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A Study Of Dispersion and Retardation Coefficient for two Li Atoms in the Presence of Core Polarization effect

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Abstract

We present here a study of the dispersion potential and retardation coefficient for Li atom, this study includes the motion of the valence electron in the field of a closed Li core with a one-electron model potential (i.e. we used Frozen Core Approximation-FCA) ; but we take the effect of the core polarization as a term added to the variational function; moreover we derived the dynamic dipole polarizability formula for the S-ground state of Li atom at imaginary frequencies through a double method (Perturbation – Variation). This polarizability formula is used to calculate the dynamic dipole polarizability $\alpha_2(\omega)$, the dispersion coefficient C_6 , and the retardation coefficient $f_6(R)$. The dispersion coefficient and retardation coefficient are described by Casimir-Polder potential between two Li atoms in the S-ground energy state. Our results are compared with other theoretical and experimental results.

دراسة معامل جهد التشتت والإعاقة لذرتي ليثيوم في وجود تأثير استقطاب اللب الأيوني

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الخلاصـــة

قمنا في هذا البحث بدراسة معامل جهد التشتت والإعاقة لذرة الليثيـوم إحـدى (الأنظمـة الذريـة القلوية)،حيث تمت دراسة حركة إلكترون التكافؤ لهذه الذرة في مجال اللب المغلق وذلك بالاعتماد علـى نموذج جهد الإلكترون المنفرد(تقريب اللب المنجمد FCA) ، وقد أخذنا بنظر الاعتبار تـأثير اسـتقطاب اللب الايوني على إلكترون التكافؤ المنفرد من خلال إضافة حد جديد الى دالة التغاير . إضافة الى ذلك تم اشتقاق صيغة لثنائي القطب الديناميكي للحالة الأرضـية S-State لـذرة الليثيـوم باسـتخدام الطريقـة المزدوجة(الاضطراب -التغاير).وقد اعتمدت هذه الصيغة لحساب معامل ثنائي القطب الـديناميكي ، ثـم استخدمنا هذا المعامل لحساب معامل جهد التشتت الطويل المدى C_6 ومعامل الإعاقة $f_6(R)$ لذرة الليثيوم . ان هذه المعاملات وصفت من خلال جهد كازمير -بولدر. تم مقارنة نتائجنا العددية مع نتـائج نظريـة وعملية مختلفة.

Introduction

The study of the long-range interactions between atoms or molecules is of fundamental importance for low-energy and low-temperature collisions. Recently, advances in laser cooling and trapping (MARINESCU & DALGARNO(1995)) have rekindled this study. Alkali atoms appear to be the most popular system for low-temperature experiments. The long-range potential between two atoms is very important in the confinement of alkali atoms at sub-Kelvin temperatures, and ultracold (<1 mK) dynamics collision (YAN & DALGARNO(1997)) . The characteristic distance is about 2000 a.u. (1 a.u. = 0.529177 A) for alkali atoms in the ultracold collisions. The long-range potential can be expanded in a power series in the inverse of the internuclear separation (R), which is represented by the van der Waals coefficients, C_6, C_8 and C_{10} .These coefficients can be obtained in the

evaluation of the electric dynamic multipole polarizabilities at imaginary frequencies. The asymptotical variation of the interaction potential (R^{-6}) becomes R^{-7} under the influence of the retardation at large internuclear separations (DEREVIANKO, JOHNSON, SAFRONOVA& BABB (1999)). However, the retardation have a very small effect at temperatures greater than a few degrees of K. Recently, very low-temperature experiments show the retarded effects may be detectable (YAN, MTAMBASCO & DRAKE(1998)). Therefore, the calculations including retardation are needed for studying very low energy collisions and very weakly bound states (CHEN (1998)).

In our work, the dynamic dipole polarizability is calculated by using a double method (variation - perturbation) (AL-SAMER(1998)) in the assumption of a model potential for the valence electron in the presence of the core polarizability effect through modifying the variational function, this change will gives a new perturbed energy formula and a new dynamic dipole polarizability relation.

In Sec.II, we present the method of determining the model potential and the wave functions for the valence electron of the S-ground state. This method is used to calculate the dynamic dipole polarizability, dispersion coefficient and retardation coefficient for Li atom.

In Sec.III, our numerical results for the dynamic dipole polarizability, dispersion coefficient and retardation coefficient are presented and compared with available experimental results and some other theoretical results.

The Used Model Calculation:

When the atomic system is placed under the influence of a weak electric field, the energy of this system will be changed such as (AL-SAMER(1998))::

$$E \Rightarrow E_o + \in (\pm w)$$

where E_o unperturbed energy,and $\in(\pm w)$ the dynamic perturbed term(which depends upon the frequency of the external electric field).Therefore ,this effect will change each of the wave function ψ: ($\psi=\psi_o+\Phi$) and the Hamiltonian operator H: ($H=H_o+U$) ,where Φ and U repersent the perturped terms .Each of the perturped terms Φ and U can be express respectively (Khalff(1997)) :

$$\Phi = \psi_o F g_c(r,\theta)$$
$$U = F r^L P_L(\cos\theta) \qquad \text{.....(1)}$$

where $g_c(r,\theta)$ is the variational function , $P_L(\cos\theta)$ Legender polynomial (L: polar degree ,L=1≡dipole ,L=2≡quadrupole ,L=3≡octupole),the external electric field intensity. The total energy of the atomic system which depends on the frequency of the external electric field represented as (AL-SAMER(1998)):

$$E_o + \in(\pm w) = \frac{\int(\psi_o^* + \Phi^*)(H_o + \hat{U})(\psi_o + \Phi)\,d\tau \pm w\int\Phi^*\Phi\,d\tau}{\int(\psi_o^* + \Phi^*)(\psi_o + \Phi^*)\,d\tau} \qquad \text{.....(2)}$$

where $\psi_0(r,\theta,\Phi) = R_{nl}(r)Y_l^m(\theta,\Phi)$

The perturbed energy equation for S-State, described in a general form which is derived previously in the reference (AL-SAMER(1998)) and (AL-SAMER and EASA(2003)). We use Schrödinger equation for one electron atomic system to described the atom under studying.

By introducing a model potential to approximate the n - electron (MARINESCU, SADEGHPOURE & DALGARNO(1994)), we have (in a.u.) :

$$V_l(r) = -\frac{Z_l(r)}{r} - \frac{\alpha_c}{2r^4}[1 - e^{-(r/r_c)^6}] \qquad \text{.....(3)}$$

where α_c is the static dipole polarizability of the positive ion core; while the radial charge $Z_{ls}(r)$ given by (MARINESCU, SADEGHPOURE & DALGARNO(1994)):

$$Z_l(r) = 1 + (z-1)e^{-a_1 r} - r(a_3 + a_4 r)e^{-a_2 r}$$

where z is the nuclear charge of the neutral atom and r_c is the cutoff radius introduced to truncate the unphysical short-range contribution of the polarization potential near the origin. The optimized parameters in above equation are listed in reference (MARINESCU, SADEGHPOURE & DALGARNO(1994)) for Li atom. In our work ,we modified the variational function $g_c(r)$, which can be expressed in terms of the variational constants (EASA & SHUKLA(1980)),to includes the effect of the core polarizability (MARINESCU, SADEGHPOURE & DALGARNO(1994)):

$$g_c(r) = g(r)\left[1 - \left\{\frac{\alpha_c^L}{r^{2L+1}}\left(1 - e^{-(r/r_c)^{2L+1}}\right)\right\}\right] \qquad \text{.....(4)}$$

where $$g(r) = \sum_n C_n(\pm w)\, r^{n+L-1}$$

α_c^L is the core 2^L tensor polarizability and r_c is a cutoff radius to be determined empirically. The numerical value of r_c is 2.3542392 for Li atom.

By substituting above form of variational function (eq.4) in the perturbed energy equation and perform the required derivations ,we give the dynamic dipole polarizability formula including the core effect, through the following identity (AL-KURTASS (1979)):

$\in(\pm\omega) = -\frac{1}{2} F^2 \alpha_2^L(\pm\omega)$

The dynamic dipole polarizability can be described in terms of variational constants and the integral of radial wave functions for S-State (AL-SAMER and EASA(2003)).

The numerical problem consists in the computation of the radial wave function which is appearing in the dynamic dipole polarizability formula,where it is invariable as an implicit wave function for multielectron atoms, as an efficient way for solving nonlinear and non homogenous differential equation , we chose the Numerov method which adopted with a tiny modification (AL-SAMER (2004)).

As be mentioned previously, we described the Alkali atoms by l–dependent model potential and so only the contribution of the valence electron is taken explicitly into account (i.e. we use FCA "Frozen Core

Approximation").On the other hand ,we use a trial values of the electron energies which required to gives an accurate wave functions that satisfy the boundary initial conditions (SZASZ(1985)).

The second order long–range interaction energy between two atoms ,a and b, can be expanded in terms of the dispersion coefficients (MARINESCU & DALGARNO(1998)):

$$V(R) = -C_6 R^{-6} - C_8 R^{-8} - C_{10} R^{-10} \qquad \text{.....(5)}$$

where R is the separation between the charge centers , By substituting in Casimir-Polder formula (AL-SAMER (1998)) , we get the dominant dispersion coefficient :

$$C_6 = \frac{3}{\pi} \int_0^\infty \alpha_2^a(iw)\, \alpha_2^b(iw)\, dw \qquad \text{.....(6)}$$

The long-range interactions between atoms can be calculated by evaluating the electric dynamic multipole polarizabilities at imaginary frequencies. These polarizabilities expressed in terms of an effective oscillation strengths f_{iL} and effective transition frequencies w_{iL} such us (YAN, BABB & DRAKE(1996)) :

$$\alpha_{2^L}(w) = \sum_{i=1}^{} \frac{f_{iL}}{w_{iL}^2 - w^2} \qquad \text{.....(7)}$$

where (i) referring to the number of variational constants, and w is the frequency of the external electric field. In our study ,we interested for the dominant long-rang interaction coefficients (C_6 & $f_6(R)$) only, therefore our calculating for transition frequencies and oscillation strengths includes five only of variational constants.:

$$C_6 = \frac{3}{2} \sum_{i=1} \sum \frac{f_{iLa} f_{iLb}}{w_{iLa} w_{jLb} (w_{iLa} + w_{jLb})} \qquad \text{.....(8)}$$

For the long-range interaction between atoms , Casimir and Polder have obtained the electric dipole interaction,Au and Feinberg generalized the electric dipole interaction to all electric and magnetic multipoles by using the method of Feinberg and Sucher. Considering the electric multipole

interactions, the retardation potentials between two Li atoms can be expressed as follows (MARINESCU, BABB & DALGARNO(1994)):

$$V(R) = -\frac{C_6 f_6(r)}{R_6} - \frac{C_8 f_8(r)}{R_8} - \frac{C_{10} f_{10}(r)}{R_{10}} \quad \text{.....(9)}$$

where $f_6(r)$ $f_8(r)$ and $f_{10}(r)$ are retardation coefficients. The distance between the charge centers, R, is sufficiently large that the overlap of the two atoms.Charge distributions can be neglected. Here, the dominant retardation coefficient are given as:

$$f_6(R) = \frac{1}{\pi C_6} \int_0^\infty \alpha_2^2(iw)\ \exp(-2w\alpha_{fs}R)\ P_1(\alpha_{fs}wR)\ dw \quad \text{.....(10)}$$

where $P_1(x)$ is the given as (MARINESCU, BABB & DALGARNO(1994)):

$$P_N(x) = \sum_{M=0}^{2(N+1)} \beta_{NM} X^M \quad , (N=1)$$

where β_{NM} are constants given in the same reference (MARINESCU, BABB & DALGARNO(1994)).

Results and Conclusions

In table-I- the dynamic dipole polarizabilities for two Li atom are given, our result is in a close agreement with the experimental value (CHEN (1998)) and theoretical results (MARINESCU, SADEGHPOURE& DALGARNO(1994)) and (YAN, BABB, DALGARNO& DRAKE(1996)) ,which includes the effect of the core polarizability in the calculations. Also our result is compared with other theoretical results, but in the absence the effect of the core polarization (i.e. they have neglected the core polarization term in variational function form $g_c(R)$ $g(R)$ at $\alpha_c=0$) (Khalff (1997)) and (AL-SAMER and EASA(2003)).

All researchers mentioned above have assumed a model potential to describe the motion of the valence electron in the presence of a frozen core,

and used the double method(Perturbation – Variation) to derive the dynamic dipole polarizability at imaginary frequencies (*iw*), except (YAN, BABB, DALGARNO& DRAKE(1996)),they have used the variational method.

The values of table-I- displays the importance of modifying the variational function by adding the core polarization effect to be more accurate in the theoretical derivations ,which leads to the dynamic dipole polarizabilities so closed the experimental values.

Table I : The Dipole Polarizabilities for Li Atom

OUR RESULT **	1.6104(2)
MODEL-POTENTIAL (MARINESCU,	1.6391(2)
VARIATIONAL (YAN, BABB, DALGARNO&	1.6411(2)
DOUBLE (PERTURBATION-VARIATION)	1.3878(2)
(K-P-S (Khalff (1997)	1,1993(2)
(EXPERIMENT (CHEN (1998)	1.6400(2)

NOTE: The sign "**" refer to inserting the core polarization effect into the calculations.

In Table-II-,we give the dispersion forces coefficient C_6(van der Walls coefficient), including a selection of previous researchers .The result of C_6 are in a close agreement among the different theoretical methods except for the results of AL-SAMER & EASA and Khalff,for the same reason as mentioned above, where AL-SAMER & EASA and Khalff assumed a model-potential for the motion of the valence electron in the presence of a frozen core,and used a general form of variational function without any effect of electronic core.(i.e. eliminating the core polarization),which leads to inaccurate results.

Table II: The van der Walls C_6 Coefficient for Li Atom

OUR RESULT **	1.3738(3)
MODEL-POTENTIAL (MARINESCU, SADEGHPOURE& DALGARNO(199))**	1.3600(3)
VARIATIONAL(YAN, BABB, DALGARNO& DRAKE(1996)) **	1.3933(3)
DOUBLE (PERTURBATION-VARIATION) (AL-SAMER and EASA(2003)).	1.2058(3)
K-P-S (Khalff (1997))	1.0599(3)

Finally, we investigated the effect of the retardation effect under various separation distances between two Li-atoms. Fig-1- shows the shape for the retardation coefficient $f_6(R)$. The retardation curve starts with a unity at very small separation distance R ,then damps with an increasing of R and takes a saturation level at R >=200000(a.u.).The curve behavior is the same as in other studies of the retardation coefficients (AL-SAMER and EASA(2003)). The numerical values of the retardation coefficients are given in table -III-.

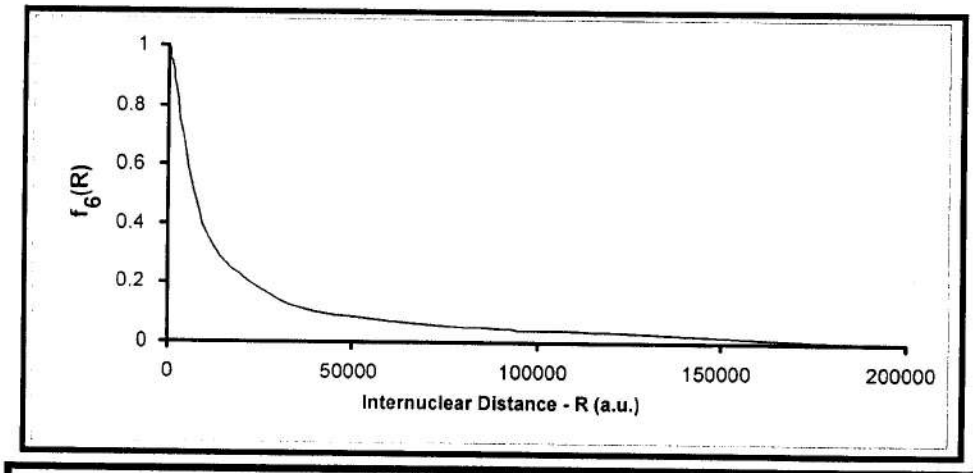

Fig-1-Retardation coefficient f_6 (R) for Two Li - Atom

Table -III-, the retardation coefficient, f_6, for Li atom are listed.

Table III: Retardation Coefficient $f_6(R)$ for Li Atom

1	1.000847494
2	1.000847482
3	1.000847452
4	1.000847393
5	1.000847296
6	1.000847151
7	1.000846949
8	1.000846680
9	1.000846336
10	1.000845906
15	1.000842165
20	1.000834963
25	1.000823267
30	1.000806138
35	1.000782745
40	1.000752372
45	1.000714429
50	1.000668455
60	1.000551177
70	1.000399236
80	1.000212979
90	0.999994042
100	0.999744960
300	0.991955884
500	0.981221564
700	0.967049984
900	0.950273513
1000	0.941248001
10000	0.373539164
30000	0.139605347
50000	0.084741002
70000	0.060729258
90000	0.047298662
100000	0.042585842

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