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TABLE OF EIGENVALUES FOR PURE QUADRUPOLE SPECTRA, SPIN 5/2

Ralph Livingston and Henry Zeldes

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TABLE OF EIGENVALUES FOR PURE QUADRUPOLE SPECTRA, SPIN 5/2

Ralph Livingston and Henry Zeldes

INTRODUCTION

The table in this report contains eigenvalues for use in nuclear quadrupole spectroscopy for the spin $\frac{5}{2}$ case and allows asymmetries and quadrupole couplings to be obtained from experimentally measured frequencies. The roots of the spin $\frac{5}{2}$ secular equation[1]

$$E^3 - (84 + 28\eta^2)\,E - 160 + 160\eta^2 = 0$$

have been calculated for preset values of η ranging from 0 to 1 in increments of 0.001, where η is defined in the usual way with respect to derivatives of the electric field along the principal axes directions,

$$\frac{(\partial E_x/\partial x) - (\partial E_y/\partial y)}{\partial E_z/\partial z} .$$

Each of the roots has been multiplied by the factor $1[4I(2I - 1)] = \frac{1}{40}$ for $I = \frac{5}{2}$; this gives tabular entries that can be applied to experimentally measured frequencies in a very direct manner, as outlined below.

The calculation was coded for the high-speed digital computer (the Oracle) at the Oak Ridge National Laboratory by the Mathematics Panel. E. C. Long and A. S. Householder handled the main burden of the work. The problem was coded so that for a given η value each of the three roots was separately calculated and then tested to see that the three summed to zero, as required by the secular equation, before the next η value was used. As a further check, the entire calculation was performed twice, and the output tapes were compared. The calculations are tabulated essentially as they were printed from the machine output tape, so as to involve a minimum of labor and eliminate chances of error. Consequently, some interpretation of the printed numbers is required, as explained below.

USE OF THE TABLE

The numbers in the E_1, E_2, E_3, and R columns must be interpreted as follows:

1. The last digit (zero) is not significant and should be ignored.
2. All entries are the significant figures after the decimal point; hence every entry should be regarded as having a decimal point preceding it.
3. Although the entries are used for magnitudes of couplings, E_1 and E_2 must be regarded as having the same sign, and E_3 *as having the opposite sign.* Thus

$$E_1 + E_2 + E_3 = 0$$

for every value of η.

4. Unity should be added to every value in the R column. Thus the value of R for $\eta = 0$ is 1.999999999 or 2; R is the magnitude of $(E_3 - E_2)/(E_2 - E_1)$.

The following example should make the use of the table clear. An iodine ($I = \frac{5}{2}$) quadrupole resonance in a crystalline solid was found to have resonant frequencies at 202.8696 and 325.8298 Mc. The frequency ratio is 1.6061046. The R column immediately gives $\eta = 0.451$. The magnitude of the z component of the coupling is found by dividing 202.8696 Mc by $|E_2 - E_1| = 0.180087105$, giving 1126.508 Mc, or, alternatively, by dividing 325.8298 Mc by $|E_3 - E_2| = 0.289238701$, giving 1126.508 Mc, the same answer as before. In the above example the frequencies were adjusted so that interpolation was not needed.

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[1]See, for example, R. Bersohn, *J. Chem. Phys.* 20, 1505 (1952).

η	E_1	E_2	E_3	R
.000	1999999990	0499999990	2500000000	9999999990
.001	2000000080	0499999240	2500000130	9999974070
.002	2000003550	0499997000	2500000550	9999896290
.003	2000007990	0499993250	2500001250	9999766670
.004	2000014220	0499988000	2500002220	9999585190
.005	2000022220	0499981250	2500003470	9999351880
.006	2000031990	0499973000	2500005000	9999066720
.007	2000043550	0499963250	2500006800	9998729730
.008	2000056880	0499952000	2500008880	9998340920
.009	2000071990	0499939250	2500011250	9997900290
.010	2000088880	0499925000	2500013800	9997407850
.011	2000107540	0499909250	2500016800	9996863610
.012	2000127990	0499892000	2500020000	9996267580
.013	2000150200	0499873260	2500023470	9995619780
.014	2000174200	0499853010	2500027220	9994920210
.015	2000199970	0499831270	2500031250	9994168900
.016	2000227520	0499808030	2500035550	9993365860
.017	2000256840	0499783290	2500040130	9992511100
.018	2000287950	0499757050	2500045000	9991604640
.019	2000320820	0499729310	2500050130	9990646500
.020	2000355480	0499700070	2500055550	9989636700
.021	2000391900	0499669340	2500061250	9988575260
.022	2000430110	0499637110	2500067220	9987462200
.023	2000470090	0499603380	2500073470	9986297550
.024	2000511840	0499568150	2500080000	9985081330
.025	2000555370	0499531430	2500086800	9983813560
.026	2000600670	0499493210	2500093890	9982494270
.027	2000647740	0499453500	2500101250	9981123480
.028	2000696590	0499412290	2500108890	9979701230
.029	2000747220	0499369580	2500116810	9978227540
.030	2000799610	0499325380	2500125000	9976702450
.031	2000853780	0499279690	2500133470	9975125970
.032	2000909720	0499232500	2500142220	9973498160
.033	2000967440	0499183810	2500151250	9971819030
.034	2001026920	0499133630	2500160560	9970088630
.035	2001088180	0499081960	2500170140	9968306990
.036	2001151200	0499028800	2500180010	9966474140
.037	2001216000	0498974140	2500190150	9964590120
.038	2001282570	0498917990	2500200570	9962654980
.039	2001350910	0498860350	2500211260	9960668740
.040	2001421010	0498801220	2500222240	9958631460
.041	2001492890	0498740600	2500233490	9956543170
.042	2001566530	0498678480	2500245020	9954403910
.043	2001641940	0498614880	2500256830	9952213720
.044	2001719120	0498549790	2500268910	9949972660
.045	2001798060	0498483210	2500281270	9947680770
.046	2001878780	0498415140	2500293920	9945338090
.047	2001961250	0498345580	2500306840	9942944670
.048	2002045500	0498274530	2500320030	9940500560
.049	2002131500	0498202000	2500333510	9938005810

η	E_1	E_2	E_3	R
.050	2002219280	0498127980	2500347260	9935460470
.051	2002308810	0498052480	2500361290	9932864590
.052	2002400110	0497975490	2500375600	9930218220
.053	2002493170	0497897010	2500390190	9927521410
.054	2002588000	0497817060	2500405060	9924774230
.055	2002684580	0497735620	2500420200	9921976730
.056	2002782930	0497652690	2500435620	9919128950
.057	2002883030	0497568290	2500451320	9916230970
.058	2002984900	0497482400	2500467300	9913282830
.059	2003088520	0497395030	2500483560	9910284600
.060	2003193900	0497306180	2500500090	9907236340
.061	2003301040	0497215850	2500516900	9904138110
.062	2003409940	0497124050	2500533990	9900989960
.063	2003520590	0497030760	2500551360	9897791970
.064	2003633000	0496936000	2500569010	9894544200
.065	2003747170	0496839760	2500586930	9891246710
.066	2003863080	0496742040	2500605130	9887899570
.067	2003980750	0496642850	2500623610	9884502840
.068	2004100180	0496542190	2500642370	9881056600
.069	2004221350	0496440050	2500661410	9877560910
.070	2004344280	0496336440	2500680730	9874015840
.071	2004468960	0496231360	2500700320	9870421460
.072	2004595390	0496124800	2500720190	9866777840
.073	2004723560	0496016770	2500740340	9863085060
.074	2004853490	0495907280	2500760770	9859343190
.075	2004985160	0495796310	2500781480	9855552310
.076	2005118570	0495683880	2500802460	9851712480
.077	2005253740	0495569980	2500823720	9847823790
.078	2005390640	0495454620	2500845260	9843886310
.079	2005529300	0495337780	2500867080	9839900120
.080	2005669690	0495219490	2500889180	9835865300
.081	2005811830	0495099730	2500911560	9831781920
.082	2005955710	0494978500	2500934210	9827650070
.083	2006101320	0494855820	2500957150	9823469840
.084	2006248680	0494731670	2500980360	9819241300
.085	2006397780	0494606060	2501003850	9814964530
.086	2006548610	0494479000	2501027620	9810639620
.087	2006701180	0494350470	2501051660	9806266650
.088	2006855490	0494220490	2501075990	9801845720
.089	2007011530	0494089050	2501100590	9797376900
.090	2007169310	0493956160	2501125470	9792860290
.091	2007328820	0493821810	2501150630	9788295970
.092	2007490060	0493686010	2501176070	9783684030
.093	2007653030	0493548760	2501201790	9779024560
.094	2007817730	0493410050	2501227790	9774317650
.095	2007984160	0493269900	2501254060	9769563400
.096	2008152320	0493128290	2501280610	9764761890
.097	2008322200	0492985240	2501307450	9759913230
.098	2008493810	0492840740	2501334560	9755017490
.099	2008667150	0492694790	2501361940	9750074790

η	E_1	E_2	E_3	R
.100	2008842210	0492547400	2501389610	9745085210
.101	2009018990	0492398560	2501417560	9740048850
.102	2009197490	0492248280	2501445780	9734965810
.103	2009377720	0492096560	2501474290	9729836180
.104	2009559660	0491943400	2501503070	9724660070
.105	2009743320	0491788800	2501532130	9719437570
.106	2009928700	0491632760	2501561470	9714168790
.107	2010115800	0491475290	2501591090	9708853820
.108	2010304610	0491316370	2501620990	9703492770
.109	2010495130	0491156030	2501651160	9698085740
.110	2010687370	0490994240	2501681620	9692632840
.111	2010881320	0490831030	2501712350	9687134160
.112	2011076970	0490666380	2501743360	9681589820
.113	2011274340	0490500310	2501774650	9675999910
.114	2011473420	0490332800	2501806220	9670364550
.115	2011674200	0490163870	2501838070	9664683840
.116	2011876690	0489993510	2501870200	9658957890
.117	2012080880	0489821730	2501902610	9653186810
.118	2012286770	0489648520	2501935300	9647370710
.119	2012494370	0489473890	2501968260	9641509690
.120	2012703670	0489297830	2502001510	9635603870
.121	2012914660	0489120360	2502035030	9629653370
.122	2013127360	0488941470	2502068830	9623658280
.123	2013341750	0488761160	2502102910	9617618720
.124	2013557840	0488579430	2502137270	9611534820
.125	2013775620	0488396290	2502171910	9605406680
.126	2013995090	0488211730	2502206830	9599234410
.127	2014216260	0488025760	2502242030	9593018130
.128	2014439110	0487838390	2502277510	9586757960
.129	2014663660	0487649600	2502313260	9580454020
.130	2014889890	0487459400	2502349300	9574106420
.131	2015117810	0487267790	2502385610	9567715270
.132	2015347420	0487074780	2502422210	9561280710
.133	2015578700	0486880370	2502459080	9554802840
.134	2015811680	0486684550	2502496230	9548281790
.135	2016046330	0486487330	2502533660	9541717680
.136	2016282660	0486288710	2502571370	9535110620
.137	2016520670	0486088690	2502609370	9528460750
.138	2016760350	0485887280	2502647640	9521768180
.139	2017001710	0485684470	2502686180	9515033030
.140	2017244750	0485480260	2502725010	9508255430
.141	2017489450	0485274660	2502764120	9501435510
.142	2017735830	0485067670	2502803510	9494573380
.143	2017983880	0484859290	2502843180	9487669180
.144	2018233600	0484649520	2502883130	9480723020
.145	2018484980	0484438370	2502923350	9473735040
.146	2018738030	0484225830	2502963860	9466705360
.147	2018992740	0484011900	2503004640	9459634110
.148	2019249110	0483796590	2503045710	9452521420
.149	2019507150	0483579900	2503087050	9445367410

η	E_1	E_2	E_3	R
.150	2019766840	0483361830	2503128680	9438172210
.151	2020028200	0483142380	2503170580	9430935960
.152	2020291200	0482921560	2503212770	9423658780
.153	2020555870	0482699360	2503255230	9416340810
.154	2020822180	0482475790	2503297980	9408982170
.155	2021090150	0482250840	2503341000	9401583000
.156	2021359770	0482024530	2503384310	9394143430
.157	2021631040	0481796850	2503427890	9386663590
.158	2021903950	0481567800	2503471750	9379143610
.159	2022178510	0481337380	2503515900	9371583630
.160	2022454720	0481105600	2503560320	9363983790
.161	2022732560	0480872460	2503605020	9356344210
.162	2023012050	0480637950	2503650010	9348665030
.163	2023293170	0480402090	2503695270	9340946380
.164	2023575940	0480164870	2503740810	9333188410
.165	2023860340	0479926300	2503786640	9325391250
.166	2024146370	0479686370	2503832740	9317555030
.167	2024434040	0479445080	2503879130	9309679890
.168	2024723340	0479202450	2503925790	9301765980
.169	2025014270	0478958470	2503972740	9293813420
.170	2025306820	0478713140	2504019960	9285822350
.171	2025601000	0478466460	2504067470	9277792920
.172	2025896810	0478218440	2504115250	9269725270
.173	2026194240	0477969080	2504163320	9261619520
.174	2026493290	0477718370	2504211660	9253475830
.175	2026793960	0477466330	2504260290	9245294330
.176	2027096250	0477212950	2504309200	9237075170
.177	2027400150	0476958230	2504358390	9228818480
.178	2027705670	0476702180	2504407850	9220524400
.179	2028012800	0476444800	2504457600	9212193090
.180	2028321540	0476186080	2504507630	9203824670
.181	2028631900	0475926040	2504557940	9195419300
.182	2028943860	0475664670	2504608530	9186977110
.183	2029257420	0475401980	2504659400	9178498240
.184	2029572590	0475137960	2504710560	9169982850
.185	2029889360	0474872620	2504761990	9161431080
.186	2030207740	0474605960	2504813700	9152843060
.187	2030527710	0474337980	2504865700	9144218950
.188	2030849280	0474068690	2504917970	9135558890
.189	2031172440	0473798080	2504970530	9126863020
.190	2031497200	0473526160	2505023360	9118131480
.191	2031823550	0473252920	2505076480	9109364430
.192	2032151490	0472978380	2505129880	9100562010
.193	2032481020	0472702530	2505183560	9091724370
.194	2032812140	0472425380	2505237520	9082851650
.195	2033144840	0472146920	2505291760	9073944000
.196	2033479120	0471867160	2505346280	9065001560
.197	2033814990	0471586100	2505401090	9056024490
.198	2034152430	0471303740	2505456170	9047012920
.199	2034491450	0471020080	2505511540	9037967020

η	E_1	E_2	E_3	R
.200	2034832050	0470735130	2505567190	9028886920
.201	2035174220	0470448890	2505623110	9019772770
.202	2035517960	0470161360	2505679320	9010624730
.203	2035863270	0469872540	2505735820	9001442940
.204	2036210160	0469582430	2505792590	8992227540
.205	2036558600	0469291030	2505849640	8982978690
.206	2036908620	0468998360	2505906980	8973696550
.207	2037260190	0468704400	2505964590	8964381240
.208	2037613330	0468409160	2506022490	8955032940
.209	2037968020	0468112650	2506080670	8945651780
.210	2038324270	0467814860	2506139130	8936237910
.211	2038682080	0467515790	2506197880	8926791500
.212	2039041440	0467215460	2506256900	8917312670
.213	2039402350	0466913850	2506316210	8907801600
.214	2039764820	0466610980	2506375800	8898258420
.215	2040128830	0466306840	2506435670	8888683290
.216	2040494380	0466001430	2506495820	8879076380
.217	2040861480	0465694770	2506556250	8869437770
.218	2041230120	0465386840	2506616970	8859767690
.219	2041600300	0465077660	2506677970	8850066260
.220	2041972020	0464767220	2506739250	8840333630
.221	2042345280	0464455520	2506800810	8830569960
.222	2042720070	0464142580	2506862650	8820775390
.223	2043096390	0463828380	2506924780	8810950090
.224	2043474240	0463512940	2506987180	8801094190
.225	2043853620	0463196250	2507049870	8791207850
.226	2044234530	0462878310	2507112840	8781291230
.227	2044616960	0462559130	2507176100	8771344470
.228	2045000910	0462238720	2507239630	8761367730
.229	2045386390	0461917060	2507303450	8751361160
.230	2045773380	0461594170	2507367550	8741324910
.231	2046161890	0461270040	2507431940	8731259140
.232	2046551910	0460944680	2507496600	8721163990
.233	2046943450	0460618100	2507561550	8711039630
.234	2047336500	0460290280	2507626780	8700886190
.235	2047731050	0459961240	2507692290	8690703840
.236	2048127120	0459630970	2507758090	8680492730
.237	2048524680	0459299480	2507824170	8670253010
.238	2048923750	0458966770	2507890530	8659984830
.239	2049324320	0458632850	2507957170	8649688350
.240	2049726390	0458297700	2508024100	8639363710
.241	2050129960	0457961350	2508091310	8629011050
.242	2050535020	0457623780	2508158800	8618630600
.243	2050941570	0457285000	2508226580	8608222420
.244	2051349610	0456945020	2508294630	8597786700
.245	2051759140	0456603830	2508362970	8587323600
.246	2052170160	0456261430	2508431600	8576833260
.247	2052582660	0455917840	2508500500	8566315040
.248	2052996650	0455573040	2508569690	8555771490
.249	2053412110	0455227050	2508639170	8545200360

η	E_1	E_2	E_3	R
.250	2053829060	0454879860	2508708920	8534602600
.251	2054247480	0454531480	2508778960	8523978380
.252	2054667370	0454181910	2508849290	8513327830
.253	2055088740	0453831150	2508919890	8502651120
.254	2055511570	0453479200	2508990780	8491948390
.255	2055935880	0453126070	2509061950	8481219810
.256	2056361650	0452771760	2509133410	8470465510
.257	2056788880	0452416260	2509205150	8459685650
.258	2057217580	0452059590	2509277170	8448880390
.259	2057647730	0451701740	2509349480	8438049880
.260	2058079340	0451342720	2509422070	8427194270
.261	2058512410	0450982520	2509494940	8416313710
.262	2058946930	0450621160	2509568100	8405408350
.263	2059382910	0450258630	2509641540	8394478340
.264	2059820330	0449894930	2509715260	8383523850
.265	2060259200	0449530070	2509789270	8372545010
.266	2060699520	0449164050	2509863570	8361541990
.267	2061141270	0448796860	2509938140	8350514920
.268	2061584470	0448428530	2510013000	8339463970
.269	2062029110	0448059030	2510088150	8328389280
.270	2062475180	0447688390	2510163580	8317291010
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