subset of the Euclidean space that illustrates a property called self-similarity, which means that appears the same at different scales and exhibits similar patterns at increasingly smaller scales.

1.2.5 Sierpiński carpet

The Sierpiński carpet is a plane fractal that was first described by Wacław Sierpiński in 1916, as a two dimensions generalization of the Cantor set, that was discovered in 1874 by Henry John Stephen Smith and introduced by German mathematician Georg Cantor in 1883.

The Cantor ternary set is created by iteratively deleting the open middle third from a set of line segments.

Figure 1: First six steps of Cantor ternary set

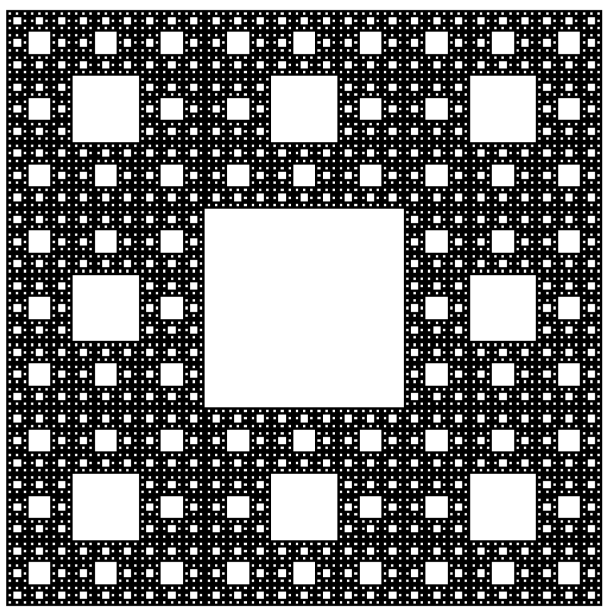

Figure 2: Sierpiński carpet with 5 levels of recursion

2 Justification

The interdisciplinary aspect of this project is what attracts me the most. Quantum mechanics is a complicated field that we do not study on the GEI degree. That is why this project really interested me personally, as it gives me the opportunity to learn and work on a subject that is quite different to what I am used to, and I am also able to contribute on a physics research project applying my computation knowledge, something I would enjoy doing as a future job.

There have been recent experiments [2] that have shown how it is possible to produce a Bose-Einstein condensate. In the last few years, new experimental techniques have been developed, and it became feasible to create two-dimensional Fermi or Bose gas in highly controllable external potential. The projected potential can be chosen essentially in any desired shape, fractal shapes included. This means that our work could be verified by experimentation.

3 Objectives

The aim of the project is to study the properties of quantum particles in a fractal external potential. The main goal is to obtain a detailed description of such a system in terms of energetic, structural and dynamic properties. In particular, the energetic properties can be quantified by evaluation of the ground state energy and the excitation spectrum. The structural property of interest is the density profile. The dynamic property to be calculated is the diffusion coefficient.

We consider the external potential in the shape of a Sierpiński carpet. It has a fractal structure with the fractal dimensionality between 1 (i.e. a line) and 2 (i.e. a plane). The strength of the external potential is considered to be infinite (i.e. hard walls) in the positions where the fractal is present. It means that the particles cannot diffuse freely in the system. At the same time, the phase space is joined, that is the particle is allowed to move between any two points where the external field is absent. The fractal shape is defined in a simple recursive procedure and depends on the recursion level.

One of our goals is to provide a detailed description of the properties of quantum particles in fractal external potential. In particular, we plan to verify the existence of a simple scaling law between the recursion number of the zero-point energy of the system and the number of iterations of the fractal.

This is an interdisciplinary problem, based on application of mathematical concepts to the field of quantum physics, and relies on the use of numerical methods. This project requires carrying out a scientific investigation and a priori it is not clear which quantum system is going to be the best to study these properties.

4 Scope

We plan to execute this study considering different types of atoms confined to an external fractal potential. In particular we will consider:

- One quantum particle
- Ideal Fermions
- Interacting Bosons

In this way we cover the major typical experimental conditions. In experiments with ultracold atoms, the atoms obey either Bose-Einstein statistics (bosons) or Fermi-Dirac statistics (fermions). A proper simulation of the properties requires an implementation of different methods used to address the system's properties such as:

1. Exact diagonalization technique, applicable to one particle and many-body system composed of fermions.
2. Random Walk stochastic method, applicable to one particle.
3. Gross-Pitaevskii equation, applicable to many-body system composed of bosons.

Method 1 allows to obtain energetic and structural properties, while method 2 the structural and dynamic ones. Method 3 can be used to obtain energetic, structural and dynamic properties of the system.

5 Potential obstacles and risks

The biggest obstacle to me is the fact that I have to really comprehend all the physical concepts to be able to properly implement the techniques to model and solve the quantum systems that we propose. I am a computer science student and I have not been taught quantum mechanics, what means that this project involves a lot of self-studying by my part.

Another obstacle/risk is the possibility that some of the systems that we propose are not good to observe the properties we are searching for. That is why we want to try different quantum systems and compare the viability of studying them when applying an external field with a fractal shape.

6 How the project will be developed

As our goal is to study the effect of the external potential field on a quantum system, we must compute the ground state energy of the quantum system that we present.

To do so, for the case of a single particle in an infinitely high external potential box mathematically described by zero boundary conditions, we must solve the time-independent Schrödinger equation while we apply the external potential field to the box. We implement a Matlab code that generates a Sierpiński carpet given a recursion number and we apply the field to the particle by defining the potential energy part of the Hamiltonian operator using this fractal. This potential is described by the function $V(x, y)$, which checks if the position (x, y) of the fractal is filled or empty. With this done, we solve the time-independent Schrödinger equation on a discretized two-dimensional space, and we obtain the ground state energy and the wavefunction of the particle. In Figure 3 it can be seen the wavefunction obtained as a result of first experiments using this method.

We are going to repeat this process using a different number of iterations of the fractal, so we can deduce the relation that this parameter has with the zero-point energy.

We want to obtain a result, and as memory and computation resources are limited, we must define some discretization of the space that reflects in a computable problem. An option is to solve the problem with different values for N (being N the number of fractions the space is divided in) and study how this evolves when N goes to infinity, or analogously, when $1/N$ goes to 0.

As this first case involves a relatively simple quantum system, we can define a way of obtaining an exact solution of the system's properties that we are interested in. But as I previously mentioned on this document, there are a lot of systems without exact solutions, as we do not know how to solve them. To handle this, we are going to use numerical methods such as random walks to approximate solutions for the system's properties.

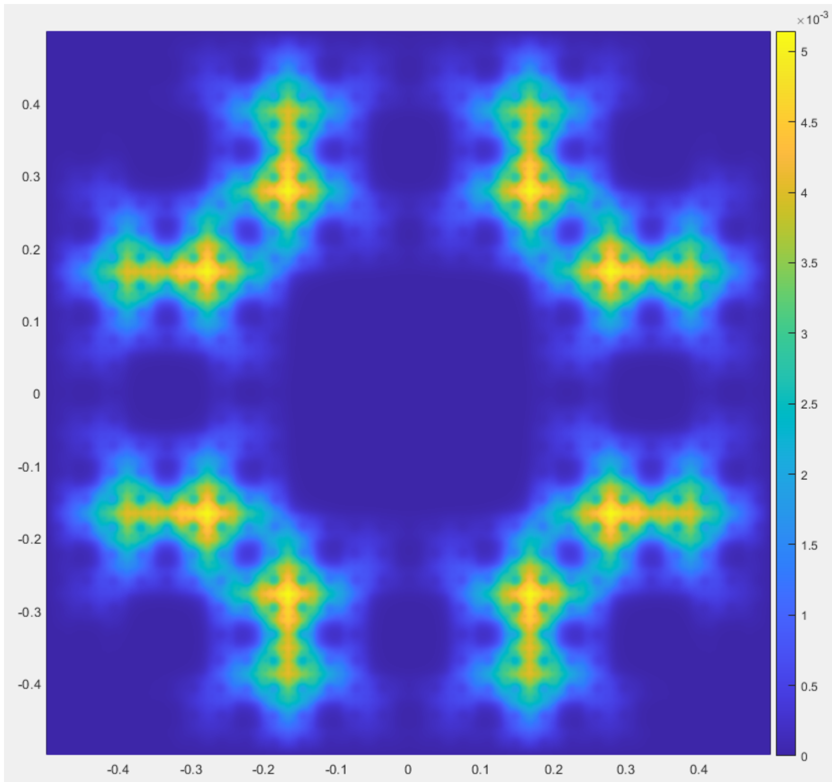

Figure 3: Wavefunction of a particle in a box with Sierpinski shaped external potential

6.1 Methodology and rigour

As this is a research project, every step we take is going to be vastly justified. Every modelling of a system is going to be verified by computing some properties that we know in advance, such as that the ground energy of a particle in a box without an external potential has to be equal to $\frac{\pi^2\hbar}{2mL^2}$.

All the techniques followed to model and solve the systems are going to be referenced and explained in detail on the thesis documentation.

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