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Four-parameter analytical local model potential for atoms*

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Analytical local model potential for modeling the interaction in an atom reduces the computational effort in electronic structure calculations significantly. A new four-parameter analytical local model potential is proposed for atoms Li through Lr, and the values of four parameters are shell-independent and obtained by fitting the results of X_a method. At the same time, the energy eigenvalues, the radial wave functions and the total energies of electrons are obtained by solving the radial Schrödinger equation with a new form of potential function by Numerov's numerical method. The results show that our new form of potential function is suitable for high, medium and low Z atoms. A comparison among the new potential function and other analytical potential functions shows the greater flexibility and greater accuracy of the present new potential function.

Keywords: analytical local potential, atomic structure
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1. Introduction

In recent years, a lot of work has been done to investigate the properties of ground and excited states of atoms.[1−5] Numerical methods, such as Hartree–Fock (HF), X_a and density functional theory (DFT) methods give good results for atomic structure calculations.[6−9] An alternative to the HF method is given by the optimized effective potential (OEP) method proposed by Sharp and Horton[10] as a variational alternative to Slater's simplified treatment of the exchange term in the HF equations on average in the occupied orbitals.[11] In the OEP method the orbitals must satisfy a single particle equation with a certain local potential, which is the same for all the electrons. At first, the OEP was reformulated[12] and implemented[13,14] by numerically solving the integral equation (NOEP). Latter, the OEP equations were solved based on an analytical parameterization of the potential (POPE).[15−18] Sarsa[18] has obtained good results in the calculation of the ground state of atoms with POEP method , but its analytical potential function contains many adjustable parameters.

Analytical local potentials for modeling the electron-electron interaction in an atom reduce significantly the computational effort in electronic structure calculation. With these local potentials, Hartree–Fock-like equations for the determination of orbitals are easily solvable. The development of these potentials has a long history. In 1969[19] Green *et al* presented a very successful shell-independent model potential with a simple analytical form, which has been used for calculating the electron-atom scattering and the atom-ion scattering,[20,21] electron-impact excitation and ionization,[22−24] oscillator strengths,[22] antiproton-atomic collisions[25] and electron-capture processes.[26,27] However, due to its simple form, there are obvious differences between Green's eigenvalues and HF eigenvalues for neutral atoms, especially for outer shell electrons, though the parameters of Green's potential are obtained by fitting the HF eigenvalues. In 2002[28,29] Neugebauer *et al* explored a shell-dependent parameterization of Green's potential, and the results showed that shell-dependent analytical model potentials could improve orbitals and energy expectation values. However, the shell-dependent an-

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alytical potentials contain a large number of fitting parameters.

It is clear that the form of Green's potential function is too simple to give accurate results and the analytical potential of numerical parametrized optimized effective potential (POEP) method contains many adjustable parameters though good results are obtained. Both of them are inconvenient to extend and use. Thus, the development of an accurate analytical model potential in a simple form is highly desirable.

A new four-shell-independent parameter analytical local model potential is proposed in the present work. The values of four-adjustable parameters are fixed by fitting the results of X_a method. We systematically make calculations for the ground state configuration of the Li through Lr atoms with a new potential function. The energy eigenvalues, the radial wave functions and the total energies of the electrons are obtained by solving the radial Schrödinger equation with Numerov's method. Calculation results are consistent with the results of X_a method, which demonstrates that the new potential function is suitable for low, medium and high Z atoms. A comparison between the present potential function and the Green's potential function shows the greater flexibility and greater accuracy of the present potential function.

The rest of the present paper is organized as follows. In Section 2, the key equations and Green's potential function are summarized briefly; the analysis of the present new potential function is carried out. In Section 3, the energy eigenvalues, the radial wave functions and the total energies of electrons are obtained by the numerical solution of Schrödinger equation with a new form of potential function, and the results are presented and analysed. Finally, a conclusion will be given in Section 4. Atomic units are used throughout the present paper.

2. Analytical local model potential

2.1. The Green's potential

In the independent particle model approximation, the one-electron radial Schrödinger equation is

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l\left(l_+1\right)}{2r^2}+V\left(r\right)-E_{nl}\right)P_{nl}\left(r\right)=0, \quad (1)$$

where n is principal quantum number, l is angular momentum quantum number, r is the radial variable, E_{nl} is the energy eigenvalue, and $V(r)$ is a central atomic potential due to the Z units of nuclear charge and the average effect of the remaining core electrons.

The analytical local potential proposed by Green *et al* in 1969[19] is as follows:

$$V^{\mathrm{Green}}\left(r\right)=-\frac{1}{r}\left[1+\frac{Z-1}{H\left[\exp\left(r/d\right)-1\right]+1}\right], \quad (2)$$

where Z is the number of nuclear charges, r is the radial variable, and H and d are adjustable parameters. The adjustable parameters H and d are evaluated by the HF eigenvalues. For neutral atoms, it is convenient to express H in the form

$$H=d\alpha N^{0.4}, \quad (3)$$

where d is adjusted for each element and the parameter $\alpha=1.05$ for Hatree–Foch–Slater (HFS) and 1.00 for HF models respectively.

2.2. The new potential

The new potential function has the form

$$V\left(r\right)=-\frac{Z-1}{r}\left[1-\alpha+\alpha\exp\left(\beta r^{\delta}+\gamma r^{2\delta}\right)\right]^{-1}-\frac{1}{r}, \quad (4)$$

where Z is the number of nuclear charges, r is radial variable, and δ, α, β and γ are adjustable parameters. The corrcet short- and long-range asymptotic potentials

$$V\left(r\right)\to-\frac{Z}{r} \quad \text{as} \quad r\to 0, \quad (5)$$

$$V\left(r\right)\to-\frac{1}{r} \quad \text{as} \quad r\to\infty, \quad (6)$$

are simultaneously satisfied.

In order to investigate the accuracy of new potential function, we make calculations for neutral atoms from Z=3 to Z=103. The values of four parameters are fixed by fitting the results of X_a method, because a rather accurate central potential is given by the X_a method.[7] Calculation results are compared with those obtained by the Green and X_a methods. Listed in Table 1 are the values of four parameters and the average relative deviations among two kinds of analytical local potentials and X_a potential. It can be seen from Table 1 that the values of Δ_G are larger than the values of Δ_N for each atom. For the Green's potential function, the value of Δ_G varies nearly 5% for light atoms with $Z\leq 57$ and varies nearly 2% for heavy atoms with $Z\geq 58$. The average value of Δ_G is 2.0779% for all calculated atoms. While, for a new potential function, the average value of Δ_N is 1.0440%. More importantly, for all calculated atoms, the value of Δ_N changes nearly 1%, which means that the new

potential function is suitable for high, medium and low Z atoms.

For making a clear comparison between the new potential function and Green's potential function, the absolute values of the product of the radial coordinate and the potential $|rV(r)|$ for neutral atoms with Z=10, 30, 50, 70 are shown in Fig.1. Further, in Fig.2, the values of relative deviation η_i among two kinds of

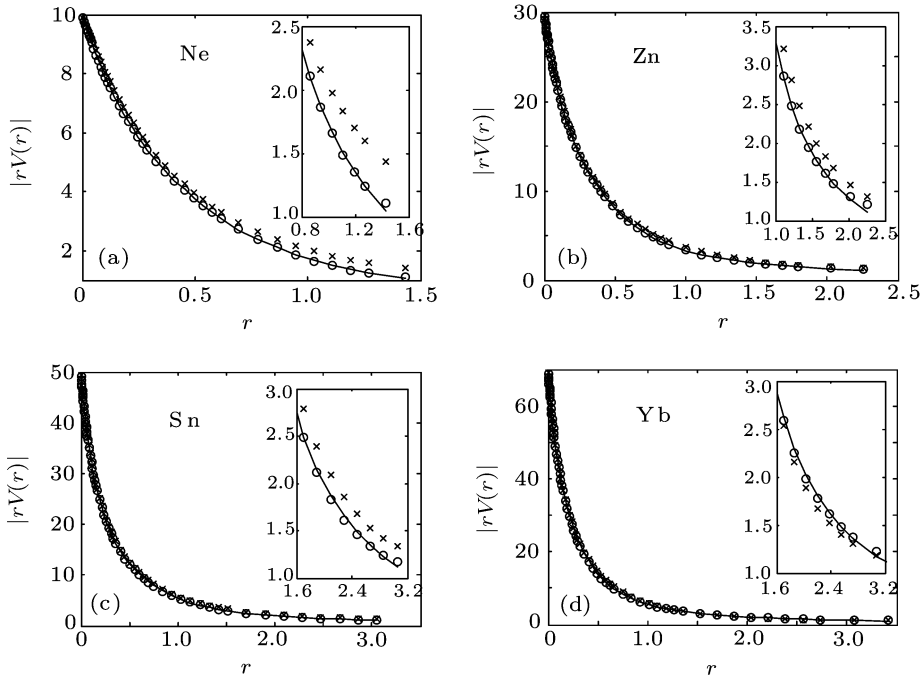


Fig.1. Absolute values of the product of the radial coordinate and the potential $|rV(r)|$ for neutral atoms with Z = 10, 30, 50, 70. Comparison among Green's potential[19] (cross), present new potential (open circles) and X_a potential[7] (solid line). Data are in atomic units (a.u.).

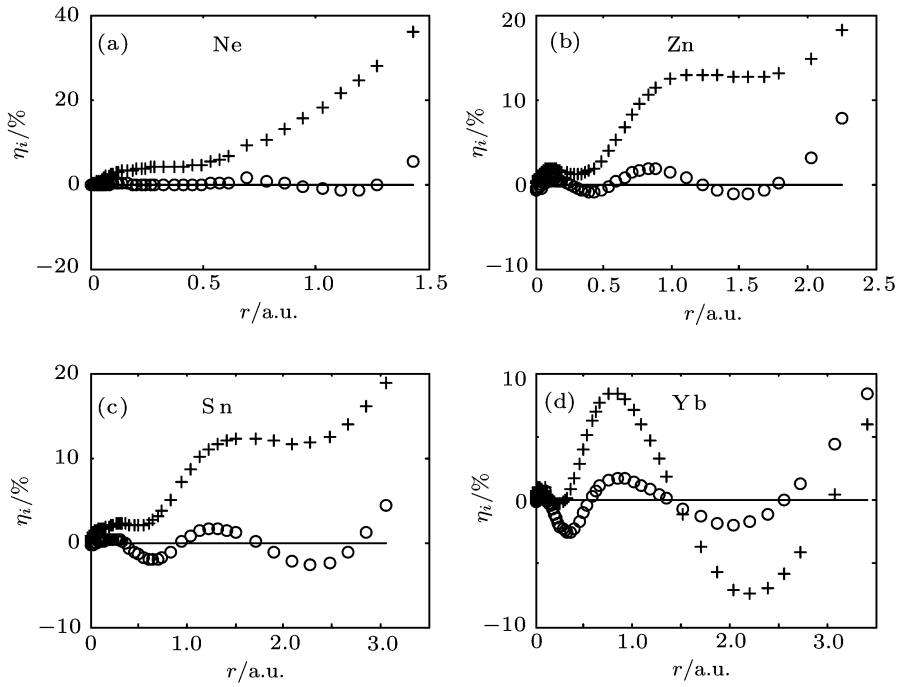


Fig.2. Values of Relative deviations η_i (i=G, N) among two kinds of analytical local potentials and X_a potential[7] for neutral atoms with Z = 10, 30, 50, 70. $\eta_i = [V_i(r_k) - V_{Xa}(r_k)]/V_{Xa}(r_k)$, i=G denotes Green's potential[19] (cross), and i=N denotes the present new potential (open circles).

Table 1. Values of four parameters δ, α, β and γ to fit X_a potential and the average relative deviations among two kinds of analytical local potentials and X_a potential for neutral atoms with $3 \leq Z \leq 103$. Δ_i (i=G, N), $\Delta_{\rm G}$ (Green's potential),[19] $\Delta_{\rm N}$ (New potential), $\Delta_i = 100\% \times \frac{1}{M}\sum_{K=1}^{M} |[V_i(r_k) - V_{Xa}(r_k)]/V_{Xa}(r_k)|$, where M is the total number of data points.

Z	symbol	δ	α	β	γ	$\Delta_{\rm G}$/%	$\Delta_{\rm N}$/%
3	Li	1.0255	1.7402	1.0543	0.7165	8.8849	0.8306
4	Be	1.0560	3.2043	0.6541	0.1994	6.6840	0.5569
5	B	0.9963	2.6683	0.7537	0.1432	5.5881	1.1800
6	C	1.0092	2.6421	0.7999	0.1703	4.5672	1.2389
7	N	0.9093	2.2503	0.7809	0.4286	5.1119	1.5765
8	O	0.8714	1.4099	1.1924	0.5415	6.7901	1.7691
9	F	0.8740	1.4315	1.2471	0.6790	5.6759	1.4557
10	Ne	0.8468	1.2742	1.3428	0.9436	6.3688	1.5090
11	Na	0.9729	2.5434	1.0406	0.4685	6.4675	0.6983
12	Mg	1.0173	5.7432	0.5362	0.2861	4.3097	0.5401
13	Al	1.0422	2.9955	1.1566	–0.02379	3.7862	0.6184
14	Si	1.0289	6.8858	0.5011	0.1153	3.9867	1.1020
15	P	1.0362	5.9601	0.6015	0.0781	3.9314	1.0416
16	S	0.9821	5.6607	0.5642	0.1545	4.6158	1.5816
17	Cl	0.9463	3.9064	0.7593	0.2144	5.4848	2.0779
18	Ar	0.9458	3.4947	0.8528	0.2209	5.6621	2.0143
19	K	0.9172	4.1728	0.6845	0.2280	6.2515	1.5744
20	Ca	0.9110	4.8667	0.5935	0.1864	6.1920	1.4321
21	Sc	0.9192	4.2164	0.7007	0.1804	6.0075	1.2366
22	Ti	0.9134	3.8597	0.7557	0.2050	5.7316	0.8872
23	V	0.9084	3.7757	0.7757	0.2386	5.8935	0.7754
24	Cr	0.8902	3.0923	0.9032	0.3309	5.3174	0.8495
25	Mn	0.9241	3.2710	0.9481	0.2527	5.5597	0.6321
26	Fe	0.9293	3.1737	1.0041	0.2719	5.5954	0.7038
27	Co	0.9210	4.7646	0.6539	0.3964	5.5174	0.8050
28	Ni	0.9061	5.5142	0.5386	0.4692	5.3910	0.8997
29	Cu	0.9135	4.0060	0.7733	0.5658	5.1467	0.9304
30	Zn	0.8856	6.0057	0.4627	0.5901	4.7065	0.9326
31	Ga	0.8975	10.9018	0.2594	0.4183	3.5218	1.1650
32	Ge	0.9076	12.9730	0.2311	0.3480	3.0695	1.2882
33	As	0.8714	13.9804	0.1930	0.3502	3.0640	1.3536
34	Se	0.9449	11.8586	0.3023	0.2962	3.1735	1.4896
35	Br	0.9527	11.9754	0.3129	0.2879	3.0104	1.2482
36	Kr	0.9920	8.8218	0.4895	0.2594	3.3763	1.3933
37	Rb	0.9708	13.9706	0.2909	0.2215	3.0079	1.2982
38	Sr	0.9959	16.9567	0.2648	0.1439	3.2482	1.2723
39	Y	1.0198	10.9673	0.4502	0.1130	3.1249	1.3042
40	Zr	1.0107	9.9255	0.4873	0.1224	2.7347	1.0472
41	Nb	0.9962	6.9426	0.6734	0.1432	3.1703	1.2363
42	Mo	0.9764	7.8890	0.5602	0.1967	3.4722	1.0612
43	Tc	0.9806	7.0921	0.6387	01749	3.9185	1.0384
44	Ru	0.9691	5.0607	0.8689	0.1929	4.2709	0.9905
45	Rh	0.9503	5.1819	0.8065	0.2652	4.8541	1.1091
46	Pd	0.9400	4.3169	0.9246	0.3200	5.4245	1.5915
47	Ag	0.9323	4.9035	0.8144	0.3462	5.3769	0.9593
48	Cd	0.9498	4.9570	0.8603	0.2844	5.5811	0.7135
49	In	0.9478	8.7841	0.4815	0.2901	5.0954	0.7817
50	Sn	0.9553	9.5168	0.4589	0.2546	4.4701	0.7503
51	Sb	0.9546	10.1522	0.4319	0.2403	4.4536	0.7327

Table 1. (*Continued*).

Z	symbol	δ	α	β	γ	Δ_G/%	Δ_N/%
52	Te	0.9528	9.9821	0.4402	0.2369	4.7533	0.7183
53	I	0.9628	7.0326	0.6522	0.2070	5.2517	0.7619
54	Xe	0.9577	5.9994	0.7593	0.1939	5.9755	0.8798
55	Cs	0.9447	14.7149	0.2944	0.1934	5.4734	0.9492
56	Ba	0.9586	15.9839	0.2867	0.1494	4.5790	1.0465
57	La	0.9609	16.9743	0.2735	0.1361	4.7615	0.9295
58	Ce	0.9370	18.9196	0.2268	0.1591	3.7953	0.8293
59	Pr	0.9455	18.9519	0.2321	0.1744	3.3165	0.9774
60	Nd	0.9324	17.9913	0.2367	0.1969	3.2979	1.0216
61	Pm	0.9109	19.9928	0.1973	0.2134	3.0245	0.9440
62	Sm	0.8876	19.9646	0.1798	0.2433	2.8517	0.9181
63	Eu	0.8986	19.9884	0.1893	0.2435	2.7037	0.9546
64	Gd	0.8940	19.9819	0.1864	0.2450	2.9361	1.0818
65	Tb	0.8703	19.9931	0.1678	0.2899	4.1306	1.0640
66	Dy	0.8824	20.9639	0.1673	0.2862	2.2504	1.1253
67	Ho	0.8676	21.0008	0.1580	0.3063	2.2862	1.1645
68	Er	0.8707	21.9785	0.1507	0.3092	2.3481	1.2076
69	Tm	0.8860	23.0001	0.1539	0.3008	2.4213	1.2542
70	Yb	0.8704	22.0040	0.1513	0.3306	2.5397	1.3173
71	Lu	0.8751	25.9884	0.1303	0.2872	2.8092	1.1707
72	Hf	0.8580	24.0050	0.1344	0.3089	2.7918	1.1099
73	Ta	0.8795	23.9716	0.1483	0.2950	2.6436	1.0711
74	W	0.8780	22.0139	0.1634	0.3097	2.5165	1.0893
75	Re	0.8992	20.0287	0.1970	0.3175	2.3756	1.1335
76	Os	0.9028	19.9898	0.2017	0.3162	2.1327	0.8190
77	Ir	0.8968	17.0599	0.2365	0.3538	2.4899	0.8439
78	Pt	0.9418	13.9300	0.3418	0.3649	3.5052	0.7789
79	Au	0.9177	12.8450	0.3406	0.4211	3.9776	0.7361
80	Hg	0.9355	13.9998	0.3382	0.3671	3.9305	0.7628
81	Ti	0.8475	16.1516	0.2104	0.4142	2.8517	0.6893
82	Pb	0.8906	20.9939	0.1898	0.3111	2.2279	0.5490
83	Bi	0.9678	24.9990	0.1892	0.2383	2.2061	0.5520
84	Po	0.6864	12.4817	0.1174	0.5990	2.2086	0.7329
85	At	0.9581	24.9772	0.2087	0.2084	2.2554	0.7874
86	Rn	0.9909	19.9474	0.2950	0.1967	2.5749	0.9857
87	Fr	0.9678	26.9093	0.2026	0.1711	2.5461	1.0731
88	Ra	0.6315	14.0044	0.06418	0.5459	3.1269	1.1678
89	Ac	0.9976	35.9796	0.1679	0.1086	2.9454	1.4464
90	Th	1.0138	29.9907	0.2152	0.1034	2.7192	1.2741
91	Pa	0.9653	32.9949	0.1662	0.1381	2.3103	0.7947
92	U	0.9616	30.9674	0.1755	0.1493	2.1654	0.7669
93	Np	0.9553	28.9947	0.1848	0.1630	2.1025	0.6565
94	Pu	0.9354	25.9949	0.1923	0.2038	2.1868	0.7082
95	Am	0.9223	27.9758	0.1694	0.2107	2.3375	0.8055
96	Cm	0.9338	25.9827	0.1923	0.2058	2.3393	0.7009
97	Bk	0.9214	23.9906	0.1985	0.2450	3.9202	0.9282
98	Cf	0.9061	23.0046	0.1965	0.2690	2.7545	0.8686
99	Es	0.8988	21.9993	0.2004	0.2885	2.9034	0.9814
100	Fm	0.8965	21.9932	0.1977	0.3004	3.0476	1.1001
101	Md	0.8994	22.0035	0.1990	0.3073	3.1821	1.2182
102	No	0.8781	21.0196	0.1921	0.3421	3.3146	1.3409
103	Lr	0.9013	24.9899	0.1764	0.2863	3.1196	1.3850
average						3.9194	1.0440

analytical local model potentials and the X_a potential for neutral atoms with Z=10, 30, 50, 70 are plotted. As can be seen from Figs.1 and 2, in these cases, the differences among three kinds of potentials are small in a region of small atomic radius r and increase with atomic radius r increasing. On the whole, the relative deviations between the Green's potential and the X_a potential $\eta_{\rm G}$ are larger than those between the new potential and the X_a potential $\eta_{\rm N}$. In summary, our new form of potential function is better than Green's potential function in the sense of the accuracy of potential, and it is suitable for high, medium and low Z atoms.

3. Energy eigenvalues, radial wave functions and total energies of electrons

In order to demonstrate the accuracy of our new potential further, the new form of potential function is used for solving the radial Schrödinger equation by Numerov's method.[30−32] The energy eigenvalues, the radial wave functions and the total energies of electrons are obtained. A comparison between the energy eigenvalues and the total electronic energies for atoms with Z=10, 30, 50 and 70 are listed in Table 2 and Table 3 respectively. Radial wave functions and their comparisons with the results obtained from the X_a method for Yb atom are shown in Fig.3.

As can be seen from Table 2, there are obvious differences between Green's energy eigenvalues and HF eigenvalues especially for out-shell electrons, despite the fact that the parameters of Green's functions are fixed by fitting the energies of the HF equations. The average relative deviation of energy eigenvalues between the Green's model and the HF method is 5.14% for all calculated electronic shells listed in Table 2. While the energy eigenvalues obtained with our model accord well with the results from the X_a method and the POEP method. The accuracy of energy eigenvalues of outer-shell electrons is improved greatly. For all calculated electronic shells listed in Table 2, the average relative deviation of energy eigenvalues between our model and the X_a method is only 1.44%. It should be noted that X_a energy eigenvalues are found to be appreciably different from the eigenvalues obtained by the HF method: the difference increases with further going into the inner shells of the atom. The above differences were caused by the difference between the relations for the total energy and energy eigenvalues in the X_a method, and that in the HF method.[33] This is why our energy eigenvalues are consistent with the results obtained by the X_a method and the PEOP methods, but differ from the results obtained by the Green' model and the HF method. However, these differences do not influence the calculation of the total electronic energies of atoms, which has been proved by total electronic energy calculations for atoms with Z=10, 30, 50 and 70, and the results are listed in Table 3. The differences of total energies between our model and the HF method are small. The new local model potential has almost as accurate as the X_a method. From Fig.3, we can see that the radial wave functions of Yb atoms are consistent with the results of X_a method. The accuracy of new potential has been proved again. In summary, the eigenvalues, the radial wave functions and the total energies of electrons obtained by our new local model potential are in consistent with the results obtained by the X_a method. Moreover, our calculations involve heavy, medium and light atoms, for which almost the same accuracy are achieved.

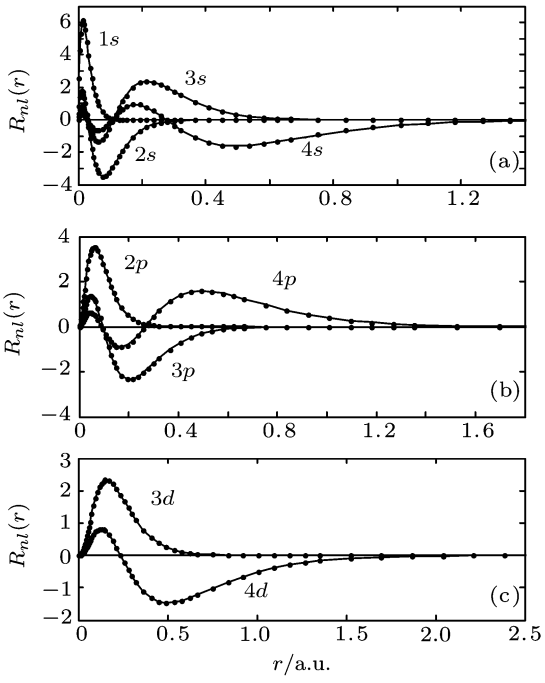


Fig.3. Comparison among radial wave functions $R_{nl}(r)$ of Yb atom. Solid lines denote results of this work and dot lines denote results obtained by X_a method [7]. (a): n=1, 2, 3, 4, l=0, (b): n= 2, 3, 4, l=1, (c): n= 3, 4, l=2.

Table 2. Comparison among energy eigenvalues for Z=10, 30, 50 and 70.

shell	HFS[a]	HF[b]	Green[c]	POEP[d]	X_a[e]	this work
			Z=10, Ne			
1s	–31.50	–32.77	–32.12	–30.87	–30.68	–30.57
2s	–1.59	–1.93	–1.77	–1.72	–1.42	–1.39
2p	–0.74	–0.85	–0.94	–0.85	–0.60	–0.60
			Z=30, Zn			
1s	–349.20	–353.30	–352.80	–345.27	–345.50	–343.82
2s	–42.56	–44.36	–43.18	–41.69	–41.66	–41.47
2p	–37.78	–38.93	–38.77	–36.75	–36.78	–37.05
3s	–4.90	–5.64	–5.25	–4.82	–4.62	–4.60
3p	–3.33	–3.84	–3.70	–3.24	–3.06	–3.09
3d	–0.63	–0.79	–0.88	–0.55	–0.43	–0.39
4s	–0.31	–0.30	–0.36	–0.28	–0.27	–0.27
			Z=50, Sn			
1s	–1034.50	–1041.00	–1042.50	–1028.35	–1028.00	–1024.82
2s	–153.90	–157.00	–156.50	–151.80	–151.80	–151.45
2p	–144.40	–146.50	–147.80	–141.96	–142.10	–142.03
3s	–30.03	–31.61	–30.76	–29.40	–29.21	–29.06
3p	–26.04	–27.22	–26.90	–25.36	–25.21	–25.11
3d	–18.58	–19.17	–19.39	–17.88	–17.74	–17.67
4s	–4.88	–5.52	–5.17	–4.70	–4.58	–4.55
4p	–3.53	–3.98	–3.83	–3.36	–3.25	–3.23
4d	–1.27	–1.38	–1.52	–1.15	–1.03	–1.04
5s	–0.46	–0.48	–0.54	–0.48	–0.39	–0.38
5p	–0.22	–0.25	–0.27	–0.25	–0.17	–0.17
			Z=70, Yb			
1s	–2095.00	–2104.50	–2108.00	–	–2085.00	–2077.73
2s	–341.45	–346.00	–343.25	–	–338.20	–340.04
2p	–277.00	–330.20	–330.25	–	–323.40	–327.31
3s	–76.70	–79.20	–76.30	–	–75.55	–74.00
3p	–70.00	–71.95	–69.75	–	–68.78	–67.59
3d	–57.35	–56.60	–56.70	–	–56.11	–55.28
4s	–14.80	–16.10	–15.40	–	–14.33	–13.96
4p	–12.04	–13.09	–12.67	–	–11.58	–11.29
4d	–7.01	–7.66	–7.56	–	–6.59	–6.35
4f	–0.51	–0.74	–0.97	–	–0.30	–0.29
5s	–1.87	–2.10	–1.93	–	–1.69	–1.68
5p	–1.13	–1.21	–1.14	–	–0.97	–0.96
6s	–0.19	–0.18	–0.18	–	–0.16	–0.17

[a]Results of Hatree–Fock method were cited from Ref.[19].
[b]Results of Hatree–Fock–Slater method were cited from Ref.[19].
[c]Results of Green's local potential method were cited from Ref.[19].
[d]Results of parametrized optimized effective potential method were cited from Ref [18].
[e]Results of X_a method were cited from Ref.[7].

Table 3. Total elecrtonic energies for neutral atoms with Z=10, 30, 50 and 70.

Z	symbol	HF[a]	X_a[b]	this work
10	Ne	–128.55	–128.51	–128.50
30	Zn	–1777.85	–1777.74	–1777.67
50	Sn	–6022.90	–6022.78	–6022.84
70	Yb	–13391.46	–13391.00	–13390.07

[a] Exact HF energies were cited from Ref.[6].
[b]X_a energies were cited from Ref.[7].

4. Conclusion

There are obvious differences between Green's eigenvalues and the HF eigenvalues especially for outer-shell electrons, though the parameters of Green's potential are obtained by fitting the HF eigenvalues. It means the Green's potential is neither an accurate electrostatic potential, nor an accurate central potential. A new four-parameter analytical local model potential is proposed in the present work, and the parameters are shell-independent and can be obtained easily. For neutral atoms, analytical potentials, eigenvalues, radial wave functions and total electronic energies are obtained and accord well with the results obtained by the X_a method. The results show that our new form of potential function gives an accurate central potential for the calculations on atomic structure and is better than the Green's potential function. The flexibility and accuracy of the new analytical potential are proved. To a certain extent, the new analytical potential remedies the disadvantages of other analytical potentials. What is more, the new potential function is suitable for high, medium and low Z atoms though it contains only four parameters. Due to its accuracy and simple form, the new potential function can be easily extended to and used in the calculation of other atomic properties. In addition, it can also be used in self-consistent-field calculation, and may serve as an effective potential used in OEP methods. Finally, it should be pointed out that it is very important to consider the exponential term parameter δ as an adjustable parameter, thereby improving the accuracy of potential function greatly. This would be helpful for the future research on finding other good analytical potential functions.

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