Studies of quantum dots

Quantum-mechanical systems in traps and density functional theory

by

Jørgen Høgberget

THESIS
for the degree of
MASTER OF SCIENCE

(Master in Computational Physics)

Faculty of Mathematics and Natural Sciences
Department of Physics
University of Oslo

June 2013

Preface

blah blah

Contents

Chapter 1

Introduction

blah blah

Part I

Theory

Chapter 2

Quantum Mechanics

Although classical mechanics succeeds at describing the visual objects of the world to great presicion, it does not function as a general framework for the entire universe. The universe consist, physically, of objects of all scales: From galaxies and black holes, stars and planets, to people and everyday objects, all the way down to electrons and light. Whenever we make a change in the scale of our system, there is a chance that our current set of mechanics will not produce a satisfying result. The complexity of a given mechanics is usually reflected in the complexity of the systems it can describe; a statement which should prove true in the case of quantum mechanics, when it early in the 20th century came to scientists attention that the building blocks of nature was, and still is, incomprehensibly complex.

2.1 Fundamentals

A quantum mechanical system is described by a statistical ensamble of possible states. Unlike other ensambles in statistical mechanics, an object described by quantum mechanics has the possibility to occupy several physical states simultaneously. Each of these states (i.e. the energy levels of hydrogen) is described by a *wavefunction*. The full state of a system is constructed by a weighted superposition of all the possible physical states, exactly like a basis expansion in linear algebra. Performing a measurement on a system will, obviously[1], give only one value corresponding to the value of one of the constituent states. The probability of measuring a spesific value equals the absolute square of it's weight in the superposition [1].

This mathematical model is rigid, and works in the sence that it gives accurate results. How to interpret it physically, however, is a completely different question. We will come back to this topic in more detail in section **??**.

2.1.1 Wavefunctions

$$\psi$$

[1]Measuring the energy of hydrogen is practically measuring the (averaged) location of it's electron. The electron, when observed, cannot be in several places at once.

2.1.2 The road to Quantum Mechanics

Ever since mankind first started asking questions about the mechanisms behind the events of the earth, physics has been in development. The revolution of physics however, came in the language of mathematics. As important as the question “why does the apple fall”, was the question “at what speed” and “at what time”. The framework containing not only explairnations to general phenomenon, but also the tools needed to calculate properties of special events, are often named some type of mechanics.

For instance, we have the classical mechanics, explaining conservation of evergy, momentum, etc. It’s fortresses are Newton’s Equations, Lagrange’s equations and so on. Written in the language of mathematics, it is extremely effective at describing the motion of systems like i.e. the pendulum. The behaviour calculated lives up to *our expectations* of the system from the “real-world”.

However, as time passed and classical physics became a well known topic, it’s flauds arose. The perhaps most famous of these are the *ultraviolet catastrophe*: The energy in high frequency radioation was simply counter intuitive. If this radiation followed classical electrodynamics, we would all be fried centuries ago. Something was off. Max Planch served the solution: Energy is *quantized*. You do not have a continous energy spectre in a system. Some energies are high, some are low, but they are not continiously connected as in classical physics. This time classical physics did not do well, but it couldn’t be all wrong! It serves perfect solutions to systems like the pendulum mentioned above; it lives up to our expectations at some level.

So what does expectations have to do with anything? And what’s this level where we cannot trust it anymore? Let us assume that Newton’s second law only holds for expectation values of quantities:

$$\vec{F} = m\vec{a} \Longrightarrow \langle F \rangle = \langle ma \rangle$$

$$\vec{F} = -\vec{\nabla} V \qquad m\vec{a} = \frac{d\vec{p}}{dt}$$

$$\langle -\vec{\nabla} V \rangle = \langle \frac{d\vec{p}}{dt} \rangle.$$

So, whatever more complex mathematical framework lies behind our classical physics, it should obey this relation. It must produce what we expect from the real world. “Changing” the fundamental theory should not make the pendulum swing any different. As stated by Ehrenfest in his theorem:

Expectation values of variables follows classical paths.

Thinking of it, if only some of the gazillions of particles making up the pendulum behaves non-classical, it doesn’t make a difference. It’s neglectable in the bigger picture, since most of them will behave classicly. In other words: When you throw an apple, you don’t throw one object, you throw trillions of atoms.

So, what’s the underlying equation which, when taken the expectationvalue of, becomes the equation derived from Newton’s second law above? It’s the fortress of Quantum Mechanics; *the Schrödinger Equation*:

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r)\psi(r,t)$$

The $\psi(r,t)$ is called the *wavefunction*. It's the goal of the computation. Once you have the wavefunction, you have everything. It acts as the probability amplitude of the system. The probability distribution function is the square of the amplitude:

$$P(r,t) = |\psi(r,t)|^2 .$$

This basically means that the outcome of a measurement is not given in forehand. All you can calculate is the probability of measuring a certain value (remember that values, like i.e. energy, is quantized), not what one measurement will yield. This, however, is a mathematical formulation. What makes up the physics is how we interpret it. Either, the measurement is indeed given in forehand, we just do not have the rights to know, or, on the other hand, we follow Niels Bohr's interpretation, and say that the wavefunction is a superposition of all possible states with different weights, and a measurement will simply collapse it into one of them.[1]

Part II

Results

Bibliography

[1] D. Griffiths, *Introduction to Quantum Mechanics*, 2nd ed. Pearson, 2005.