МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
ОДЕСЬКИЙ ДЕРЖАВНИЙ ЕКОЛОГІЧНИЙ УНІВЕРСИТЕТ

Methodical instructions for practical work, test performance, distance learning of PhD students in the discipline "Computational Methods of optics and dynamics of quantum and laser systems. Part 4".

(Training of PhD students of the specialty:
104 –"Physics and astronomy")

«Затверджено»
на засіданні групи забезпечення спеціальності
Протокол №1 від 28/08/2021 Голова групи________Свинаренко А.А.

«Затверджено»
на засіданні кафедри вищої та прикладної математики
Протокол №1 від 28/08/2021 Зав. кафедри________ Глушков О.В.

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THE MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
ODESSA STATE ENVIRONMENTAL UNIVERSITY

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PREFACE

The discipline "Computational methods of optics and dynamics of quantum and laser systems" is a mandatory discipline in the cycle of professional training of graduate students (3rd level of education) in the specialty 104- Physics and astronomy.

It is aimed at mastering (providing) a number of planned competencies, including the study of the modern apparatus of optics and dynamics of quantum and laser systems, as well as the development of new computational methods and algorithms for numerical study of energy and spectroscopic characteristics of atoms, molecules, solids , the main properties of quantum and laser systems, systems in general in the field of optics and laser physics and new developed computational methods in order to achieve scientific results that create potentially new knowledge in computational applied mathematics.

The place of the discipline in the structural and logical scheme of its teaching: the knowledge gained in the study of this discipline is used in writing dissertations, the subject of which is related to the development of new computational methods and algorithms for studying energy and spectroscopic characteristics of atoms, molecules, solids, basic properties quantum and laser systems. The basic concepts of the discipline are the basic tools of a specialist in the field of optics and laser physics.

The purpose of the discipline is to master (provide) a number of competencies, in particular, to achieve relevant knowledge, understanding and ability to use methods of data analysis and statistics at the latest level, the ability to use standard and build new software based on new mathematical approaches.
-study, adapt, improve computational methods and algorithms for numerical study of the characteristics of linear and nonlinear processes in complex quantum and classical systems.

The total amount of study time for the study of the discipline is 150 hours. for full-time and part-time education, respectively.

After mastering this discipline, the graduate student must be able to use modern or personally developed new computational methods, in particular, to analyses, model, predict, program the dynamics of classical and quantum systems with the formulation of appropriate computer experiments.

The main topics: Numerical algorithms of methods of self-consistent field theory, approximate methods of model potential, quantum defect, and density functional

Topics: Numerical algorithms of methods of self-consistent field theory, approximate methods of model potential, quantum defect, and density functional

Топіки: Чисельні алгоритми методів теорії самоузгодженого поля, наближених методів модельного потенціалу, квантового дефекту, Томаса-Фермі та функціонала густини (ЗБ- Л2.7)

1. Introduction

At present time a density functional theory (DFT) became by a powerful tool in studying the electron structure of different materials, including atomic and molecular systems, solids, semiconductors etc. [1-42]. A construction of the correct energy functionals of a density for multi-body systems represents very actual and important problem of the modern theory of semiconductors and solids, thermodynamics, statistical physics (including a theory of non-equilibrium thermodynamical processes), quantum mechanics and others.

In last time a development of formalism of the energy density functional has been considered in many papers (see [1–7]). Its application is indeed based on the two known theorems by Hohenbreg-Kohn ($\tau = 0$, where τ is a temperature) and Mermin ($\tau \neq 0$) [1,2]. According to these theorems, an energy and thermodynamical potential of the multi-body system are universal density functionals. Though these theorems predict an existence of such a density functional, however its practical realization is connected with a number of the significant difficulties (see [1-3,8-17]). The problem is complicated under consideration of the non-stationary tasks (the known theorem by Runge-Gross about 1-1 mapping between time-dependent densities and the external potentials [2]).

Let us remind some important results of the density functional theory. It should be mentioned a constructive approach to delivering optimal representations for an exact density functional [1,2,8-16], which has been used for generalization of the Hohenberg-Kohn theorem in order to get an effective density functional for large molecules. As alternative version one could consider a quasiparticle conception of Kohn-Sham and the Levi-Valone method [2,3]. In fact it has been done an attempt practically to realize an idea of the Hohenberg-Kohn theorem.

More advanced analogous approach with account of the multi-particle correlations is developed in ref. [8,17,18].

The quasiparticle Fermi-liquid version of the DFT has been earlier developed in Refs. [1-3,8,17] and based on the principles of the Landau-Migdal Fermi liquids theory. In refs. [4,5] it has been firstly developed a consistent relativistic quasiparticle theory of a density functional formalism and constructed an optimized one-quasiparticle representation in a theory of multi-electron systems. The lowest order multi-body effects, in particular, the gauge dependent radiative contribution for the certain class of the photon propagators calibration are treated in QED formulation and new density functional integral-differential equations are derived. The minimal value of the gauge dependent radiative contribution is considered to be the typical representative of the multi-electron correlation effects, whose minimization is a reasonable criteria in the searching for the optimal QED perturbation theory one-electron basis. In this paper we present the optimized version of the quasiparticle DFT (a Fermi-liquid version of the DFT), based on the principles of the Landau-Migdal Fermi-liquids theory and performance of the gauge invariant principle.

The elaborated approach to construction of the eigen-functions basis can be characterized as an improved one in comparison with similar basises of other one-particle representations, namely, in the HF, the standard Kohn-Sham approximations [12-17] etc.

Below we present only the key points of the theory for multielectron atomic systems.

2. Quasiparticle density functional formalism

According to Refs. [1-5], the master equations can be obtained on the basis of variational principle, if we start from a Lagrangian of an atomic system L_q. It should be defined as a functional of quasiparticle densities:

$$\begin{aligned} \nu_0(r) &= \sum_\lambda n_\lambda \,|\Phi_\lambda(r)|^2, \\ \nu_1(r) &= \sum_\lambda n_\lambda \,|\nabla\Phi_\lambda(r)|^2, \\ \nu_2(r) &= \sum_\lambda n_\lambda [\Phi_\lambda^* \Phi_\lambda - \Phi_\lambda^* \Phi_\lambda]. \end{aligned} \tag{1}$$

The densities ν_0 and ν_1 are similar to the HF electron density and kinetical energy density correspondingly; the density ν_2 has no an analog in the Hartree-

Fock (HF) or the standard DFT theory and appears as result of account for the energy dependence of the mass operator Σ. The functions Φ_λ are the solutions of the master equations for multielectron atomic systems with a nuclear charge Z (in atomic units) as follows:

$$\begin{aligned}&[p^2/2-\sum_\alpha Z_\alpha/r_\alpha+\sum{}_0(x)+\\&p(\partial\sum/\partial p^2)p]\Phi_\lambda(x)=\\&(1-\partial\sum/\partial\varepsilon)\varepsilon_\lambda\Phi_\lambda(x)\end{aligned} \qquad \mathbf{(2)}$$

The functions Φ_λ in (5) are orthogonal with a weight

$$\rho_k{}^{-1}=a^{-1}=[1-\partial\sum/\partial\varepsilon]. \qquad (3)$$

Now one can introduce the wave functions of the quasiparticles

$$\varphi_\lambda=a^{-1/2}\Phi_\lambda, \qquad (4)$$

which are, as usually, orthogonal with weight 1. For complete definition of $\{\varphi_\lambda\}$ it should be determined the values $\sum{}_0,\partial\sum/\partial p^2,\partial\sum/\partial\varepsilon$.
A Lagrangian L_q can be written as a sum of a free Lagrangian and Lagrangian of interaction:

$$L_q = L_q{}^0 + L_q{}^{int}, \qquad (5)$$

where a free Lagrangian L_q^0 has a standard form:

$$L_q^0=\int dr\sum_\lambda n_\lambda\Phi^*_\lambda(i\partial/\partial t-\varepsilon_p)\Phi_\lambda, \qquad (6)$$

The interaction Lagrangian is defined in the form, which is characteristic for a standard (Kohn-Sham) density functional theory (as a sum of the Coulomb and exchange-correlation terms), however, it takes into account for the energy dependence of a mass operator $\sum$:

$$L_q^{\mathrm{int}}=L_K-\frac{1}{2}\sum_{i,k=0}^{2}\int\beta_{ik}F(r_1,r_2)\nu_i(r_1)\nu_k(r_2)dr_1dr_2 \qquad (7)$$

where β_{ik} are some constants (look below), F is an effective potential of the exchange-correlation interaction

In the local density approximation in the density functional the potential F can be expressed through the exchange-correlation pseudo-potential V_{XC} as follows [1-5]:

$$F(r_{1,}r_2) = \delta V_{XC} / \delta v_0 \cdot \delta(r_1 - r_2). \tag{8}$$

According to ref. [1-4], one can get the following expressions for $\sum_i = -\delta L_q^{\text{int}} / \delta v_1$:

$$\begin{aligned}
&\sum\nolimits_0 = (1 - \sum\nolimits_e) V_K + \sum\nolimits_0^{ex} + \\
&\frac{1}{2}\beta_{00}\delta^2 V_{XC} / \delta v^2 \cdot v_0^2 + \beta_{00}\delta V_{XC} / \delta v_0 \cdot v_0 + \\
&+ \beta_{01}\delta V_{XC} / \delta v_0 \cdot v_1 + \beta_{01}\delta^2 V_{XC} / \delta v_0^2 \cdot v_0 v_1 + \\
&\beta_{02}\delta^2 V_{XC} / \delta v_0^2 \cdot v_0 v_2 + \beta_{02}\delta V_{XC} / \delta v_0 \cdot v_2 \\
&\sum\nolimits_1 = \beta_{01}\delta V_{XC} / \delta v_0 \cdot v_0 + \\
&+ \beta_{12}\delta V_{XC} / \delta v_0 \cdot v_2 + \beta_{11}\delta V_{XC} / \delta v_0 \cdot v_1; \\
&\sum\nolimits_2 = \beta_{02}\delta V_{XC} / \delta v_0 \cdot v_0 + \\
&+ \beta_{12}\delta V_{XC} / \delta v_0 \cdot v_1 + \beta_{22}\delta V_{XC} / \delta v_0 \cdot v_2;
\end{aligned} \tag{9}$$

Here V_K is the Coulomb term (look above), $\sum_0^{ex}$ is the exchange term. Using the known canonical relationship:

$$H_q = \Phi_\lambda^* \delta L_q / \delta\Phi_\lambda^* + \Phi_\lambda \delta L_q / \delta\Phi_\lambda - L_q \tag{10}$$

after some transformations one can receive the expression for the quasiparticle Hamiltonian, which is corresponding to a Lagrangian L_q:

$$\begin{aligned}H_q &= H_q^0 + H_q^{\text{int}} = H_q^0 - L_K + \\ &+ \frac{1}{2}\beta_{00}\delta V_{XC}/\delta v_0 \cdot v_0^2 + \\ &+ \beta_{01}\delta V_{XC}/\delta v_0 \cdot v_0 \cdot v_1 + \\ &\frac{1}{2}\beta_{11}\delta V_{XC}/\delta v_0 \cdot v_1^2 - \\ &- \frac{1}{2}\beta_{22}\delta V_{XC}/\delta v_0 \cdot v_2^2\end{aligned} \tag{11}$$

It is obvious that omitting the energy dependence of the mass operator (i.e. supposing $\beta_{02} = 0$) the quasiparticle density functional theory can be resulted in the standard Kohn-Sham theory.

Further let us give the corresponding comments regarding the constants β_{ik}. Without a detailed explanation, we note here that the corresponding constants in our theory approximately possess the same universality as ones in the Landau Fermi-liquid theory and Migdal finite Fermi-systems theory. Though it is well known that the entire universality is absent. First of all, it is obvious that the terms with constants $\beta_{01}, \beta_{11}, \beta_{12}, \beta_{22}$ give omitted contribution to the energy functional (at least in the zeroth approximation in comparison with others), so they can be equal to zero in the simple approximation. The value for a constant β_{00} in some degree is dependent upon the definition of the potential V_{XC}. If as V_{XC} it is use one of the correct exchange-correlation potentials from the standard density functional theory, then without losing a community of statement, the constant β_{00} can be equal to 1. The constant β_{02} can be in principle calculated by analytical way, but it is very useful to remember its connection with a spectroscopic factor F_{sp} of atomic or molecular system (it is usually defined from the ionization cross-sections) [5]:

$$F_{sp} = \left\{1 - \frac{\partial}{\partial \in} \sum_{kk} \left[-(I.P.)_k\right]\right\} \tag{12}$$

where I.P. is a ionization potential. It is easily to understand the this definition is in fact corresponding to the pole strength of the corresponding Green's function [62]. The simple approximation for the I.P. is as follows [2-4]:

$$(I.P.)_k = -(\in_k + F_k), \tag{13}$$

$$F_k = \Sigma_{kk}(-(I.P.)_k) \approx \frac{1}{1-\partial\Sigma_{kk}(\in_k)/\partial_{\in}} \Sigma_{kk}(\in_k). \tag{14}$$

It is well known that can be determined by the following standard expression (in the second order of the perturbation theory):

$$\sum\nolimits_{kk}^{(2)}(\in) = \sum_{\substack{i,j \\ s\notin F}} \frac{(V_{ksij}-V_{ksji})V_{ksij}}{\in+\in_s-\in_i-\in_j} + \sum_{\substack{i,j \\ s\notin F}} \frac{(V_{ksij}-V_{ksji})V_{ksij}}{\in+\in_s-\in_i-\in_j}$$

(15)

Other details can be found in Refs. [1-10]).

3. As application of the quasiparticle theory we present the estimates for the atomic spectroscopic factors. Using the above written formula, one can simply define the values (3)-(12) one could the quantity (12). In the concrete calculation as potential V_{XC} we use the exchange-correlation pseudo-potential which contains the correlation (Gunnarsson-Lundqvist) potential and relativistic exchanger Kohn-Sham one [4,5].

As example in table 1 we present our calculational data for spectroscopic factors of some atoms.

Table 1.Spectroscopic factors of the external ns^2 shells of some atoms and ions

Atom, ion	N	F_{sp}	Atom, ion	n	F_{sp}
Ar	3	0.58	As	6	0.30
Exp.	3	0.56	As$^-$	6	0.31
RPA	3	0.70	Rn	6	0.29
TI $^{(IV)}$	3	0.60	Fr$^+$	6	0.28
Xe	6	0.36	Fr	6	0.28
TI	6	0.36	Ra	7	0.43
Pb	6	0.34	Ac	7	0.42
Bi	6	0.33	Th	7	0.42
Po+	6	0.31	Pa	7	0.42
Po	6	0.31	U	7	0.42

There are also listed for the argon atom the experimental value of the spectroscopic factor and the value, obtained in the random phase approximation (RPA) with exchange. It should be noted that the Hartree-Fock theory gives the value of 1. In conclusion let us remind that the presented approach to definition of the functions basis $\{\Phi_\lambda\}$ of a Hamiltonian H_q can be treated as an improved in comparison with similar basises of other one-particle representations (for example, the HF, the Hatree-Fock-Slater, the standard Kohn-Sham approximations etc.). Naturally, this advancement can be manifested during studying those properties of the multi-electron systems, when an accurate account for the complex exchange-correlation effects, including the continuum pressure, energy dependence of a mass operator etc, is critically important [28-40].

Tests performance

Task Option 1.

1). Give the key definitions in theory of optimized one-quaiparticle density functional theory for atomic systems and explaine the main computational details of their realization: i) construction of the optimized one-quaiparticle density functional for atomic systems; ii) computing the Dirac-Kohn-Sham equations and analysis of the corresponding solutions under asymptotic; iii). The numerical features of accounting for the exchange-correlation effects; iv). The numerical features of accounting for the relativistic effects; v) The numerical features of accounting for the nuclear effects; vi) the technical details of the computation code.

2).Explain the key ideas of the numerical estimation of the energy and spectroscopic characteristics of atomic systems, namely, ionization potentials and spectroscopic factors in application to computing of the caesium atom.

3). To carry out and apply the numerical algorythm of **density functional theory** for concrete atomic system such **as an alkali atom Cs.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Task Option 2.

1). Give the key definitions in theory of optimized one-quaiparticle density functional theory for atomic systems and explaine the main computational details of their realization: i) construction of the optimized one-quaiparticle density functional for atomic systems; ii) computing the Dirac-Kohn-Sham equations and analysis of the corresponding solutions under asymptotic; iii). The numerical features of accounting for the exchange-correlation effects; iv). The numerical features of accounting for the relativistic effects; v) The numerical features of accounting for the nuclear effects; vi) the technical details of the computation code.

2).Explain the key ideas of the numerical estimation of the energy and spectroscopic characteristics of atomic systems, namely, ionization potentials and spectroscopic factors in application to computing of the rubidium atom.

3). To carry out and apply the numerical algorythm of **density functional theory** for concrete atomic system such **as an alkali atom Rb.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: "Superatom" (all necessary numerical parameters should be self-taken).

Test Option 3.

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1). Give the key definitions in theory of optimized one-quaiparticle density functional theory for atomic systems and explaine the main computational details of their realization: i) construction of the optimized one-quaiparticle density functional for atomic systems; ii) computing the Dirac-Kohn-Sham equations and analysis of the corresponding solutions under asymptotic; iii). The numerical features of accounting for the exchange-correlation effects; iv). The numerical features of accounting for the relativistic effects; v) The numerical features of accounting for the nuclear effects; vi) the technical details of the computation code.

2).Explain the key ideas of the numerical estimation of the energy and spectroscopic characteristics of atomic systems, namely, ionization potentials and spectroscopic factors in application to computing of the magnesium atom.

3). To carry out and apply the numerical algorythm of **density functional theory** for concrete atomic system such **as atom of Mg.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” (all necessary numerical parameters should be self-taken).

Test Option 4.

1). Give the key definitions in theory of optimized one-quaiparticle density functional theory for atomic systems and explaine the main computational details of their realization: i) construction of the optimized one-quaiparticle density functional for atomic systems; ii) computing the Dirac-Kohn-Sham equations and analysis of the corresponding solutions under asymptotic; iii). The numerical features of accounting for the exchange-correlation effects; iv). The numerical features of accounting for the relativistic effects; v) The numerical features of accounting for the nuclear effects; vi) the technical details of the computation code.

2).Explain the key ideas of the numerical estimation of the energy and spectroscopic characteristics of atomic systems, namely, ionization potentials and spectroscopic factors in application to computing of the sodium atom.

3). To carry out and apply the numerical algorythm of **density functional theory** for concrete atomic system such **as an alkali atom Na.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” (all necessary numerical parameters should be self-taken).

Test Option 3.

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1). Give the key definitions in theory of optimized one-quaiparticle density functional theory for atomic systems and explaine the main computational details of their realization: i) construction of the optimized one-quaiparticle density functional for atomic systems; ii) computing the Dirac-Kohn-Sham equations and analysis of the corresponding solutions under asymptotic; iii). The numerical features of accounting for the exchange-correlation effects; iv). The numerical features of accounting for the relativistic effects; v) The numerical features of accounting for the nuclear effects; vi) the technical details of the computation code.

2).Explain the key ideas of the numerical estimation of the energy and spectroscopic characteristics of atomic systems, namely, ionization potentials and spectroscopic factors in application to computing of the francium atom.

3). To carry out and apply the numerical algorythm of **density functional theory** for concrete atomic system such **as the atom of Fr.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” (all necessary numerical parameters should be self-taken).

Test Option 6.

1). Give the key definitions in theory of optimized one-quaiparticle density functional theory for atomic systems and explaine the main computational details of their realization: i) construction of the optimized one-quaiparticle density functional for atomic systems; ii) computing the Dirac-Kohn-Sham equations and analysis of the corresponding solutions under asymptotic; iii). The numerical features of accounting for the exchange-correlation effects; iv). The numerical features of accounting for the relativistic effects; v) The numerical features of accounting for the nuclear effects; vi) the technical details of the computation code.

2).Explain the key ideas of the numerical estimation of the energy and spectroscopic characteristics of atomic systems, namely, ionization potentials and spectroscopic factors in application to computing of the lithium atom.

3). To carry out and apply the numerical algorythm of **density functional theory** for concrete atomic system such **as an alkali atom Li.** To perform its pracrical realization (using Fortran Power Station , Version 4.0; PC Code: “Superatom” (all necessary numerical parameters should be self-taken).

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