How do electrons move in atoms?
From the Bohr model to quantum mechanics

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Abstract

It is argued that two ontological assumptions in Bohr's original atomic model are actually supported by the latter quantum mechanics. They are: (1) electrons are particles; and (2) they undergo discontinuous jumps.

1   Introduction

Niels Bohr proposed what is now called the Bohr model of the atom in 1913 (Bohr 1913). He suggested that electrons are particles and they undergo two kinds of motion in atoms; they either move continuously around the nucleus in certain stationary orbits or discontinuously jump between these orbits. This gives a visualizable picture of motion of the electrons in atoms. The Bohr model was latterly replaced by quantum mechanics, in which the physical state of an electron is described by a wave function. What, then, does the wave function represent? Exactly what are electrons? And how do they move in atoms?

The physical meaning of the wave function has been an important interpretative problem of quantum mechanics. The standard assumption is that the wave function of an electron is a probability amplitude, and its modulus squared gives the probability density of finding the electron in a certain location at a given instant. This is usually called the probability interpretation of the wave function. Notwithstanding its great success, this interpretation is not wholly satisfactory because of resorting to the vague concept of measurement (see, e.g. Bell 1990). Recently a new analysis strongly suggests that the wave function not only gives the probability of getting different outcomes, but also may offer a faithful representation of reality (Pusey, Barrett and Rudolph 2012). This analysis confirms the earlier result obtained based on protective measurements (Aharonov and Vaidman 1993; Aharonov, Anandan and Vaidman 1993), and shows that the standard probability interpretation of the wave function is ripe for rethinking. In fact, the realistic view of the wave function is already a common assumption in the main alternatives to quantum mechanics such as the de Broglie-Bohm theory and the many-worlds interpretation (de Broglie 1928;

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Bohm 1952; Everett 1957; DeWitt and Graham 1973). Unfortunately, however, the precise meaning of the wave function is still an unresolved issue in these theories.

In this article, we will demonstrate that a deep analysis of protective measurements and the mass and charge distributions of a quantum system may help answer the above questions[1]. It turns out that microscopic particles such as electrons are indeed particles, but their motion is never continuous but always discontinuous and random. Moreover, the wave function represents the state of random discontinuous motion of particles, and in particular, the modulus squared of the wave function gives the probability density for particles being in certain locations. In some sense, this new picture of quantum reality may be regarded as an extension to Bohr's discontinuous quantum jumps.

2 Measuring the state of a quantum system

The meaning of the wave function in quantum mechanics is often analyzed in the context of conventional (impulsive) measurements, for which the coupling interaction between the measured system and the measuring device is of short duration and strong. As a result, even though the wave function of a quantum system is in general extended over space, an ideal position measurement can only detect the system in a random position in space. Then it is unsurprising that the wave function is assumed to be related to the probability of the random measurement result by the standard probability interpretation. This also indicates that conventional measurements cannot obtain enough information about a single quantum system to determine what physical state its wave function represents.

Fortunately, it has been realized that the physical state of a single quantum system can be protectively measured (Aharonov and Vaidman 1993; Aharonov, Anandan and Vaidman 1993; Aharonov, Anandan and Vaidman 1996; Vaidman 2009)[2]. A general method is to let the measured system be in a nondegenerate eigenstate of the whole Hamiltonian using a suitable protective interaction (in some situations the protection is provided by the measured system itself), and then make the measurement adiabatically so that the state of the system neither collapses nor becomes entangled with the measuring device appreciably. In general, the measured state needs to be known beforehand in order to arrange a proper protection. In this way, such protective measurements can measure the expectation values of observables on a single quantum system, and in particular, the mass and charge distributions of a quantum system as one part of its physical state can be measured as expectation values of certain observables. Since the principle of protective measurement is independent of the controversial collapse postulate and only based on the linear Schrödinger evolution (for microscopic systems such as electrons) and the Born rule[3], which are two established parts of quantum mechanics, its result as predicted by quantum mechanics can be

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[1]For a more detailed analysis see Gao (2011a, 2011b, 2013a, 2013b).

[2]Note that the earlier objections to the validity and meaning of protective measurements have been answered (Aharonov, Anandan and Vaidman 1996; Dass and Qureshi 1999; Vaidman 2009; Gao 2012).

[3]It is worth noting that the possible existence of very slow collapse of the wave function for microscopic systems does not influence the principle of protective measurement.

used to investigate the meaning of the wave function[4].

According to protective measurement, the charge of a charged quantum system such as an electron is distributed throughout space, and the charge density in each position is proportional to the modulus squared of the wave function of the system there[5]. Historically, the charge density interpretation for electrons was originally suggested by Schrödinger when he introduced the wave function and founded wave mechanics (Schrödinger 1926). Schrödinger clearly realized that the charge density cannot be classical because his equation does not include the usual classical interaction between the densities. Presumably since people thought that the charge density could not be measured and also lacked a consistent physical picture, this initial interpretation of the wave function was soon rejected and replaced by Born's probability interpretation (Born 1926). Now protective measurement re-endows the charge distribution of an electron with reality by a more convincing argument. The question then is how to find a consistent physical explanation for it. Our following analysis can be regarded as a further development of Schrödinger's original idea to some extent. The twist is: that the charge distribution is not classical does not imply its non-existence; rather, its existence may point to a new, non-classical picture of quantum reality that hides behind the wave function.

3   Electrons are particles

The key to unveil the meaning of the wave function is to find the physical origin of the charge distribution. The charge distribution of a quantum system such as an electron has two possible existent forms: it is either real or effective. The distribution is real means that it exists throughout space at the same time, e.g. there are different charges in different positions at any instant. The distribution is effective means that at every instant there is only a localized, point-like particle with the total charge of the system, and its motion during an infinitesimal time interval forms the effective distribution. Concretely speaking, at a particular instant the charge density of the particle in each position is either zero (if the particle is not there) or singular (if the particle is there), while the time average of the density during an infinitesimal time interval gives the effective charge density. Moreover, the motion of the particle is ergodic in the sense that the integral of the formed charge density in any region is required to be equal to the expectation value of the total charge in the region.

If the charge distribution is real, then any two parts of the distribution (e.g. the two wavepackets in box 1 and box 2 in the example given in the Appendix), like two electrons, will also have the same form of electrostatic interaction as that between two electrons, which is described by the potential term in the Schrödinger equation. The existence of such electrostatic self-interaction for individual quantum systems contradicts the superposition principle of quantum mechanics (at least for microscopic systems such as electrons). Moreover, the existence of the electrostatic self-interaction for the charge distribution of an electron is incompatible with experimental observations either. For example, for the electron in the hydrogen atom, since the potential of the electrostatic

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[4]It can be expected that protective measurements will be realized in the near future with the rapid development of quantum technologies (cf. Lundeen et al. 2011).

[5]See the Appendix for an introduction of this important result.

self-interaction is of the same order as the Coulomb potential produced by the nucleus, the energy levels of hydrogen atoms would be remarkably different from those predicted by quantum mechanics and confirmed by experiments if there existed such electrostatic self-interaction. By contrast, if the charge distribution is effective, then there will exist no electrostatic self-interaction of the effective distribution, as there is only a localized particle at every instant. This is consistent with the superposition principle of quantum mechanics and experimental observations.

To sum up, we have argued that the superposition principle of quantum mechanics requires that the charge distribution of a quantum system such as an electron is not real but effective; at every instant there is only a localized particle with the total charge of the system, while during an infinitesimal time interval the ergodic motion of the particle forms the effective charge distribution, and the charge density in each position is proportional to the modulus squared of the wave function of the system there. In short, electrons are particles, and their charge distributions in space, which are measureable by protective measurements, are formed by the ergodic motion of these particles.

4   Particles move in a discontinuous and random way

The next question is which sort of ergodic motion the particles undergo. If the ergodic motion of a particle is continuous, then it can only form the mass and charge distributions during a finite time interval. But the mass and charge distributions of a quantum system at each instant, which is proportional to the modulus squared of the wave function of the system at the instant, is required to be formed during an infinitesimal time interval near the instant[6]. Thus it seems that the ergodic motion of the particle cannot be continuous. This conclusion can also be reached by analyzing a specific example. Consider an electron in a superposition of two energy eigenstates in two boxes $\psi_1(x) + \psi_2(x)$. In this example, even if one assumes that the electron can move with infinite velocity, it cannot *continuously* move from one box to another due to the restriction of box walls. Therefore, any sort of continuous motion cannot generate the effective charge distribution $e|\psi_1(x) + \psi_2(x)|^2$[7].

On the other hand, in order that the ergodic motion of a particle forms the right mass and charge distributions, for which the mass and charge density in each position is proportional to the modulus squared of its wave function there, the (objective) probability density for the particle to appear in each position must be proportional to the modulus squared of its wave function there too (and for normalized wave functions they should be equal)[8]. This is understandable,

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[6]For instance, in the example given in the Appendix, the trajectory of the electron wave packet is influenced by the effective charge in box 1 during an arbitrarily short time interval according to quantum mechanics.

[7]One may object that this is merely an artifact of the idealization of infinite potential. However, even in this ideal situation, the ergodic model should also be able to generate the effective charge distribution by means of some sort of ergodic motion of the electron; otherwise it will be inconsistent with quantum mechanics.

[8]Besides, for normalized wave functions, the (objective) probability current density must also equal to the formed mass or charge flux density divided by the mass or charge of the particle.

since that the mass and charge density is large in a position requires that the frequency of the particle appearing there is high. Moreover, from a logical point of view, the particle must also have an instantaneous property (as a probabilistic instantaneous condition) which determines the probability density for it to appear in every position in space; otherwise the particle would not "know" how frequently it should appear in each position in space. This property is usually called indeterministic disposition or propensity in the literature[9].

In summary, we have argued that the consistency of the formed mass and charge distribution with that predicted by quantum mechanics requires that the ergodic motion of a particle is discontinuous, and the probability density for the particle to appear in every position is equal to the modulus squared of its wave function there. In other words, the ergodic motion of the particle is random and discontinuous.

5   Meaning of the wave function

According to the above analysis, microscopic particles such as electrons are indeed particles. Here the concept of particle is used in its usual sense. A particle is a small localized object with mass and charge, and it is only in one position in space at an instant. Moreover, the motion of these particles is not continuous but discontinuous and random in nature. We may say that an electron is a quantum particle in the sense that its motion is not continuous motion described by classical mechanics, but random discontinuous motion described by quantum mechanics.
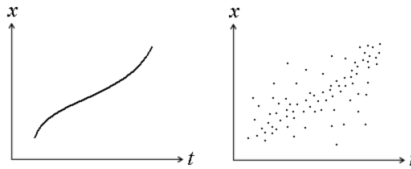

Fig.1. Continuous motion vs. discontinuous motion

Unlike the deterministic continuous motion, the trajectory function $x(t)$ can no longer provide a useful description for random discontinuous motion. It has been shown that the strict description of random discontinuous motion of a particle can be given based on the measure theory (Gao 2011). Loosely speaking, the random discontinuous motion of the particle forms a particle "cloud" extending throughout space (during an infinitesimal time interval), and the state of motion of the particle is represented by the density and flux density of the cloud, denoted by $\rho(x,t)$ and $j(x,t)$, respectively, which satisfy the continuity equation $\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0$. This is similar to the description of a classical fluid in hydrodynamics. But their physical meanings are different. The particle cloud is formed by the random discontinuous motion of a single particle, and the density of the cloud, $\rho(x,t)$, represents the probability density for the particle

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[9]Note that the propensity here denotes single case propensity. In addition, it is worth stressing that the propensities possessed by particles relate to their objective motion, not to the measurements on them.

to appear in position x at instant t, and it satisfies the normalization condition $\int_{-\infty}^{+\infty} \rho(x,t)dx = 1$.

As we have argued in the last section, for a charged particle such as an electron, the cloud will be an electric cloud, and $\rho(x,t)$ and $j(x,t)$, when multiplied by the total charge of the particle, will be the (effective) charge density and electric flux density of the cloud, respectively. Thus we have the following relations:

$$\rho(x,t) = |\psi(x,t)|^2, \tag{1}$$

$$j(x,t) = \frac{\hbar}{2mi}[\psi^*(x,t)\frac{\partial \psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial \psi^*(x,t)}{\partial x}]. \tag{2}$$

Correspondingly, the wave function $\psi(x,t)$ can be uniquely expressed by $\rho(x,t)$ and $j(x,t)$ (except for an overall phase factor):

$$\psi(x,t) = \sqrt{\rho(x,t)}e^{im\int_{-\infty}^{x}\frac{j(x',t)}{\rho(x',t)}dx'/\hbar}. \tag{3}$$

This means that the wave function $\psi(x,t)$ also provides a description of the state of random discontinuous motion of a particle.

This picture of motion of a single particle can be extended to the motion of many particles. The extension may also help explain the multi-dimensionality of the wave function (cf. Monton 2002; Lewis 2004). At a given instant, a quantum system of N particles can be represented by a point in a $3N$-dimensional configuration space. During an infinitesimal time interval near the instant, these particles perform random discontinuous motion in the real space, and correspondingly, this point performs random discontinuous motion in the configuration space and forms a cloud there. Then, similar to the single particle case, the state of the system is represented by the density and flux density of the cloud in the configuration space, $\rho(x_1, x_2, ...x_N, t)$ and $j(x_1, x_2, ...x_N, t)$, where the density $\rho(x_1, x_2, ...x_N, t)$ represents the probability density of particle 1 appearing in position x_1 and particle 2 appearing in position x_2, ..., and particle N appearing in position x_N[10]. Since these two quantities are defined not in the real three-dimensional space, but in the 3N-dimensional configuration space, the many-particle wave function, which is composed of these two quantities, is also defined in the 3N-dimensional configuration space.

One important point needs to be stressed here. Since the wave function in quantum mechanics is defined at a given instant, not during an infinitesimal time interval, it should be regarded not simply as a description of the state of motion of particles, but more suitably as a description of the dispositional property of the particles that determines their random discontinuous motion at a deeper level[11]. In particular, the modulus squared of the wave function determines the probability density of the particles appearing in certain positions in space. By contrast, the density and flux density of the particle cloud, which are defined during an infinitesimal time interval near a given instant, are only a description of the state of the resulting random discontinuous motion of particles, and they

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[10]When these N particles are independent, the density $\rho(x_1, x_2, ...x_N, t)$ can be reduced to the direct product of the density for each particle, namely $\rho(x_1, x_2, ...x_N, t) = \prod_{i=1}^{N} \rho(x_i, t)$.

[11]For a many-particle system in an entangled state, this dispositional property is possessed by the whole system.

are determined by the wave function. In this sense, we may say that the motion of particles is "guided" by their wave function in a probabilistic way.

6 Conclusions

In this article, we have argued that two ontological assumptions in Bohr's original atomic model, which are (1) electrons are particles; and (2) they undergo discontinuous jumps, are actually supported by quantum mechanics. There are three main steps to reach this conclusion.

First of all, protective measurement, whose principle is based on the established parts of quantum mechanics, shows that the charge of a charged quantum system such as an electron is distributed throughout space, and the charge density in each position is proportional to the modulus squared of its wave function there. Next, the superposition principle of quantum mechanics requires that the charge distribution is effective, that is, it is formed by the ergodic motion of a localized particle with the total charge of the system. Lastly, the consistency of the formed distribution with that predicted by quantum mechanics requires that the ergodic motion of the particle is discontinuous, and the probability density of the particle appearing in every position is equal to the modulus squared of its wave function there.

Therefore, quantum mechanics seems to imply that microscopic particles such as electrons are indeed particles, and their motion is discontinuous and random. Moreover, the wave function describes the state of random discontinuous motion of particles, and at a deeper level, it represents the dispositional property of the particles that determines their random discontinuous motion. In particular, the modulus squared of the wave function not only gives the probability density of the particles *being found* in certain locations as the standard probability interpretation assumes, but also gives the probability density of the particles *being* there[12]. This new picture of quantum reality may be regarded as an extension to the discontinuous quantum jumps assumed by Bohr in his atomic model.

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[12]It will be interesting to see how this new interpretation of the wave function can be extended to quantum field theory and what it implies for the solutions to the measurement problem. For an initial analysis see Gao (2013a, 2013b).

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Appendix: Protective measurement of the charge distribution of a charged quantum system

Since the existence of the charge distribution of a charged quantum system is the basis of our analysis of the meaning of the wave function, we will briefly introduce this important result here. For a more detailed analysis see Aharonov and Vaidman (1993), Aharonov, Anandan and Vaidman (1993, 1996), and Gao (2013).

Consider a protective measurement of the charge of a quantum system with charge Q in a small spatial region V having volume v. This is equivalent to measuring the following observable:

$$A = \begin{cases} Q, & \text{if } x \in V, \\ 0, & \text{if } x \notin V. \end{cases} \tag{4}$$

A protective measurement of A in a general superposition state $\psi(x,t)$ yields

$$\langle A \rangle = Q \int_V |\psi(x,t)|^2 dv, \tag{5}$$

which gives the charge of the system in the region V. When $v \to 0$ and after performing measurements in sufficiently many regions V, we can find the charge density everywhere in space, which turns out to be $\rho_Q(x,t) = Q|\psi(x,t)|^2$[13].

This result can be illustrated by a specific example. Consider a quantum system with charge Q whose spatial wave function is

$$\psi(x,t) = a\psi_1(x,t) + b\psi_2(x,t), \tag{6}$$

where $\psi_1(x,t)$ and $\psi_2(x,t)$ are two normalized wave functions respectively localized in their ground states in two small boxes 1 and 2, and $|a|^2 + |b|^2 = 1$. A measuring electron, whose initial state is a Gaussian wave packet narrow in both position and momentum, is shot along a straight line near box 1 and perpendicular to the line of separation between the boxes. The electron is detected on a screen after passing by box 1. Suppose the separation between the boxes is large enough so that a charge Q in box 2 has no observable influence on the electron. Then if the system is in box 2, namely $|a|^2 = 0$, the trajectory of the electron wave packet will be a straight line as indicated by position "0" in Fig.2, indicating that there is no charge in box 1. If the system is in box 1, namely $|a|^2 = 1$, the trajectory of the electron wave packet will be deviated by the electric field of the system by a maximum amount as indicated by position "1" in Fig.2, indicating that there is a charge Q in box 1. These two measurements are conventional measurements of the eigenstates of the system's charge in box 1, and their results can reveal the actual charge distribution in box 1. However, when $0 < |a|^2 < 1$, i.e. when the measured system is in a superposition of two eigenstates of its charge in box 1, it is well known that such conventional measurements cannot detect the actual charge distribution in box 1.

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[13]Similarly, we can protectively measure another observable $B = \frac{\hbar}{2mi}(A\nabla + \nabla A)$. The measurements will give the electric flux density $j_Q(x,t) = \frac{\hbar Q}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$ everywhere in space. According to the Schrödinger equation, the charge density and electric flux density satisfy the continuity equation $\frac{\partial \rho_Q(x,t)}{\partial t} + \nabla \cdot j_Q(x,t) = 0$.
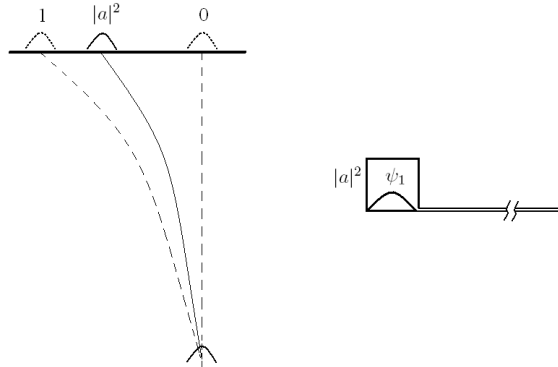
Fig.2. Scheme of a protective measurement of the charge distribution of a quantum system

Now let's make a protective measurement of the charge of the system in box 1 for the general superposition state. Since the state $\psi(x,t)$ is degenerate with its orthogonal state $\psi'(x,t) = b^*\psi_1(x,t) - a^*\psi_2(x,t)$, we need an artificial protection procedure to remove the degeneracy, e.g. joining the two boxes with a long tube whose diameter is small compared to the size of the box[14]. By this protection $\psi(x,t)$ will be a nondegenerate energy eigenstate. The adiabaticity condition and the weakly interacting condition, which are required for a protective measurement, can be further satisfied when assuming that (1) the measuring time of the electron is long compared to $\hbar/\Delta E$, where ΔE is the smallest of the energy differences between $\psi(x,t)$ and the other energy eigenstates, and (2) at all times the potential energy of interaction between the electron and the system is small compared to ΔE. Then the measurement by means of the electron trajectory is a protective measurement, and the trajectory of the electron wave packet is only influenced by the expectation value of the charge of the system in box 1. As a result, the electron wave packet will reach the position "$|a|^2$" between "0" and "1" on the screen as denoted in Fig.2, indicating that there is a charge $|a|^2Q$ in box 1.

In conclusion, protective measurement shows that the charge of a charged quantum system is distributed throughout space, and the charge density in each position is proportional to the modulus squared of its wave function there.

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[14]It is worth stressing that the added protection procedure depends on the measured state, and different states need different protection procedures in general. This means that a protective measurement with an artificial protection procedure requires that the wave function of the measured system is known beforehand.