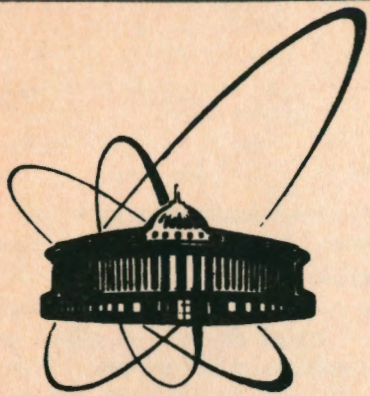

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THE NONPERTURBATIVE SHIFT OF THE ENERGY LEVELS INDUCED BY THE STATIC COULOMB SELF-INTERACTION

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1. Introduction

The present consideration is initiated by the interesting paper /1/ that has recently been published in this Journal. Its authors have dealt with the removal of divergences from the vacuum charge density of a hydrogen (H)-like atom. These divergences arise from the electrons that fill the Dirac sea (DS) states. Regretfully, no concrete figures concerning level shifts were obtained in /1/. Here we consider the nonrelativistic (NR) one-electron atoms with the self-interaction (SI). The latter is taken into account in the framework of the theory developed by A.O.Barut and his colleagues /2/. We limit ourselves to the NR version of this theory. Its applicability is justified by the small velocities of atomic electrons and by the fact that the original NR Bethe calculations /3/ of the Lamb shift are almost exactly reproduced by the more refined relativistic ones /4/. There is no DS levels in this case and no divergences appear. The plan of our exposition is as follows. In §2 the main facts and Eqs. concerning SI are presented.The positions of the lowest energy levels and the corresponding wave functions (WF) are evaluated in §3. The short discussion of the results obtained is given in §4.

2. Main Facts Concerning the Self-Interaction

In the relativistic case, the following Lagrangian describes the interaction of the electromagnetic field with electrons /5/:

$$\mathbf{L}(x) = \bar{\Psi}(x)(i\nabla - e\mathbf{A}(x) - m)\Psi(x) - \frac{1}{4}\mathbf{F}^{\mu\nu}(x)\mathbf{F}_{\mu\nu}(x), \qquad (2.1)$$

$$\mathbf{A} = \mathbf{A}_\mu\gamma^\mu, \qquad \nabla = \gamma^\mu\frac{\partial}{\partial x^\mu}, \qquad \bar{\Psi}(x) = \Psi^+(x)\gamma_o,$$

$$\mathbf{A}^\mu = (\Phi, \mathbf{A}), \qquad \gamma = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}, \qquad \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

By varying $\mathbf{L}(x)$ wrt Ψ and $\mathbf{A}$ we get the following coupled system of equations:

$$(i\nabla - m)\Psi = e\mathbf{A}\Psi, \qquad \frac{\partial \mathbf{F}^{\mu\nu}}{\partial x^\nu} = e\bar{\Psi}\gamma^\mu\Psi.$$

When considering the electron motion in the external field one should add it to the radiation field. Then:

$$(i\nabla - m)\Psi = e(\mathbf{A} + \mathbf{A}_{\text{ext}})\Psi, \qquad (2.2)$$

$$\Box\mathbf{A}^\mu = -e\bar{\Psi}\gamma^\mu\Psi, \qquad \frac{\partial \mathbf{A}^\mu}{\partial x^\mu} = 0. \qquad (2.3)$$

Barut et al./ 2/ proposed to find $\mathbf{A}$ from (2.3), substitute it into (2.2) and to solve thus obtained highly nonlinear equation. The WF Ψ satisfying (2.2) may be developed into the Coulomb eigenfunctions Ψ_c of the Hamiltonian without SI. The complete set of these states consists of scattering states ($E > mc^2$), bound states ($-mc^2 < E < mc^2$) and DS states ($E < -mc^2$). The latter ones should be completely filled /6/(in order to prevent the particle penetration into DS states and their subsequent transition to the infinite negative energy states). DS states give divergent contribution to the charge and current densities. It was the main goal of ref./1/ to remove these divergences. Usually /7/ SI effects are taken into account in the framework of the perturbation theory (PT). The divergent integrals arising in it are handled by the suitable cut-off procedure. An alternative approach to take into account SI interaction without using the PT has been suggested by A.O.Barut and his colleagues /2/. The present treatment may be viewed as a practical realization of their ideas. To escape the infinite contribution of DS states we consider the NR electron with SI. The corresponding Lagrangian is given by /8/

$$\mathbf{L} = \mathbf{L}_e + \mathbf{L}_f, \mathbf{L}_e = \Psi^*(i\hbar\frac{\partial}{\partial t} - e\Phi)\Psi - \frac{\hbar^2}{2m}(\nabla + \frac{ie}{\hbar c}\mathbf{A})\Psi^*(\nabla - \frac{ie}{\hbar c}\mathbf{A})\Psi ,$$

$$\mathbf{L}_f = (\mathbf{E}^2 - \mathbf{H}^2)/8\pi, \qquad \mathbf{E} = -\nabla\Phi - \dot{\mathbf{A}}/c, \qquad \mathbf{H} = \text{ rot } \mathbf{A}.$$

By varying it over $\Psi, \Phi, \mathbf{A}$ we arrive at the following coupled system of equations:

$$(i\hbar\frac{\partial}{\partial t} - e\Phi)\Psi + \frac{\hbar^2}{2m}(\nabla - \frac{ie}{\hbar c}\mathbf{A})^2\Psi = 0, \tag{2.4}$$

$$\Delta\Phi - \frac{1}{c^2}\ddot{\Phi} = -4\pi\rho, \qquad \Delta\mathbf{A} - \frac{1}{c^2}\ddot{\mathbf{A}} = -\frac{4\pi}{c}\mathbf{J}. \tag{2.5}$$

The Lorentz gauge condition div $\mathbf{A} + \Phi/c = 0$ was used in deriving (2.5). NR charge and current densities entering into (2.5) are

$$\rho = e \mid \Psi \mid^2, \mathbf{J} = -\frac{ie\hbar}{2m}(\Psi^*\nabla\Psi - \nabla\Psi^*\Psi) - \frac{e^2}{mc}\mathbf{A} \mid \Psi \mid^2.$$

We limit ourselves to the static potentials Φ , $\mathbf{A}$. In this case the time dependence may be separated from Ψ : $\Psi = \exp(\text{iEt}/\hbar)U(r)$. Then

$$-\frac{\hbar^2}{2m}(\nabla - \frac{ie}{\hbar c}\mathbf{A})^2U + e\Phi U = EU, \tag{2.6}$$

$$\Delta\Phi = -4\pi\rho, \qquad \Delta\mathbf{A} = -\frac{4\pi}{c}\mathbf{J}, \qquad div\mathbf{A} = 0.$$

Consider now a particular case when $\mathbf{A} = 0$, while the scalar potential Φ is spherically symmetric :

$$-\frac{\hbar^2}{2m}\Delta U + e\Phi U = EU, \qquad \Delta\Phi = -4\pi\rho, \qquad \rho = e \mid \Psi \mid^2 .$$

We realize that disregarding solutions with $\mathbf{A} \neq 0$ we lose the major part of physically interesting effects (Lamb shift, etc.). However, the solution found here (as far as we know) is the first nonperturbative one. Further, we limit ourselves to the states with zero angular momentum, i.e., to the s states ($U = R(r)$)

$$-\frac{\hbar^2}{2m}(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}) + e\Phi R = ER, \tag{2.7}$$

$$\frac{d^2\Phi}{dr^2} + \frac{2}{r}\frac{d\Phi}{dr} = -4\pi eR^2. \tag{2.8}$$

We are interested in studying the SI influence on the electron in the field of the fixed Coulomb center. For this we should add its energy into the rhs of Eq.(2.7). This gives

$$-\frac{\hbar^2}{2m}(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}) - \frac{Ze^2}{r}R + e\Phi R = ER. \tag{2.9}$$

Following the idea suggested by A.O.Barut and his colleagues/2/ we find Φ from (2.8) :

$$\Phi = e(\frac{1}{r}\int_0^r dr'R^2(r')r'^2 + \int_r^\infty dr'R^2(r')r') \tag{2.10}$$

and substitute it into (2.9).As a result we obtain the nonlinear Hartree-Fock type equation (2.9) with Φ given by (2.10). It is convenient to express the radial coordinate r and energy E in the dimensionless variables: $x = Zr/a_0, \epsilon = \hbar^2E/Z^2\text{me}^4$.
Here $a_0 = \hbar^2/\text{me}^2$ is Bohr's radius. In these units the energies and eigenfunctions of the H -like atoms without SI are the same for any Z. Particularly, for the treated s states they are

$$\epsilon_n^c = -1/2n^2, R_n^c = (2/n^{3/2})_1F_1(1-n, 2, 2x/n)\exp(-x/n). \tag{2.11}$$

These functions are orthonormal:

$$\int_0^\infty dxR_n^c(x)R_{n'}^c(x)x^2 = \delta_{nn'}.$$

3. Numerical Results

The solutions of the nonlinear Eq.(2.9) were obtained as follows. The starting point is the eigenfunction (2.11) corresponding to the particular (ns) state of the H -like atom without SI. We substitute R_n^c into Φ and solve $Eq(2.9)$ with such a Φ . Let $\epsilon_n^{(1)}$ and $R_n^{(1)}$ be the solutions of (2.9). We repeat this procedure by substituting $R_n^{(1)}$ into Φ and solving again Eq.(2.9). This process stops when

two successive iterations give practically the same energy and WF. Three lowest absolute values of the energy levels are collected in the Table .

Table . The lowest energy levels of H -like atoms with SI

$n\backslash Z$	2	4	6	8	10	82	
1	0.232	0.354	0.400	0.424	0.439	0.492	0.500
2	0.057	0.089	0.101	0.107	0.110	0.123	0.125
3	0.026	0.039	0.044	0.047	0.048	0.05475	0.055

In the last column of this table we present the energies of the H -like atoms without SI ($|\ \epsilon_n^c\ | = 1/2n^2$). One may wonder why this Table does not contain the energy levels of the hydrogen atom($Z = 1$). The reason is that SI in this case turns out to be so strong that it pushes out hydrogen bound states into the continuum. This is also confirmed by the naive application of the PT. In fact, averaging the SI term over the unperturbed ground state WF (given by $Eq(2.11)$ with $n = 1$ in it) we obtain for the energy shift $\Delta\epsilon_1 = 5/4Z$. Adding it to the nonperturbative energy of the same state ($\epsilon_1^c = -1/2$) we find that the total energy falls for $Z = 1$ into the continuum. It does not follow from this Table that deviations of E_n from E_n^c are smaller for large values of Z. With the account of factor Z^2 in the definition of ϵ_n they are in fact larger. The WF corresponding to the energy levels of the Table are shown in Figs.1-3. The point-like curves are related to the WF without SI. For states with $n = 2$ and 3 there are shown WF only with the lowest values of Z (the WF with higher Z cannot be discriminated on these Figs.). To make the effective potential energy more visualable we present Φ in the form

$$\Phi = -\frac{Ze^2}{r}V_{\rm eff}, \qquad V_{\rm eff} = 1 - \frac{1}{Z}\left(\int_0^r dr' R^2(r')r'^2 + r\int_r^\infty dr' R^2(r')r'\right).$$

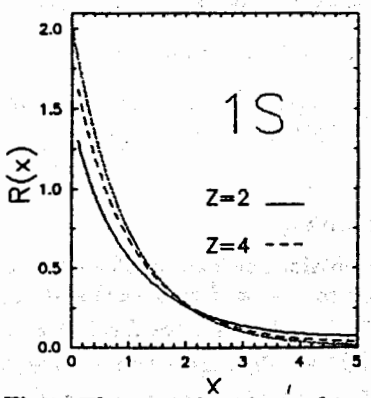

Fig.1. The wave functions of $1s$ states with self interaction (full and broken curves) and without it (point-like curve).

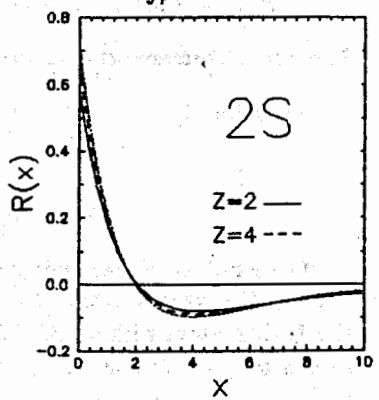

Fig.2. The same as in Fig.1,but for $2s$ states.

Figs.4-6 show $V_{\rm eff}$ for different Z and different eigenfunctions. The deviation of $V_{\rm eff}$ from unity measures the power of SI.

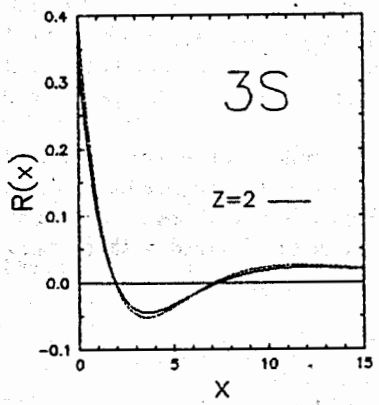

Fig.3. The same as in Fig.1, but for $3s$ states.

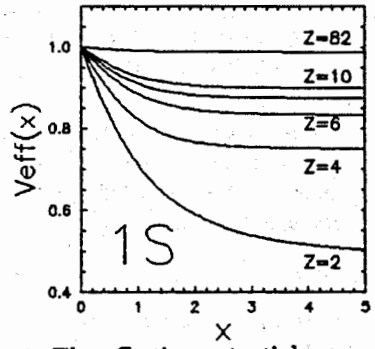

Fig.4. The effective potential energy for $1s$ states.

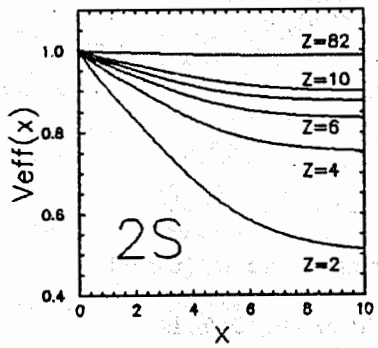

Fig.5. The same as in Fig.4, but for $2s$ states.

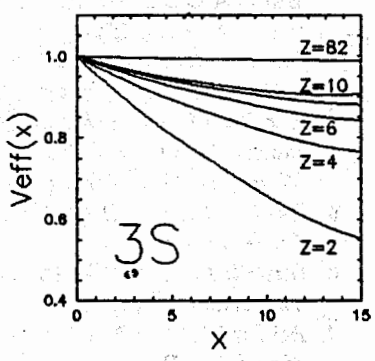

Fig.6. The same as in Fig.4, but for $3s$ states.

4. Discussion and Conclusion

It follows from the previous section that SI should destroy an atom as a bound system. But such an atom exists in Nature with its energies not very far from those of the H atom without SI. However, one cannot simply discard SI terms as they are responsible for such well established effects as Lamb shift, anomalous magnetic moment of the electron, radiative corrections to the Coulomb scattering, etc.(see, e.g., /7/). Usually, it is believed (Cf. /2,4,5,7/)

that a static SI considered here does not lead to the observable effects (it renormalizes the atomic levels and does not contribute to the radiative corrections mentioned above). If we adopt this viewpoint, then the Table gives the values of these renormalizations. Usually, they are evaluated by means of PT which is not free from divergences. The special subtraction and cut-off procedures are used to get rid off them. We have succeeded in obtaining the finite renormalizations of atomic levels without using PT.

To the end, using ideas of A.O.Barut and his colleagues we have evaluated nonperturbative renormalizations of atomic levels and wave functions of the hydrogen-like atoms with self-interaction. This raises one's hope that more realistic observable effects (Lamb shift, etc.) can be obtained without using perturbation theory.

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