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# SOME PUZZLES IN QUANTUM MECHANICS

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**Abstract**

Two fundamental problems of non-relativistic quantum mechanics are considered. These are the electromagnetic self-action of an atomic electron and the quantization of angular motion of electrons in a helium atom. The state of the art in the theory and experiment is briefly presented.


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## Introduction

Atomic physics is mainly the interweaving of quantum mechanics and electrodynamics. The electromagnetic field is the relativistic and, consequently, Lorentz-invariant matter. It can exist separately of charged particles, but not vice-versa. The concept of a charged particle in quantum mechanics is rather vague. On the one hand, a charged particle must create a field around itself, and the system "particle - field" cannot be considered as a localized point-like object any more. On the other hand, the theory of relativity is not well correlated with diffused objects in both classical and quantum physics. In quantum electrodynamics, the transition from a bare (point-like) to a dressed (by the field) electron is realized by means of a unitary transformation containing the sum over so-called "longitudinal" non-physical photons (see, for example, [1]). However, even this trick does not obviate all difficulties of the theory and leads to divergences, and Dirac honestly emphasizes this statement in his book.

In this paper, the problem of "diffused" charged particles is discussed at the level of the non-relativistic theory of a hydrogen atom. Even in this archetypical case, unexpected results can be obtained which, perhaps, might shed light on the whole problem.

Another interesting problem is also discussed, that was first formulated by Heisenberg in 1922 and stays still unsolved. It is quantization of angular motion of electrons in a helium atom [2]. Being guided by these ideas, Zommerfeld had formulated one of the best semiclassical models of the correlated motion of electrons in helium. It gives a practically exact single ionization potential of 24.6 eV and a zero magnetic moment [3]. The ideas of this part were published earlier in [4].

The atomic units $|e| = \hbar = m_e = 1$ are used throughout the paper for the sake of convenience.

## Nonlinear hydrogen atom?

Let us apply the system of the Heisenberg equations for interacting electrons and photons, which can be found in any textbook on quantum electrodynamics, to the hydrogen atom. Since on an atomic scale the nucleus (proton) has very small size, it can be considered as a classical external source of a field. There are no electron-positron pairs in non-relativistic physics, therefore the single-particle

wave function becomes a simple $C$-number in the operator sense. The analogue of the Dirac equation for the electron motion in an atom in the non-relativistic limit acquires the form

$$\left[\frac{1}{2}\triangle - \varepsilon + V(\vec{r})\right]\psi(\vec{r}) = 0; \quad \varepsilon > 0, \quad \int |\psi(\vec{r})|^2 d\vec{r} = 1. \qquad (1)$$

The equation for the potential follows from the Poisson equation

$$\triangle V(\vec{r}) = -4\pi\rho(\vec{r}). \qquad (2)$$

In non-relativistic physics, the charge density of the system composed of a point-like classical field source and a quantum electron might be determined as follows

$$\rho(\vec{r}) = Z\delta(\vec{r}) - |\psi(\vec{r})|^2. \qquad (3)$$

Eqs. (2) and (3) give

$$V(\vec{r}) = \frac{Z}{r} - \int \frac{d\vec{r}\,'}{|\vec{r} - \vec{r}\,'|}|\psi(\vec{r}\,')|^2, \qquad (4)$$

what points at the essentially nonlinear character of eq. (1) in the potential (4). This potential is a short-range one at $Z = 1$, as it should be for a neutral atom. If one omits the second term in eq. (3), which is responsible for the self-action of the electron, then the standard Schrödinger equation (SE) for the hydrogen atom derives. Let us recall that in classical electrodynamics this term is just thrown away by hand.

The self-action term obviously presents in the system of the Heisenberg operator equations in quantum electrodynamics (see any textbook), and its role is vigorously discussed in the already cited monograph by Dirac [1]. The Heisenberg and Schrödinger representations are related through the unitary transformation which includes the sum over nonphysical "longitudinal" photons. These photons are introduced into the theory by hand for convenience of working in 4D space. However, the infinite number of virtual electron-positron loops leads to well-known divergencies in higher Born terms, and rules of their removing (renormalization) are also introduced into practice by hand. In non-relativistic physics, the primitive perturbation theory

cannot be applied to the solution of eq. (1), and bound states must be obtained on the basis of its numerical solution.

There is a question: Whether we have self-action of an electron in non-relativistic quantum mechanics or not? Spectroscopy of atomic levels is a high-accuracy experimental field of science and therefore eq. (1) must yield the same transition energies and the ionization potential both with and without nonlinear term. This means that both equations (linear and nonlinear) must be related through a unitary transformation whose particular form is not known.

Another methodological question arises as to whether an absolute square of the electron wave function being multiplied by its charge can be interpreted as the charge density or not? And what to do with the probability interpretation in this case?

It is worthwhile to note that "constructions" of the type (1)÷(4) appear now and then in special literature. For example, there are some attempts to find a fully positive quantum distribution function, as opposed to the Wigner function [5]. Alike equations also arise in condensed matter physics and describe the so-called autolocalized states of an electron (one can familiarize with this problem in the review paper [6]). Recently, I've known about ideas of Sapogin *et al* who include the appropriate bilinear combination of the wave functions in the Dirac-like equation instead of mass [7].

## Quantization of angular motion of electrons in helium?

Let us consider the helium atom as an example of the simplest many-electron stable quantum system. It is well known that an analytical solution of the SE can not be obtained. Any reasonable small parameter to consider the perturbation decomposition of bound (ground) wave functions is lacking as well. The variational method allows to get a wealth of trial wave functions, which are quite different and, of course, contain no indication of the quantization of angular motion of electrons. Since the ground state of parahelium is a $S$-state, the 6D SE can be transformed into the 3D Hylleraas equation. Fock proposed to solve it on the surface of a 4D sphere and obtained an infinite system of coupled differential equations [8]. Calculations within this approach were realized by Ermolaev [9], however no quan-

tization of angular motion of both electrons was obtained, again due to the approximate character of the solution.

As it was mentioned in Introduction, Heisenberg surmised such quantization in a letter to Zommerfeld in the twenties of the last century (the idea was never published). In turn, Zommerfeld proposed one of the best semiclassical models of synchronous motion of electrons in helium along two oblong elliptic orbits. According to him, "one electron is taken to be at perihelion when the other is at aphelion, so that collisions are avoided and symmetry and periodicity are further as much as possible" [3].

The Hylleraas equation for the ground $S$-state of parahelium takes the form

$$\left[\frac{1}{2}\frac{\partial^2}{\partial\rho^2} + \frac{5}{2\rho}\frac{\partial}{\partial\rho} + \frac{1}{2\rho^2}\hat{T}(\varphi,\xi) + \frac{1}{\rho}Z(\varphi,\xi)\right]\Phi = \varepsilon\Phi. \qquad (5)$$

Here

$$r_1 = \rho\,\cos\varphi, \qquad r_2 = \rho\,\sin\varphi, \qquad r_{12} = \sqrt{2}\,\rho\,\cos\xi, \qquad (6)$$

where $\hat{T}(\varphi,\xi)$ and $Z(\varphi,\xi)$ are known angular operators. By analogy with hydrogen, we seek a solution in the form

$$\Phi(\vec{r}_1,\vec{r}_2) = A(\rho,\varphi,\xi)\;e^{-\chi(\varphi,\xi)\;\rho}\;. \qquad (7)$$

For the eikonal $\chi(\varphi,\xi)$ a nonlinear first-order differential equation can be written, and all its physical solutions can be found analytically [10]. In particular, $\chi_0\rho = \sqrt{2\varepsilon}\rho$ and $\chi_1\rho = p_1r_1 + p_2r_2$, where $p_1^2 + p_2^2 = 2\varepsilon$. One easily obtains a linear differential equation for the amplitude function $A$ [10]. Studies of its asymptotic behavior with respect to $\rho$ again lead to a simple linear differential equation in angle variables, and its integral of motion is the angle between electrons for the eikonal $\chi_1\rho$ (!) The amplitude function $A$ can be decomposed into the series with respect to the hyperradius $\rho$ which, according to Fock [8], includes products of powers and logarithms. General mathematical considerations suggest that this series must exhibit, at least, a powerlike growth at large $\rho$, otherwise we obtain an exponentiallike growth. This asymptotical limitation should give us energies of all bound $S$-states and, presumably, some rules of the electrons' angular motion. Unfortunately, serious mathematical difficulties wait for us

here, and only rather crude analytical models can be obtained. For example, applying the diagonal approximation one gets $\varepsilon \approx 2.72$ for the helium ground state ($\varepsilon_{exp} = 2.904$) [10].

At the same time, there is a number of experimental data which can be interpreted as indication of a preferable angle between velocities of electrons escaping from the atom. In Fig.1, which is borrowed from [11], the double differential cross section of the double ionization of helium by electron impact (the so-called $(e, 3e)$ process) is presented. The X-axis is the reduced energy sharing between the electrons, whilst the Y-axis is their mutual angle. In this experiment the incoming fast electron transfers very small parts of its energy and momentum to the helium atom, which are still enough to release both atomic electrons. The escaping electrons have relatively small energies $E_b$ and $E_c$ and $E_b + E_c \leq 20$ eV. The in-plane angle between them is denoted as $\Phi$. One readily sees that the distribution has a rather wide peak at $\Phi \sim 120^\circ \div 150^\circ$ and $x = E_b/(E_b + E_c) \approx 0.5$. Its $x$-position signalizes strong correlation between the electrons. If the correlation was weak, the distribution would have maxima at $x \sim 0$ and 1. Perhaps, we see these in Fig. 1 too. The fast projectile electron can interact effectively only with one atomic electron and eject it. Another electron is released due to either mutual correlations or shake off effects in the residual ion. All corresponding 3 peaks are seen, but the angle $\Phi$ is practically the same in all three cases (?).

Fig. 2 is borrowed from [12]. Here the differential cross section of the $(e, 3e)$ reaction is also presented as a function of the angle between velocities of the slow escaped electrons. In this experiment their energies are fixed, $E_b = E_c = 4$ eV. The peaks around the angles $\Phi \sim 120^\circ \div 140^\circ$ are also well seen. These peaks can be reproduced within the model which takes into account the correlated motion of both helium electrons after a direct collision of one of them with the incident fast electron. These calculations are purely numerical and based on the closed-coupling method [13]. But even this theory does not enable to reproduce the growth of the cross section at the relative angle $\Phi \sim 60^\circ$ (this growth is absent at the energies $E_b = E_c = 10$ eV). Until now there is no serious theoretical explanation of this observation.

Finally, in Fig. 3, which was borrowed from [14], a case of a capture process is presented. It is the so-called transfer ionization re-

action where a fast projectile ion (proton) captures an electron from the helium target, while another bound electron is ejected simultaneously. The deflection angle of the produced fast hydrogen atom is rather small (few milliradians), what indicates a very large impact parameter. This means that the proton picks up an electron mainly from the asymptotical part of the electron cloud where the relative angle $\Phi$ is fixed (the integral of motion). According to classical physics, the maximal probability for the proton to pick up an electron occurs when both particles move concurrently and with the same velocity [15]. If one accepts this classical mechanism, the angle between the momentum of one electron $\vec{k}_{e1}$ and the other electron $\vec{k}_{e2}$ is again equal approximately $120^\circ \div 140^\circ$ within a wide range of proton energies. The value of the mutual angle $\Phi$, which should be asymptotically fixed in helium and which we are not able to calculate from the theory, probably lies in the range $\Phi \sim 120^\circ \div 150^\circ$. But the issue remains open.

## Discussion

Only two examples of unsolved problems in quantum mechanics are presented in this paper. The first one should either confirm the hydrogen spectrum, which is measured with high precision and calculated without self-action of the electron in eq. (1), or shake ... the theory of quantum electrodynamics (!) Some preliminary and rather crude numerical calculations of eq. (1) with the potential (4) were performed and gave few lowest $s$-states [16], and this problem needs more attention. And the question remains open: Does the unitary transformation exist which removes the self-action term from the potential?

The second example clearly demonstrates that even the simplest two-electron atom (helium) cannot be exhaustively explored without numerical calculations. However, such calculations do not allow us to study fine effects which follow only from exact analytical solutions. Increasing the number of electrons only strengthens the problem. We are doomed to investigate more or less suitable models which fill a gap between the SE and atomic-molecular-chemical-biological world. Moreover, to find a particular solution of the SE we have to supply it with appropriate boundary conditions. These are the symmetries,

geometry of a molecule, asymptotic behavior of the wave function and etc. Obviously, these boundary conditions must be borrowed from outside (experiment, "general considerations"). The more complex the system, the more of boundary conditions is needed. Consequently, the SE is not complete without boundary conditions, even in the case of a hydrogen atom.

Regarding the experiments presented above, they actually do not allow to make univocal conclusions in favor of quantization of electrons' motion in helium. The process of escape of both slow electrons from the atom after a direct collision with the fast projectile particle is very complicated. The final wave function has negative impact: it considerably overshadows any information on the electrons' distribution in helium. Even the method of quasi-elastic knock-out (the so-called Electron Momentum Spectroscopy [17]), which is the most direct method for investigating the ground states of targets, does not lend a possibility to see any features beyond the trial wave functions. Though recent (e,3-1e) experiments of this type allow to exclude from further consideration the simplest ones [18]. However, if some optimist interprets the results of the considered experiments in favor of the fixed mutual angle between the electron velocities, he would find its value in the range $120^\circ \div 150^\circ$, what coincides with the semiclassical predictions by Gryzinsky [19]. In short, we need further experimental and theoretical efforts to learn more about atoms.

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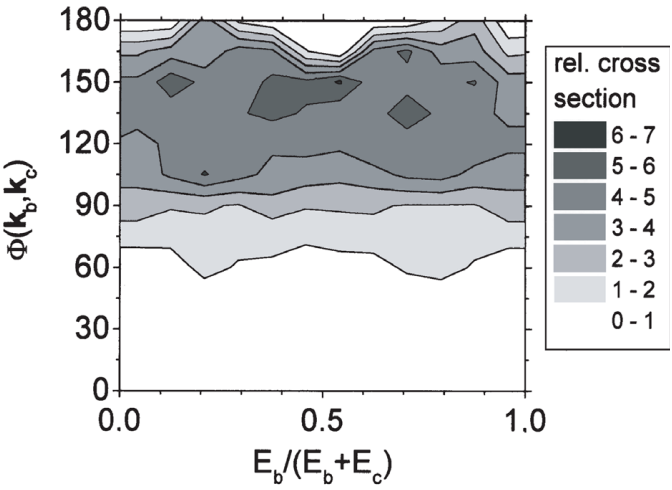


Figure 1: Double differential cross section of the reaction $\mathrm{He} + e \rightarrow \mathrm{He}^{++} + 3e$ as a function of the reduced sharing parameter $x = E_b/(E_b + E_c)$ and the in-plane relative angle between velocity vectors of two slow escaping electrons. The energy of the incoming electron is $E_0 = 3$ KeV. The cross section is integrated over the energies of slow electrons within the range $E_b + E_c \leq 20$ eV.

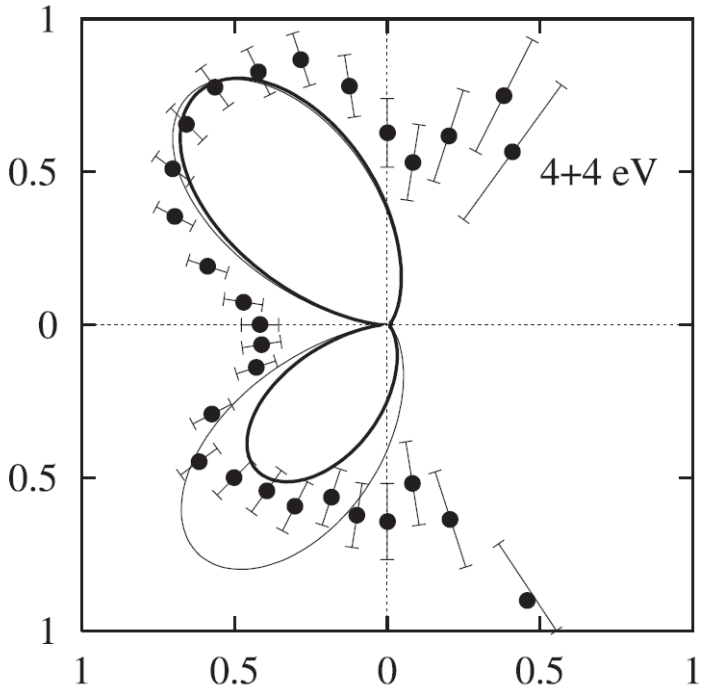


Figure 2: Double differential cross section of the reaction $\mathrm{He} + e \rightarrow \mathrm{He}^{++} + 3e$ as a function of the in-plane relative angle between velocity vectors of two slow escaping electrons with fixed energies $E_b = E_c = 4$ eV. The energy of the fast incident electron is $E_0 = 5587$ eV. The curves represent the results of calculations, and their details are given in [12].

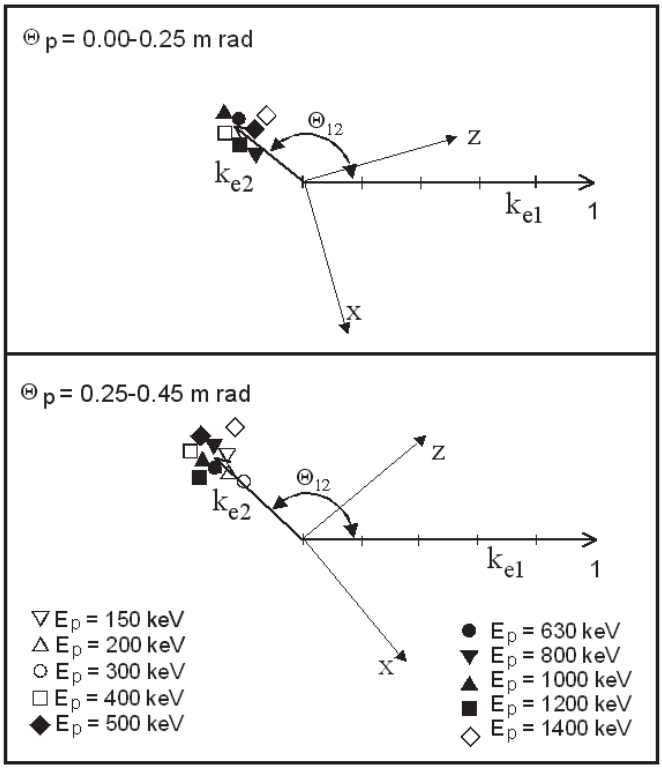


Figure 3: Momentum distribution of the electron $e_1$ captured by the passing proton, and of the ionized electron $e_2$ in the reaction $\mathrm{He} + p \rightarrow \mathrm{He}^{++} + e + \mathrm{H}$ at different proton energies and its azimuthal angle $\Theta_p$. Details of the experiment and theoretical considerations one can find in [14].

Comment

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# Comment on SOME PUZZLES IN QUANTUM MECHANICS

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The problem of selfenergy (SE) for bounded electrons is well elaborated. This is a part of the general problem of shifting of atomic levels (see, for example, the book by Akhiezer and Berestecky). One simply takes the standard QED and splits the electromagnetic field into classical and quantum parts. The linear problem of Dirac particle in classical em field is solved first and the effect of quantum em field is taken into account perturbatively. This allows for neglecting the selfinteraction contribution to the electron mass by renormalizing it for freely moving electron and taking systematically corrections following from the fact that electron is bounded. The equation proposed by the author is written ad hoc. The proper approach is most clearly seen if one uses the Columb gauge in the formalism sketched above.

Consider now the helium problem. I agree that the many-electron atoms cannot be exhaustively explored without numerical calculations. It is also true that the SE is not complete without boundary

conditions. This is, however, rather obvious. One should keep in mind that the quantum mechanical operators, in particular an energy operator, are given as selfadjoint operators related to some formal differential operators and their proper definition needs a careful determination of the domain. This is well known and can be found in Kato, Thirring or Simon & Reed books. As fur as helium atom is concerned most of its qualitative properties are well understood . In order to classify its eigenstates one has to find the complete set of commuting observables . In general case this problem is quite interesting. If the classical counterpart of quantum system is integrable and the integrability property survives quantisation the problem is solved automatically; moreover, for generic nonsuperintegrable system the complete set of commuting observables may be smaller than the number of degrees of freedom indicate; in fact it can reduce to the energy itself if there is no degeneracy. For nonintegrable systems the number of commuting observables in complete set is smaller than the number of degrees of freedom.

In the nonintegrable case of, say, parahelium there are nine degrees of freedem end six commuting intergrals only (total momentum, energy, total angular momentum and one of its components). The resulting equation is, therefore, there dimensional. It cannot be solved exactly but there are no conceptual problems. These only arise if one wants to quantize helium energy by the methods of old quantum theory; the latter demands complete integrability on classical level which is not the case here.