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Soliton Model of Atom

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The Einstein–de Broglie soliton concept is applied to simulate stationary states of an electron in a hydrogen atom. According to this concept, the electron is described by the localized regular solutions to some nonlinear equations. It is shown that the electron–soliton center travels along some stationary orbit around the Coulomb center. The electromagnetic radiation is absent as the Poynting vector has non-wave asymptote $O(r^{-3})$ after averaging over angles.

1. INTRODUCTION

From the history of quantum mechanics it is known that as early as 1927, in the framework of his "theory of double solution," Louis de Broglie made an attempt to represent the electron as a source of waves obeying the Schrödinger equation.[1] Later he modified his model showing that the electron should be described by regular solutions to some nonlinear equation coinciding with the Schrödinger one in the linear approximation. This scheme became famous as a causal nonlinear interpretation of quantum mechanics.[2] Developing this concept, de Broglie remarked that it has much in common with Einstein's ideas about unified field theory according to which particles were to be considered as clots of some material fields obeying the nonlinear field equations.[3] In recent years, these types of field configurations, known as soliton or particle-like solutions, came into active use to model extended elementary particles.[4]

In this paper the Einstein–de Broglie soliton concept is employed to model stationary states of the electron in a hydrogen atom.

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2. BOHM PROBLEM ABOUT NONLINEAR RESONANCE AND ITS POSSIBLE SOLUTION

As a starting point, we will consider an interesting problem posed by D. Bohm. Long ago, in his book[5] Bohm discussed the possible connection between the wave–particle dualism in quantum mechanics and the hypothetical nonlinear origin of fundamental equations in a future theory of elementary particles. To illustrate the line of Bohm's argument we will consider a simple scalar model in the Minkowski space-time given by the Lagrangian density

$$\mathscr{L} = \partial_i \phi^* \, \partial_j \phi \eta^{ij} - (mc/h)^2 \, \phi^* \phi + F(\phi^* \phi) \tag{1}$$

Here $i, j = 0, 1, 2, 3$; $\eta^{ij} = \mathrm{diag}(1, -1, -1, -1)$, the nonlinear function $F(s)$ behaves at $s \to 0$ as s^n, $n > 1$, and it is assumed as such that the corresponding field equations allow the existence of particle-like (soliton) solutions, i.e., regular configurations localized in space and endowed with finite energy. In particular, it can be shown that if one chooses $F(s) = ks^{3/2}$, $k > 0$, the model (1), known as the Synge model,[6] admits the following stationary solutions:

$$\phi_0 = u(r) \exp(-i\omega_0 t), \qquad r = |\mathbf{r}| \tag{2}$$

Here, the real radial function $u(r)$ is regular everywhere and exponentially decreases as $r \to \infty$, which provides finiteness of energy of the configuration

$$E = \int d^3x \, T^{00}(\phi_0) \tag{3}$$

where T^{ij} is the corresponding energy-momentum tensor.

Moreover, the model mentioned is intriguing due to the fact that nodeless solitons turn out to be stable by Liapunov provided that their charge is fixed.[7] So there exist perturbed solitons slightly differing from the stationary solitons (2):

$$\phi = \phi_0 + \xi(t, \mathbf{r}) \tag{4}$$

Note that the perturbation ξ in (4) is small as compared with ϕ_0 only in the area of localization of the soliton, where ϕ_0 significantly differs from zero. Nonetheless, far from the soliton center, where ϕ_0 is negligibly small, one can put $\phi \approx \xi$, i.e., the *tail* of the soliton is completely defined by perturbation ξ.

Bohm posed the following question: Does there exist any nonlinear model for which the spatial asymptote (as $r \to \infty$) of a perturbed soliton-like solution represents oscillations with characteristic frequency $\omega = E/\hbar$? In other words, for the model in question the principal Fourier amplitude in the expansion of the field $\phi \approx \xi$ as $r \to \infty$ should correspond to the frequency ω connected with the soliton energy (3) by the Planck–de Broglie formula

$$E = \hbar\omega \tag{5}$$

Note that for the model (1) at spatial infinity, where $\phi \to 0$, the field equation reduces to the linear Klein–Gordon equation

$$[\Box - (mc/\hbar)^2]\,\phi = 0 \tag{6}$$

and therefore the relation (5) holds only for solitons with unique energy $E = mc^2$ defined by the mass m fixed in (1). Thus, the universality of the relation (5) breaks down in the model (1), thus forcing its modification. In the light of the above universality, since the frequency ω in (5) is defined by the mass of the system, it seems natural that in the new, modified model one should use the gravitational field, the spatial asymptote of which is also defined by the mass of the considered localized system. Thus, to solve the Bohm problem the possibility to invoke the gravitational field comes into reality.[8]

So we will describe the new model with the Lagangian density $\mathscr{L} = \mathscr{L}_m + \mathscr{L}_g$, where

$$\mathscr{L}_g = c^4 R/16\pi G$$

corresponds to Einstein's theory of gravity, and $\mathscr{L}_m$ is chosen as

$$\mathscr{L}_m = \partial_i \phi^* \, \partial_j \phi g^{ij} - I(g_{ij})\, \phi^* \phi + F(\phi^* \phi) \tag{7}$$

The crucial point of this scheme is to build up the invariant $I(g_{ij})$ depending on the metric tensor g_{ij} of the Riemannian space-time and its derivatives. This invariant should possess such properties that in the vicinity of the soliton with mass m, the relation

$$\lim_{r \to \infty} I(g_{ij}) = (mc/\hbar)^2 \tag{8}$$

should hold. It is easy to see that on the basis of (8) one can asymptotically deduce Eq. (6) from the Lagrangian (7).

We argue that the invariant I can be built from the curvature tensor R_{ijkl} and its covariant derivatives $R_{ijkl;n}$:

$$I = (I_1^4/I_2^3)\, c^6 h^{-2} G^{-2} \tag{9}$$

where G is Newton's gravitational constant and the invariants I_1 and I_2 take the form

$$I_1 = R_{ijkl} R^{ijkl}/48, \qquad I_2 = -R_{ijkl;n} R^{ijkl;n}/432$$

Estimating R^{ijkl} at large distance r with the help of the Schwarzschild metric, one finds

$$I_1 = G^2 m^2/(c^4 r^6), \qquad I_2 = G^2 m^2/(c^4 r^8)$$

So from (9) follows immediately (8). Thus, within the modified model (7) for all massive particles the Planck–de Broglie relation (5) is automatically fulfilled. This means that in the framework of the scheme mentioned the principle of wave–particle dualism is valid, according to wich the relation (5) is realized as a condition of the nonlinear resonance.

To verify the fact that solitons can really possess wave properties, the thought diffraction experiment with individual electron–solitons was realized.[9] Solitons with some velocity were dropped into a rectilinear slit, cut in the impermeable screen, and the transverse momentum that they gained while passing the slit whose width significantly exceeded the size of the soliton, was calculated. As a result, the picture of distribution of the centers of scattered solitons was restored on the registration screen by considering their initial distribution to be uniform over the transverse coordinate. It was explained that although the center of each soliton fell into a definite place of the registration screen (depending on the point of crossing of the slit and the initial soliton profile), the statistical picture in many ways was similar to the well-known diffraction distribution in optics, i.e., Fresnel's picture at short distances from the slit and Fraunhofer's picture at large distances.[10,11]

Fulfillment of the quantum mechanics correspondence principle for the Einstein–de Broglie's soliton model was discussed in Refs. 12–15. In these papers it was shown that in the framework of the soliton model all quantum postulates were regained at the limit of point particles so that from the physical fields one can build the amplitude of probability and the average can be calculated as a scalar product in the Hilbert space by introducing the corresponding quantum operators. In this paper, we will show that in the framework of the Einstein–de Broglie soliton model a hydrogen atom can be simulated.

3. FUNDAMENTAL EQUATIONS AND STRUCTURE OF SOLUTIONS

As physical fields we choose the complex scalar field ϕ interacting with the electromagnetic one $F_{ik} = \partial_i A_k - \partial_k A_i$. The nucleus field is assumed to be the Coulomb field: $A_i^{ext} = \delta_i^0 Ze/r$. The Lagrangian density is taken in the form

$$\mathscr{L} = -\frac{1}{16\pi}(F_{ik})^2 + |[\partial_k - i\varepsilon(A_k + A_k^{ext})]\phi|^2 - (mc/\hbar)^2 \phi^*\phi + F(\phi^*\phi) \quad (10)$$

where $\varepsilon = e/(\hbar c)$ is the coupling constant and $F(\phi^*\phi)$ is some nonlinear function, decreasing faster than $|\phi|^2$ as $\phi \to 0$ and chosen so that the field equation at $A_i^{exp} = 0$ allows the existence of stable stationary soliton-like solutions of the type (2), describing configurations with mass m and charge e.

Note that for simplicity we do not write down the terms corresponding to the gravitational field, which will be taken into account implicitly with the help of the nonlinear resonance condition (5).

Let us consider the nonrelativistic approximation assuming that

$$\phi = \psi \exp(-imc^2 t/\hbar) \quad (11)$$

neglecting in the equations of motion higher derivatives of ψ with respect to time and retaining only linear terms in A_i. As a result, taking (11) into account we get the following system of equations:

$$\begin{aligned} i\hbar\partial_t\psi &+ (\hbar^2/2m)\,\Delta\psi + (Ze^2/r)\psi \\ &= -(\hbar^2/2m)[2i\varepsilon(\mathbf{A}\nabla)\psi + 2(\varepsilon mc/\hbar)\,A_0\psi + i\varepsilon\psi \operatorname{div}\mathbf{A} + F'(\psi^*\psi)\psi] \\ &\equiv -(\hbar^2/2m)\hat{f}(\mathbf{A}, A_0, \psi^*\psi)\psi \end{aligned} \quad (12)$$

$$\Box A_0 = (8\pi me/\hbar^2)\,|\psi|^2 \equiv -4\pi\rho \quad (13)$$

$$\Box\mathbf{A} = 4\pi[2\varepsilon^2\mathbf{A}\,|\psi|^2 - i\varepsilon(\psi^*\nabla\psi - \psi\,\nabla\psi^*)] \equiv -(4\pi/c)\,\mathbf{j} \quad (14)$$

Moreover, in Eqs. (12)–(14) it is supposed that the 4-potential A_i of the proper electromagnetic field of the soliton obeys the Lorentz condition

$$\partial_t A_0 + c \operatorname{div}\mathbf{A} = 0$$

which is consistent with Eqs. (12)–(14) owing to the conservation of electric charge.

We will seek the solutions to Eqs.(12)–(14) describing the stationary state of an atom when the electron–soliton center is assumed to be moving along a circular orbit of radius a_0 with some angular velocity Ω. In this problem there arise two characteristic lengths: the size of the soliton $l = \hbar/(mc)$ and the Bohr's radius $a = \hbar^2/(mZe^2)$. It is obvious that $a_0 \sim a \gg l$.

Let us first consider the area near the soliton center where $r - a_0 \sim l$. Suppose the soliton center trajectory is $\mathbf{r} = \zeta(t)$. Putting into (12) the configuration

$$\psi = u(\mathbf{r} - \zeta(t)) \exp(i\mathscr{S}/\hbar)$$

neglecting the contribution of the proper electromagnetic field, and separating the real and imaginary parts, we get

$$\partial_t \mathscr{S} - \frac{Ze^2}{r} + \frac{1}{2m} (\nabla \mathscr{S})^2 - \frac{\hbar^2}{2m} \left(\hat{f} + \frac{\Delta u}{u} \right) = 0 \tag{15}$$

$$\Delta \mathscr{S} + 2(\nabla \mathscr{S} - m\dot{\zeta}) \cdot \nabla u/u = 0 \tag{16}$$

Assuming S to be a slowly varying function of a point in the vicinity of the soliton center, from (16) we deduce

$$\mathscr{S} \approx m\dot{\zeta} \cdot (\mathbf{r} - \zeta) + C_0 t + \chi(t), \qquad C_0 = \text{const} \tag{17}$$

Taking into account the classical equations of motion of a charged particle in the Coulomb field

$$m\ddot{\zeta} = -Ze^2 \zeta/\zeta^3$$

and using the expansion

$$\frac{1}{r} \approx \frac{1}{\zeta} - \frac{\zeta \cdot (\mathbf{r} - \zeta)}{\zeta^3}$$

from (15) and (17) we derive

$$\partial_t \chi = \frac{m}{2} \dot{\zeta}^2 + \frac{Ze^2}{\zeta} \equiv \mathscr{L}(t)$$

where $\mathscr{L}(t)$ is the Lagrangian of a particle in the Coulomb field. Thus, the function χ is the classical action on the trajectory:

$$\chi(t) = \int_0^t \mathscr{L}(t)\, dt \tag{18}$$

and the function u is the soliton-like solution to the quasi-stationary problem

$$\hbar^2(\hat{f} + \Delta u/u) = 2mC_0 \tag{19}$$

In this case according to (3.4) and (3.5)

$$\rho = -(2me/\hbar^2)u^2, \qquad \mathbf{j} = -2\varepsilon c u^2(\varepsilon\mathbf{A} + m\dot{\zeta}/\hbar)$$

which makes it possible, using the common solutions to Eqs. (13), (14), and (15), to calculate the potentials A_i of the electromagnetic field in the vicinity of the soliton center:

$$A_0 = A_0(\mathbf{r} - \zeta(t)), \qquad c\mathbf{A} = \dot{\zeta}(t)\, A_0(\mathbf{r} - \zeta(t))$$

where the terms $\dot{\zeta}^2/c^2$ are neglected.

To find the field ψ far from the soliton center, we rewrite equation (12) in the integral form

$$\psi(t, \mathbf{r}) = C_n\psi_n(\mathbf{r}) \exp(-i\omega_n t) + \frac{1}{2\pi}\int d\omega \int dt' \int d^3x'$$
$$\times \exp[-i\omega(t-t')]\, G(\mathbf{r}, \mathbf{r}'; \omega + i0)\, \hat{f}\psi(t', \mathbf{r}') \tag{20}$$

where $\psi_n(\mathbf{r})$ is the eigenfunction of the Hamiltonian of a hydrogen atom for a stationary state of number n with energy $E_n = \hbar\omega_n$, $C = \text{const}$, and $G(\mathbf{r}, \mathbf{r}'; \omega)$ is the Hamiltonian's resolvent having the form[16]

$$G(\mathbf{r}, \mathbf{r}'; \omega) = \frac{\Gamma(1-i\nu)}{4\pi R} \begin{vmatrix} W_{i\nu,1/2}(-ikr_+) & M_{i\nu,1/2}(-ikr_-) \\ \dot{W}_{i\nu,1/2}(-ikr_+) & \dot{M}_{i\nu,1/2}(-ikr_-) \end{vmatrix} \tag{21}$$

Here, the following notation is used:

$$k = (2m\omega/\hbar)^{1/2}, \qquad \operatorname{Im} k > 0, \qquad \nu = (ka)^{-1}$$
$$r_{\pm} = r + r' \pm |\mathbf{r} - \mathbf{r}'|$$

and the Whittaker functions $W_{i\nu,1/2}$, $M_{i\nu,1/2}$ and their derivatives $\dot{W}_{i\nu,1/2}$, $\dot{M}_{i\nu,1/2}$ are introduced. To find the field ψ at large distances from the electron–soliton center, i.e., at $|r - a_0| \gg l$, it is sufficient to put in (20)

$$\hat{f}\psi(t, \mathbf{r}) = g \exp(-i\omega_n t)\, \delta(\mathbf{r} - \zeta(t)), \qquad g = \text{const} \tag{22}$$

where the relation (5) is taken into account. As a result, we get

$$\psi(t, \mathbf{r}) = C_n \psi_n(\mathbf{r}) \exp(-i\omega_n t) + \frac{1}{2\pi} \int d\omega \int dt'$$
$$\times \exp[-i\omega t + it'(\omega - \omega_n)]\, G(\mathbf{r}, \mathbf{r}'; \omega + i0) \tag{23}$$

It is easy to verify that the field (23) decreases exponentially at large distances.

With the help of (23) and Eqs. (13) and (14), one can evaluate the electromagnetic field outside the soliton. In doing this, we notice that for large times $|\omega_n| t \gg 1$ the 4-potential A_k will contain only stationary part $A_k = (A_k^{ret} + A_k^{adv})/2$. In this case, in the wave zone, the field strengths are

$$\mathbf{E} = \tfrac{1}{2}(\mathbf{E}_+ + \mathbf{E}_-), \qquad \mathbf{B} = \tfrac{1}{2}([\mathbf{n}_- \mathbf{E}_-] - [\mathbf{n}_+ \mathbf{E}_+]) \tag{24}$$

where $\mathbf{E}_- = \mathbf{E}^{ret}$, $\mathbf{E}_+ = \mathbf{E}^{adv}$, $\mathbf{n}_\pm = \mathbf{R}_\pm / R_\pm$, $\mathbf{R}_\pm = \mathbf{r} - \zeta(t_\pm)$, and $t_\pm$ are the roots of the equations $t_\pm = t \pm R_\pm / c$.

From (24) it follows that the projection of the Poynting vector $\mathbf{S}$ in the direction of the vector $\mathbf{N} = (\mathbf{n}_+ + \mathbf{n}_-)/2$, coinciding with $\mathbf{n} = \mathbf{r}/r$, as $r \to \infty$ takes the form

$$S_N = \frac{c}{16\pi\sqrt{2}} (E_-^2 - E_+^2)(1 + \mathbf{n}_+ \cdot \mathbf{n}_-)^{1/2} \tag{25}$$

Since $\mathbf{n}_\pm = \mathbf{n} + O(r^{-1})$, after averaging expression (3.16) over the sphere, we find

$$\langle S_N \rangle = \frac{c}{16\pi} (\langle E_-^2 \rangle - \langle E_+^2 \rangle) = O(r^{-3}) \tag{26}$$

Thus according to (26) the electromagnetic radiation from the system is absent. In particular, for the circular motion in the spherical coordinates r, θ, and ϕ we have the following components of the Poynting vector $\mathbf{S}$:

$$S_r = \frac{\kappa}{r^2} \sin^2\theta \sin 2(\phi - \Omega t) \sin(2\Omega r/c)$$
$$S_\theta = \sin(\Omega r/c)\, O(r^{-3}), \qquad S_\phi = \sin(\Omega r/c)\, O(r^{-3}) \tag{27}$$

where $\kappa = e^2 a_0^2 \Omega^4 / (16\pi c^3)$. From (27) it is obvious that there exist spherical surfaces where either $S_r = 0$ or $\mathbf{S} = 0$, thus once again confirming the fact that in the stationary states described, radiation is absent.

4. CONCLUSION

In the considered soliton model of a hydrogen atom the stability condition of spatial stationary motions of electrons in the field of the Coulomb center is fulfilled. The existence of this kind of motion was mentioned by Boguslavsky[17] and Chetaev.[18] In particular, due to the fulfillment of the nonlinear resonance condition (5) the energy spectrum of these stationary states coincides with that of a hydrogen atom. This fact indicates the role of nonlinearity in the formation of extended micro-objects, whose laws of evolution agree with quantum mechanics.

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