

**DIPOLE DYNAMIC POLARIZABILITY OF  $Zn_n$ :  
AN RPAE CALCULATIONS**

Aleksandar R. Tančić\*  
Miroslav R. Nikolić°  
Miron Ya. Amusia\*

\* Institute for Nuclear Sciences Vinča, Laboratory for Theoretical Physics,  
PO Box 522, 11001 Belgrade, Yugoslavia

° The Faculty of Philosophy, Department of Physics,  
University of Niš, PO Box 92, 18000 Niš, Yugoslavia

\* A. F. Ioffe Physico-Technical Institute 194021 St. Petersburg, Russia

**Abstract:** The dipole dynamic polarizability of Zn atom is calculated within the framework of the Hartree-Fock method (HF) and by taking into account the correlations in the random phase with exchange (RPAE) approximation. The importance of taking into account the many-electron correlations, especially for heavier atoms, are pointed here.

There are many theoretical calculations of the dipole dynamical polarizability of some atoms. In these calculations, sum rule for the oscillator strength [1,2], variational method [3-5] and many-body method [6-8] were generally used. The calculations considered mainly the light atoms. In this paper, we extended the work to the zinc atoms. This extension has been prompted mainly by the desirability of being able to account for induced polarization of the atom core and for accurate interpretation of experimental data. It is therefore that we present our extensive and, we believe, very accurate results.

Generally polarizability, in linear approximation, originates from additional dipole electric momentum that is induced by the action of external time dependent electromagnetic field on the system of electric charges. Let us define polarizabilities of arbitrary multipolarity [1]

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

where  $M_{2L}$  is the operator of the  $L$ -pole moment of a system, and  $\omega_n = E_n - E_0$  - the excitation energy. Summation over  $n$  includes integration over the continuous spectrum and summation over the occupied states. Atomic units system is used in the present paper and all notations follow those in [11].

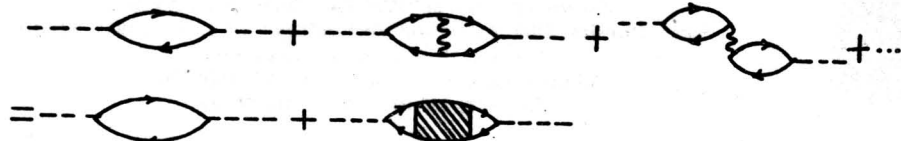


FIGURE 1. Some RPAE diagrams corresponding to the  $\alpha_d(\omega)$ .

If the length of light that interacts with atom is greater than the dimensions of atom, and the electric field intensity  $\vec{\epsilon}$  is smaller than the intensity of the inner-atom field, 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  $\alpha_d$  describes the corresponding energy shift of an atom:

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

The dynamic dipole polarizability is determined by the following expression:

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

where  $f_n$  is either oscillator strength for discrete transition or density of oscillator strength in the continuous spectrum (in both cases  $f_n$  is determined by the length form  $-\alpha_d^r$ , or velocity form  $-\alpha_d^v$ )

It is possible to find  $\alpha_d$  if the cross section in the dipole approximation for photoelectric effect is known. The polarizability is determined by diagram' row (fig. 1.) in the RPAE. Shadow part in fig. 1. represents  $2L$ -pole matrix element that is calculated by taking into account many electron's correlations. The dipole matrix element in the RPAE satisfies the relation

$$\begin{aligned} \langle k_1 | D(\omega) | k_2 \rangle &= \langle k_1 | d | k_2 \rangle + \\ &+ \left( \sum_{\substack{k_3 \leq F \\ k_4 > F}} - \sum_{\substack{k_3 > F \\ k_4 \leq F}} \right) \frac{\langle k_4 | D(\omega) | k_3 \rangle \langle k_3 k_1 | \mathcal{U} | k_4 k_2 \rangle}{[\omega - E_{k_4} + E_{k_3} + i\delta(1 - 2n_{k_4})]}, \end{aligned} \quad (4)$$

where  $k_i$  denotes quantum numbers set  $n, \ell, m$  and  $s$ , and

$$\langle k_3 k_1 | \mathcal{U} | k_4 k_2 \rangle = \langle k_3 k_1 | V | k_4 k_2 \rangle - \langle k_3 k_1 | V | k_2 k_4 \rangle. \quad (5)$$

Coulomb's matrix elements are

$$\langle k_3 k_1 | V | k_4 k_2 \rangle = \int \varphi_{k_3}^*(\vec{r}_1) \varphi_{k_1}^*(\vec{r}_2) \varphi_{k_4}(\vec{r}_1) \varphi_{k_2}(\vec{r}_2) \frac{d\vec{r}_1 d\vec{r}_2}{|\vec{r}_1 - \vec{r}_2|} \quad (6)$$

and

$$n_{k_4} = \begin{cases} 1, & k_4 \leq F \\ 0, & k_4 > F. \end{cases} \quad (7)$$

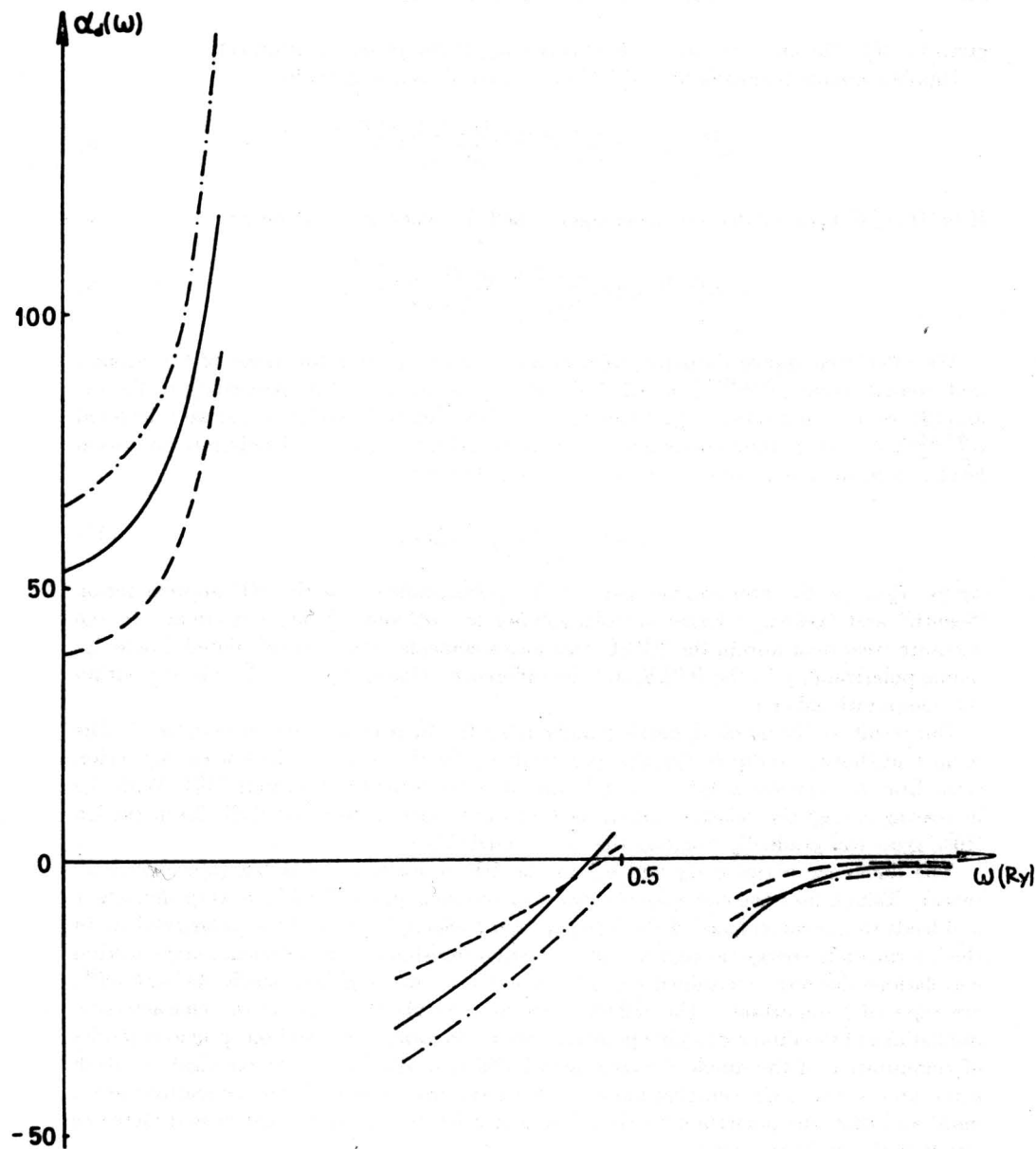


FIGURE 2. The dipole dynamic polarizability  $\alpha_d(\omega)$  for Zn:  $\cdots$   $\alpha_d^\sigma$ ,  $\cdots$   $\alpha_d^\gamma$  (HF approximation);  $\text{---}$   $\alpha_d^{\text{RPAE}}$  (RPAE).

The condition  $k_4 \leq F$  means the summation over occupied states, and  $k_4 > F$  means the summation over free states and integration over continuous spectra states. Functions  $\varphi_k$  are solutions of the HF equations. A detailed discussion of the choice of wave functions is

given in [10]. The calculations are done according to the programs from [11].

Dipole dynamic polarizability,  $\alpha_d^{RPAE}(\omega)$ , in the RPAE is given by

$$\alpha_d^{RPAE}(\omega) = \sum_n \frac{2\omega_n \langle n | D(\omega) | 0 \rangle \langle 0 | d | n \rangle}{\omega_n^2 - \omega^2}. \quad (8)$$

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

$$\alpha_d^{RPAE}(\omega) = \sum_n \frac{2\omega_n |\langle n | D(\omega_n) | 0 \rangle|^2}{\omega_n^2 - \omega^2}. \quad (9)$$

We calculated dipole dynamic polarizability by using wave functions of the ground and excited states  $\varphi^{N(LS)}$  obtained in the HF approximation [11]. According to the (2) and (3) we obtained values  $\alpha_d^r(\omega)$  and  $\alpha_d^v(\omega)$ . According to the relation (9) we calculated  $\alpha_d^{RPAE}(\omega)$ . Used method allows to calculate polarizability, also near the discrete excitation levels, when the polarizability may be represented in the form:

$$\alpha_d(\omega) = \frac{f_n}{\omega_n^2 - \omega^2} + \alpha_d'(\omega) \quad (10)$$

where  $\alpha_d'(\omega)$  is the nonresonant part of the polarizability. In the HF approximation "length" and "velocity" forms of polarizability ie.  $\alpha_d^r$  and  $\alpha_d^v$  are not equal. In the accurate treatment also in the RPAE, this forms coincide. We have calculated dipole dynamic polarizability in the RPAE and the difference between  $\alpha_d^r$  and  $\alpha_d^v$  is in the within the computational error.

Our results of the dipole dynamic polarizability for Zn atom are presented in fig. 2. The main contribution to dipole dynamic polarizability for this atom at the low energy region came from the transition  $4s^2 \rightarrow 4s^1 4p^1$  (the same holds for the Ca atom [10]). With the increasing energy the relative contribution of the transition from 3d shell (3p in the Ca [10]), grow and gradually becomes the main contribution.

The difference between  $\alpha_d^r$  and  $\alpha_d^v$  in the HF approximation is big (approximately twice). Taking into account many-electron correlations in the RPAE, is very important and leads to the coincidence of the "length" and "velocity" forms of the polarizability. In the intermediate energy range, near the ionization threshold of the 3d shell, many-electron correlations that are determined by the interaction of two neighbour shells,  $4s^2$  and  $3d^{10}$ , are especially important. The influence of the next shell is seen as the characteristic oscillations of the dipole dynamic polarizability of Zn atom. This and our previous results of computation of the dipole dynamic polarizability [9,10] shows that for alkali or alkali earth atoms, the main contribution came from the first discrete level (or another levels ones) and that, the polarizability above the ionization threshold is negative and increases slowly with energy increasing.

#### References:

- [1] Dalgarno A., *PERTURBATION THEORY AND ITS APPLICATIONS IN QUANTUM MECHANICS* ed. by C.H. Wilcox, J. Wiley, (New York, 1966.).
- [2] Balnukov M. D., Tulub A. V., *Opt. i Spektro.*, **31**, (1971.), 574. (in Russian).
- [3] Karplus M., Kolker H. J., *J. Chem. Phys.*, **38**, (1963.), 1263.

- [4] Karplus M., Kolker H. J., *J. Chem. Phys.*, **39**, (1963.), 1493.
- [5] Kaveeshwar V. G., Chang T., Hurst R. P., *Phys. Rev.*, **172**, (1968.) 35.
- [6] Kelly H. P., *Phys. Rev.*, **152**, (1966.) 62.
- [7] Kelly H. P., *Phys. Rev.*, **182**, (1968.) 84.
- [8] Kelly H. P., *Adv. Theor. Phys.*, **2**, (1968.) 162.
- [9] Amusia M. Ya., Cherepkov N. A., Shapiro S. G., *ŽETF*, **63**, (1972.) 889.
- [10] Amusia M. Ya., Cherepkov N. A., *Case Studies in Atomic Physics*, **5**, 2, (1975.).
- [11] Amusia M. Ya., Cherepkov N. A., Chernisheva L. V. *Preprint FTI*, (1971.) N.335 N.337 (in Russian)

## DIPOLNA DINAMIČKA POLARIZABILNOST CINKA

A. R. Tančić, M. R. Nikolić, M. Ya. Amusia

U radu je računata dipolna dinamička polarizabilnost atoma cinka primenom Hartree-Fockovog metoda sa uzimanjem u obzir korelacija primenom aproksimacije slučajnih faza sa izmenom. Posebna pažnja se poklanja pokazivanju da je za teže atome veoma bitno uzimanje u obzir višeelektronskih korelacija.