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Model Potential Calculations for Various Electronic Excited States of Li^- and Na^-

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Energies and wave functions for the ground state and several excited electronic states are reported for Li^- and Na^- negative ions. Calculations have been achieved in the framework of a model potential method using s, p, d, and f atomic Slater-type basis orbitals. The electronic correlation has been considered through configuration interaction calculations. Present results are compared with available experimental and theoretical data.

1. Introduction

During the past decade, the knowledge of alkali dimers spectroscopy has been remarkably improved, in particular for the long-range part of potential energy curves. With the development of spectroscopy experiments by photoassociation in magnetooptical traps, lifetimes for the first excited atomic states may be presently deduced with a high accuracy.[1,2] Part of this data can be compared straightforwardly to long-range calculations, and such comparisons are very useful to check the accuracy of theoretical models and to perform the subsequent improvements.

Our goal is to develop a model able to substitute asymptotic calculations to ab initio ones in a smooth way at large internuclear distances. Usual long-range calculations are based on the evaluation of exchange and Coulomb interaction energies between separated atoms. Up to now, comparisons with experiment for the ground and the first excited alkali dimer states have been successful, whereas for higher excited states, such long-range models are no longer satisfactory due to the neglect of ionic−covalent interactions. An improved theoretical model has been developed in which an estimation of the interaction between covalent and ionic states has been performed.[3,4] It is based on the use of a rather crude asymptotic form for the ground state of alkali negative ions, so that the improvements, while significant, are not yet sufficient. Extensions toward more elaborated functions for the ground state and excited states of the negative alkali ion are then required.

In a recent paper,[5] we suggested the use of a two-electron correlated wave function to compute easily the ground-state energy of alkali negative ions. In this approach, which is based on the formalism developed with success for H^-,[6] the electronic correlation is taken into account through a trial function explicitly dependent on the interelectronic distance r_{12}. By this way, variational calculations with one configuration were seen to be of a very good accuracy.[7] Nevertheless, extensions of this approach to the determination of excited state wave functions, easily tractable in subsequent calculations, is not straightforward. So, presently, we have chosen to describe the excited states of Li^- and Na^- negative ions by taking into account the electronic correlation through configuration interaction calculations (CI).

2. Method

Basically, alkali negative ions M^- may be treated as systems with two outermost electrons moving in the field of an ionic core M^+. Energies and relevant wave functions are obtained by solving the Schrödinger model equation:

$$\left[-\frac{1}{2}\vec{\nabla}_1^2 - \frac{1}{2}\vec{\nabla}_2^2 + V(r_1) + V(r_2) + V_{\mathrm{pol}}(r_1,r_2) + \frac{1}{r_{12}}\right]\psi_{^{2S+1}\mathrm{L}}(r_1,r_2) = \mathrm{E}_{^{2s+1}\mathrm{L}}\Psi_{^{2s+1}\mathrm{L}}(r_1,r_2) \quad (1)$$

Interaction between the ionic core M^+ and a valence electron is described by a model potential $V(r_i)$ proposed by Klapisch[8,9] to which core polarization effects between the core M^+ and each valence electron have been added:

$$V(r_i) = -\frac{1}{r_i} - \frac{[(Z-1)\mathrm{e}^{-\gamma_1 r_i} + \gamma_2 r_i \mathrm{e}^{-\gamma_3 r_i}]}{r_i} - \frac{\alpha_\mathrm{d}}{2r_i^4}(1 - \mathrm{e}^{-(r_i/\rho)^4}) \quad (2)$$

where Z is the nuclear charge and α_d is the static dipole polarizability of the ionic core M^+. The parameter ρ is an *l*-dependent cutoff radius adjusted in order to reproduce the experimental atomic energy of the lowest state of each symmetry L.[10] For Li, values of parameters involved in eq 2 are $\gamma_1 = 7.908\,75$, $\gamma_2 = 10.321$, $\gamma_3 = 3.900\,06$, $\alpha_\mathrm{d} = 0.1915a_0^3$,[11] $\rho(s) = 3.50a_0$, and $\rho(p,d,f) = 3.70a_0$. In the case of Na, we used $\gamma_1 = 7.887\,47$, $\gamma_2 = 23.541\,02$, $\gamma_3 = 2.691\,55$, $\alpha_d = 0.9965a_0^3$,[12] $\rho(s) = 6a_0$, $\rho(p) = 6.50a_0$, and $\rho(d,f) = 8a_0$, respectively.

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TABLE 1: Couples of Parameters (n_j, ϑ_j) for Slater-type Orbital Basis in the Case of *ns*, *np*, *nd*, and *nf* Atomic States[a]

Li
ns atomic levels; $n_{\text{couple}} = 20$
(2,4.70) (3,2.48) (3,1.73) (3,0.80) (3,0.66) (3,0.51) (3,0.45) (3,0.38) (3,0.34) (4,0.28) (5,0.25) (5,0.22) (6,0.20) (6,0.18) (6,0.16) (7,0.14) (8,0.12) (9,0.10) (9,0.09) (9,0.08)
np, *nd*, and *nf* atomic levels; $n_{\text{couple}} = 19$
(2,4.70) (3,2.48) (3,1.73) (3,0.80) (3,0.66) (3,0.45) (3,0.38) (3,0.34) (3,0.33) (4,0.28) (5,0.25) (5,0.22) (6,0.20) (6,0.18) (6,0.16) (7,0.14) (9,0.12) (9,0.09) (7,0.08)
Na
ns, *np*, *nd*, and *nf* atomic levels; $n_{\text{couple}} = 24$
(2,12.66) (2,11.01) (3,8.36) (3,5.74) (3,3.61) (3,2.25) (3,1.11) (4,0.71) (3,0.61) (3,0.47) (3,0.37) (3,0.31) (3,0.27) (4,0.25) (5,0.20) (5,0.18) (7,0.16) (7,0.14) (8,0.13) (8,0.12) (9,0.11) (9,0.09) (9,0.08) (5,0.06)

[a] The number of couples n_{couple} is indicated.

TABLE 2: Electronic Energies (in Atomic Units) for the Ten Lowest $^{1,3}S$ and $^{1,3}P$ States and the Seven Lowest $^{1,3}D$ States of Li^{-}[a]

$\text{Li}^-(^1S)$	$\text{Li}^-(^3S)$	$\text{Li}^-(^1P)$	$\text{Li}^-(^3P)$	$\text{Li}^-(^1D)$	$\text{Li}^-(^3D)$
−0.220850					
Li(2s): −0.198142	**Li(2s): −0.198142**	**Li(2s): −0.198142**	**Li(2s): −0.198142**	**Li(2s): −0.198142**	**Li(2s): −0.198142**
−0.197068	−0.197286	−0.196427	−0.196700	−0.195060	−0.195061
−0.192793	−0.193658	−0.192464	−0.194781	−0.189108	−0.189118
−0.181366	−0.184279	−0.184083	−0.189782	−0.175255	−0.175254
−0.132337	−0.141510	−0.160010	−0.176643	−0.132060	
Li(2p): −0.130235	**Li(2p): −0.130235**	**Li(2p): −0.130235**	**Li(2p): −0.130235**	**Li(2p): −0.130235**	**Li(2p): −0.130235**
−0.128554	−0.128518	−0.128758	−0.129568	−0.128568	−0.128516
−0.128375	−0.128389	−0.128568	−0.128387	−0.128369	−0.128406
−0.128194	−0.128200	−0.128353	−0.128220	−0.128141	−0.128220
−0.124377	−0.124040	−0.128183	−0.127664		−0.127062
−0.123890	−0.123901	−0.124438	−0.125314		
	−0.123318	−0.123561	−0.123899		

[a] Value of the atomic threshold is indicated.

The polarization of the ionic core M^+ by the two outermost electrons in eq 1 is represented by an effective potential:

$$V_{\text{pol}}(r_1,r_2) = -\frac{\alpha_{\text{d}}\vec{r}_1.\vec{r}_2}{2r_1^3\,r_2^3}(1 - e^{-(r_1/\tau)^4})(1 - e^{-(r_2/\tau)^4}) \qquad (3)$$

The parameter τ is adjusted to reproduce the known experimental energy of the negative ionic ground state M^{-} [7] (E_{Li^-} ($2s^2$) = −0.220 853 a.u. and E_{Na^-} ($3s^2$) = −0.208 994 a.u.) through a CI calculation. With $\tau_{\text{Li}^-} = 0.074\,33a_0$ and $\tau_{\text{Na}^-} = 0.1807a_0$, the computed ground-state energies are equal to −0.220 85 a.u. and −0.209 008 a.u., respectively.

For a given symmetry $^{2S+1}$L of the negative ion M^-, energies and wave functions of excited states are obtained by solving eq 1 through CI calculations including s, p, d, and f atomic Slater-type orbitals:

$$\Psi_{^{2S+1}\text{L}}(r_1,r_2) = \sum_{ab} c_{ab}(\phi_a(r_1)\phi_b(r_2) \pm \phi_a(r_2)\phi_b(r_1))[\chi(1)\beta(2) \mp \chi(2)\beta(1)] \qquad (4)$$

where χ and β are spin wave functions. The one-electron radial wave function $\phi_{a(b)}(r_i)$ has been obtained by solving the one-electron Schrödinger equation:

$$\left[-\frac{\vec{\nabla}^2}{2} + V(r_i)\right]\phi_{a(b)}(r_i) = \epsilon_{a(b)}\phi_{a(b)}(r_i) \qquad (5)$$

where $V(r_i)$ is the model potential defined in eq 2 and $\phi_{a(b)}(r_i) = \sum_{j=1}^{\text{ncouple}} c_j \sum_{p=0}^{n_j-1} r_i^{p+l} e^{-\vartheta_j r_i}$.

One-electron wave functions $\phi_{a(b)}$ are expanded on a basis set of Slater-type orbitals including typically 100 terms for Li and 114 for Na. Each basis set has been defined in order to reproduce the 10 lowest atomic levels[10] with an average accuracy of 10^{-5} a.u. (≈2 cm^{-1}). Couples of parameters (n_j,ϑ_j) are given in Table 1. As a check of the accuracy of such atomic orbitals $\phi_{a(b)}$, the static dipole polarizability of the atomic ground state has been calculated in a sum-over-states approach. We found $\alpha_{\text{d}}^{\text{Li}}(2s) = 164a_0^3$ and $\alpha_{\text{d}}^{\text{Na}}(3s) = 165a_0^3$ in excellent agreement with the experimental values ($164 \pm 3a_0^3$ for Li,[13] $159 \pm 3a_0^3$,[13] and $165 \pm 11a_0^3$ [14] in the case of Na).

For a given symmetry $^{2S+1}$L, the expansion of the trial wave function $\Psi_{^{2S+1}\text{L}}$ (eq 4) contains in average 90 two-electron configurations. These configurations are built up from the following atomic basis sets {$2s - 6s$, $2p - 6p$, $3d - 6d$, $4f - 6f$} for Li^- and {$3s - 7s$, $3p - 7p$, $3d - 7d$, $4f - 6f$} for Na^-. In this work, we have restricted our investigations to $^{2S+1}\text{L}_0$ states.

3. Results

With the aim of being able to model the ionic−covalent interaction problem, we are mainly interested in the lowest excited states of M^- which can play a role in the occurrence of structures in long-range potential energy curves of highly excited states of alkali dimers. So, we report in Tables 2 and 3 for Li^- and Na^- negative ions the energy of the ten lowest electronic excited states for $^{1,3}S$ and $^{1,3}P$ symmetries and the seven lowest ones for $^{1,3}D$.

A comparison with available theoretical calculations[15−20] is presented in Table 4. Present and previous calculated energies of various excited states provide the same order of magnitude. Discrepancies with model potential calculations of Stewart et al.[15] are due partly to the core polarization effects (V_{pol}, eq 3)

TABLE 3: Electronic Energies (in Atomic Units) for the Ten Lowest $^{1,3}S$ and $^{1,3}P$ States and the Seven Lowest $^{1,3}D$ States of Na^{-a}

Na$^-$(^1S)	Na$^-$(^3S)	Na$^-$(^1P)	Na$^-$(^3P)	Na$^-$(^1D)	Na$^-$(^3D)
−0.209008					
Na(3s): −0.188858	**Na(3s): −0.188858**	**Na(3s): −0.188858**	**Na(3s): −0.188858**	**Na(3s): −0.188858**	**Na(3s): −0.188858**
−0.187801	−0.188057	−0.187273	−0.187414	−0.187757	−0.187762
−0.183450	−0.184490	−0.183579	−0.184977	−0.182283	−0.182286
−0.172093	−0.175400	−0.176029	−0.180165	−0.173848	−0.173887
−0.113464	−0.133642	−0.154979	−0.168480	−0.158018	−0.158134
			−0.116728	−0.114161	
Na(3p): −0.111548	**Na(3p): −0.111548**	**Na(3p): −0.111548**	**Na(3p): −0.111548**	**Na(3p): −0.111548**	**Na(3p): −0.111548**
−0.110065	−0.110030	−0.110534	−0.113938	−0.110354	−0.110365
−0.109802	−0.109830	−0.110099	−0.109829	−0.110098	−0.110028
−0.109668	−0.109676	−0.109788	−0.109730		−0.109896
−0.106199	−0.105856	−0.109594	−0.109636		
−0.105620	−0.105583	−0.106309	−0.108859		
	−0.105217	−0.105204			

[a] Value of the atomic threshold is indicated.

TABLE 4: Comparison (in Atomic Units) with Relevant Theoretical Energy Determinations for Li$^-$and Na$^-$ Excited Electronic States

excited states	Stewart et al. calc[a]	Dulieu calc[b]	present work	other theoretical results
Li$^-$(^3P)			−0.129568	−0.132440[c]
Li$^-$(^1S)		−0.13470	−0.132337	
Li$^-$(^3P)			−0.113383	−0.113827[d]
Li$^-$(^1S)	−0.0844	−0.08340	−0.080956	
Li$^-$(^3P)	−0.0787	−0.07666	−0.075918	
Li$^-$(^3S)	−0.0743		−0.074093	
Li$^-$(^1P)			−0.064251	−0.06571[e]
Li$^-$(^3P)	−0.0641		−0.064068	
Li$^-$(^1S)	−0.0622	−0.06521	−0.067129	
Li$^-$(^1D)	−0.0619	−0.06292	−0.065927	
Li$^-$(^1D)	−0.0608		−0.065638	
Li$^-$(^3P)	−0.0598	−0.05938	−0.061929	
Li$^-$(^1P)	−0.0594	−0.06062	−0.057368	−0.05961[e]
				−0.05786[e]
Li$^-$(^1P)	−0.0577		−0.056511	
Li$^-$(^3S)	−0.0574		−0.057508	
Na$^-$(^3P)		−0.119600	−0.116728	−0.114598[d]
Na$^-$(^1S)	−0.0795	−0.08064	−0.080856	
Na$^-$(^3P)	−0.0735		−0.073309	
Na$^-$(^3S)	−0.0718		−0.071076	
Na$^-$(^1P)			−0.061043	−0.061460[f]
Na$^-$(^1S)	−0.0582	−0.05862	−0.055589	
Na$^-$(^1D)	−0.0579	−0.05540	−0.055115	
Na$^-$(^3P)	−0.0573	−0.05596	−0.056462	
Na$^-$(^1P)	−0.0567	−0.05829	−0.055657	
Na$^-$(^3D)	−0.0563		−0.056163	
Na$^-$(^3D)	−0.0559		−0.055442	
Na$^-$(^1P)		−0.051650	−0.051424	−0.051100[f]

[a] Reference 15. [b] Reference 16. [c] Reference 17. [d] Reference 18. [e] Reference 19. [f] Reference 20.

TABLE 5: Comparison (in Atomic Units) with Experimental Energy Determinations for Li$^-$and Na$^-$ Excited Electronic States with Previous Theoretical Values Also Reported

excited state	experiment	present work	other calculations
Li$^-$(^3P)	−0.196305[a]	−0.196700	
Li$^-$(^1S)	−0.084587[b]	−0.080956	−0.083400[g]
Li$^-$(^3P)	−0.077604[b]	−0.075918	
Li$^-$(^3S)	−0.075032[b]	−0.074093	
Li$^-$(^1P)	−0.062096[c]	−0.064251	−0.06571[h]
Li$^-$(^1P)	−0.032895[d]	−0.035903	
Li$^-$(^1P)	−0.032947[d]	−0.035793	
Li$^-$(^1P)	−0.032594[d]	−0.031171	
Li$^-$(^1P)	−0.032572[d]	−0.030378	
Li$^-$(^1P)	−0.032046[d]	−0.029393	
Na$^-$(^1S)	−0.111685[e]	−0.113464	−0.080640[g]
Na$^-$(^1P)	−0.063911[e]	−0.064966	−0.069970[g]
Na$^-$(^3P)	−0.060236[e]	−0.060286	
Na$^-$(^1D)	−0.052151[e]	−0.054254	−0.055400[g]
Na$^-$(^1P)	−0.035067[f]	−0.035138	−0.034930[i]
Na$^-$(^1P)	−0.032337[f]	−0.033873	−0.032290[i]
Na$^-$(^1P)	−0.031620[f]	−0.032380	−0.031700[i]
Na$^-$(^1P)	−0.031442[f]	−0.031991	−0.031300[i]

[a] Reference 21. [b] Reference 25. [c] Reference 22. [d] Reference 23. [e] Reference 25. [f] Reference 24. [g] Reference 16. [h] Reference 19. [i] Reference 20.

which have been neglected and partly to the size of CI calculations restricted typically to 50 two-electron functions for both negative ions. Those with Pluvinage calculations including a model potential approach[16] are due to the determination of CI basis sets which include only the first excited atomic states. Agreement with eigenchannel R-matrix calculations[19,20] appears satisfying. In particular for Li$^-$, Pan et al.[19] report results of two alternative calculations: one predicting a resonance at an energy of −0.059 61 a.u. and one giving two resonances at −0.065 71 and −0.057 86 a.u. Present results are in a satisfying agreement with the second calculations, and we predict a third resonance. Finally, we may assume that present description of highly excited states of ^3S, $^{1,3}P$ and $^{1,3}D$ symmetries is accurate.

From recent photodetachment cross section measurements, the position of various ^1P and ^3P excited states have been deduced for Li$^-$ and Na$^-$ negative ions.[21−23] A comparison with these experimental data and theoretical results is reported in Table 5. One ^3P excited-state lying below the Li(2p) threshold[21] has been identified at an energy of −0.196 305 a.u. and six ^1P states have been located below the Li(3p) and Li(4p) thresholds.[22,23] In the case of Na$^-$, four ^1P excited states lying below the Na(4d) threshold have been identified.[24] Several excited electronic states determined experimentally by Kazakov[25] and Lengyel[26] and reported in ref 16 have been also quoted in Table 5. In the experimental energy range, computed energies appear either lower or higher for the two negative ions. As these states are located at a very high energy, comparison with present calculations is rather difficult and we can only quote that a reasonable agreement is displayed with both data. Comparison with experiment can be completed by determining the character of known excited states which has been determined theoretically in some papers[20,22−24] for the ^1P symmetry. For both ions, the wave function of the ^1P states present a strong configuration mixing as observed previously by Liu and Starace.[20] For Li$^-$, an analysis of the eigenvector components (a) shows that the ^1P state located below Li(3p) threshold at an energy of −0.064 251 a.u. depends mainly on $3s3p$ ($a = 0.38$), $3s4p$ ($a = 0.38$), $3s6p$ ($a = 0.66$), $4s3p$ ($a = 0.27$), and $3p3d$ ($a = 0.20$)

configurations. Although present results are in agreement with calculations of Berzinsh et al.,[22] this state appears dominated by 3*s*6*p*, 3*s*3*p*, and 3*s*4*p* configurations and not by 3*p*3*d* and 4*s*3*p* as predicted in ref 22. Present other four Li^- (^1P) states are mainly built on the two-electron configurations 3*pns*, 3*pnp*, and 3*snd* (with $n \geq 3$); 4*pnp* (with $n \geq 5$); and 3*dnd* and 3*dnf* (with $n > 3$). This analysis is partly in agreement with that proposed by Haeffler et al.[23] (3*snp* and 4*snp*). Similar patterns are also observed for the Na^- negative ion. Haeffler et al.[24] suggested that the four ^1P states located below Na(4*d*) threshold are constructed mainly on 4*dmf* and 4*dmp* configurations. In present calculations, 3*dn*l (with $n \geq 4$ and $\mathrm{l} = 1{,}2$) and 5*snp* (with $n \geq 5$) configurations have a significant contribution ($a \geq 0.20$ and $a \geq 0.40$, respectively), whereas a small weight is observed for 4*dmf* configurations ($a \leq 0.15$). We have extended our comparison to the Na^- (^1P) state predicted by Liu and Starace[20] at $-0.061\,060$ a.u. and dominated by 4*s*4*p* and 3*d*4*p* configurations. In present work, we found it at $-\ 0.061\,043$ a.u. (see Table 4), and the same configurations 4*s*4*p* ($a = 0.39$) and 3*d*4*p* ($a = 0.20$) give a significant contribution as well as 4*s*5*p* ($a = 0.30$) and 4*s*7*p* ($a = 0.70$) configurations.

4. Conclusion

We have determined, for the first time, the energy of numerous excited states for Li^- and Na^- negative ions, following a model potential approach. Using only one adjustable parameter (the cutoff radius τ (eq 3)) determined from the known experimental ground-state energy of M^{-} [7] and performing CI calculations, we have succeeded to describe the lowest excited states of M^- with a satisfying accuracy.

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