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The Tables of Eigenvalues and Eigenvectors Useful for the Scattering Problems in a Two Centre Coulomb Field

Mikio Shimizu (清 水 幹 夫)

Department of Physics, Faculty of Science,
Ochanomizu University, Tokyo

The Schroedinger equation which describes the scattering of an electron with the kinetic energy $k^2/2$ by a pair of charges, say Z_a and Z_b, fixed at a distance R can be separated adopting the prolate spheroidal coordinates ξ, η and φ. Then the solution of this equation is of the form

$$\alpha_l^m(\xi)\beta_l^m(\eta)\begin{Bmatrix}\cos m\varphi\\ \sin m\varphi\end{Bmatrix}, \tag{1}$$

l and m being the quantum numbers and the function β satisfies the equation

$$\left[\frac{d}{d\eta}(\eta^2-1)\frac{d}{d\eta}-\frac{m^2}{\eta^2-1}+\lambda^2\eta^2+2D\eta-A_l^m\right]\beta=0, \tag{2}$$

where $2D=(Z_a-Z_b)R$, $\lambda=\dfrac{kR}{2}$ and $A_l^m(\lambda, D)$ is the separation constant.

We have expanded β in terms of the associated Legendre functions in order to obtain the constant A_l^m.

$$\beta_l^m(\eta)=\sum_{j\geqq m}^{\infty}c_j^{lm}(\lambda, D)P_j^m(\eta). \tag{3}$$

We have solved the difference equation for c_j^{lm} under a proper boundary condition. The calculated eigenvalues A_l^m and the coefficients c_j^{lm} for various sets of parameters λ and D are shown in the following tables. For convenience c_j^{lm} are normalized as $\sum_j |c_j^{lm}|^2=1$ and R is taken to be equal to 2. The details will be appeared in another paper.

In conclusion the author wishes to express his sincere thanks to Prof. Takahashi and the members of his laboratory at the University of Tokyo for helps in programming and operating the Parametron Computor No. 1.

Table 1. The eigenvalues A_l^m of the equation (2).*

$k=0\ \sqrt{e.\ V.}$

l	$m\backslash D$	1/4	1/2	1	3/2	2	5/2	4
0	0	−0.15763	−0.55727	−1.70484	−3.06023	−4.51990	−6.04508	−10.85605
1	0	2.09078	2.22872	2.60239	2.58729	2.26404	1.72334	−0.66265
2	0	6.02403	6.09845	6.41283	6.90876	7.44444	7.87937	8.14111
1	1	1.95034	1.80512	1.26986	0.48954	−0.45813	−1.15234	−5.16578
2	1	6.01159	6.04265	6.12299	6.15393	6.07635	5.86921	4.54312
3	1	12.00833	12.03321	12.13095	12.28511	12.47759	12.68108	13.07907

* We have adopted the parameter k instead of λ in units of $\sqrt{e.v.}$

$k=1\ \sqrt{e.\ V.}$

l	$m\backslash D$	1/4	1/2	1
0	0	−0.12909	−0.52420	−1.66450
1	0	2.13501	2.32583	2.63136
2	0	6.06557	6.14083	6.45673
1	1	1.96641	1.82218	1.29064
2	1	6.04482	6.07481	6.15194
3	1	12.04497	12.06982	12.16731

$k=2\ \sqrt{e.\ V.}$

l	$m\backslash D$	1/4	1/2	1
0	0	−0.04481	−0.42645	−1.54469
1	0	2.26745	2.44181	2.71858
2	0	6.19034	6.26851	6.58846
1	1	2.01429	1.87334	1.35114
2	1	6.14429	6.17113	6.23878
3	1	12.15500	12.17970	12.31498

$k=3\ \sqrt{e.\ V.}$

l	$m\backslash D$	1/4	1/2	1
0	0	0.09138	−0.26840	−1.34917
1	0	2.48742	2.63532	2.86494
2	0	6.40385	6.48303	6.80810
1	1	2.09285	1.95702	1.45142
2	1	6.30922	6.33110	6.38360
3	1	12.33866	12.36307	12.45812

Table 2. Several Components of the Eigenvectors for Some Values of D and (l, m).

$k=0\sqrt{e.V.}$

component / l	m	C_0	C_1	C_2	C_3
			$D=1/4$		
0	0	.9030	.4271	.0464	.0023
1	0	—.1552	.9736	.1671	.0101
2	0	.0055	—.0998	.9900	.0997
1	1	.9966	.0825	.0033	.0001
2	1	—.1476	.9868	.0661	.0020
3	1	.0057	—.0948	.9940	.0534
			$D=1/2$		
0	0	.7601	.6358	.1309	.0126
1	0	—.2635	.9040	.3342	.0415
2	0	.0216	—.1979	.9597	.1976
1	1	.9870	.1603	.0126	.0006
2	1	—.2822	.9506	.1291	.0080
3	1	.0224	—.1874	.9763	.1058
			$D=1$		
0	0	.5919	.7569	.2727	.0484
1	0	—.3504	.6840	.6185	.1620
2	0	.0779	—.3749	.8390	.3811
1	1	.9558	.2908	.0442	.0040
2	1	—.4857	.8399	.2402	.0291
3	1	.0866	—.3562	.9075	.2037
			$D=3/2$		
0	0	.5063	.7747	.3676	.0903
1	0	—.3480	.4502	.7599	.3081
2	0	.1429	—.4937	.6524	.5373
1	1	.9188	.3855	.0836	.0112
2	1	—.6173	.7123	.3281	.0626
3	1	.1724	—.4926	.8024	.2860
			$D=2$		
0	0	.4532	.7682	.4321	.1309
1	0	—.3242	.2752	.7877	.4303
2	0	.1981	—.5355	.4316	.6513
1	1	.8830	.4522	.1237	.0213
2	1	—.6955	.5906	.3958	.1023
3	1	·2689	—.5869	.6748	.3500

			$D=5/2$		
0	0	.4160	.7545	.4774	.1681
1	0	−.3013	.1557	.7641	.5201
2	0	.2173	−.5186	.2117	.7061
1	1	.8505	.4994	.1614	.0334
2	1	−.7426	.4789	.4442	.1453
3	1	.3602	−.6412	.5395	.3955
			$D=4$		
0	0	.3477	.7078	.5525	.2571
1	0	−.2548	.0317	.6237	.6553
2	0	.2152	−.3284	.2228	.5804
1	1	.7727	.5768	.2537	.0746
2	1	−.7947	.2105	.4971	.2655
3	1	.5576	−.6435	.1730	.4423

$k=1\sqrt{e.V.}$

$D=1/4$

component / l	m	C_0	C_1	C_2	C_3
0	0	.9054	.4229	.0380	.0008
1	0	−.1530	.9736	.1690	.0071
2	0	.0072	−.1000	.9899	.1001
1	1	.9966	.0190	.0022	.0000
2	1	−.1465	.9870	.0662	.0011
3	1	.0083	−.0947	.9940	.0534
			$D=1/2$		
0	0	.7642	.6329	.1238	.0103
1	0	−.2605	.9039	.3370	.0389
2	0	.0233	−.1982	.9595	.1984
1	1	.9872	.1594	.0115	.0004
2	1	−.2803	.9511	.1294	.0070
3	1	.0250	−.1872	.9763	.1059
			$D=1$		
0	0	.5949	.7564	.2679	.0458
1	0	−.3476	.6841	.6206	.1598
2	0	.0791	−.3747	.8383	.3827
1	1	.9062	.2895	.0429	.0037
2	1	−.4857	.8399	.2402	.0292
3	1	.0866	−.3562	.9076	.2037

$k=2\sqrt{e.V.}$

$D=1/4$

component / l	m	C_0	C_1	C_2	C_3
0	0	.9117	.4106	.0131	.0036
1	0	−.1467	.9737	.1742	.0018
2	0	.0123	−.1006	.9897	.1013
1	1	.9968	.0805	.0010	.0003
2	1	−.1434	.9874	.0666	.0018
3	1	.0162	−.0943	.9940	.0538

$D=1/2$

0	0	.7642	.6329	.1238	.0103
1	0	−.2605	.9039	.3370	.0389
2	0	.0233	−.1982	.9595	.1984
1	1	.9872	.1594	.0115	.0004
2	1	−.2803	.9511	.1294	.0070
3	1	.0250	−.1872	.9763	.1059

$D=1$

0	0	.6038	.7549	.2531	.0378
1	0	−.3392	.6847	.6264	.1532
2	0	.0824	−.3743	.8363	.3875
1	1	.9575	.2856	.0392	.0028
2	1	−.4786	.8436	.2419	.0260
3	1	.0950	−.3539	.9074	.2052

$k=2\sqrt{e.V.}$

$D=1/4$

conponent / l	m	C_0	C_1	C_2	C_3
0	0	.9203	.3901	.0283	.0104
1	0	−.1365	.9736	.1819	.0170
2	0	.0206	−.1015	.9891	.1035
1	1	.9969	.0781	.0062	.0007
2	1	−.1383	.9881	.0672	.0062
3	1	.0291	−.0936	.9937	.0542

$D=1/2$

0	0	.7916	.6076	.0649	.0075
1	0	−.2370	.9035	.3566	.0174
2	0	.0358	−.2002	.9574	.2051
1	1	.9883	.1524	.0027	.0009
2	1	−.2659	.9550	.1315	.0003
3	1	.0448	−.1850	.9758	.1074

$D=1$

0	0	.6188	.7516	.2272	.0243
1	0	−.3252	.6863	.6348	.1418
2	0	.0876	−.3730	.8330	.3956
1	1	.9597	.2792	.0330	.0012
2	1	−.4667	.8496	.2445	.0227
3	1	.1031	−.3517	.9071	.2065

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