An advanced approach to quantization of the quasistationary states of Dirac-Slater equation

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Abstract An advanced procedure for quantization of the quasi-stationary states of the relativistic Dirac-Fock equation with a local potential is developed within a gauge-invariant relativistic many-body perturbation theory ([1], [2]). New numerical local Dirac-Fock approach to calculating spectra of the quantum (atomic) systems with an account of relativistic and exchange-correlation corrections is presented. Numerical test results are presented.

Keywords Dirac-Slater equation · Quasi-stationary states · Eigen functions and eigen values of energy

Mathematics Subject Classification (2000) 55R05 · 53B05

1 Introduction

As it is known ([1]–[7]), the problems of calculating the eigen values and eigen functions of the the different quantum operators is relating to a number of the most important and actual problems of the modern quantum geometry and quantum theory of the many-body systems. In this paper we present an advanced procedure for quantization of the quasi-stationary states of the relativistic Dirac-Fock equation with introduced local Dirac-Fock potential. All consideration, as usually, is performed within gauge-invariant relativistic many-body perturbation theory ([2], [3],[7]-[10]). In our previous papers [7]-[12] the same task has been considered for a few classes of the relativistic differential equations (Dirac, Dirac-Kohn-Sham, Dirac-Slater etc). The developed approaches have been tested

on calculating a set of the energy and spectral parameters for different multi-electron systems.Here we consider the Dirac-Fock equation with a local potential. The main difference of these equations of the standard Dirac-Fock ones is that the standard equation contain non-local potential and correspondingly the calculational scheme of their solving is very complicated because of the cited non-locality (the exchange interaction term). The more details about the modern art of state concerning calculating the eigen values of energies and eigen functions for different operators (Hamiltonians) of the finite quantum (atomic) systems can be found in a number of recent books (see, for example,[1]–[7] and references therein)). we can remind such atomic multi-configuration Dirac-Fock codes as the Desclaux program, Dirac package etc (see for example, [1]–[10]). The main idea of our approach is in using the local Dirac-Fock equations, i.e. using sufficiently simplified procedure for an account of relativistic, exchange-correlation effects. The general potential in these equations includes the self-consistent local mean field potential, the electric of a nucleus (within the Fermi model). New element of the approach is connected with using ab initio consistent quantum electrodynamics approach to construction of the optimal one-quasiparticle representation in the local Dirac-Fock approach.

2 Local Dirac-Fock equation: quantization of the quasistationary states

In this section we describe the key moments of our approach to quantization of the quasistationary (stationary) states of the relativistic local Dirac-Fock equation which is indeed very similar to schemes of Refs.[7]-[10]), however contains other potentials.

One-particle wave functions are found from solution of the relativistic local Dirac-Fock equation, which can be written in the central field in a two-component form (see, for example,([1], [5]):

$$\begin{aligned} &\frac{\partial F}{\partial r} + (1+\chi)\frac{F}{r} - (\epsilon + m - V_{loc}(b,r))G = 0, \\ &\frac{\partial G}{\partial r} + (1-\chi)\frac{G}{r} - (\epsilon - m - V_{loc}(b,r))F = 0. \end{aligned} \tag{1}$$

where all notations are standard, b is the special gauge-invariant parameter (look below).Here we put the fine structure constant $\alpha = 1$. The moment number

$$\chi = \begin{cases} -(1+1), & j > 1 \\ 1, & J < 1 \end{cases} \tag{2}$$

The general potential $V_{loc}(b,r)$ includes the self-consistent local Dirac-Fock potential (see, for example,([5], [11])). Further, as usually, (see [2],[7]), at large χ the radial functions F and G vary rapidly at the origin of co-ordinates:

$$F(r), G(r) \approx r^{\gamma-1}, \qquad (3)$$
$$\gamma = \sqrt{\chi^2 - \alpha^2 Z^2}.$$

This involves difficulties in numerical integration of the equations in the region $r \to 0$. To prevent the integration step becoming too small it is convenient to turn to new functions isolating the main power dependence: $f = Fr^{1-|\chi|}$, $g = Gr^{1-|\chi|}$. The Dirac equation for F and G components are transformed as (in the Coulomb units):

$$f' = -(\chi + |\chi|)\frac{f}{r} - \alpha Z V_{loc}(b,r)g - \left(\alpha Z E_{n\chi} + \frac{2}{\alpha Z}\right) g,$$
$$g' = (\chi - |\chi|)\frac{g}{r} - \alpha Z V_{loc}(b,r)f + \alpha Z E_{n\chi} f. \qquad (4)$$

Naturally, the system of Eq. (4) has two fundamental, solutions. As usually, we are interested in the solution regular at $r \to 0$. The boundary values of the correct solution are found by the first term s of the expansion into the Taylor series (see [2]):

$$g = \frac{(V_{loc}(0) - E_{n\chi})r\alpha Z}{2\chi + 1}; \qquad f = 1 \quad \text{at} \quad \chi < 0,$$
$$f = \left(V_{loc}(0) - E_{n\chi} - \frac{2}{\alpha^2 Z^2}\right)\alpha Z; \qquad g = 1 \quad \text{at} \quad \chi > 0. \qquad (5)$$

The condition $f, g \to 0$ at $r \to \infty$ determines the quantified energies of the state $E_{n\chi}$. At correctly determined energy $E_{n\chi}$ of the asymptotic f and g at $r \to \infty$ are:

$$f, g \sim \exp\left(-r/n^*\right), \qquad (6)$$

where $n^* = \sqrt{\frac{1}{2|E_{n=\chi}|}}$ is the effective main quantum number. The Eq.(4) was solved by the Runge-Kutt method (see details in ([1], [5]).

Regarding the nuclear potential of the local Dirac-Fock equation, as in Refs.([2], [7]) we use the Gauss model for the charge distribution in the nucleus $\rho(r)$. According to [2] one could write:

$$\rho(r|R) = \frac{4\gamma^{3/2}}{\sqrt{\pi}} \exp(-\gamma r^2);$$
$$\int_0^\infty dr r^2 \rho(r|R) = 1; \qquad (7)$$
$$\int_0^\infty dr r^3 \rho(r|R) = R,$$

where $\gamma = frac4\pi R^2$, R is the effective nucleus radius. The following simple dependence of R on Z assumed:

$$R = 1.60 \cdot 10^{-13} Z^{1/3} \quad \text{(cm)}. \tag{8}$$

The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{\text{nucl}}(r|R) = -\frac{1}{r}\int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r'^2 \rho(r'|R). \tag{9}$$

It is determined by the following system of differential equations ([1], [5]):

$$\begin{aligned} V_{\text{nucl}}(r,R) = \frac{1}{r^2}\int_0^r dr' r'^2 \rho(r',R) \equiv \frac{1}{r^2} y(r,R); \\ y'(r,R) = r^2 \rho(r,R); \\ \rho'(r,R) = -8\gamma^{5/2}\frac{r}{\sqrt{\pi}}\exp(-\gamma r^2) = -2\gamma r \rho(r,R) = -\frac{8r}{\pi r^2}\rho(r,R) \end{aligned} \tag{10}$$

with the boundary conditions:

$$\begin{aligned} V_{\text{nucl}}(r,0) = -\frac{4}{\pi r}; \\ y(0,R) = 0; \\ \rho(0,R) = \frac{4\gamma^{3/2}}{\sqrt{\pi}} = \frac{32}{R^3}. \end{aligned} \tag{11}$$

The above written equations and a whole scheme determine a procedure for quantization of the quasi-stationary states of the relativistic Dirac-Fock equation with introduced local Dirac-Fock potential. The key question of any approach is performance of the gauge-invariance condition, by checking, for example, the Yord equalities.Naturallu it requires a construction of the corresponding Green's function of thew Dirac-Fock equations. More efficient and simultaneously simplified recept is connected with calculating the radiation transition probabilities (oscillator strengths)in two different transition operator (length and velocity) forms using the basis of the relativistic Dirac-Fock wave functions, in our case the local Dirac-Fock scheme. Earlier it was shown ([2], [3]) that an adequate description of the atomic characteristics requires using the optimized basis of wave functions. In Ref. [3] a new ab initio optimization procedure for construction of the optimized basis is proposed. It is reduced to minimization of the gauge dependent multielectron contribution $Im\Delta\ E_{ninv}$ of the lowest quantum-electrodynamical perturbation theory corrections to the radiation widths of atomic levels. In the fourth order of quantum-electrodynamical perturbation theory(the second order of the atomic perturbation theory) there appear the diagrams, whose contribution to the $Im\Delta\ E_{ninv}$ accounts for the correlation (polarization) effects (see,

e.g., [2]). This contribution describes the collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). All the gauge non-invariant terms are multielectron by their nature (the particular case of the gauge non-invariance manifestation is a non-coincidence of the oscillator strengths values, obtained in the approximate calculations with the "length" and "velocity" transition operator forms). The corresponding expression for the imaginary part of the electron energy has been determined in Ref. [3]. We have performed the simplified numerical test in order to check the optimality properties of the wave functions by means the minimization of the value $Im\Delta\, E_{ninv}(b)$ with the parameter b. Our test has been carried out for the radiative 3s-3p transitions in spectra of the sodium-like ions SVI and $ClVII$. The empirical values of the oscillator strengths for these ions are : 0.66 ± 0.01 and 0.604 ± 0.015. The calculation results within the local Dirac-Fock scheme (without account of the correlation effects) are 0.69 and 0.64 correspondingly (here the gauge non-invariant contribution is 10 percents). The calculation result within the local Dirac-Fock scheme (with account of the correlation effects by means of the method [3]) are 0.663 and 0.608 correspondingly. In the last case, the gauge non-invariant contribution is 0.1 percents. This numerical result has shown that our approach (without an accounting the correlation effects) can hardly provide a high (spectroscopic) accuracy, however, an implementation of the correct multi-body correlation potentials into the local Dirac-Fock equations and using the formalism of the relativistic perturbation theory with the local Dirac-Fock potential will provide a sufficiently high accuracy of calculating the energy and spectral characteristics of the multi-electron atomic systems.

3 Conclusions

In conclusion let us underline that we have proposed a new procedure for quantization of the stationary and quasistationary states of the relativistic Dirac-Fock equation with a local potential within a gauge-invariant relativistic many-body perturbation theory ([2], [3]). Further we presented a numerical local Dirac-Fock approach to calculating spectra of the quantum (atomic) systems with an account of relativistic and exchange corrections. Within a propose scheme we have carried out the test calculation of the oscillator strengths for the radiative 3s-3p transitions in spectra of the sodium-like ions SVI and $ClVII$, which shown that the local Dirac-Fock approach without an accounting of the correlation effects can hardly provide a high accuracy of calculating the energy and spectral characteristics (oscillator strengths)of the multi-electron atomic systems. However,

an implementation of the correct multi-body correlation potentials into it and using the formalism of the relativistic perturbation many-body theory with the local Dirac-Fock potential can provide a spectroscopic accuracy.

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