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The excitation energies and term energies of the excited states $1s^2ns$ (n=3,4,5) and $1s^2nf$ (n=4,5) of lithium-like systems of Z=11–20*

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In this paper, the full-core plus correlation (FCPC) and the Ritz method is extended to calculate the non-relativistic energies of $1s^2ns$ (n=3,4,5) and $1s^2nf$ (n=4,5) states and the wavefunctions of the lithium-like systems from Z=11–20. The mass-polarization and the relativistic correction including the kinetic-energy correction, the Darwin term, the electron–electron contact term, and the orbit–orbit interaction are evaluated perturbatively as the first-order correction. The contribution from quantum electrodynamic is also included by using the effective nuclear charge formula. The excited energies, the term-energy and fine structure, are given and compared with the other theoretical calculation and experimental results. It is shown that the correlative wave in the FCPC method embodies well the strong correlation between the $1s^2$ core and the valence electron.

Keywords: lithium-like systems, full core plus correlation, excited states, fine-structure
PACC: 3130, 3110, 3270

1. Introduction

The multi-configuration wavefunction, especially the Slater-type configuration-interaction (CI) wavefunction, approach to the atomic structure problem has the advantage that it can be easily applied to many-electron systems.[1] However, for systems with $1s^2$ core, high-precision results are difficult to obtain with the CI method.[2] This is because the large contributions from the high-angular-momentum components in the wavefunction make the energy convergence slow. Recently, a full-core plus correlation (FCPC) method has been applied to the atomic system with a $1s^2$-core.[3,4] The ionization potentials (IPs) of the ground states of the lithium-like from LiI to NeVIII are predicted to within 10ppm of the experimental values.[5] For an excited state, most of the calculated excitation energies for the $1s^2nl$ states from LiI to NeVIII are in agreement with the experimental data to about $1cm^{-1}$. An improved calculation made this discrepancy decrease to within 1ppm.[6] The predicted non-relativistic energies agree with the highly accurate results from the Hylleraas or configuration-interaction function. An interesting question is whether the same accurate calculation is possible for the excited states of lithium-like system with higher nuclear charges. In this paper, we extend this method to calculate the term energies, excitation energies of $1s^2ns$ (n=3,4,5) and $1s^2nf$ (n=4,5) and fine structures of $1s^2nf$ (n=4,5) of the lithium-like systems from Z=11–20.

2. Theory

The essential point of the FCPC method is to use a large predetermined $1s^2$-core wavefunction as a single term in the total wavefunction of the three-electron system. The effect of the valence electron is accounted for by multiplying the core wavefunction by a linear combination of single-electron Slater orbital. The relaxation of the core and the other possible correlations are described by another large CI wavefunction. The wavefunction of the lithium-like system with $1s^2$ core is given by

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$$\Psi(1,2,3) = A\left[\Phi_{1s1s}(1,2)\sum_i d_i r_3^i e^{-\beta r_3}\chi(3) + \sum_i C_i \Phi_{n(i),l(i)}(1,2,3)\right], \quad (1)$$

where A is the antisymmetrization operator. The second term $\Phi_{n(i)l(i)}(1,2,3)$ on the right-hand side accounts for the three-electron correlation and the relaxation of the core. The function $\Phi_{1s1s}(1,2)$ of the $1s^2$ core is given by

$$\Phi_{1s1s}(1,2) = A\sum_{k,n,l} C_{knl} r_1^k r_2^n e^{-\beta_l r - \rho_{l1} r_2} Y_l(1,2)\chi(1,2), \quad (2)$$

when $Y_l(1,2)$ and the $\chi(1,2)$ are the angular part and the singlet spin function respectively. The nonlinear parameters β_l and ρ_l are individually optimized in the energy minimization process. The LS coupling scheme is used in this paper. The non-relativistic Hamiltonian of a lithium-like system is given by (in a.u.)

$$H_0 = \sum_{i=1}^{3}\left[-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right] + \sum_{\substack{i,j=1\\ i<j}}^{3}\frac{1}{r_{ij}}. \quad (3)$$

The non-relativistic energies of the $1s^2$-core and $1s^2nl$ states are calculated by minimizing the expectation value of H_0

$$\delta E_0 = \delta\langle H_0\rangle = \delta\frac{\langle\Psi|H_0|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \quad (4)$$

The correlation from the relativistic and the mass-polarization effects is given by

$$\Delta E = \langle\Psi|H_1+H_2+H_3+H_4+H_5+H_6+H_7|\Psi\rangle. \quad (5)$$

The total energy is

$$E_{\rm tot} = E_0 + \Delta E. \quad (6)$$

The correction of the relativistic perturbation to the kinetic energy is

$$H_1 = -\frac{1}{8c^2}\sum_{i=1}^{3} p_i^4, \quad (7)$$

where c=137.036 and Darwin term is

$$H_2 = \frac{Z\pi}{2c^2}\sum_{i=1}^{3}\delta(r_i). \quad (8)$$

The electronic- electron contact term is

$$H_3 = -\frac{\pi}{c^2}\sum_{\substack{i,j=1\\ i<j}}^{3}\left[1+\frac{8}{3}\boldsymbol{s}_i\cdot\boldsymbol{s}_j\right]\delta(r_{ij}). \quad (9)$$

The orbit- orbit interaction term is

$$H_4 = -\frac{1}{2c^2}\sum_{\substack{i,j=1\\ i<j}}^{3}\frac{1}{r_{ij}}\left[\boldsymbol{p}_i\cdot\boldsymbol{p}_j + \frac{\boldsymbol{r}_{ij}(\boldsymbol{r}_{ij}\cdot\boldsymbol{p}_i)\cdot\boldsymbol{p}_j}{r_{ij}^2}\right]. \quad (10)$$

The spin–orbit interaction term is

$$H_5 = \frac{Z}{2c^2}\sum_{i=1}^{3}\frac{\boldsymbol{l}_i\cdot\boldsymbol{s}_i}{r_{ij}}. \quad (11)$$

The spin-other-orbit interaction term is

$$H_6 = -\frac{1}{2c^2}\sum_{i\neq j}^{3}\left[\frac{1}{r_{ij}}(\boldsymbol{r}_i-\boldsymbol{r}_j)\times\boldsymbol{p}_i\right]\cdot(\boldsymbol{s}_i+2\boldsymbol{s}_j). \quad (12)$$

The mass-polarization term is

$$H_7 = -\frac{1}{M}\sum_{i<j}^{3}\nabla_i\cdot\nabla_j. \quad (13)$$

In calculation of the fine structure, the LS coupling scheme is used.[7]

Table 1. Energy convergence for the $1s^2$- core and the $1s^24s$ states of lithium-like systems from Z=11–20.

Angular No. of component terms		$-\Delta E$/a.u.				
		Z=11	13	15	18	20
(0,0)	49	114.25082320	161.00074190	215.75068373	312.87562115	387.62558995
(1,1)	42	0.02571810	0.02583883	0.02592956	0.02602081	0.02606763
(2,2)	36	0.00357928	0.00362691	0.00366242	0.00370072	0.00371984
(3,3)	30	0.00095756	0.00097345	0.00098516	0.00099794	0.00100435
(4,4)	25	0.00035081	0.00035718	0.00036189	0.00036703	0.00036962
(5,5)	20	0.00015289	0.00015580	0.00015795	0.00016031	0.00016949
(6,6)	20	0.00007675	0.00007826	0.00007937	0.00008060	0.00008121
Total	222	114.28165857	161.03177231	215.78185708	312.90694855	387.65699406

Table 1 (*Continued*)

core+4s	8	116.91321085	164.93730870	221.21142028	321.09134977	397.99047408
((0,0),0)	67	0.00015638	0.00017912	0.00019833	0.00022430	0.00023961
((0,1),1)	161	0.00045355	0.00047322	0.00049222	0.00050841	0.00051455
((0,2),2)	125	0.00005357	0.00005798	0.00005851	0.00005824	0.00006065
((0,3),3)	95	0.00001446	0.00001554	0.00001596	0.00001601	0.00001588
((0,4),4)	34	0.00000519	0.00000561	0.00000535	0.00000544	0.00000553
((0,5),5)	34	0.00000249	0.00000269	0.00000282	0.00000236	0.00000238
((0,6),6)	34	0.00000140	0.00000150	0.00000151	0.00000118	0.00000118
((0,1),1)[a)]	13	0.00000117	0.00000230	0.00000237	0.00000076	0.00000133
((1,0),1)	10	0.00000083	0.00000059	0.00000099	0.00000023	0.00000027
((0,2),2)[a)]	13	0.00000026	0.00000033	0.00000032	0.00000019	0.00000032
((1,2),1)	10	0.00000024	0.00000018	0.00000014	0.00000009	0.00000008
((0,0),0)[a)]	11	0.00000009	0.00000011	0.00000030	0.00000018	0.00000048
((2,3),1)	10	0.00000003	0.00000002	0.00000001	0.00000001	0.00000001
Total	625	116.91390050	164.93804858	221.21219912	321.09216719	397.99131663

[a)] In these angular components, the spins of the first two electrons couple into a triplet.

3. Results and discussion

In this work, a 222-term core wavefunction with seven l components are used. Though the number of terms is not large enough, this does not lead to a substantial effect on our calculations because the IP is determined by subtracting the energy of the three-electron system from that of the $1s^2$ core. To calculate the $1s^2ns$ energy, we used eight d_i terms and 625 terms of $\Phi_{n(i)l(i)}$ (1,2,3) with 13 partial waves in Eq.(1). This means that one-half of 2401×2401 matrix elements have to be calculated for each secular equation.[8] The $1s^2nf$ energy converged faster than the $1s^2ns$ energy; hence fewer in $\Phi_{n(i)l(i)}$ (1,2,3) is used, about 300 terms with 11 partial waves. As typical examples, the energy convergence of the lithium-like $1s^24s$ states from Z=11–20 are given in Table 1. Note that the same $1s^2$-core wavefunctions are used in all calculations of lithium-like $1s^2ns$ (n=3,4,5) and $1s^2nf$ (n=4,5) systems. It is seen that the 'speed' of convergence of $1s^24s$ states is faster than that of $1s^2$-core.

Table 2. Non-relativistic energy, term energy of relativistic correction and mass-polarization of $1s^2nl$(l=4,5;n=3,4,5) states (in a.u).

	$< H_{\rm nonrelativistic} >$	$< H_1 + H_2 >$	$< H_3 >$	$< H_4 >$	$< H_{\rm MP} >$	$< H_5 + H_6 >_{7/2}$	$< H_5 + H_6 >_{5/2}$
Z=11							
$1s^23s$	119.02644449	–0.1779344	0.0076547	–0.0004667	0.0000337		
$1s^24s$	116.91390050	–0.1744332	0.0075615	–0.0004609	0.0000329		
$1s^25s$	115.95278318	–0.1731020	0.0075292	–0.0004590	0.0000326		
$1s^24f$	116.81300405	–0.1718913	0.0074968	–0.0004566	0.0000323	0.0000975	–0.0001300
$1s^25f$	115.90171628	–0.1718143	0.0074968	–0.0004567	0.0000323	0.0000499	–0.00006654
Z=12							
$1s^23s$	142.48595706	–0.2550372	0.0100856	–0.0005621	0.0000355		
$1s^24s$	139.89472480	–0.2498072	0.0099595	–0.0005550	0.0000346		
$1s^25s$	138.71395366	–0.2478300	0.0099157	–0.0005527	0.0000344		
$1s^24f$	139.78182394	–0.2460220	0.0098716	–0.0005497	0.0000340	0.0001486	–0.0001981
$1s^25f$	138.65678319	–0.2458897	0.0098715	–0.0005499	0.0000340	0.0000761	–0.0001014
Z=13							
$1s^23s$	168.05659174	–0.3548436	0.0129832	–0.0006663	0.0000344		
$1s^24s$	164.93804858	–0.3473524	0.0128170	–0.0006580	0.0000336		
$1s^25s$	163.51511777	–0.3445079	0.0127597	–0.0006550	0.0000333		
$1s^24f$	164.81313368	–0.3419049	0.0127015	–0.0006513	0.0000330	0.0002175	–0.0002900
$1s^25f$	163.45184042	–0.3417112	0.0127012	–0.0006516	0.0000330	0.0001114	–0.0001485

Table 2 (*Continued*)

Z=14							
$1s^2 3s$	195.73834667	−0.4814139	0.0163896	−0.0007796	0.0000359		
$1s^2 4s$	192.04387376	−0.4710131	0.0161761	−0.0007695	0.0000351		
$1s^2 5s$	190.35628271	−0.4670540	0.0161024	−0.0007660	0.0000347		
$1s^2 4f$	191.90693564	−0.4634449	0.0160274	−0.0007616	0.0000344	0.0003081	−0.0004108
$1s^2 5f$	190.28689019	−0.4631724	0.0160274	−0.0007617	0.0000344	0.0001577	−0.0002103
Z=15							
$1s^2 3s$	225.53121771	−0.6391783	0.0203453	−0.0009016	0.0000349		
$1s^2 4s$	221.21219912	−0.6250986	0.0200770	−0.0008895	0.0000341		
$1s^2 5s$	219.23744284	−0.6197108	0.0199832	−0.0008856	0.0000338		
$1s^2 4f$	221.06323092	−0.6148307	0.0198885	−0.0008805	0.0000334	0.0004243	−0.0005658
$1s^2 5f$	219.16193339	−0.6144644	0.0198884	−0.0008809	0.0000334	0.0002172	−0.0002897
Z=16							
$1s^2 3s$	257.43520630	−0.8328975	0.0248913	−0.0010325	0.0000363		
$1s^2 4s$	252.44302340	−0.8142201	0.0245574	−0.0010189	0.0000354		
$1s^2 5s$	250.15860221	−0.8070835	0.0244423	−0.0010139	0.0000350		
$1s^2 4f$	252.28202128	−0.8005908	0.0243243	−0.0010080	0.0000347	0.0005708	−0.0007610
$1s^2 5f$	250.07697182	−0.8001053	0.0243243	−0.0010084	0.0000347	0.0002922	−0.0003896
Z=17							
$1s^2 3s$	291.45030779	−1.0676743	0.0300688	−0.0011723	0.0000353		
$1s^2 4s$	285.73634925	−1.0433721	0.0296608	−0.0011566	0.0000345		
$1s^2 5s$	283.11975996	−1.0340581	0.0295196	−0.0011511	0.0000342		
$1s^2 4f$	285.56330737	−1.0255950	0.0293754	−0.0011441	0.0000338	0.0007522	−0.0010029
$1s^2 5f$	283.03200610	−1.0249713	0.0293754	−0.0011446	0.0000338	0.0003851	−0.0005134
Z=18							
$1s^2 3s$	327.57652526	−1.3488880	0.0359185	−0.0013211	0.0000329		
$1s^2 4s$	321.09216719	−1.3177782	0.0354265	−0.0013031	0.0000321		
$1s^2 5s$	318.12091541	−1.3058357	0.0352563	−0.0012968	0.0000318		
$1s^2 4f$	320.90708947	−1.2950055	0.0035082	−0.0012889	0.0000314	0.0009737	−0.0012983
$1s^2 5f$	318.02703652	−1.2942458	0.0035082	−0.0012894	0.0000314	0.0004985	−0.0006646
Z=19							
$1s^2 3s$	365.81385491	−1.6823881	0.0424831	−0.0014785	0.0000357		
$1s^2 4s$	358.51050043	−1.6430739	0.0418955	−0.0014585	0.0000348		
$1s^2 5s$	355.16206989	−1.6279843	0.0416920	−0.0014510	0.0000345		
$1s^2 4f$	358.31336871	−1.6143085	0.0414830	−0.0014422	0.0000341	0.0012409	−0.0016545
$1s^2 5f$	355.06206416	−1.6133448	0.0414833	−0.0014429	0.0000341	0.0006353	−0.0008470
Z=20							
$1s^2 3s$	406.16229504	−2.0742445	0.0498008	−0.0016449	0.0000367		
$1s^2 4s$	397.99131663	−2.0251961	0.0491066	−0.0016224	0.0000358		
$1s^2 5s$	394.24322401	−2.0063963	0.0488659	−0.0016143	0.0000355		
$1s^2 4f$	397.78214535	−1.9893424	0.0486190	−0.0016042	0.0000351	0.0015597	−0.0020795
$1s^2 5f$	394.13708933	−1.9881231	0.0486193	−0.0016049	0.0000351	0.0007985	−0.0010646

Using the wavefunctions obtained above, the expectation values of the relativistic operators, including the mass-polarization operator, are computed using Eq.(5). The relativistic energy including the kinetic-energy correction, the Darwin term, the electron–electron contact term, and the orbit–orbit interaction are evaluated perturbatively as first-order correction. The non-relativistic energy, term energy of relativistic correction and mass-polarization are shown in Table 2. The excitation energies of the $1s^2nl$ are obtained by subtracting the $1s^2nl$ energies from the $1s^22s$ energies and are given in Table 3 for $1s^2ns$ (n=3,4,5) and Table 4 for $1s^2nf$ (n=4,5). The quantum electrodynamic correction to the excitation energies is esti-

mated by using the effective nuclear charge formula of hydrogen-like atomic systems.[9] The experimental data and the other theoretical results are also listed in these tables. To sum up the comparison between our predicted excitation energies and the available experimental data in the literature, we find that our results agree better with the more recent experimental data. In the case of the $1s^2ns$, the agreement is up to the fourth significant figure. It is also found from Table 4 that our predicted excitation energies agree with the results of Vainshtein and Sofronova. In particular our results of the $1s^2nf$ states are in fairly good agreement with the experimental data. No experimental data are found for the $1s^2nf$ systems with $Z > 16$.

Table 3. Excitation energies (in cm^{-1}) of lithium-like $1s^2ns$ states and a comparison with experimental data and other theoretical results.

Z	This work	Experiment & other theory	This work	Experiment & other theory	This work	Experiment & other theory
		$1s^23s$		$1s^24s$		$1s^25s$
11	1375932.6	1375944[a]	1840302.1	1840336[a]	2051517.8	20515201[b]
		1375950[b]		1840350[b]		2051922 [a]
		1375923[c]		1840310[c]		2051230 [d]
		1375953[d]		1839910[d]		
12	1682796.1	1682700[e]	2252589.1	2252595[c]	2512148.4	2511600[a]
		1682648[a]		2252140[d]		2511600[e]
		1682786[c]				2511820[d]
		1682811[d]				
13	2020552.4	2020550[c]	2706554.0	2706589[c]	3019445.0	3019070[a]
		2020450[e]		2705600[a]		3019700[e]
		2020460[a]		2705700[e]		3019070[d]
		2020460[d]		2706060[d]		
14	2389261.8	2389293[c]	3202280.5	3202331[c]	3573493.8	3573500[a]
		2388850[a]		3202100[f]		3573450[f]
		2388870[f]		3201750[d]		3573100[d]
		2389280[d]				
15	2789032.7	2789110[c]	3739904.7	3740002[c]	4174474.7	4174020[d]
		2788600[a]		3709400[a]		
		2788650[g]		3740040[g]		
		2789056[d]		3739400[d]		
16	3219950.1	3220100[h]	4319542.0	4319701[c]	4822421.1	4822550[h]
		3231100[a]		4319700[h]		4821980[d]
		3220094[c]		4332800[a]		
		3219983[d]		4318940[d]		
17	3682125.8	3682361[c]	4941328.8	4941573[c]	5517575.7	5517100[d]
		3698000[a]		4934600[a]		
		3682163[d]		4940700[d]		
18	4175667.4	4176024[c]	5605409.2	5605760[c]	6260059.0	6259560[d]
		4175705[d]		5604710[d]		
19	4700651.9	4701197[c]	6311896.8	6312400[a]	7050002.1	7049510[d]
		4701220[a]		6312406[c]		
		4700725[d]		6311220[d]		
20	5257241.3	5258020[a]	7060995.0	7061700[a]	7887611.3	7887130[d]
		5258025[c]		7061697[d]		
		5257352[d]		7060310[d]		

[a] Ref.[11], [b] Ref.[12], [c] Ref.[10], [d] Ref.[13], [e] Ref.[14], [f] Ref.[15], [g] Ref.[16], [h] Ref.[17].

Table 4. Excitation energies (in cm^{-1}) of lithium-like $1s^2nf$ states and a comparison with experimental data.

Z	This work	Experiment	This work	Experiment
	$1s^24f$		$1s^25f$	
11	1882978.6	1882961[a]	2062995.3	
12	2278162.1	2278150[b]	2525103.3	2525045[c]
		2278110[c]		
13	2735116.1	2735100[b]	3033921.7	3033737[c]
		2734939[c]		
14	3233931.4	3233500[b]	3589543.0	3590000[b]
		3233770[d]		3589450[f]
15	3774769.9	3774427[e]	4192129.4	
16	4357765.0	4357805[f]	4841815.5	4841818[c]
17	4983080.1		5538764.6	
18	5650870.8		6283127.4	
19	6361288.2		7075068.4	
20	7114548.9		7914802.7	

[a] Ref.[13], [b] Ref.[12], [c] Ref.[14], [d] Ref.[15], [e] Ref.[16], [f] Ref.[17].

The fine-structure splits of the $1s^2nf$ states are calculated by using the same method above. They are given together with a comparison of the theory and experimental in Table 5. Our results follow a well-behaved isoelectronic regularity. For the $1s^24f$ states, our results agree with the results of Edlen[10] and with most data available in the literature.[11–18] However, the datum for Z=15 (in 140cm^{-1})[16] 20cm^{-1} smaller than that for Z=14.[15] No experimental data are available for the systems from Z=17–20. For the $1s^25f$ states, our calculated splitting values are in agreement with the data in Refs.[12] and [13]. In the case of Z=11,14,15 and 18–20. No experimental data are available. The theoretical results of the fine-structure splits for the $1s^2nf$ (n=4,5) states and some experimental data are depicted in Fig.1.

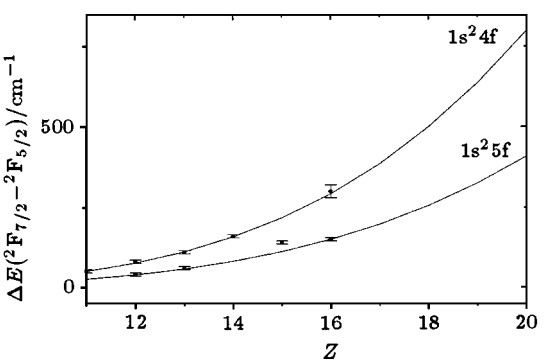


Fig.1. The fine-structure splits of $1s^2nf$ (n=4,5) for the lithium-like systems from Z=11–20. The full curve, FCPC; the experimental data refer to the literature Z=11 (Ref.[13]),12,13 (Ref.[14]), 14 (Ref.[15]), 15 (Ref.[16]), 16 (Ref.[17]).

Table 5. Fine-structure splitting ($\Delta E=E_{7/2}-E_{5/2}$) for $1s^2nf\ ^2F$ states of lithium-like systems (in cm^{-1}).

	Z	11	12	13	14	15
$1s^24f$	This work	50.039	76.265	111.658	158.139	217.812
	Experiment	50[a]	80[b]	110[b]	160[c]	140[d]
	Edlen[10]	49.9	76.1	111.4	157.7	
$1s^25f$	This work	25.616	39.042	57.161	80.959	111.509
	Experiment		40[b]	60[b]		
	Z	16	17	18	19	20
$1s^24f$	This work	292.967	386.074	499.786	636.94	800.56
	Experiment	300[e]				
$1s^25f$	This work	149.984	197.650	255.869	326.090	409.850
	Experiment	150[e]				

[a] Ref.[13], [b] Ref.[14], [c] Ref.[15], [d] Ref.[16], [e] Ref.[17].

In conclusion, we have extended the FCPC method to calculate the excitation energies, term energies and the fine-structure splits for lithium-like atomic systems from Z=11–20. Our calculated excitation energies agree closely with the theoretical results obtained by $1/Z$ expansion method in Ref.[10]. The agreement of our results with the experimental data available in the literature is usually better than a few hundred cm^{-1}. Our calculated fine-structure splits for lithium-like $1s^2nf$ (n=4,5) states follow a well behave isoelectronic trend. However, the comparison with the experimental data indicates that some data of $1s^2nf$ states deviate significantly from this isoelectronic regularity. Recently, we had calculated the excitation energies and term energies of the excited states $1s^2nd$ (n=3,4,5) of lithium-like systems from Z=11–20 by using our FCPC wavefunctions.[8,19] These results show that the FCPC method is effective for calculations involving lithium-like systems with higher nuclear charges.

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