Errata

Erratum: Hydrogen atom under a sequence of static multipole perturbations: Wave-function corrections [Phys. Rev. A 33, 717 (1986)]

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In an attempt to obtain high-order sum rules by using the solution given in Eqs. (11)–(15) in this paper, I found that when $l=0$ occurs in the midst of the iteration process, the solution as given requires a subtraction. In order to minimize the disruption of notations, I would like to correct the coefficients b_n^{Ll} as given in Eq. (14) of that paper as follows. First define

$$B_n^{Ll}=\frac{(L-l+1)!(L+l+2)!(n-1)!2^n}{2^{L+1}(L+1)!(n+l+1)!(n-l)!}\ , \tag{14a}$$

$$\beta_n^{Ll}=\begin{cases} B_n^{Ll} \text{ for } L+1\geq n\geq l+2\delta_{l0} \\ -\sum_{i=2}^{L+1} B_i^{L0}\frac{(i+2)!}{2^{i+1}} \text{ for } l=0 \text{ and } n=0 \\ 0 \text{ otherwise ;} \end{cases} \tag{14b}$$

then

$$b_n^{Ll}=-A_{Ll}\beta_n^{Ll}\ . \tag{14c}$$

Equations (14a), (14b), and (14c) should replace Eq. (14) in the paper. Subsequently in Eqs. (18) and (20), the lower limits of the summation range should be l instead of $l+2\delta_{l0}$. I would like to assure the readers that in subsequent publications in which I have utilized this method, I only consider cases for which $l=0$ does not occur in the midst of the iteration and so the final results are unaffected.

I would like to thank R. J. Drachman for discussion.

Erratum: Atomic-charge convexity and the electron density at the nucleus [Phys. Rev. A 42, 641 (1990)]

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We have found a computational error in the evaluation of the second derivative $\rho''(r)$, mainly due to the normalization of the density (which is done to N^2 in the paper instead of N, where N is the electron number of the system). This results in a modification of the absolute values of the quantities represented in Fig. 1 and in the second and third columns of Table I.

Here, we present the new Fig. 1 and Table I with the correct "normalized to N" density $\rho(r)$. The rest of the contents and the conclusions of the paper continue to remain fully valid.

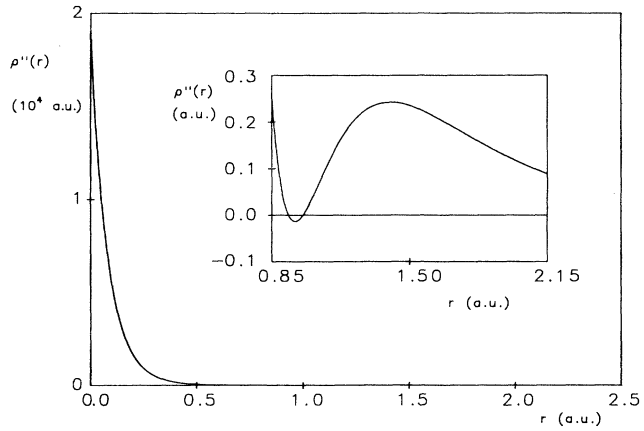

FIG. 1. Second derivative of the charge density, $\rho''(r)$, of carbon. The region of negative $\rho''(r)$ is shown separately to illustrate its small width and magnitude.

TABLE I. Values of $\rho''(r)$ at the origin $\rho''(0)$, and at the minimum r_0 of the negativity region $\rho''_{\min}=\rho''(r_0)$, and their mutual ratio are given for all the atoms with $Z \leq 54$ which are not strictly convex. Also, the width Δ of that region is shown. Numbers in square brackets denote the corresponding power of 10, i.e., 5.2892[+2] means 5.2892×10^2. Atomic units are used throughout. See text for further details.

Z	$\rho''(0)$	$-\rho''_{\min}$	$-\frac{\rho''_{\min}}{\rho''(0)}$	r_0	Δ
3	5.2892[+2]	4.3606[−4]	8.2[−7]	2.500	0.56
4	2.3778[+3]	1.0320[−2]	4.3[−6]	1.590	0.44
5	7.4775[+3]	2.9232[−2]	3.9[−6]	1.195	0.24
6	1.8968[+4]	1.3994[−2]	7.4[−7]	0.960	0.07
16	2.7691[+6]	1.6763[−1]	6.1[−8]	1.315	0.31
17	3.7530[+6]	1.2115[−1]	3.2[−8]	1.205	0.18
18	5.0320[+6]	3.5779[−1]	7.1[−8]	1.080	0.21
19	6.6136[+6]	7.5369[−1]	1.1[−7]	0.980	0.20
20	8.5922[+6]	1.3763	1.6[−7]	0.895	0.19
21	1.1016[+7]	2.0204	1.8[−7]	0.835	0.18
22	1.3934[+7]	2.7409	2.0[−7]	0.780	0.15
23	1.7464[+7]	3.5719	2.0[−7]	0.730	0.14
24	2.1638[+7]	3.7463	1.7[−7]	0.695	0.12
25	2.6576[+7]	5.2865	2.0[−7]	0.655	0.11
26	3.2480[+7]	6.0261	1.9[−7]	0.620	0.10
27	3.9319[+7]	6.2588	1.6[−7]	0.590	0.08
28	4.7190[+7]	6.1480	1.3[−7]	0.565	0.07
29	5.6296[+7]	3.5784	6.4[−8]	0.540	0.04
30	6.6813[+7]	3.3736	5.0[−8]	0.515	0.04
31	7.8596[+7]	2.4610	3.1[−8]	0.495	0.02
32	9.2300[+7]	9.3183[−1]	1.0[−8]	0.470	0.01
45	5.1604[+8]	7.1666[−1]	1.4[−9]	0.910	0.08
46	5.7659[+8]	1.8448	3.2[−9]	0.875	0.11
47	6.4281[+8]	3.2567	5.1[−9]	0.835	0.12
48	7.1568[+8]	5.4906	7.7[−9]	0.805	0.13
49	7.9519[+8]	8.0546	1.0[−8]	0.770	0.14
50	8.7919[+8]	1.1264[+1]	1.3[−8]	0.740	0.14
51	9.7156[+8]	1.5351[+1]	1.6[−8]	0.710	0.13
52	1.0718[+9]	2.0353[+1]	1.9[−8]	0.685	0.13
53	1.1802[+9]	2.6302[+1]	2.2[−8]	0.665	0.13
54	1.2970[+9]	3.4035[+1]	2.6[−8]	0.640	0.13