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Retarded long-range potentials for the alkali-metal atoms and a perfectly conducting wall

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Abstract

The retarded long-range potentials for hydrogen and alkali-metal atoms in their ground states and a perfectly conducting wall are calculated. The potentials are given over a wide range of atom-wall distances and the validity of the approximations used is established.

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The long-range interaction potential of an atom and a surface characterizes the physics of many actual systems. For ground state alkali-metal atoms it has been measured by deflection of atomic beams in scattering [1], reflection of atoms in atomic fountains [2,3], and by combinations of deflection and spectroscopy [4,5]. As the atom-wall separation increases the interaction potential weakens due to retardation arising from the finite speed of light [6,7]. A retarded potential has been observed for Na atoms between parallel metallic plates [5] and for the hydrogen atom inclusion of retardation in theoretical calculations of hydrogen-liquid helium film sticking coefficients dramatically improves the agreement with experiment [8,9]. In the present paper we present calculations of the retarded long-range potentials for hydrogen and alkali-metal atoms and a perfectly conducting wall. When a metallic wall has high reflectivity at the atomic resonance transition wavelengths in the atomic electric dipole polarizability it can be treated as a perfectly conducting wall [10] for atom-wall separations large enough that higher multipoles in the interaction and overlap with the surface electrons are unimportant. Approximations proportional to the retarded potential for an atom and a perfectly conducting wall have been given for the corresponding retarded potential for a dielectric wall [11,12]. Thus the present results may be useful in analyzing the interactions of atoms with dielectric or metallic walls for spectroscopy or atom interferometry experiments [13].

The retarded long-range potential $V(R)$ of a spherically-symmetric ground state atom and a perfectly conducting wall, where R is the atom-wall distance, was derived in 1948 by Casimir and Polder [14]. It can be written [12]

$$V(R) = \frac{-1}{4\pi\alpha_{\text{fs}}R^4} \int_0^\infty dx \alpha(ix/\alpha_{\text{fs}}R) \exp(-2x)[2x^2 + 2x + 1], \quad (1)$$

where $\alpha(i\omega)$ is the atomic dynamic electric dipole polarizability evaluated at imaginary frequency $i\omega$ and $\alpha_{\text{fs}} = 1/137.0359895$ is the fine structure constant. We use atomic units throughout. For small distances Eq. (1) has the limiting form

$$V(R) \sim -C_3/R^3, \quad R \rightarrow 0, \quad (2)$$

where

$$C_3 = \frac{1}{4\pi} \int_0^\infty d\omega \alpha(i\omega). \quad (3)$$

As the distance increases, retardation arising from the finite speed of light becomes increasingly important and $V(R)$ approaches its asymptotic form, a simple power law,

$$V(R) \sim V_\infty(R) \equiv -K_4/R^4, \quad R \rightarrow \infty, \quad (4)$$

where

$$K_4 = 3\alpha(0)/8\pi\alpha_{\text{fs}} = 16.36\alpha(0). \quad (5)$$

A method has been developed to calculate directly the dynamic electric dipole polarizability corresponding to an electron in the presence of a central core field [15]. It gives the function $\alpha(i\omega)$ for hydrogen exactly. Combined with a correction reflecting the polarization of the alkali-metal core by the valence electron [15,16], we used it with a model potential for the field of the positive-ion core seen by the atomic valence electron [15] to obtain the functions $\alpha'(i\omega)$ for the alkali-metal atoms, where the prime has been introduced to indicate the results for the alkali-metal atoms obtained using this method. In determining the correction, measured values of $\alpha(0)$ were adopted. For Li, K, Rb, and Cs the values of $\alpha(0)$ are those given in Ref. [17]. For Na the value $\alpha(0) = 162.7$ [13] was used, yielding a value of the cutoff radius $r_c = 2.860\,812\,8$ in the core-polarization correction compared to the values $\alpha(0) = 159.2$ and $r_c = 0.379\,266\,0$ of Ref. [15]. The values of $\alpha(0)$, and the corresponding values of K_4 , are listed in Table I.

The calculated values for $V(R)$ for hydrogen and the alkali-metal atoms are given in Table II. Eq. (1) was integrated with a Gauss-Laguerre quadrature method. The results for H are exact. In Fig. 1 plots of $V(R)$ are presented for hydrogen and the alkali-metal atoms.

Hinds and Sandoghdar [10] calculated the discrete valence electron contributions to $\alpha(\omega)$ and evaluated the retarded long-range energy shift for ground state Rb. They presented the results graphically for atom-wall distances from about 0.1 to 0.7 μm . For example, they give a potential energy of -1.15 MHz at 0.106 μm ($2000a_0$), in agreement with our value of

-1.162 MHz, obtained from Table I and Figure 1, where the energy, in MHz, was obtained by multiplying the value of $V(R)$ in a.u. by 6.580×10^9 .

The function $\alpha'(i\omega)$ is an excellent approximation to the exact dynamic polarizability $\alpha(i\omega)$ for photon energies ω greater than the first excitation threshold of the core [18,19], which means, accordingly, that $V(R)$ will be most accurate for values of $R \gtrsim 1/(\alpha_{\text{fs}} E_{\text{opt}})$, where in atomic units, E_{opt} is the energy of the first excitation transition. The model potential method does not completely account for inner shell contributions to the oscillator strength distribution and the resulting error in $\alpha'(i\omega)$ leads to a corresponding error in the evaluation of $V(R)$ for small R .

For Na, Kharchenko *et al.* [20] constructed a semi-empirical representation of the function $\alpha(i\omega)$, which explicitly included core contributions, using a combination of theoretical and experimental photoionization and photoabsorption cross sections, and evaluated $V(R)$ using Eq. (1). To determine the accuracy of the potentials in the present work, the ratio of the potential obtained using $\alpha'(i\omega)$ to the potential obtained using the empirical $\alpha(i\omega)$ was calculated. It is given in Fig. 2. For Na, the optical transition energy is $E_{\text{opt}} \sim 0.077$, suggesting that the ratio should be near unity for $R \gtrsim 1800$, which it is, as seen in Fig. 2. The potential calculated using $\alpha'(i\omega)$ underestimates the true potential by 5% at $R = 200$ and by 2% at $R = 500$.

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TABLES

TABLE I. Static electric dipole polarizabilities $\alpha(0)$ for the atoms and asymptotic Casimir coefficients K_4 for the alkali-atom-wall interactions.

Quantity	Ref.	H	Li	Na	K	Rb	Cs
$\alpha(0)/a_0^3$	Present ^a	4.500	164.0	162.7	292.8	319.2	402.2
K_4/a_0^4	Present	73.62	2683	2662	4789	5221	6579

^aSame as Ref. [15], Table II, line labeled “b”, except for Na.

TABLE II. Values of $-R^3V(R)$, where $V(R)$ is the atom-wall potential, Eq. (1), for the hydrogen-wall and alkali-atom-wall interactions, in atomic units. Numbers in square brackets represent powers of ten.

R/a_0	H	Li	Na	K	Rb	Cs
1.0	2.4981[-1]	1.4468	1.5753	2.1521	2.2903	2.5882
1.5	2.4951[-1]	1.4466	1.5750	2.1518	2.2900	2.5879
2.0	2.4912[-1]	1.4462	1.5746	2.1514	2.2896	2.5875
2.5	2.4868[-1]	1.4457	1.5742	2.1510	2.2892	2.5871
3.0	2.4824[-1]	1.4453	1.5737	2.1506	2.2888	2.5867
4.0	2.4742[-1]	1.4445	1.5729	2.1498	2.2880	2.5860
5.0	2.4674[-1]	1.4438	1.5723	2.1492	2.2873	2.5854
6.0	2.4616[-1]	1.4432	1.5717	2.1486	2.2868	2.5849
8.0	2.4518[-1]	1.4422	1.5707	2.1477	2.2859	2.5840
1.0[1]	2.4423[-1]	1.4412	1.5698	2.1468	2.2849	2.5831
1.5[1]	2.4158[-1]	1.4385	1.5672	2.1443	2.2824	2.5806
2.0[1]	2.3872[-1]	1.4356	1.5643	2.1415	2.2795	2.5779
2.5[1]	2.3589[-1]	1.4326	1.5614	2.1387	2.2767	2.5752
3.0[1]	2.3316[-1]	1.4298	1.5586	2.1360	2.2739	2.5725
4.0[1]	2.2795[-1]	1.4242	1.5530	2.1306	2.2684	2.5671
5.0[1]	2.2295[-1]	1.4187	1.5475	2.1252	2.2629	2.5618
6.0[1]	2.1811[-1]	1.4132	1.5420	2.1198	2.2573	2.5564
8.0[1]	2.0892[-1]	1.4024	1.5309	2.1089	2.2462	2.5456
1.0[2]	2.0038[-1]	1.3919	1.5199	2.0981	2.2349	2.5346
1.5[2]	1.8156[-1]	1.3662	1.4927	2.0708	2.2068	2.5070
2.0[2]	1.6567[-1]	1.3417	1.4659	2.0436	2.1787	2.4791
2.5[2]	1.5211[-1]	1.3180	1.4397	2.0166	2.1507	2.4512
3.0[2]	1.4042[-1]	1.2951	1.4141	1.9898	2.1228	2.4233

4.0[2]	1.2136[-1]	1.2515	1.3646	1.9372	2.0681	2.3680
5.0[2]	1.0653[-1]	1.2106	1.3176	1.8862	2.0148	2.3136
6.0[2]	9.4707[-2]	1.1720	1.2729	1.8368	1.9632	2.2606
8.0[2]	7.7144[-2]	1.1011	1.1905	1.7433	1.8654	2.1590
1.0[3]	6.4810[-2]	1.0374	1.1165	1.6568	1.7747	2.0636
1.5[3]	4.5911[-2]	9.0333[-1]	9.6172[-1]	1.4683	1.5762	1.8515
2.0[3]	3.5345[-2]	7.9700[-1]	8.4053[-1]	1.3130	1.4122	1.6728
2.5[3]	2.8659[-2]	7.1098[-1]	7.4384[-1]	1.1839	1.2754	1.5214
3.0[3]	2.4069[-2]	6.4023[-1]	6.6535[-1]	1.0755	1.1601	1.3923
4.0[3]	1.8199[-2]	5.3139[-1]	5.4651[-1]	9.0469[-1]	9.7795[-1]	1.1849
5.0[3]	1.4616[-2]	4.5218[-1]	4.6156[-1]	7.7725[-1]	8.4153[-1]	1.0269
6.0[3]	1.2206[-2]	3.9236[-1]	3.9829[-1]	6.7922[-1]	7.3628[-1]	9.0342[-1]
8.0[3]	9.1748[-3]	3.0869[-1]	3.1107[-1]	5.3949[-1]	5.8578[-1]	7.2426[-1]
1.0[4]	7.3473[-3]	2.5346[-1]	2.5428[-1]	4.4556[-1]	4.8430[-1]	6.0173[-1]
1.5[4]	4.9032[-3]	1.7400[-1]	1.7361[-1]	3.0815[-1]	3.3541[-1]	4.1944[-1]
2.0[4]	3.6787[-3]	1.3200[-1]	1.3140[-1]	2.3452[-1]	2.5542[-1]	3.2034[-1]
2.5[4]	2.9435[-3]	1.0619[-1]	1.0559[-1]	1.8897[-1]	2.0587[-1]	2.5859[-1]
3.0[4]	2.4531[-3]	8.8763[-2]	8.8202[-2]	1.5811[-1]	1.7228[-1]	2.1659[-1]
4.0[4]	1.8400[-3]	6.6780[-2]	6.6313[-2]	1.1906[-1]	1.2976[-1]	1.6329[-1]
5.0[4]	1.4721[-3]	5.3501[-2]	5.3110[-2]	9.5433[-2]	1.0402[-1]	1.3095[-1]
6.0[4]	1.2267[-3]	4.4620[-2]	4.4286[-2]	7.9611[-2]	8.6777[-2]	1.0927[-1]
8.0[4]	9.2008[-4]	3.3492[-2]	3.3236[-2]	5.9772[-2]	6.5156[-2]	8.2066[-2]
9.0[4]	8.1785[-4]	2.9777[-2]	2.9548[-2]	5.3146[-2]	5.7934[-2]	7.2975[-2]
1.0[5]	7.3607[-4]	2.6804[-2]	2.6597[-2]	4.7842[-2]	5.2153[-2]	6.5696[-2]
1.0[6]	7.3609[-5]	2.6826[-3]	2.6613[-3]	4.7894[-3]	5.2212[-3]	6.5788[-3]

FIGURES

FIG. 1. For H, Li, Na, K, Rb, and Cs, values of $R^3V(R)$, where $V(R)$ is the atom-wall potential, Eq. (1), as a function of the atom-wall distance R in a_0 .

FIG. 2. For Na, ratio of the atom-wall potential calculated in the present work to the more accurate potential calculated by Kharchenko *et al.* [20].

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