1. INTRODUCTION

1.1 OVERVIEW

The Scope of Quantum Mechanics

Quantum mechanics is a theory originally developed to describe the phenomena of atomic and molecular physics, where dimensions range from 10^{-12} to 10^{-4} meters, where energies are usually well below 10^5 eV, and where processes are dominated by the electromagnetic interaction. Quantum mechanics is astonishingly successful in this regime, with the agreement between calculation and experiment often better than one part per million, a level of agreement vastly superior to that shown by any other physical theory at any scale.

The essence of quantum mechanics is the maintenance of distinction between observable quantities and theoretical constructs. This distinction enables one to retreat from the classical, highly literal view (e.g. the electron trajectory as a single line in space-time) and to accept more abstract representations for the unseen atomic world. We demand that these abstractions be in harmony with our actual observations but we liberate them from the constraints of our unverifiable preconceptions. These abstractions provide a manner of calculating probabilities that unifies the quantum theory of atomic phenomena. Moreover these abstractions, strongly based on fundamental and very general symmetries, can be applied over ranges of size and energy that far exceed the usual domain of atomic physics: In fact the eventual reach of quantum mechanics extends from the statistical world of gases at pico-Kelvin temperatures to the high energy elementary particle physics done at the largest accelerators.

Some Characteristic Sizes

10^{-20} m	distances in TeV scattering events
10^{-15} m	nuclear radii
10^{-10} m	atomic radii
10^{-6} m	visible light wavelength
10^{-4} m	naked eye limit
10^{-1} m	everyday objects
10^{+3} m	diameter of a small town
10^{+7} m	earth diameter
10^{+11} m	earth-sun distance
10^{+13} m	solar system diameter
10^{+16} m	to nearest star
10^{+20} m	diameter of our galaxy
10^{+22} m	distance to nearest galaxy
10^{+26} m	apparent radius of Universe

Objective of Our Work

Our objective here is to present non-relativistic quantum mechanics, a theory that describes the behavior of microscopic systems at moderate energies. We concentrate on the behavior of individual particles (particularly electrons, protons, and neutrons) and aggregates of particles (mainly atoms and simple molecules), and we describe the electromagnetic radiation field as a quantum mechanical system so that we may begin to understand the way an atom interacts with its surroundings. Whenever possible we show how quantum mechanical processes are fundamental to fields such as condensed matter physics, astrophysics, and coherent optics.

1.2 EXPERIMENTS AND PARADIGMS

Normal Science vs. Paradigm Changes

Progress in physics, both classical and modern, comes from a careful exploration of contradictions between accepted theory and careful observations. In most cases, the contradictions are resolved by adding new features to the currently-accepted theoretical framework or paradigm [Kuhn, *The Structure of Scientific Revolutions,* 1962]; this is regarded as normal science and is considered more interesting if the resolutions of contradiction are accompanied by new, testable predictions. As two (admittedly spectacular) examples we may cite the discovery in 1846 of the planet Neptune from apparent anomalies in the orbit of Uranus, and the discovery in 1894 of the element argon from discrepancies in the measured densities of air, nitrogen and oxygen.

In a very few cases, the differences between theory and experiment are not resolved until a revolutionary change occurs and a new paradigm is adopted.

The prototype for this is the understanding of planetary trajectories brought about when Copernicus introduced a heliocentric theory of the solar system that gave quantitative agreement with observations. The impact of Copernican theory spread beyond astronomy to every aspect of human affairs; indeed it is from the title of his 1543 book *De Revolutionibus Orbium Coelestium* [On the Revolution of Heavenly Bodies] that we have the terms "revolution" and "revolutionary" that are applied to drastic changes of any sort.

Paradigm Changes Define "Modern" Physics

Twice in the early years of the 20th century the accumulated weight of evidence compelled drastic revision of thought in physics: Relativity unified the previously disparate concepts of space and time (1905), and Quantum Mechanics fundamentally changed the way we calculate probabilities (1925). These changes in viewpoint are revolutionary in the Copernican sense; they represented new paradigms for our science. It is still too early to tell whether the analysis of non-linear and chaotic systems will lead us to new paradigms for the descriptions of nature.

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1.3 EXPERIMENTS CHALLENGE CLASSICAL ATOMIC THEORY

19th Century Spectroscopy

Already by 1840 it seemed clear that atoms in their gas phase would absorb and emit radiation with a sharply-defined line spectrum characteristic of the atomic species involved, but the mechanism for producing such line spectra was not known. Nor was there a way of understanding the broad spectral distribution of radiation from a hot object (the so-called "black body" radiation). Many scientists struggled to get a reasonable theory for discrete and continuous spectra, but the first minimally satisfying results were not available until the theories by Planck and by Bohr were published in first decade of the 1900's.

19th Century Electromagnetic Theory

Meanwhile, progress in electromagnetism was substantial. Maxwell's conceptual unification of light, electricity, and magnetism (1873) was stunningly confirmed in 1887 by Hertz who generated radiofrequency radiation and showed that it could be reflected, refracted, and polarized in ways familiar from experiments with visible light.

Maxwell's theory described the flow of electricity as a smooth current and the phenomenon of light as an undivided flux.. This continuum view of electromagnetic theory came to a certain maturity before physicists had to confront the conceptual problems that arose from the discovery of the electron (1897), from the development of the photon theory (1905), and from the quantitative measurements of the photoelectric effect (1900-1915).

Puzzles did remain. Theorists wanted to understand the spectrum of radiation from a hot object (the so-called *black body* radiation] and they very much wanted to understand atomic spectra on the basis of an electro-mechanical model for the atom.

Bohr's Theory of Atomic Structure

Bohr (1913) postulated the quantization of angular momentum, thereby obtaining discrete energy levels in atoms and explaining the existence of line spectra with the hypothesis that electrons, moving in orbits without losing energy, emit radiation only when jumping from a larger orbit to a smaller. The Bohr theory did lead to some useful results but there is no way to reconcile classical electrodynamics with the notion of an orbiting electron that does not lose energy. Moreover, there is no satisfactory classical or semi-classical theory that explains interference phenomena as seen in situations when the flux is so weak that less than one photon (or electron) is in the apparatus at any one time.

Patching classical theory with ad hoc assumptions was useful for coming to terms with some of the outstanding problems, but a satisfactory theory was not available until the revolutionary advent of quantum mechanics in the mid 1920's.

1.4 WHAT IS QUANTUM MECHANICS?

Predicting the Future from the Present

Quantum Mechanics is a formalism that helps us answer question such as:

> Given a system at time t_1 with a set of observed values and conditions $\{x_1, C_1,\}$ what are the chances of having the observed values and conditions $\{x_2, C_2\}$ at a later time t_2?

The quantum theorist first chooses a model for the general type of system under consideration and then writes an equation of motion that expresses the way in which the system develops in time. The theorist then uses the information available about the particular system as parameters and initial conditions for the model in order to predict that system's state at some future time.

Predictions are for Probabilities

The predictions are given in the form of relative probabilities, not certainties. The probabilities may be specified either as functions of a continuous variable (e.g. position, momentum) or of a discrete variable (e.g. spin state), depending on the nature of the quantity being predicted.

This statistical nature of quantum mechanics corresponds to the experimental finding that measurements on individual particles done under identical conditions need not yield the same observable results from one particle to the next. There have been attempts to attribute variations in observed values (for example where a given electron lands in a two-slit diffraction experiment)to hidden variables not under the experimenter's control, but these augmentations to the conventional quantum mechanics paradigm have not proven useful.

Quantum mechanics is thus a theory of probabilities; it differs from classical probabilistic theories (e.g. the kinetic theory of gases) in that calculations are made in terms of "probability amplitudes" that are converted to observable probabilities only in the last stages of the calculations: It is the absolute magnitude of a net probability amplitude, when squared, that corresponds to classical probability. This concept is not novel but is familiar from calculations of radiation in electromagnetic theory where the energy density at a particular location is proportional to the square of the total field amplitude at that location.

The change from a deterministic to a probabilistic approach leads us to

–describing PREDICTIONS in terms of continuous functions

but

–describing OBSERVATIONS in terms of a discrete set of points.

1.5 QUANTUM MECHANICS AND ELECTROMAGNETIC THEORY

Equations for electrons and for photons

The similarity between electromagnetic theory and quantum mechanics is not accidental but rather the source for a satisfying intellectual unification:

Electromagnetic Wave Equation

$$\frac{\partial^2 E}{\partial t^2} = \left(\frac{\omega}{k}\right)^2 \frac{\partial^2 E}{\partial x^2}$$

derived from Maxwell Field Equations
describes propagation in free space

Schrödinger Equation

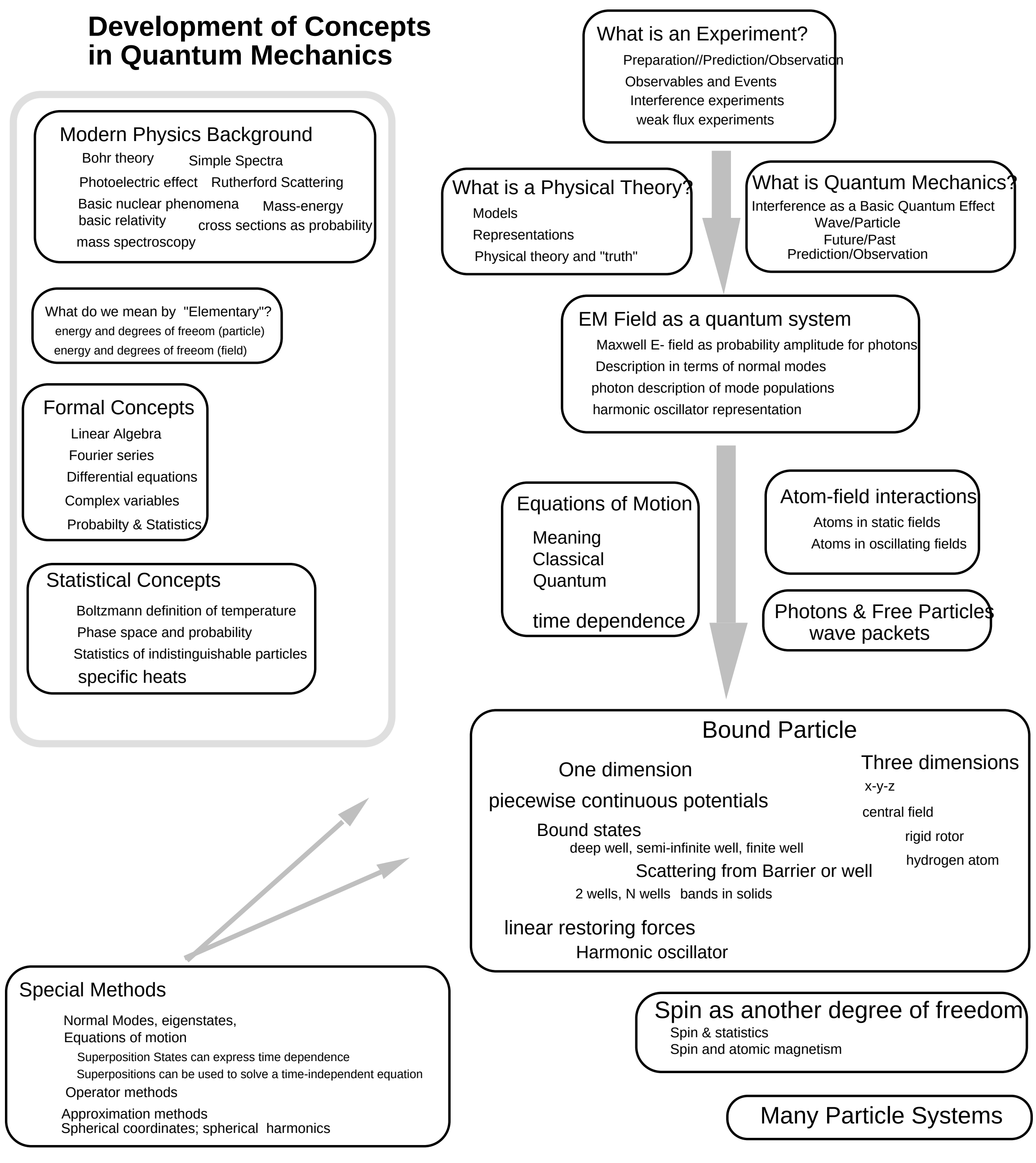
$$-i\hbar\frac{\partial \Psi}{\partial t} = \left(\frac{\hbar^2}{2m}\right)\frac{\partial^2 \Psi}{\partial x^2}$$

describes motion in free space

The electromagnetic wave equation which emerges from Maxwell's field equations is an equation of motion; it has solutions E(x,t) that represent the probability amplitude for zero-mass photons.

The Schrödinger equation of motion has solutions Ψ(x,t) that represent the probability amplitude for finite mass particles.

The general flow and outline of our study of Quantum Mechanics is shown on the diagram below. We will find it useful to re-examine the concepts of *experiment*, *observation* and *measurement.* We will then show how results from experiments on free particles and on simple atoms at low energies require a revision of our ideas about the behavior of matter on this scale.



1.6 LIMITS TO QUANTUM MECHANICS

Not an Ultimate Theory

Contemporary quantum mechanics is a theory that allows us to represent a wide range of phenomena in a unified, consistent, and satisfying manner.

It must be said, however, that we do not expect quantum mechanics to be an ultimate theory. Experience tells us that fundamentally new behaviors of nature are to be expected whenever the scales of size or energy change by more than a few orders of magnitude. New interactions become evident in experiments that reach beyond the conventional limits, and new theoretical structures may be needed to handle the new observations.

The High energy Frontier

Conventional exposition of this point is directed toward the higher energies.... nuclear physics and the growth of a new elementary periodic table... mesons etc. and finally elementary particles at the level of new standard model in which quarks are the elementary constituents

Additional, pragmatic comment: It may be that the press toward higher energies has come from financial limitations. so it may be that the search at very low energies will, in the immediate future be most fruitful. It is paradoxical in a sense that information previously thought to be particularly relevant to high energy may come form searches at low energies. the parity violation studies are one example; the cosmic background temperature is another.

The Low-Energy Frontier

Much attention is focused on the new information on particles and interactions found from research done at higher and higher energies, but tests of our understanding also come from the low energy frontier of kilometer-wave spectroscopy and nano-Kelvin thermodynamics made accessible by newer refrigeration techniques (notably the laser cooling of atoms) and by modern signal processing methods.

In the limit of low energy we can expect new behaviors from particles as their deBroglie wavelengths become comparable to mean free path of atoms in the experiment, and as kinetic energies drop to the level of the potential energy between two very distant atoms. BOSE EINSTEIN CONDENSATION

We can also expect new behaviors from radiation as its wavelength goes far beyond the scale where photon properties have been measured. Of course the conventional assumption is that results found in the visible and infrared regimes also characterize the photons of VLF 10 m) radiation. But experience suggests that surprises are in store when we extrapolate any theory over more than ten orders of magnitude.

The Non-Linear Frontier

Because linear differential equations are friendlier than the non-linear ones, less attention has been paid to non-linear phenomena. In recent years, however, improvement in mathematical techniques and increases in computing power have made it possible to explore non-linear and chaotic phenomena in considerable detail. We can anticipate more new physics as the frontiers of non-linear studies are extended.

Comparison of Classical, Quantum, and Chaotic Situations

Classical Mechanics

Deterministic in the sense that the ***exact*** same initial conditions will lead to the same outcome

Predictable in the sense that ***almost exactly*** the same initial conditions will lead to almost the same outcomes.

Convergent in the sense that a slight variation of the input values about some set of central values yields an output that varies in a corresponding way about a central output value.

Quantum Mechanics

Probabilistic in that the exact same intiial conditions yield the same *probabilities* for final outcomes, but results for *individual events* may vary.

Predictable in that ***almost exactly*** the same initial conditions will lead to almost the same probabiltiies as predictions for the outcomes.

Convergent in the sense that a slight variation of the input values about some set of central values yields an output that varies in a corresponding way about a central output value.

Chaos

Deterministic in that the ***exact*** same initial conditions will lead to the same outcome

Unpredictable in that ***almost exactly*** the same initial conditions may lead to drastically different outcomes.

Divergent in the sense that a slight variation of the input values about some set of central values yields an output that varies in an unpredictable way with no obvious central output value.
F(x) is known but **dF/dx** is large and not well determined .

---------Exercise for fun-----------

One can get a feel for some behaviors of non linear systems by calculating several dozen terms of each of the following sequences:

$$Sequence\ 1: \quad x_{n+1} = x_n^2 + 0.1 \quad try\ with\ x_0 = 0.887298\ and\ x_0 = 0.887299$$

$$Sequence\ 2: \quad x_{n+1} = x_n^3 + C \quad with\ x_0 = 0, \quad try\ C = 0.385, \quad C = 0.388\ and\ C = 0.3895$$

A spreadsheet is very convenient for making the calculation and displaying the results.