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Wave Functions for Quadrupole Antishielding Factors*

Supplement to the paper: "Quadrupole Antishielding Factors of Ions", Phys. Rev. 130, (1963)

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INTRODUCTION

The purpose of this paper is to present tables of the perturbed¹ wave functions which have been recently obtained in a calculation of the quadrupole antishielding factors² γ_{∞} for the Mn^{+2} , Fe^{+3} , Ga^{+3} , and Ag^{+} ions. The wave functions $v_1'(nl \rightarrow l)$ which are tabulated represent the effect of the perturbation due to a nuclear quadrupole moment Q on the wave functions of the outermost electrons of the ion core.

The functions $v_1'(nl \rightarrow l)$ are the solutions of the following equation:

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V_0 - E_0 \right] v_1'(nl \rightarrow l) = u_0' \left(\frac{1}{r^3} - \left\langle \frac{1}{r^3} \right\rangle_{nl} \right) v_1'$$

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where u'_0 is r times the unperturbed radial wave function for the nl shell; u'_0 is normalized according to:

$$\int_0^\infty u_0'^2 dr = 1. \quad (2)$$

In Eq. (1), V_0 and E_0 are the unperturbed (spherical) effective potential and the unperturbed eigenvalue for the state nl . $v'_1(nl \rightarrow l)$ is completely determined by Eq. (1) and by the orthogonality condition:

$$\int_0^\infty u'_0 v'_1(nl \rightarrow l) dr = 0. \quad (3)$$

We note that $v'_1(nl \rightarrow l)$ is the same as the function $u'_1(nl \rightarrow l)$ of reference 1. We use the notation v'_1 in order to be consistent with the notation of two previous tabulations³ of perturbed wave functions, in which the perturbed functions pertaining to the effect of the nuclear Q are called v'_1 , [while u'_1 denotes the functions pertaining to an external (dipole or quadrupole) perturbation].

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According to a method previously employed by the author

$V_0 - E_0$ is obtained from the unperturbed wave function u'_0 by means of the relation:

$$V_0 - E_0 = \frac{1}{u'_0} \frac{d^2 u'_0}{dr^2} - \frac{l(l+1)}{r^2}. \quad (4)$$

The method of solution of Eq. (1) has been described in reference

1. The unperturbed wave functions u'_0 used in this work were the Hartree-⁵⁻⁷Fock functions for the four ions considered.

The contribution to the total antishielding factor γ_∞ due to the $n\ell \rightarrow \ell$ mode of excitation of the $n\ell$ shell is given by:

$$\gamma_\infty(n\ell \rightarrow \ell) = C_{\ell\ell}^{(2)} \int_0^\infty u_0' v_1'(n\ell \rightarrow \ell) r^2 dr, \quad (5)$$

where the coefficient $C_{\ell\ell}^{(2)}$ represents the effect of the integration over the angular variables and the summation over magnetic substates. For a completed p shell, $C_{11}^{(2)} = 48/25$; for a completed d shell, $C_{22}^{(2)} = 16/7$. For the cases of Mn^{+2} and Fe^{+3} , in which the 3d shell is half-filled, we have $C_{22}^{(2)} = 8/7$.

The resulting functions $v_1'(np \rightarrow p)$ and $v_1'(nd \rightarrow d)$ are presented in Tables I-IV. The perturbation $v_1'(4d \rightarrow d)$ for Ag^+ has been obtained previously, and is included in Table IV for the sake of convenience. In Tables I and II pertaining to Mn^{+2} and Fe^{+3} , we have also given the unperturbed functions $u_0'(3p)$ and $u_0'(3d)$ of Watson which were used in the calculations.

At the bottom of each table, we have listed the values of $\langle r^{-3} \rangle_{n\ell}$ (in units a_H^{-3}), $\gamma_\infty(n\ell \rightarrow \ell)$ and of $J(n\ell \rightarrow \ell)$ defined as:

$$J(n\ell \rightarrow \ell) \equiv \int_0^\infty u_0' v_1'(n\ell \rightarrow \ell) r^{-3} dr. \quad (6)$$

As previously discussed in reference 8, $J(n\ell \rightarrow \ell)$ enters into the calculation of the second-order quadrupole effect for the hyperfine structure. It is estimated that the accuracy of the functions $v_1'(n\ell \rightarrow \ell)$ and of the resulting values of $\gamma_\infty(n\ell \rightarrow \ell)$ and $J(n\ell \rightarrow \ell)$ is generally within 3%.

for the given zero-order (Hartree-Fock) wave functions used in the calculations.

TABLE I, Wave functions $v_1'(3p \rightarrow p)$ and $v_1'(3d \rightarrow d)$ for Mn^{+2} . The
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unperturbed wave functions $u_0'(3p)$ and $u_0'(3d)$ of Watson are
also listed.

r	$v_1'(3p \rightarrow p)$	$v_1'(3d \rightarrow d)$	$u_0'(3p)$	$u_0'(3d)$
0.01	+0.98	+0.004	+0.0147	+0.00012
0.02	1.98	0.014	0.0520	0.00083
0.03	2.81	0.032	0.1036	0.00259
0.04	3.47	0.056	0.1631	0.00571
0.05	3.94	0.087	0.2257	0.01037
0.06	4.22	0.124	0.2877	0.01668
0.07	4.33	0.165	0.3464	0.02468
0.08	4.27	0.210	0.4001	0.03435
0.09	4.06	0.258	0.4474	0.04565
0.10	3.74	0.309	0.4876	0.0585
0.12	2.80	0.415	0.5451	0.0884
0.14	1.58	0.524	0.5721	0.1232
0.16	+0.21	0.632	0.5706	0.1619
0.18	-1.21	0.735	0.5440	0.2035
0.20	-2.61	0.832	0.4964	0.2471
0.22	-3.93	0.920	0.4316	0.2919
0.24	-5.15	0.999	0.3536	0.3371
0.26	-6.23	1.070	0.2658	0.3822
0.28	-7.14	1.131	0.1713	0.4267
0.30	-7.90	1.181	+0.0729	0.4700
0.35	-9.28	1.270	-0.1764	0.5716
0.40	-9.86	1.306	-0.4113	0.6610
0.45	-9.78	1.294	-0.6169	0.7368
0.50	-9.19	1.247	-0.7866	0.7987
0.55	-8.23	1.171	-0.9190	0.8474
0.60	-7.05	1.076	-1.0158	0.8839
0.7	-4.33	0.840	-1.1174	0.9251
0.8	-1.74	0.587	-1.1260	0.9324
0.9	+0.45	0.339	-1.0745	0.9148

TABLE I (cont'd).

1.0	2.13	+0.110	-0.9889	0.8800
1.1	3.33	-0.091	-0.8873	0.8340
1.2	4.11	-0.263	-0.7817	0.7818
1.4	4.76	-0.530	-0.5848	0.6716
1.6	4.57	-0.696	-0.4237	0.5666
1.8	4.00	-0.785	-0.3006	0.4737
2.0	3.30	-0.820	-0.2099	0.3938
2.2	2.62	-0.814	-0.1446	0.3259
2.4	2.005	-0.779	-0.0984	0.2684
2.6	1.498	-0.725	-0.0662	0.2197
2.8	1.094	-0.660	-0.0440	0.1786
3.0	0.781	-0.590	-0.0290	0.1441
3.2	0.550	-0.517	-0.0189	0.1153
3.4	0.378	-0.447	-0.0122	0.0915
3.6	0.258	-0.381	-0.0078	0.0721
3.8	0.173	-0.323	-0.0049	0.0563
4.0	0.116	-0.272	-0.00311	0.0437
4.5	0.041	-0.173	-0.00095	0.0226
5.0	0.015	-0.110	-0.00028	0.0112
5.5	0.005	-0.070	-0.00008	0.0054
6.0	0.002	-0.045	-0.00002	0.0026
6.5		-0.029		0.0012
7.0		-0.018		0.0005
7.5		-0.012		0.0002
8.0		-0.007		
8.5		-0.005		
9.0		-0.003		
$\langle r^{-3} \rangle_{ns}$	46.58	4.250	-----	-----
γ_{∞}	-9.15	-2.55	-----	-----
J	822.1	9.325	-----	-----

TABLE II. Wave functions $v_1'(3p \rightarrow p)$ and $v_1'(3d \rightarrow d)$ for Fe^{+3} . The unperturbed wave functions $u_0'(3p)$ and $u_0'(3d)$ of Watson are also listed.

r	$v_1'(3p \rightarrow p)$	$v_1'(3d \rightarrow d)$	$u_0'(3p)$	$u_0'(3d)$
0.01	+1.13	+0.005	+0.0168	+0.00015
0.02	2.27	0.019	0.0593	0.00110
0.03	3.20	0.042	0.1173	0.00343
0.04	3.91	0.073	0.1835	0.00750
0.05	4.40	0.112	0.2523	0.01354
0.06	4.66	0.158	0.3196	0.02165
0.07	4.70	0.209	0.3825	0.03186
0.08	4.57	0.264	0.4390	0.04412
0.09	4.26	0.322	0.4877	0.05834
0.10	3.82	0.383	0.5280	0.07441
0.12	2.64	0.507	0.5822	0.1115
0.14	+1.17	0.631	0.6017	0.1541
0.16	-0.43	0.749	0.5896	0.2009
0.18	-2.05	0.860	0.5504	0.2508
0.20	-3.62	0.962	0.4888	0.3025
0.22	-5.07	1.052	0.4096	0.3552
0.24	-6.36	1.129	0.3172	0.4079
0.26	-7.47	1.194	0.2155	0.4600
0.28	-8.38	1.246	+0.1081	0.5109
0.30	-9.11	1.286	-0.0022	0.5601
0.35	-10.30	1.341	-0.2749	0.6736
0.40	-10.59	1.334	-0.5235	0.7707
0.45	-10.16	1.278	-0.7336	0.8500
0.50	-9.21	1.183	-0.8998	0.9115
0.55	-7.93	1.060	-1.0225	0.9563
0.60	-6.45	0.921	-1.1052	0.9858
0.7	-3.30	0.609	-1.1722	1.0063
0.8	-0.50	0.301	-1.1458	0.9879
0.9	+1.70	+0.023	-1.0644	0.9440
1.0	3.27	-0.215	-0.9561	0.8853
1.1	4.28	-0.408	-0.8390	0.8192

TABLE II (cont'd).

1.2	4.84	-0.559	-0.7237	0.7508
1.4	5.02	-0.758	-0.5196	0.6185
1.6	4.49	-0.841	-0.3604	0.5001
1.8	3.67	-0.843	-0.2435	0.3980
2.0	2.83	-0.789	-0.1609	0.3118
2.2	2.083	-0.704	-0.1042	0.2404
2.4	1.479	-0.603	-0.0663	0.1825
2.6	1.018	-0.500	-0.0415	0.1365
2.8	0.684	-0.404	-0.0256	0.1006
3.0	0.450	-0.320	-0.0156	0.0732
3.2	0.289	-0.247	-0.0094	0.0526
3.4	0.183	-0.189	-0.0056	0.0374
3.6	0.114	-0.143	-0.00328	0.0264
3.8	0.071	-0.107	-0.00191	0.0184
4.0	0.044	-0.081	-0.00111	0.0127
4.5	0.013	-0.040	-0.00027	0.0049
5.0	0.004	-0.020	-0.00007	0.0018
5.5	0.001	-0.010	-0.00002	0.0007
6.0		-0.005		0.0002
6.5		-0.002		0.0001
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$\langle r^{-3} \rangle_{n\ell}$	56.17	5.724	-----	-----
γ_{∞}	-7.89	-1.59	-----	-----
J	1034	12.18	-----	-----

TABLE III. Wave functions $v_1^i(3p \rightarrow p)$ and $v_1^i(3d \rightarrow d)$ for Ga^{+3} .

r	$v_1^i(3p \rightarrow p)$	$v_1^i(3d \rightarrow d)$
0.01	+1.93	+0.010
0.02	3.77	0.043
0.03	5.15	0.095
0.04	6.06	0.166
0.05	6.52	0.252
0.06	6.56	0.351
0.07	6.22	0.460
0.08	5.57	0.575
0.09	4.66	0.694
0.10	3.57	0.815
0.12	+1.00	1.055
0.14	-1.79	1.281
0.16	-4.51	1.485
0.18	-7.01	1.662
0.20	-9.19	1.809
0.22	-10.97	1.925
0.24	-12.37	2.012
0.26	-13.38	2.069
0.28	-14.04	2.099
0.30	-14.40	2.103
0.35	-14.14	2.027
0.40	-12.64	1.849
0.45	-10.38	1.604
0.50	-7.81	1.323
0.55	-5.20	1.027
0.60	-2.75	0.734
0.7	+1.46	+0.179
0.8	4.34	-0.286
0.9	5.99	-0.651
1.0	6.81	-0.923
1.1	6.97	-1.113
1.2	6.71	-1.235

TABLE III (cont'd).

1.4	5.51	-1.321
1.6	4.11	-1.270
1.8	2.88	-1.145
2.0	1.929	-0.988
2.2	1.256	-0.825
2.4	0.800	-0.673
2.6	0.497	-0.539
2.8	0.305	-0.424
3.0	0.186	-0.329
3.2	0.113	-0.253
3.4	0.068	-0.192
3.6	0.041	-0.144
3.8	0.025	-0.109
4.0	0.015	-0.082
4.5	0.004	-0.040
5.0	0.001	-0.019
5.5		-0.009
6.0		-0.005
6.5		-0.002
7.0		-0.001
<hr/>		
$\langle r^{-3} \rangle_{ng}$	108.1	11.83
γ_{∞}	-6.42	-3.29
J	2433	34.18

TABLE IV. Wave functions $v_1^i(4p \rightarrow p)$ and $v_1^i(4d \rightarrow d)$ for Ag^+ .

r	$v_1^i(4p \rightarrow p)$	$v_1^i(4d \rightarrow d)$
0.01	+3.03	+0.036
0.02	5.90	0.142
0.03	7.87	0.299
0.04	8.82	0.464
0.05	8.74	0.610
0.06	7.74	0.765
0.07	6.08	0.918
0.08	3.95	1.061
0.09	+1.54	1.185
0.10	-0.98	1.288
0.11	-3.48	1.366
0.12	-5.86	1.420
0.14	-9.95	1.448
0.16	-12.79	1.379
0.18	-14.22	1.227
0.20	-14.33	1.004
0.225	-12.99	0.650
0.25	-10.55	+0.252
0.275	-7.45	-0.170
0.30	-3.96	-0.597
0.35	+3.10	-1.392
0.40	9.58	-2.051
0.45	14.62	-2.543
0.50	17.96	-2.872
0.55	18.39	-3.053
0.60	17.62	-3.112
0.7	14.02	-2.951
0.8	8.93	-2.543
0.9	+3.83	-2.016
1.0	-0.52	-1.447
1.1	-3.90	-0.894
1.2	-6.30	-0.387

TABLE IV (cont'd).

1.4	-8.84	+0.440
1.6	-9.16	1.014
1.8	-8.32	1.374
2.0	-7.05	1.574
2.2	-5.71	1.657
2.4	-4.50	1.657
2.6	-3.46	1.599
2.8	-2.60	1.505
3.0	-1.916	1.391
3.2	-1.415	1.263
3.4	-1.023	1.134
3.6	-0.733	1.008
3.8	-0.525	0.888
4.0	-0.373	0.777
4.5	-0.161	0.542
5.0	-0.070	0.368
5.5	-0.030	0.245
6.0	-0.013	0.161
6.5	-0.006	0.105
7.0	-0.002	0.068
7.5		0.044
8.0		0.029
8.5		0.019
9.0		0.012
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$\langle r^{-3} \rangle_{nl}$	88.53	8.11
γ_{∞}	-20.39	-13.14
J	4009	39.48

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