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Analytical transition-matrix treatment of electric multipole polarizabilities of hydrogen-like atoms

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HIGHLIGHTS

- A new description for electric polarization of hydrogen-like atoms.
- Expression for multipole polarizabilities in terms of off-shell scattering functions.
- Derivation of integral equation determining the off-shell scattering function.
- Rigorous analytic solving the integral equations both for ground and excited states.
- Study of contributions of virtual multiple scattering to electric polarizabilities.

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ABSTRACT

The direct transition-matrix approach to the description of the electric polarization of the quantum bound system of particles is used to determine the electric multipole polarizabilities of the hydrogen-like atoms. It is shown that in the case of the bound system formed by the Coulomb interaction the corresponding inhomogeneous integral equation determining an off-shell scattering function, which consistently describes virtual multiple scattering, can be solved exactly analytically for all electric multipole polarizabilities. Our method allows to reproduce the known Dalgarno–Lewis formula for electric multipole polarizabilities of the hydrogen atom in the ground state and can also be applied to determine the polarizability of the atom in excited bound states.

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1. Introduction

The phenomenon of polarization (deformation) under the action of an external electromagnetic field is inherent in all composite quantum systems containing one or more charged components (to molecules, atoms, nuclei, nucleons and other complexes) and is indisputably an universal property of the system.

Theoretical studies of influence of the electric and magnetic fields on structure of spectra of the simplest atoms were in the center of attention while becoming of modern quantum mechanics [1,2]. The Stark effect of the second order for hydrogen-like atoms was first calculated by Epstein [3], Wentzel [4] and Waller [5] based on the separation of the Schrödinger equation in parabolic coordinates and by using the perturbation theory.

Later on, the electric dipole polarizability of the simplest atomic systems were calculated directly using the traditional method by the formula for the energy shift in the second order of the Rayleigh–Schrödinger perturbation theory [2,6,7] in the applied electric field. As an example, employing this method, the contributions of the excited virtual states to the electric dipole polarizability of the hydrogen atom were investigated in Ref. [8]. However, in general case this method is too cumbersome and nonpracticable because of the necessity of taking into account of virtual excited states, both discrete and from the continuum, that are coupled with the ground state by the perturbated interaction, especially for the systems with three and more particles.

The modification of the Rayleigh–Schrödinger perturbation theory proposed by Dalgarno and Lewis [9] (see also [10–12]) permits to avoid difficulties associated with allowance for all possible intermediate bound and continuum states by the prior determination of the first-order correction to the wave function of the unperturbated state which satisfies an inhomogeneous differential equation. In the case of the hydrogen atom Dalgarno and Lewis managed to solve analytically the differential equation and first derive a general formula for all electric multipole polarizabilities of the atom in the ground bound state. With the use of the O(4)-symmetry of the energy operator of the hydrogen-like atom [13] and Dalgarno–Lewis perturbative technique [9] purely algebraic approach to the calculation of the second-order Stark effect for the atom has been developed in Ref. [14].

The object of this paper is to elaborate a new method of the analytical solution of the electric multipole polarizabilities of the hydrogen-like atom on the basis of the transition matrix approach, which has been applied by us earlier in nuclear physics to calculate the electric dipole polarizabilities of systems with the S-wave finite-range interaction—the deuteron [15–18] and two-cluster models of the triton and lambda hypertriton [19,20]. In the preceding paper [21] the t-matrix formalism was firstly applied to calculate numerically the dipole, quadrupole and octupole polarizabilities of the hydrogen atom using the representation of the Coulomb t-matrix with explicitly removed singularities [22].

In this paper we demonstrate that the integral equations, which appear in the framework of the t-matrix formalism, permit in the case of the Coulomb interaction exact analytical solution for all the electric multipole polarizabilities of the hydrogen-like atom. Section 2 is devoted to description of the t-matrix formalism of the polarization interaction of a two-particle bound complex placed in a external electric field of a charged particle. In Section 3 the proposed approach is applied for derivation of the main integral equation that determines the electric multipole polarizabilities of the hydrogen-like atom. Strictly analytical solving of the obtained integral equation is performed in Section 4 in the case of the ground bound state. In Section 5 the general formula for the electric multipole polarizabilities of the hydrogen-like atom in the ground state is derived and discussed. Section 6 is concerned with the analytical derivation of the electric dipole polarizability of the hydrogen-like atom in the excited $2S$-state. Conclusions and outlook are presented in Section 7.

2. Transition matrix description of polarization interaction for a two-particle bound complex

Let us consider scattering of a two-particle complex formed from charged particles 1 and 2 in the ground bound state by an external electric field of a charged particle 0. The total Hamiltonian of the