

PROBING THE (EMPIRICAL) QUANTUM STRUCTURE EMBEDDED IN THE PERIODIC TABLE WITH AN EFFECTIVE BOHR MODEL

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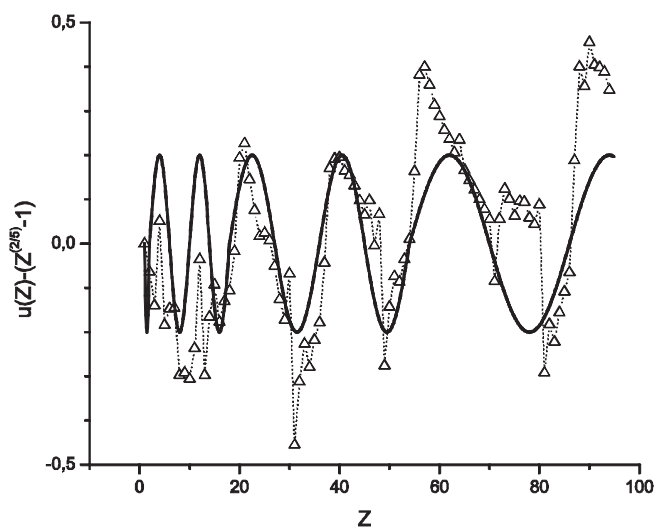


Figure 1S. - $u(Z) - \bar{u}(Z) \approx (1/5) \sin[2\pi y(Z)]$ (solid line), where $y(Z) = Z/2$ to $Z \leq 2$, $y(Z) = (Z - 2)/8$ to $2 \leq Z \leq 18$, $y(Z) = Z/18$ to $18 \leq Z \leq 54$, and $y(Z) = (Z + 10)/32$ to $Z \geq 54$; $u(Z) - \bar{u}(Z)$ (triangle) as function of Z for complete PT

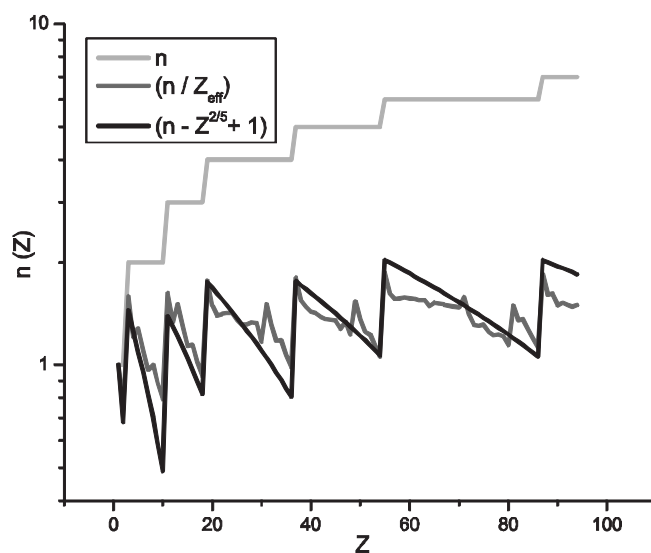


Figure 2S. The $n(Z)$, $n^*(Z) = n(Z)/Z_{\text{eff}}(Z) = n(Z) - u(Z)$, and $\bar{n}^*(Z) = n(Z) - Z^{2/5} + 1$ as function of Z for complete PT

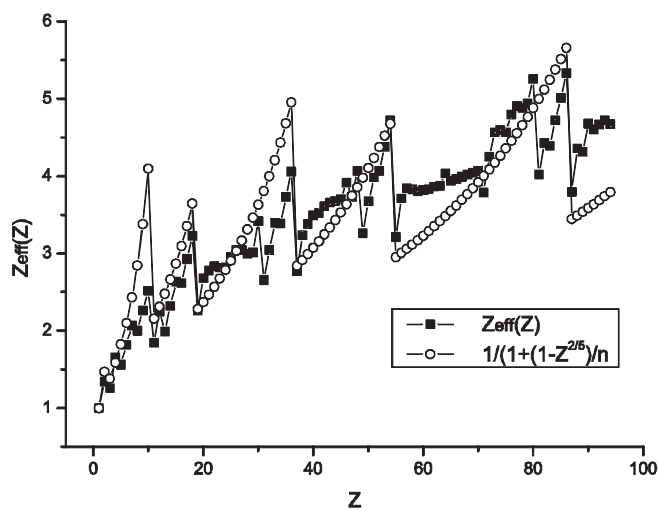


Figure 3S. Experimental Z_{eff} (square) and $\bar{Z}_{\text{eff}} = 1/(1 + (1 - Z^{2/5})/n(Z))$ (circle) as function of Z for complete PT

Table 1S. Experimental Ionization Potential (IP), Adjusted Ionization Potential $\overline{IP} = 13.6/(n(Z)-Z^{2.5}+I)^2$, Experimental Effective Charge (Z_{eff}), Adjusted Effective Charge $\overline{Z}_{eff} = I/(1+(1-Z^{2.5})/n(Z))$, Experimental Effective Quantum defect (u), and Adjusted Effective Quantum Defect $\overline{u} = Z^{2.5}-I$. Data considered in Figures 1 to 5 and 3S

Z	IP (eV)	\overline{IP} (eV)	Z_{eff}	\overline{Z}_{eff}	u	\overline{u}
1	13.598	13.598	1	1	0	0
2	24.587	29.365	1.34467	1.4695	0.25632	0.31951
3	5.392	6.4840	1.25941	1.3811	0.41196	0.55185
4	9.322	8.5801	1.65595	1.5887	0.79223	0.74110
5	8.298	11.313	1.56235	1.8242	0.71988	0.90365
6	11.26	14.994	1.81996	2.1001	0.90107	1.0477
7	14.534	20.120	2.06769	2.4328	1.03274	1.1779
8	13.618	27.546	2.00147	2.8466	1.00073	1.2974
9	17.422	38.830	2.26382	3.3797	1.11654	1.4082
10	21.564	57.073	2.51859	4.0974	1.20590	1.5119
11	5.139	7.0329	1.84426	2.1575	1.37333	1.6095
12	7.646	8.0700	2.24958	2.3111	1.66642	1.7019
13	5.986	9.2850	1.99045	2.4790	1.49281	1.7898
14	8.151	10.720	2.32268	2.6637	1.70839	1.8738
15	10.486	12.432	2.63444	2.8686	1.86124	1.9542
16	10.36	14.495	2.61857	3.0974	1.85434	2.0314
17	12.967	17.008	2.92957	3.3551	1.97596	2.1058
18	15.759	20.109	3.22959	3.6482	2.07109	2.1777
19	4.341	4.4257	2.26005	2.2820	2.23012	2.2471
20	6.113	4.7862	2.68194	2.3731	2.50854	2.3144
21	7.00	5.1799	2.77848	2.4688	2.54143	2.3798
22	6.828	5.6110	2.83445	2.5695	2.58879	2.4432
23	6.746	6.0842	2.81738	2.6756	2.58024	2.5050
24	6.766	6.6053	2.82155	2.7879	2.58234	2.5652
25	7.434	7.1808	2.95756	2.9068	2.64753	2.6239
26	7.902	7.8184	3.04924	3.0331	2.68820	2.6812
27	7.881	8.5271	3.04518	3.1676	2.68645	2.7372
28	7.64	9.3177	2.99826	3.3111	2.66589	2.7920
29	7.726	10.203	3.01509	3.4649	2.67334	2.8456
30	9.939	11.198	3.41975	3.6300	2.83032	2.8981
31	5.999	12.323	2.65682	3.8078	2.49444	2.9495
32	7.899	13.598	3.04866	4.0000	2.68795	3.0000
33	9.81	15.052	3.39748	4.2085	2.82266	3.0495
34	9.752	16.720	3.38742	4.4355	2.81916	3.0982
35	11.841	18.644	3.73264	4.6837	2.92837	3.1460
36	13.999	20.878	4.05855	4.9564	3.01443	3.1930
37	4.177	4.3857	2.77118	2.8396	3.19571	3.2392
38	5.695	4.6213	3.23578	2.9148	3.45478	3.2846
39	6.217	4.8722	3.38083	2.9929	3.52107	3.3294
40	6.634	5.1397	3.49237	3.0740	3.56831	3.3734
41	6.759	5.4254	3.52512	3.1583	3.58161	3.4169
42	7.092	5.7310	3.61091	3.2460	3.61531	3.4596
43	7.28	6.0582	3.65846	3.3374	3.63330	3.5018
44	7.36	6.4091	3.67851	3.4327	3.64075	3.5434
45	7.459	6.7859	3.70316	3.5321	3.6498	3.5844
46	8.337	7.1914	3.91505	3.6361	3.72288	3.6249
47	7.576	7.6283	3.73209	3.7449	3.66027	3.6649
48	8.994	8.0998	4.06639	3.8590	3.77041	3.7043
49	5.786	8.6098	3.26153	3.9786	3.46698	3.7433
50	7.344	9.1624	3.6745	4.1043	3.63927	3.7818
51	8.641	9.7624	3.98579	4.2365	3.74554	3.8198
52	9.009	10.415	4.06978	4.3759	3.77143	3.8574
53	10.451	11.127	4.3834	4.5229	3.85933	3.8945
54	12.13	11.905	4.7224	4.6784	3.94122	3.9313
55	3.894	3.2919	3.21079	2.9522	4.1313	3.9676
56	5.212	3.4115	3.71463	3.0053	4.38477	4.0035
57	5.577	3.5363	3.8425	3.0598	4.43852	4.0391
58	5.539	3.6667	3.82939	3.1157	4.43317	4.0742
59	5.464	3.8029	3.80337	3.1730	4.42245	4.1091
60	5.525	3.9454	3.82455	3.2319	4.43119	4.1435

Table 1S. continuation

Z	IP (eV)	\overline{IP} (eV)	Z_{eff}	\overline{Z}_{eff}	u	\overline{u}
61	5.55	4.0946	3.83319	3.2924	4.43472	4.1776
62	5.644	4.2507	3.86551	3.3546	4.44781	4.2114
63	5.67	4.4143	3.87441	3.4186	4.45138	4.2449
64	6.15	4.5859	4.03507	3.4844	4.51304	4.2780
65	5.864	4.7659	3.94013	3.5521	4.47721	4.3109
66	5.939	4.9550	3.96525	3.6219	4.48685	4.3434
67	6.022	5.1536	3.99286	3.6938	4.49732	4.3756
68	6.108	5.3625	4.02127	3.7679	4.50793	4.4076
69	6.184	5.5823	4.04621	3.8443	4.51713	4.4393
70	6.254	5.8138	4.06905	3.9232	4.52545	4.4706
71	5.426	6.0579	3.79013	4.0048	4.41694	4.5018
72	6.825	6.3155	4.25075	4.0890	4.58848	4.5326
73	7.89	6.5874	4.57038	4.1761	4.6872	4.5633
74	7.98	6.8749	4.59637	4.2663	4.69462	4.5936
75	7.88	7.1791	4.56748	4.3596	4.68637	4.6237
76	8.7	7.5012	4.79925	4.4563	4.7498	4.6536
77	9.1	7.8427	4.90834	4.5567	4.77759	4.6832
78	9	8.2051	4.88129	4.6608	4.77082	4.7126
79	9.226	8.5902	4.9422	4.7689	4.78597	4.7418
80	10.438	8.9997	5.25681	4.8812	4.85862	4.7708
81	6.108	9.4359	4.02127	4.9981	4.50793	4.7996
82	7.416	9.9010	4.43097	5.1198	4.64589	4.8281
83	7.289	10.398	4.39286	5.2466	4.63415	4.8564
84	8.42	10.928	4.72139	5.3789	4.72919	4.8845
85	9.5	11.497	5.01505	5.5170	4.8036	4.9124
86	10.748	12.106	5.3343	5.6613	4.8752	4.9402
87	4	3.2923	3.79656	3.4444	5.15623	4.9677
88	5.279	3.3828	4.3615	3.4914	5.39505	4.9950
89	5.172	3.4763	4.31708	3.5393	5.37853	5.0222
90	6.084	3.5731	4.68226	3.5883	5.50499	5.0492
91	5.887	3.6733	4.60583	3.6382	5.48019	5.0760
92	6.1941	3.7771	4.67031	3.6893	5.50117	5.1026
93	6.2657	3.8846	4.72211	3.7414	5.51761	5.1290
94	6.063	3.9961	4.67417	3.7947	5.50241	5.1553

Table 2S. Experimental Effective Charge (Z_{eff}), Slater Effective Charge (Z_{eff}^*), and Adjusted Effective Charge $\overline{Z}_{eff} = I/(1+(1-Z^{2.5})/n(Z))$ and their IP (eV) for some Z . Data considered in Figure 6

Z	Z_{eff}	IP	Z_{eff}^*	IP^*	\overline{Z}_{eff}	\overline{IP}
1	1	13.598	1	13.598	1	13.598
3	1.2594	5.392	1.3	5.75	1.381	6.4840
4	1.6560	9.322	1.95	12.93	1.589	8.5801
5	1.5624	8.298	2.6	23.0	1.824	11.313
6	1.8200	11.26	3.25	35.91	2.100	14.994
7	2.0677	14.534	3.9	51.7	2.433	20.120
8	2.0015	13.618	4.55	70.38	2.847	27.546
9	2.2638	17.422	5.2	91.9	3.380	38.830
10	2.5186	21.564	5.85	116.3	4.097	57.073
11	1.8443	5.139	2.2	7.31	2.157	7.0329
19	2.2601	4.341	2.2	4.11	2.281	4.4257
37	2.7712	4.177	2.2	2.63	2.839	4.3857
55	3.2108	3.894	2.2	1.83	2.952	3.2919