QUANTUM SYSTEMS

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Summary

A description of the origin and development of quantum mechanics is given, together with Wigner distributions and tomograms. Applications of atomic, molecular and solid state quantum systems to Bose-Einstein condensates and the quantum information theory are presented.

1. Introduction

At the beginning of the twentieth century the first quantum revolution occurred with the appearance of new principles of physics which finally yielded the formalism of quantum mechanics. Actually we are in the dawn of a new quantum revolution, because it is possible to manipulate and control sets of atoms or individual atoms trapped in electromagnetic cavities. There is the ability to observe individual atoms and learn how they form larger structures, which has been possible because new tools have been developed by means of which one can manipulate positions and velocities of atoms. This progress has moved to the level of quantum engineering, that is, the design of structures having desired optical, magnetic, and electronic properties. Among these new tools, one can mention the scanning tunneling microscope. The optical microscope resolution is limited by the wavelength of light, around one tenth of a millimeter. Modern electron microscopes have a resolution 10^5 times larger and with them it is possible to see things of the size of an atom.

To design materials with desired physical properties, it is very important to know deeply the properties of solids, by means of a quantum mechanical approach. Although a complete theoretical description is very complicated because it involves a huge number of electrons and ions, many properties such as electric conductivity and optical absorption, can be well-described with single particle models moving in relatively simple periodic potentials, which represent electron-electron effective interactions.
The low-dimensional systems have attracted attention for their potential to realize new electronic device architectures. The fabrication of low dimensional structures with molecular-beam epitaxy machines have made it possible to generate quantum systems that remember one dimensional potentials like the square well, the one-dimensional harmonic oscillator, or periodic square well potentials.

Although a fundamental feature of quantum mechanics is that complementary observables of quantum systems cannot be measured simultaneously and precisely, due to the Heisenberg uncertainty relation, there is no problem to measure complementary aspects in a series of distinct experiments or identically prepared quantum objects. It is well known that computer aided tomography lets us to get information of hidden objects. For example a cross section of a human body can be scanned by a X -ray beam whose attenuated intensity is recorded by a detector. Generally, the apparatus is rotated to yield many intensity distributions at different angles. Finally a computer analysis of the data can be done to build a picture of the human body in the form of a spatial distribution of the absorption coefficient.

Is it possible to translate this procedure to the quantum case? The answer is affirmative. In quantum mechanics one can picture the shape of an object by means of quasiprobability distributions as the Wigner function. In this case the transmission profiles correspond to marginal distributions associated to quasiprobability distributions which are also called quadrature component distributions. These can be measured by homodyne detection. From a set of these distributions the Wigner function, or more generally the quantum state, can be reconstructed. These gave rise to the existence of different tomographic schemes: optical, symplectic, and photon number tomographies, all of them expressing in different forms the quadrature components of a radiation field. These types of studies have also given rise to a new probability representation of quantum mechanics where the concepts of wave function or density matrix are not

needed. This is a classical-like description of a quantum state by means of measurable positive probability distributions. This representation has been constructed for continuous and discrete observables, such as position and spin, respectively.

The phenomenon of Bose-Einstein condensation was predicted for liquid Helium in 1924 as a necessary consequence of the work of S. N. Bose about the new rule to count correctly the distinct arrangements of indistinguishable photons or quanta of light. This new statistics, now called Bose-Einstein statistics, was extended to other particles having integral spin. Thus in a system of particles satisfying the Bose-Einstein statistics and where the total number of particles is conserved, there should be a temperature below which a finite fraction of the system occupies the same lowest energy of single particle state. In the past this was reached partially only for a few exotic systems such as $^4\mathrm{He}$, a mixture of $^4\mathrm{He}$ and $^3\mathrm{He}$, the semiconductor Cu_2O, the spin-polarized hydrogen, and the Cooper pairs in a superconductor. The control and manipulation of BEC have let us to explore the quantum behavior of dissipation, the coupling of a quantum state with an environment and the role of the entanglement. These concepts have played a fundamental role in the future of the quantum information theory and quantum computation.

Quantum information is radically different from its classical counterpart, which anyway forms the basis of the current information age. Notice that in each new generation of computer machines, the components are smaller than they were in its predecessor, so at this miniaturization and speed, it is probable that soon a point will be reached at which the quantum effects are unavoidable and the components themselves will be on the scale of atoms. The smallest quantity of the classical information is the binary digit (bit) which represent the “yes" or “no" answer to a question, i.e., it can take two values: on, which is denoted by (1), and off, denoted by (0). These bits are realized practically by simple electrical switches that are opened (0) or closed (1); in this manner the computer work is done.

The quantum bit of information, in contrast, can take the value 0 with probability p and the value 1 with a probability $1-p$, i.e., a coherent superposition of the open and close possibilities of an electric switch. Then, at first sight, it seems that from a qubit it is impossible the get a precise output, however in the last decade advances in establishing quantum algorithms have shown that this is not the case. In particular, one can mention the quantum algorithm that is able to factorize large numbers in a very efficient form, which constitutes the basis of the modern encryption codes.

The existence of a quantum computer must be based on the management of many qubits which must be realized by quantum systems of two level states. These must involve the control and manipulation of electrons, atoms, ions or nanoscale material objects. It is important to enhance elementary computations that have been performed using combinations of laser light with trapped atoms. The advantage of a quantum computer is related with the number of calculations it can do in parallel; for example a quantum computer with two qubits can run four calculations simultaneously while twenty qubits could run $2^{20} \simeq 10^6$ calculations in parallel. It is this geometric scaling that makes the potential of quantum computing so attractive.

In this chapter we discuss the origin and development of quantum mechanics together with the revision of a formulation which has impacted deeply several fields of physics and its discussion in elementary books is not normally given. This is the phase space formulation originated on the concept of Wigner function and later on developed by J. E. Moyal as a reformulation of quantum mechanics in purely statistical terms. From this formulation, a new approach has emerged in which a state is described by probability distribution functions called tomograms. Next we describe the formation of Bose-Einstein condensates, starting with a discussion of identical particles, Bose-Einstein statistics, and the mechanism for cooling atoms in order to achieve BEC. Finally, an introduction to quantum information theory is presented, i.e., how information is stored, transmitted (communication) and also processed (computation). In particular, the entanglement phenomenon is discussed for a bipartite quantum system, due to its importance in quantum computations.

2. Origin and Development of Quantum Mechanics

In the nineteenth century and at the beginning of the twentieth century, a physical system was described by a set of dynamical variables, each one of these with a well defined value which establishes the state of the system at a given time. Afterwards it was postulated that the evolution in time of the system is entirely determined if one knows its state at an initial time. This is so because the dynamical variables satisfy a first order system of differential equations in time. However, this must be taken carefully because since a century ago it was discovered that mechanical systems can have complicated motions, very sensitive to the initial conditions together with unpredictability over its movement over large intervals of time. This phenomenon is called chaos and it has become a very popular research area since the 1980s.

In the Universe one could distinguish two types of entities, matter and radiation. The first one is made of localizable particles subject, in the non-relativistic domain, to the Newtonian mechanics, each one described by six dynamical variables, the position and its velocity or momentum. The radiation obeys Maxwell's electromagnetic laws, with an infinite number of dynamical variables defined by the electric and magnetic fields at each point of space. However since 1900, it was evident that atomic and subatomic phenomena can not fit into this framework. It was soon recognized that the explanation of these phenomena required new principles. One can say that the foundations of quantum mechanics were established in the period between 1900 and 1927, which advanced our understanding of nature and formed the basis of numerous technologies. As examples one has semiconductors in computer chips, lasers in compact-disc players, and magnetic resonance imaging in hospitals. Between 1923 and 1927 almost simultaneously two equivalent formulations of quantum mechanics emerged: the matricial and wave theories.

The matricial mechanics was developed by Heisenberg, Born, and Jordan who emphasize that a physical theory must distinguish quantities that are physically observables from those which are not. This means that one should not use classical orbits, since there was no experiment showing their existence in the microscopic world. Therefore, they consider exclusively physical quantities which are observables like the

frequencies and intensities of the radiations emitted by atoms. The formalism associates matrices with physical quantities which in general obey a non-commutative algebra. Then the equations of motion of the dynamical variables are equations relating the matrices. These ideas lead Dirac to realize the analogy of this version of quantum mechanics with Poisson brackets in Hamiltonian mechanics in 1926. This similarity led him to formulate a mathematically consistent general theory of quantum mechanics in correspondence with Hamiltonian mechanics. In his new formulation, Dirac did not try to specify precisely these basic physical quantities; he considered only abstract mathematical objects. For example, the position, x_i, and momentum, p_j, coordinates must satisfy special commutation relations which must reduce to the classical Poisson brackets when the Planck constant, $\hbar$, is negligible, i.e.,

$$\left[x_i, p_j\right] = i\hbar\,\delta_{i,j}, \qquad \left[x_i, x_j\right] = \left[p_i, p_j\right] = 0, \tag{1}$$

where $\left[A, B\right] = AB - BA$. The same commutation relations were satisfied by the matrices used by Heisenberg, Jordan, and Born. The last expressions establish the Dirac quantization rule, that is, to replace the Poisson brackets of two dynamical variables $\{A, B\}$ by its commutator $(1/i\hbar)\left[A, B\right]$.

The wave mechanics of Schrödinger begins from an entirely different point of view; it is originated from the works of Louis de Broglie on the matter waves. When he proposed that the macroscopic objects satisfied the wave-particle duality, he was searching for a unified theory of radiation and matter. By means of these ideas Schrödinger discovered the equations of motion of the wave function, $\Psi(\vec{r}, t)$, representing a given quantum system; a very simple rule let us to deduce this equation from the knowledge of the Hamiltonian function of the corresponding classical system.

At the end of 1926, Dirac and Schrödinger explained the coincidence of these formulations by showing an exact mathematical equivalence between the two approaches, i.e.,

$$(x_k)_{nm} = \int \psi_n^*(\vec{r}, t)\, x_k\, \psi_m^*(\vec{r}, t)\, d^3r,$$

$$(p_k)_{nm} = \int \psi_n^*(\vec{r}, t) \frac{\hbar}{i} \frac{\partial}{\partial x_k} \psi_m^*(\vec{r}, t)\, d^3r, \tag{2}$$

with $k = 1, 2, 3$. These expressions establish the relation between the wave functions, $\psi_n(\vec{r}, t)$, and the matrices of Heisenberg. Besides, it is possible to consider the wave function as some kind of vector with the position and momentum variables acting like matrices upon this vector. This leads to the quantum mechanics formulation in a space of states, which will be discussed later on.

In 1926, Max Born discovered the empirical meaning of the wave function, by analyzing what happens when an electron collides with an atom before being detected by a Geiger counter. That is, the electron can be at any place where the wave function is

different from zero. This interpretation was generalized to any physical system. Then the wave function becomes a probability amplitude, and the probability of finding a system in any vicinity of a point in the space is given by

$$P(\vec{r}+d\vec{r}) = \left|\psi(\vec{r},t)\right|^2 d\vec{r}\,, \tag{3}$$

which immediately leads to a wave function satisfying the normalization condition.

2.1. Wave-particle Duality

All the mysteries of the quantum theory are found in the double slit Young experiment, in which the behavior of light is observed when it passes through two narrow slits and goes onto an observation screen and forms a pattern of lights and shadows. It demonstrates the wave behavior of light and from the pattern, the wavelength of the source can be measured. The more interesting aspects emerge when one considers that the intensity of the light source is diminished until it is sending almost photon by photon. If this is the case, the corpuscular model predicts that there is no interference pattern because there are no interactions between the photons while wave model always prognosticates an interference pattern. Therefore, the corposcular model fails in the short observation times while the wave case misses for long observation times. From this experiment, the following can be concluded:

- The photon travels like a wave and arrives as a particle on the screen.
- When a measurement is made on a microscopic system, it is perturbed in a fundamental way.
- It is impossible to see the interference pattern and know, at the same time, at which slit the photon went through.
- The wave and particle aspects of the light are inseparable, where the wave behavior lets us to calculate the probability of finding their corpuscular character. Thus the predictions of the behavior of the photons can only be probabilistic.

Bohr's complementarity principle established that quantum systems possess properties that are real but mutually excluding; this is the case of the wave-particle aspects of matter and radiation. The probabilistic interpretation mentioned above agrees with the existence of interferences, because the Schrödinger equation is linear and thus if ψ_1 and ψ_2 are among its solutions, their sum $\psi_1+\psi_2$ is another solution. The corresponding probability is proportional to $\left|\psi_1+\psi_2\right|^2$, and it shows interference effects. This quantum probabilities are different from the corresponding classical ones because the latter express ignorance or lack of information whereas the quantum ones assume that a more precise knowledge is impossible as a matter of principle.

Other consequences of the wave behavior of matter are the famous uncertainty relations of Heisenberg. Measurements of position and momentum taken in several identical copies of a system in a given state will vary according to known probability distributions, as $\left|\psi(\vec{r},t)\right|^2$ or $\left|\psi(\vec{p},t)\right|^2$. If we compute the uncertainty x of the position

measurements and the standard deviation p_x of the momentum measurements, then

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}. \tag{4}$$

Then one can not know with precision both position and momentum of a quantum system.

The wave-duality of massive objects has been a very important issue; however this phenomenon has never been observed in our daily experience. Superposition of de Broglie matter waves has been observed for particles with finite mass at rest such as electrons, in the experiment of Davisson and Germer about the scattering of electrons by a crystal of nickel, atoms, molecules and neutrons. In fact, there are current experiments to establish the limits to observe the quantum wave nature of massive objects. These studies have given rise to the development of electron and neutron optics and later on to molecular and atom optics. Recently , by means of a near-field diffraction scheme, the wave nature of molecules as large as the fullerenes, C_{60} molecules, and the fluorofullerenes, which are composed by 108 atoms has been demonstrated.

2.2. Quantum Mechanics in a Space of States

In many physical problems is more convenient to consider the wave function as some sort of a vector, with the position and momentum acting like matrices upon this vector, being one of the best examples the treatment of the spin of a particle. This is the reason to study the formulation of quantum mechanics within the geometrical framework of Hilbert spaces, which is due mainly to John von Neumann. A Hilbert space is a vector space formed by two sets of elements, the state vectors which can be added and the complex numbers which can multiply them.

This can be done following Dirac by defining a space of states $\mathcal{E}$ and its dual space, $\mathcal{E}^*$ through the mathematical concept of a functional, which is a function that associates a complex number to each vector. Thus the elements of $\mathcal{E}$ are the kets $|\psi\rangle$ while those of $\mathcal{E}^*$ are the so called bras $\langle\chi|$. Given these vectors one can define the scalar product given a complex number, which satisfies the following properties:

$$\langle\chi|\psi\rangle^* = \langle\psi|\chi\rangle,$$

$$\langle\chi|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1\langle\chi|\psi_1\rangle + \lambda_2\langle\chi|\psi_2\rangle,$$

$$\langle\lambda_1\chi_1 + \lambda_2\chi_2|\psi\rangle = \lambda_1^*\langle\chi_1|\psi\rangle + \lambda_2^*\langle\chi_2|\psi\rangle, \langle\psi|\psi\rangle \geq 0,$$

where the last expression is equal to zero only for $|\psi\rangle = 0$. These properties are similar to those of a scalar product in a Euclidean space, except for the occurrence of complex numbers. Then a complex Euclidean space can be considered an analogue of a Hilbert

space. For example, a vector in a complex Euclidean space can be expressed in terms of the components of a basis, i.e.,

$$\vec{A} = a_1\vec{e}_1 + a_2\vec{e}_2 + \cdots + a_n\vec{e}_n, \tag{5}$$

where the coefficients $(a_1, a_2, \cdots, a_n)$ constitute the components of the vector $\vec{A}$.

In the space of states the dynamical variables of a physical system are represented by linear operators, which besides are Hermitian. A Hermitian operator A is defined by $\langle \chi | A\psi \rangle = \langle A\chi | \psi \rangle$ whenever the scalar product exists.

In the case of a finite dimensional Hilbert space and a Hermitian operator A, the spectral theorem establishes that there exists an orthonormal basis consisting of the eigenvectors of A and that their eigenvalues are real. This spectral theorem yields the set of equations:

$$A = \sum_{k=1}^{n} a_k |e_k\rangle\langle e_k|, \qquad I = \sum_{k=1}^{n} |e_k\rangle\langle e_k|, \tag{6}$$

where the set $\{|e_j\rangle\}$ denotes the eigenstates of A.

For infinite dimensional Hilbert spaces, there are Hermitian operators, with infinite dimensional basis states, that satisfy the last equations by replacing the sums by integrals with respect to the continuous eigenvalues of these operators. This is the case of the momentum and position operators, which have infinite dimensional bases. This extension of the spectral theorem was done by von Neumann. In the general case, it is possible to have an operator with a spectrum consisting of two parts, one of them discrete and the other continuous, which satisfy the relations

$$A = \sum_{k=1}^{n} a_k |e_k\rangle\langle e_k| + \int_D \alpha |\alpha\rangle\langle\alpha| d\alpha, \qquad I = \sum_{k=1}^{n} |e_k\rangle\langle e_k| + \int_D |\alpha\rangle\langle\alpha| d\alpha. \tag{7}$$

By means of the analogy mentioned above, with the eigenstates of the position operator as a basis, the components of the state vectors constitute the wave functions and similarly if the basis states are associated to the momentum operator one has the wave functions in the momentum space. These are called the position and momentum representations of quantum mechanics. The wave functions in the momentum and position representations are connected through a Fourier transform. Actually we can use any physical observable to construct a representation of quantum mechanics.

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Biographical Sketches

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