

**DYNAMIC RESPONSE OF SOME ATOMS:
MANY-BODY CALCULATIONS***UDC 530.145; 539.183***A. R. Tančić¹, M. Nikolić²**¹VINČA Institute for Nuclear Sciences, P.O. Box 522, Belgrade, Serbia and Montenegro²Faculty of Science and Mathematics, P.O. Box 224, 18001 Niš, Serbia and Montenegro

Abstract. *The frequency-dependent polarizability in the Hartree-Fock (HF) approximation has been corrected for true correlation effects by means of many-body theory. The polarizability has been computed in the Random Phase Approximation with Exchange (RPAE) for He, Ar, Xe, Kr, Li, Ca through the second (and some higher) order in the correlation potential. With this polarizability as input we obtained the values of some atomic interaction constants.*

Key words: *dynamic polarizability, static polarizability, random phase approximation*

INTRODUCTION

The interaction of electromagnetic radiation with atoms (molecules) is the source of much of our experimental knowledge of their properties. Although a rigorous treatment of this interaction should be on the quantization of electromagnetic field, the semi classical approach yields correct results for many problems of the interest. The clear review of the time-dependent perturbations in atomic physics has been given, for example, in [1] [2]. Theoretical treatments of the electron-atom scattering, the long-range dispersion energy coefficients between atoms and/or molecules, interatomic potentials, optical properties of materials, and collision induced spectral shifts, all use polarizability [3] [4] [5] [6]. Despite their importance, values of the polarizability $\alpha(\omega)$ are not well established for all the atoms.

From the experimental point of view, the situation is not so good. For example, the dipole polarizability has been measured only for some alkali, alkaline-earth, noble gas and other atoms [3,4,5].

All this suggests that the interest for theoretical description of the many time-dependent properties of atomic systems involving harmonic perturbations is not decreased. This is primarily because of the recently discovered techniques for solving time-dependent problems.

The most notable of these methods are the oscillator sum rules [1], the variation-perturbation method [2,7], the R-matrix approach [4] (based on the procedure which com-

bined the summation techniques [1] with the R-matrix solution methods by first replacing the sum over intermediate states by differential equations and then solving these equations by the R-matrix method [8] - and the many-body theory with appropriate diagrammatic techniques [5,6, 9,10]. The correlation effects which are important in the treatment of corresponding time dependent problem can be successfully obtained with help of the Brueckner-Goldstone perturbation theory [6,9] and the Random Phase Approximation with Exchange RPAE [5,9,10].

One of the most important requirements of the conventional perturbation theory (PT) is that the exact solution to the unperturbed problem for the ground state, as it is well known, cannot be obtained and excited states cannot be known. However, as is well known, one cannot obtain exact solutions to the unperturbed problem for any atoms except hydrogen. Thus, an important practical requirement of a successful approach is that the perturbation method be able to use only an approximate unperturbed solution and the excited states need not be explicitly obtained. In the time-independent case several approximate methods satisfying these requirements have been formulated [2]. Namely, the **static** second order properties can be calculated with good precision by using the finite field method [11], but part of many-electron interaction is not taken into account.

Many of these methods have been carried over in the time-dependent case. The Hartree-Fock (HF) method is such one approximation. From the computational as well as purely theoretical point of view the HF scheme provides us with one of the most widely extendable methods for solving many-body problems. The coupled HF method for calculation of polarizability (and shielding factors, for example) is the most elaborate approximation within HF framework and generally yields more accurate values than simpler approximations such Sternheimer or uncoupled HF approximations. Thus, it is often used as a benchmark against which more refined calculations are measured and which, for example, elaborate variation methods or the many-body theory.

The interelectron interaction in the HFA is not properly taken into account. The part of the interaction not taken into account is called direct or residual. V_{res} This interaction manifests itself in significant corrections to the independent single particle motion of electrons (correlations) [5,6, 12,8]. There are two different approaches to the account V_{res} . The first one is known as the perturbation approach to the V_{res} - for example the Brueckner-Goldstone perturbation theory [1,12]. The other approach is often used under which terms of all powers of V_{res} matrix elements are accounted for, but in each order q a limited number of this expansion is retained. A version of this method is the RPAE method [5,9,10].

The main problem of this method is to find the effective interaction that may be obtained as a sum of a certain sequence of perturbation theory diagrams. In this paper we calculated dynamic polarizability for atoms by using improved version of the RPAE method [13].

Atomic units system is used throughout the article, unless otherwise stated; all notations follow those in ref. [13].

2. THEORY

2.1. Polarizability

Generally, polarizability, in linear approximation, originates from additional dipole electric momentum that is induced by the action of an external time dependent electromagnetic field of the system of electric charges. The dynamic multipole polarizabilities $\alpha(\omega)$ is defined as [1]:

$$\alpha_{2^L}(\omega) = \sum_n \frac{2\omega_n \langle n | M_{2^L} | 0 \rangle}{(\omega_n^2 - \omega)} \quad (1)$$

where M_{2^L} is an operator for the $2L$ -pole of the system, while $\omega_n = E_n - E_0$ denotes the excitation energy and ω is the photon energy ($\omega(\text{au}) = 45.5633 / \lambda(\text{nm})$). Summation over n includes integration over continuous spectrum and summation over the occupied states.

If the length of the light that interacts with the atom is greater than the dimension of the atom ($\lambda \gg a_0 \sim 10^{-8}$ cm), the electric field intensity E is smaller than the intensity of the inner atom field ($E \ll E_0 \sim e^2/a_0^2 \sim 10^9$ V/cm), and the frequency ω is not so close to the absorption frequency, then we can describe the interaction of field with atom by adding perturbation energy that contains dipole electric momentum of atom's electrons to the basic Hamiltonian. The dipole polarizability (DP) α_d describes the corresponding energy shift of an atom:

$$\Delta E = -\frac{1}{2} \alpha_d E^2 \quad (2)$$

The dynamic dipole polarizability (DDP) is based on the Cramers-Kroning relations

$$\alpha_d(\omega) = \sum_n \frac{F_n}{\omega_n^2 - \omega^2} \quad (3)$$

where the polarizabilities are expressed in au ($\alpha(\text{au}) = 6.74832 \alpha(A^3)$). $F_n = 2\omega_n |\langle 0 | d | n \rangle|^2$ is either oscillator strength (OS) for discrete transition or density of OS in the continuous spectrum; d is the momentum operator of the system.

The static DP is given by the expression (3) with $\omega = 0$.

If the following relations are used

$$\begin{aligned} -i\hat{v} &= \hat{H}\hat{r} - \hat{r}\hat{H} \\ \langle k | \hat{v} | \ell \rangle &= \langle k | \hat{p} | \ell \rangle = i(E_k - E_\ell) \langle k | \hat{r} | \ell \rangle \end{aligned}$$

where \hat{v} , \hat{H} and \hat{r} are operators of velocity, total system Hamiltonian and coordinate, respectively. The other form of DDP can be written as:

$$\alpha_d(\omega) = \sum_n \frac{2 |\langle n | \hat{p} | 0 \rangle|^2}{\omega_n (\omega_n^2 - \omega^2)} \quad (4)$$

This form of DDP is velocity form α_d^v , and expression (3) represents length form α_d^r . When we use eigenfunction of the exact Hamiltonian as basic functions, expressions for

α_d^r and α_d^∇ are identical. In the HFA α_d^r and α_d^∇ are not equivalent and difference between them is the measure of the non-locality of the self-consistent potential. These two forms coincide in the RPAE. In the one-electron approximation DP can be represented by diagram Fig. 1.

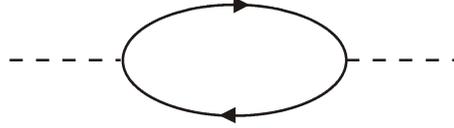


Fig. 1. The dipole polarizability in one-electron approximation.

The solid line with arrow to the right (or left) corresponds to particle (or vacancy). Dashed line represents the external field.

DDP can be found if the cross section for the photo ionization in dipole approximation is known. The transition is determined by $v_1\ell_1(\text{hole}) \rightarrow n_2(E_2)\ell_2$ (an electron in an excited or continuous spectrum state). Namely, if we introduce the spectral distribution function $g(\omega) \equiv \sum_n F_n \delta(\omega - \omega_n) = (2\omega/\pi) \text{Im} \alpha_d(\omega)$, then the dispersion relations between the real and imaginary part of DDP may be obtained; that leads to the expression [5,6]:

$$\text{Re} \alpha_d(\omega) = \sum_{v_1 v_2} \frac{F_{v_1 v_2}}{\omega^2 - \omega_{v_1 v_2}^2} + (c/2\pi^2) P \int_I^\infty \frac{\sigma(\omega') d\omega'}{\omega'^2 - \omega^2} \quad (5)$$

where c is the light velocity. The photo-ionization cross section and the oscillator strength are defined by [6]:

$$\sigma(\omega) = \sum_{v_1 v_2} \sigma_{v_1 v_2}(\omega) = \sum_{v_1 v_2} 2.689 [\omega N_1 / (2\ell_1 + 1)] \left| d_{v_1 v_2} \right|^2 (10^{-18} \text{ cm}^2) \quad (6)$$

$$F_{v_1 v_2} = [\omega_{v_1 v_2} N_1 / 3(2\ell_1 + 1)] \left| d_{v_1 v_2} \right|^2 \quad (7)$$

where N_1 is the electron number of the v_1 th sub shell and $d_{v_1 v_2}$ is the reduced dipole matrix element in the HFA or RPAE.

The knowledge of polarizability makes it possible to find the interaction potential of a heavy particle with an atom. In the first two orders of perturbation theory in Coulomb interaction this potential is determined by diagrams, part of which being presented in Fig. 2.

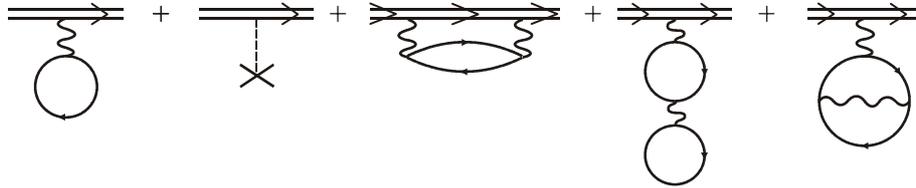


Fig. 2. The interaction of a heavy particle (double line) with an atom (the first two orders of the perturbation theory). The wavy line with a cross at the end represents the Coulomb interaction with the nucleus.

At large distances from an atom the contribution of the first, forth and fifth diagrams (Fig. 2) lead to a potential that decreases exponentially. The contribution of the third diagram defines the polarization potential (at large and at small distances):

$$U(r) = \begin{cases} -\alpha_d / (2r^4)_{(r \rightarrow \infty)}, \\ -\sum_n \left| \langle n | r^{-1} | 0 \rangle \right|^2_{(r \rightarrow 0)}, \equiv -\alpha_m(0) / 2 \end{cases} \quad (8)$$

$\alpha_m(0)$ is called the **static monopole** polarizability. By using this quantity, the interaction potential of the heavy particle with the atom at small distances can be defined. Also, using $\alpha_m(0)$, one can calculate the constant d in the expression of the phenomenological polarization potential $U(r) = -\alpha_d(0) / [2(r^2 + d^2)]$ (where $d = \sqrt{\alpha_d(0) / \alpha_m(0)}$). The solution of the Schrödinger equation with the potential (8) gives the scattering length $L = \sqrt{1 + \alpha_d(0) / d^2} \operatorname{ctg}(\pi d) / 2$ and according to the experimental values, we may test the validity of our calculated values of $\alpha_m(0)$.

The correction to the HF energy of a deep hole, which occurred because of the interaction with outer sub shells, is determined by the monopole polarizability of the outer shells, too [12]:

$$\Delta E_i = \sum_{\ell, m} \left| \langle m | r^{-1} | \ell \rangle \right|^2 / (E_m - E_\ell) = (1/2) \alpha_m(0) \quad (9)$$

2.2 Atomic interaction constants

Although more than seventy years have elapsed since the first quantum-mechanical interpretation of dispersion force by London [14] the importance of the theory of interatomic (molecular) force is now receiving much recognition due to recent developments in physical methods for observing various long-range interactions [5]. When attempting to find the interaction potential of atoms, the basic problem is the nonconvergency involved in the series expansion in reciprocal powers of interatomic distance R . Knowledge of the distribution of the dipole oscillator strengths F allows us to find the interaction potential of two neutral atoms at large distances. The dispersion interaction of the pair of non-excited atoms at large distances R may be presented by:

$$U_{disp}^{(2)} = -C_6 / R^6 (\text{dip. int.}) - C_8 / R^8 (\text{dip.} - \text{quadr. int.}) - C_{10} / R^{10} (\text{quadr.} - \text{quadr. int.}) - \dots \quad (10)$$

In the case of the three-body interaction, the first term in the series expansion of the energy is given by

$$U_{disp}^{(3)} = C_9 (1 + 3 \cos \psi_{A_1} \cos \psi_{A_2} \cos \psi_{A_3}) R_{A_1 A_2}^{-3} R_{A_2 A_3}^{-3} R_{A_1 A_3}^{-3} \quad (11)$$

where ψ_{A_i} are the angles of the triangle $A_1 A_2 A_3$.

Due to the electro neutrality of atoms (A_1 and A_2 , for example) the total contribution of first and second order diagrams presented in Fig. 3a,b (excluding the last diagrams in Fig.3) leads to a potential that decreases exponentially.

With some simplifications the contribution of the last diagram (Fig. 3b) is [5]:

$$U(R) = -3/(2R^{-6}) \left\{ \sum_{n_{A_1} n_{A_2}} F_{n_{A_1}}^{A_1} F_{n_{A_2}}^{A_2} [\omega_{n_{A_1}}^{A_1} \omega_{n_{A_2}}^{A_2} (\omega_{n_{A_1}}^{A_1} + \omega_{n_{A_2}}^{A_2})^{-1}] \right\} \equiv -C_6 / R^6 \quad (12)$$

where the notations are the same as in ref. [13]. Substituting the dipole matrix elements, we find the coefficients C_6 in RPAE [8], or C_6^{im} in improved RPA (imRPA). This version of RPAE includes some contribution of the higher order diagrams [5,13]. The next term in the expansion of the interatomic potential is proportional to $R^{-8} - C_8 R^{-8}$. That is the result of the quadruple – dipole interaction between atoms. There are significant difficulties in calculating C even in the case of simple atoms. Because of that, different semi-empirical methods have been developed.

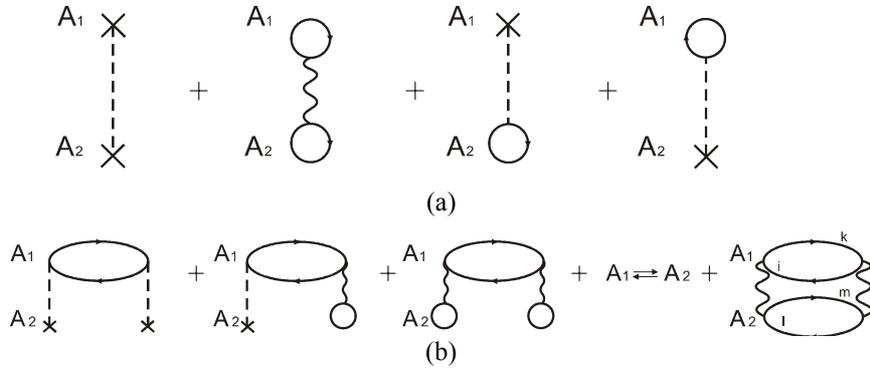


Fig. 3. The first (a) and second (b) order of the perturbation theory in the Coulomb interaction between two neutral atoms.

When we recognize the polarizability as a function of imaginary frequencies, we can calculate the dispersion coefficients with the help of the Casimir-Polder integral [15]

$$C_6 = F(\alpha_{A_1}, \alpha_{A_2}) = (3/\pi) \int_0^\infty \alpha_{A_1}(i\omega) \alpha_{A_2}(i\omega) d\omega \quad (13)$$

DDP with imaginary argument can be calculated over density of oscillator strength or over adequate analytical approximation. In the second case, the problem can be solved by Pade approximants [16].

2.3. The RPAE method

A lot of calculations of DDP in HFA have been done. Many of them are not good because there are great differences between α_d^r and α_d^∇ . The agreement with experiments is also bad. There are a few calculations of quadruple and octopole DP. Some conclusions are valid for HF calculation of the interatom constants.

In our calculation we used RPAE method with HF as basic approximation [8]. In the approximation RPAE, polarizability is determined by the infinite series of the diagrams, which are presented in Fig. 4.

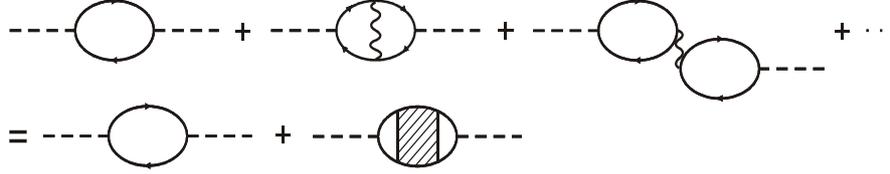


Fig. 4. The dynamic dipole polarizability in the RPAE.
The shaded part denotes the 2^L -pole matrix element [5].

The dipole matrix element in the RPAE approximation satisfied the relation [5]:

$$\langle v_1 | D(\omega) | v_2 \rangle = \langle v_1 | d | v_2 \rangle + \left(\sum_{\substack{v_3 \leq F \\ v_4 > F}} - \sum_{\substack{v_3 > F \\ v_4 \leq F}} \right) \frac{\langle v_4 | D(\omega) | v_3 \rangle \langle v_3 v_1 | U | v_4 v_2 \rangle}{[\omega - E_{v_4} + E_{v_3} + i\delta(1 - 2n_{v_4})]} \quad (14)$$

where v_i denotes the quantum numbers (n, ℓ, m, σ) , U are the antisymmetrised Coulomb matrix elements and F is the Fermi level. Detailed discussion of the choice of the wave function and calculations are given in ref. [5,6,8,13]. DDP, $\alpha_d^{RPAE}(\omega)$, in the RPAE is given by

$$\alpha_d^{RPAE}(\omega) = \sum_n 2\omega_n \langle n | D(\omega) | 0 \rangle \langle 0 | d | n \rangle (\omega_n^2 - \omega^2)^{-1} \quad (15)$$

If $\langle n | D(\omega) | 0 \rangle$ is calculated on the energetic shell (i.e. when $\omega \approx \omega_n$) we get:

$$\alpha_d^{RPAE}(\omega) = \sum_n 2\omega_n \left| \langle n | D(\omega) | 0 \rangle \right|^2 (\omega_n^2 - \omega^2)^{-1} \quad (16)$$

We calculated DDP by using wave functions of the ground and excited states $\phi^{N(LS)}$ obtained in the HF approximation [6].

The method we used allows us to calculate the polarizability near the discrete excitation levels too, using the expression:

$$\alpha_d(\omega) = F_n (\omega_n^2 - \omega^2)^{-1} + \alpha'_d(\omega) \quad (17)$$

where $\alpha'_d(\omega)$ is the non-resonant part of the polarizability.

3. RESULTS AND DISCUSSION

The calculations of DDP are performed in the following way: first the wave functions of the basic and excitation atomic state are calculated $\alpha_d^{r,\nabla}(\omega)$ in HF approximation.

Table 1. The static polarizability of atoms

Atom	Dipole polarization	Quadruple polarization	Oktopol polarization
He			
[5]	1.256		
Our res. RPAE	1.34	2.23	8.34
[19]	1.30	2.27	9.50
Exp. [18]	1.38		
Ne			
[5]	2.30	5.64	
Our res. RPAE	2.47	6.21	28.5
[19]	2.36	6.36	33.9
Exp. [18]	2.66		
Ar			
[5]	10.70	40.04	
Our res. RPAE	10.82	45.50	418
[19]	10.75	48.00	515
Exp. [18]	11.10		

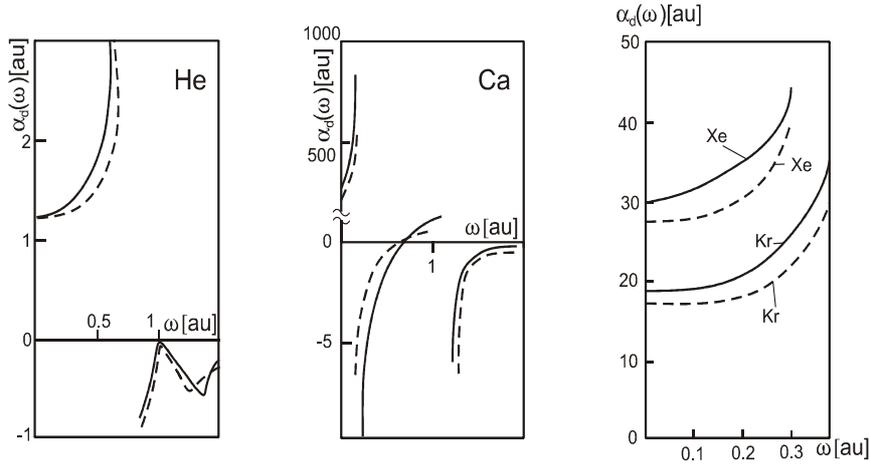


Fig. 5. Results of calculations DDP $\alpha_d^{RPAE}(\omega)$ for He, Ca, Xe and Kr atoms. Solid line denotes our improved calculation; dashed line [5].

After that integral equation for DDP (14) is solved. In this way we calculated $\alpha_d^{RPAE}(\omega)$. The programs used are given in [6]. This method makes it possible to calculate the polarizabilities in the energies ω greater than the ionization potential when $\text{Im}\alpha_d(\omega) = [c/(4\pi)]\sigma(\omega)$. In this paper, contrary to our earlier results in [17] (in Tamm-Dancof approximation) we take into account the contributions of some higher order diagrams [13]. In Tab. 1, calculations and some experimental values are given of static polarizability for He, Ne and Ar atoms (dipole, quadruple and octopole).

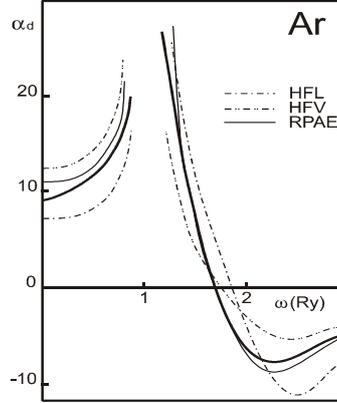


Fig. 6. Results of calculations $\alpha_d^{RPAE}(\omega)$ for Ar atom: the full fat line represents our improved calculations; dashed lines are DDP in $\langle\langle r \rangle\rangle$ and $\langle\langle \nabla \rangle\rangle$ (i.e. length L and velocity V form, respectively), and thin solid line represents the RPAE calculation [5].

Contributions of different transitions in calculation of DDP for atom Ne are shown in Tab 2.

Table 2. Contributions of different transitions to $\alpha_d(\omega)$.
(Numbers in the brackets are power of 10)

Transitions	$\omega = 0.0$			$\omega = 0.4$		
	α_d^r	α_d^0	α_d^{RPAE}	α_d^r	α_d^{RPAE}	α_d^{RPAE}
$2p^6-2p^53d^1$	0.3685(-1)	0.2832(-1)	0.3645(-1)	0.4934(-1)	0.3794(-1)	0.4887(-1)
$2p^6-2p^54d^1$	0.1869(-1)	0.1428(-1)	0.1833(-1)	0.2451(-1)	0.1873(-1)	0.2412(-1)
$2p^6-2p^55d^1$	0.1016(-1)	0.7735(-2)	0.9885(-2)	0.1322(-1)	0.1007(-1)	0.1247(-1)
$2p^6-2p^5\epsilon d$	0.1788 (1)	0.1265 (1)	0.1634 (1)	0.1956 (1)	0.1394 (1)	0.1801 (1)
$2p^6-2p^53s^1$	0.3438 (0)	0.3151 (0)	0.3502 (0)	0.5303 (0)	0.4867 (0)	0.5403 (0)
$2p^6-2p^54s^1$	0.4545(-1)	0.4157(-1)	0.4500(-1)	0.6157(-1)	0.5622(-1)	0.6095(-1)
$2p^6-2p^55s^1$	0.1497(-1)	0.1367(-1)	0.1491(-1)	0.1974(-1)	0.1805(-1)	0.1966(-1)
$2p^6-2p^5\epsilon s$	0.1904 (0)	0.1735 (0)	0.2041 (0)	0.2191 (0)	0.2001 (0)	0.2337 (0)
$2s^2-2s^13p^1$	0.2903(-2)	0.2025(-2)	0.1887(-2)	0.3015(-2)	0.2133(-2)	0.1981(-2)
$2s^2-2s^14p^1$	0.7525(-3)	0.6467(-3)	0.6365(-3)	0.7885(-3)	0.6773(-3)	0.6672(-3)
$2s^2-2s^15p^1$	0.3345(-3)	0.2862(-3)	0.2853(-3)	0.3501(-3)	0.2994(-3)	0.2994(-3)
$2s^2-2s^1\epsilon p$	0.5020(-1)	0.4433(-1)	0.4932(-1)	0.5118(-1)	0.4916(-1)	0.5033(-1)

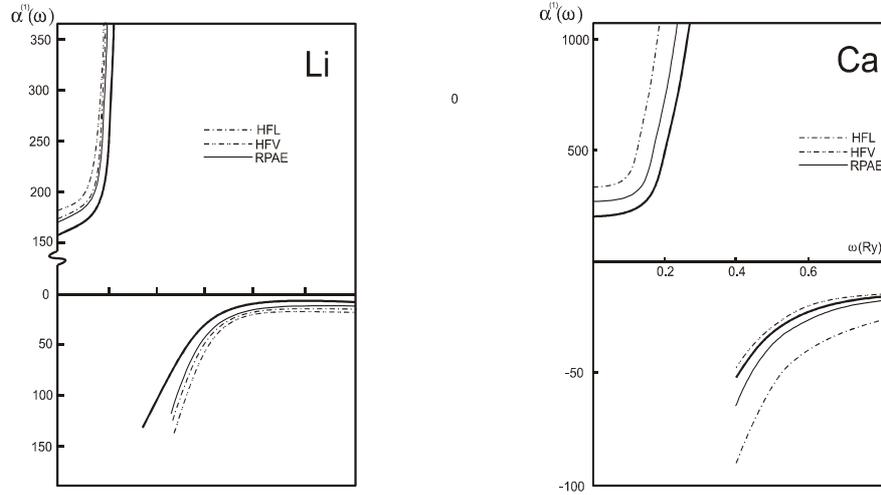


Fig. 7. Results of calculations $\alpha_d^{RPAE}(\omega)$ for Li and Ca atoms. The solid fat lines represent our improved RPAE calculations, while the other curves are the earlier RPAE results [5].

Also, in Fig. 8 DDP is presented as a function of imaginary frequency: the solid fat lines are our RPAE results, while other curves are semi-empirical results from ref. [16].

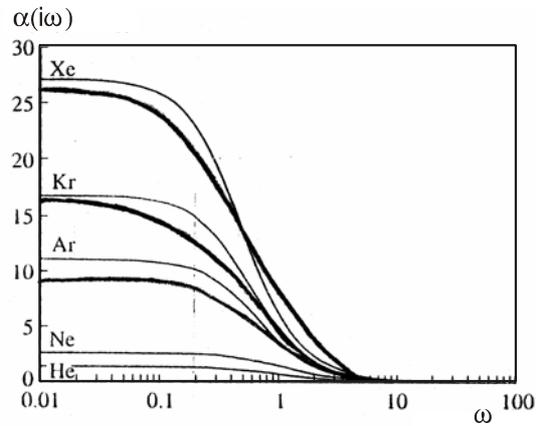


Fig. 8. $\alpha(i\omega)$ for some atoms. The solid fat lines are our RPAE result (Xe,Kr,Ar); other curves are from ref. [16].

The main conclusions after DDP calculations are as follows:

- The principal contribution comes from the main transition of the outer sub shell.
- The role of the discrete excitations (for small energies ω , especially) in noble gas atoms is negligible, whereas for alkali and alkali-earth atoms it is decisive [5,7].
- According to the results of DDP for He, we can see that the main contribution at low-level energies gives transition $1s^2 \rightarrow 1s^1 2p^1$. At higher energies, contributions of the

resonant transitions become negative and contributions of transitions in the continuum remain positive when energies increase. When energies keep increasing, DDP decreases by absolute values.

– In Fig. 5., we see oscillations occurring from differences in contributions of discrete transition and transitions in continuum spectra.

– The main contributions to DDP in Ne, Kr, Xe atoms give transitions $np^6 \rightarrow np^5\epsilon d$. The contributions of electron transitions on discrete levels are about 25%. In the case of a Ne atom, the main transitions are transitions from the highest p sub shells to the lowest discrete s levels.

– In the case of alkali and alkali-earth atoms the main contributions in DDP give discrete excitations (low energies). In the case of a Ca atom the main contribution originates from the transition $4s^2 \rightarrow 4s^1 4p^1$.

– The calculations of the quadruple and oktopole polarizability for Ne, Ar, Kr and Xe atoms show that the greatest contribution to polarizability results from transitions from the above-filled np^6 subshell in the continuum in the f state. The contributions of the electron transitions in the discrete spectrum are about 20% of the total $\alpha(\omega)$.

By indirect comparison it may be seen that our calculation of DDP for He, Ne, Ar, Kr, Xe, Li and Ca atoms are in good agreement with other theoretical results [2,3] and experimental data [21].

By using the improved RPAE approximation we calculated C_6 coefficients for some pairs of atoms (C_6^{im}). Results of calculations show that it is very important to take into account the contribution of the higher order diagram. A better agreement with experiments is obtained (Tab. 3).

Table 3. Coefficients C_6

Pair of atoms	C_6 [22]	C_6 [23]	C_6^{im}	C_6 [24]	C_6 [25]	C_6 [19]
He-He	1.24	1.46	1.35	1.4	1.82	1.43
Ca-Ca	2370		2035	1600		
Ar-Ar	52.0	64.7	65.1	62	69.9	64.5

4. CONCLUSION

We may conclude that the **static** second order properties can be calculated, for example, with good precision by the use of the finite field method [11], but the correlation effects, which can contribute significantly to the property values, can be incorporated by the finite MBPT by the finite configuration interaction method [7] or by the presented RPAE method.

For **dynamic** properties, reasonable results can be obtained by the use of time – dependent coupled HF method [2,26], but this method only incorporates "apparent" (or self-consistency) effects, while true correlation effects are often by no means negligible. True correlation effects in frequency-dependent polarizability can be obtained by MBPT methods, or with the help of diagrammatic techniques used in the RPAE method the results of which are presented in this article.

The results of our calculations DDP and coefficients of the long-range interaction between atoms suggest that it is necessary that many-electron correlations be taken into account. The improved RPAE is more consistent with experiments compared to earlier results which are performed in the simplified version of the RPAE method.

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DINAMIČKE KARAKTERISTIKE NEKIH ATOMA. MNOGOČESTIČNA IZRAČUNAVANJA

A. R. Tančić, M. Nikolić

U radu se istražuje frakventna zavisnost dinamičke polarizabilnosti u Hartri-Fokovoj aproksimaciji i korekcije koje nastaju zbog korelacija. Polarizabilnosti su računane i u aproksimaciji slučajnih faza sa izmenom za atome He, Ne, Ar, Kr, Xe, Li I Ca sa uključivanjem dijagama drugog reda (i nekih viših) pri izračunavanju korelacionog potencijala. Dobijene polarizabilnosti su iskorišćene da se izračunaju vrednosti nekih atomskih interakcionih konstanti.