Nuclear mass relations and equations

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Relations among the masses of neighboring nuclei provide an accurate and convenient method for the estimation of unknown masses. A set of such relations is "derived" and their structure as partial difference equations is discussed. These considerations lead to a set of mass equations (solutions of the difference equations) that can be ordered such that each successive member gives a potentially more nearly accurate representation of nuclear ground-state energies as functions of N and Z. The first two members of this ordered set are the mass equations considered originally by Garvey *et al.* The results obtained by fitting the third member of this set to the known masses are discussed in this paper. This third mass equation is shown to satisfy the principle of charge symmetry to a good approximation. As a consequence, it gives predictions for the masses of proton-rich nuclei.

[NUCLEAR STRUCTURE Relations among ground-state energies of neighboring nuclei.]

I. INTRODUCTION

Considerable effort has been devoted to the construction of formulas that give the ground-state energies of all nuclei. Originally these formulas were based on a simple physical model of the nucleus. These results involve a small number of parameters and reproduce only the main features and trends of nuclear energies. Today there are many investigations that require considerably more accurate predictions than can be obtained from these few parameter equations.

One approach,[1,2] which has been found to give reasonably reliable ground-state masses, is based on relations of the form

$$\sum_{ij} a_{ij} M(N+i, Z+j) \simeq 0, \tag{1.1}$$

where $M(N+i, Z+j)$ is the mass, or mass excess, of the nucleus with $N+i$ neutrons and $Z+j$ protons. The sum in Eq. (1.1) is to be made approximately equal to zero by a judicious choice of the coefficients a_{ij}. Specifically, these coefficients are to be chosen such that there is first-order cancellation in Eq. (1.1) of all single-particle energies and of all two-body interactions between nucleons. Recently it was shown[3] that these conditions define a set of mass relations, each member of which is satisfied over the known masses with essentially equal accuracy. A "derivation" of these relations and a discussion of their structure is given in Sec. II.

The essential physical observation[4] that leads to these relations is that the empirical neutron-proton interaction is generally weak and that the strength of this interaction is strongly correlated separately for neighboring even-A and odd-A nuclei. An attempt to take into account possible higher-order correlations in the n-p interaction energy is also described in Sec. II. This leads to another set of mass relations. The solutions of these relations (partial difference equations) give rise to a corresponding set of mass equations. This set is characterized by the property that the members of the set can be ordered to give an increasingly accurate description of the n-p interaction as a function of $A = N + Z$ and $T_z = \frac{1}{2}(N - Z)$.

This set of mass equations is described in Sec. III and the results of fitting the first three members of the (ordered) set are compared in Sec. IV. The first two members of the set are the equations considered originally by Garvey *et al.*[2] Numerical results for the third members of this set are discussed in Sec. IV. As shown in Secs. III and IV, this "third equation" is (to a good approximation) consistent with the principle of charge symmetry of nuclear forces and, as a consequence, initial conditions can be chosen such that this equation should give reliable predictions for the excesses of proton-rich nuclei.

The results of Sec. IV suggest that the mass equations in the ordered set fit the known masses with about the same accuracy. This would seem to indicate that this set is of little or no interest. However, a principal measure of the value of a mass equation is its usefulness as an extrapolation formula. As discussed in Sec. V, the present results suggest that successive members of this ordered set may be systematically more accurate extrapolation formulas.

A few properties of singular matrix equations, which proved to be particularly useful in the present investigations, are given in an Appendix.

II. STRUCTURE OF MASS RELATIONS

It is convenient to introduce the displacement operators E_N^n and E_Z^n, where

$$E_N^n M(N,Z) = M(N+n,Z), \tag{2.1a}$$

$$E_Z^n M(N,Z) = M(N,Z+n). \tag{2.1b}$$

Here n is a positive or negative integer. Equations (1.1) can be written as a polynomial in these operators acting on the function $M(N,Z)$, i.e.,

$$\sum_{ij} a_{ij} M(N+i,Z+j) = P(E_N,E_Z)M(N,Z), \tag{2.2}$$

where

$$P(E_N,E_Z) = \sum_{ij} a_{ij} E_N^i E_Z^j. \tag{2.3}$$

Equations (2.2) are to be made approximately equal to zero by a "proper" choice of the polynomial (2.3). Clearly, a minimum condition is that this polynomial be chosen such that the numbers of neutron-neutron, proton-proton, and neutron-proton interactions cancel in Eq. (2.2). This condition is satisfied if, and only if, the polynomial (2.3) contains a factor of the form $(E_N^l E_Z^m - 1)^\gamma (E_Z - 1)^\beta (E_N - 1)^\alpha$ with $\alpha+\beta+\gamma \geq 3$. Here α, β, and γ are non-negative integers; l and m are arbitrary integers.

Since it is desirable to have mass relations that involve only a small number of nuclei, consider the relations with the smallest value of $\alpha+\beta+\gamma$, i.e.,

$$(E_N^l E_Z^m - 1)^\gamma (E_Z - 1)^\beta (E_N - 1)^\alpha M(N,Z) \simeq 0, \quad \alpha+\beta+\gamma = 3. \tag{2.4}$$

For fixed values of l and m there are 10 distinct relations defined by Eqs. (2.4). These were evaluated over the known masses for a range of values of l and m and the relations defined by Eqs. (2.4) with $\alpha=\beta=\gamma=1$ and $l+m$ an even integer were found to have values considerably closer to zero than any of the others.

The resulting set of mass relations, namely

$$O^{lm}M(N,Z) \equiv (E_N^l E_Z^m - 1)(E_Z - 1)(E_N - 1)M(N,Z) \simeq 0, \quad l+m = \text{even} \tag{2.5}$$

have been discussed in Ref. 3. Over a considerable range of values of l and m, each member of this set gives a prediction of nearly equal statistical accuracy for a single unknown mass in Eq. (2.5). The average of this set is statistically more reliable than is the prediction obtained from any single relation. Also, the dispersion in the set gives a measure of the uncertainty of this average. With $l=\pm m=1$, Eqs. (2.5) are the Garvey-Kelson[1,2] relations.

A "physical" explanation of the accuracy of Eqs. (2.5) can be found in a discussion of mass equations given by Jänecke and Behrens.[4] The quantity

$$I_{np}(N+1,Z+1) = (E_Z - 1)(E_N - 1)M(N,Z) \tag{2.6}$$

is defined to be the effective residual n-p interaction energy in the nucleus with $N+1$ neutrons and $Z+1$ protons. In terms of this energy Eqs. (2.5) become

$$O^{lm}M(N,Z) = I_{np}(N+l+1,Z+m+1) - I_{np}(N+1,Z+1). \tag{2.7}$$

The energies I_{np} are generally small, but more importantly, they are strongly correlated separately for neighboring even-A and odd-A nuclei. Thus, with $l+m$ an even integer, $O^{lm}M(N,Z)$, as given in Eq. (2.7), is the difference between two small quantities that are of comparable magnitude.

The derivation of mass relations based on correlations in the values of I_{np} can be carried a step further. There is evidence[4] for a smooth long-range dependence of I_{np} on $A=N+Z$ and/or $T_z = \frac{1}{2}(N-Z)$. Assume that any such behavior can be represented by a polynomial of the form

$$I_{np}(N,Z) = \sum_{\kappa=0}^{k-1} f_\kappa(A) T_z^\kappa + \sum_{\sigma=0}^{s-1} g_\sigma(T_z) A^\sigma, \tag{2.8}$$

where the f_κ are arbitrary functions of A and the g_σ are arbitrary functions of T_z. For any function $f_\kappa(A)$, $(E_N E_Z^{-1} - 1)f_\kappa(A) = 0$ and for any function $g_\sigma(T_z)$, $(E_N E_Z - 1)g_\sigma(T_z) = 0$; furthermore, $(E_N E_Z^{-1} - 1)T_z^\kappa$ is a polynomial of order $\kappa - 1$ in T_z and $(E_N E_Z - 1)A^\sigma$ is a polynomial of order $\sigma - 1$ in A. It follows that, if I_{np} is described by Eq. (2.8), $(E_N E_Z^{-1} - 1)^k (E_N E_Z - 1)^s I_{np}(N,Z) = 0$. Thus the difference equations

$$(E_N E_Z^{-1} - 1)^k (E_N E_Z - 1)^s (E_Z - 1)(E_N - 1)M(N,Z) = 0 \tag{2.9}$$

take into account any behavior of the residual n-p interaction energy that can be represented by functions of the form of Eq. (2.8).

Let the set of relations (2.9) be ordered according to the value of (k,s). The first two relations $(k,s) = (0,1)$ and $(1,0)$ are the relations considered by Garvey *et al.*[2] To the extent that the behavior of the n-p interaction energy is represented by higher-order terms in Eq. (2.8), the successive members of this set are more nearly accurate relations among the masses of neighboring nuclei. However, for different values of s and k, the masses of differing numbers of nuclei are related by Eqs. (2.9) and it is difficult to judge the relative accuracy of these relations. This difficulty is easily circumvented if, instead of the difference equations (2.9), the associated solutions (mass

equations) are compared. This is discussed in Secs. III and IV.

III. MASS EQUATIONS

A mass relation is a partial difference equation, the solution of which is a mass equation.

The mass equations that arise as solutions of several of the relations (2.5) were discussed briefly in Ref. 3. As mentioned previously, the members of Eq. (2.5) are very nearly equivalent statistically and there is no *a priori* reason to believe that the more complex solutions of the higher-order difference equations are significantly more accurate than the lowest-order ones ($l=\pm m=1$) considered originally by Garvey *et al.*[2]

On the other hand, as the values of k and s are increased, the difference equations (2.9) take into account more accurately some of the long-range behavior of the excesses as functions of A and T_z. The corresponding mass equations possess the same property. Consequently, it is of some interest to investigate these equations. From their "derivation" it is easily seen that the general solutions of the difference equations (2.9) are

$$M(N,Z)=M_0+h_1(N)+h_2(Z)+\sum_{\kappa=0}^{k-1}f_\kappa(A)E^\kappa + \sum_{\sigma=0}^{s-1}g_\sigma(E)A^\sigma , \tag{3.1}$$

where h_i, f_κ, and g_σ are arbitrary functions of their arguments, M_0 is a constant independent of N and Z, and $E=N-Z$.

To make use of a mass equation of this kind, the point functions h_i, f_κ, and g_σ are evaluated by fitting the equation to the known masses (or mass excesses). The resulting equation is then used to evaluate the excesses of nuclei that are not included in the fit. The existing body of accurately known nuclear masses covers a range in Z, N, A, and E of about 100, 150, 250, and 60 values, respectively. Thus, for example, Eq. (3.1) with $(k,s)=(1,1)$ contains ~560 free parameters and yields predictions for the excesses of ~15000 nuclei.

In Sec. IV the results of fitting Eqs. (3.1) with $(k,s)=(0,1)$, $(1,0)$, and $(1,1)$ to the known masses are compared. Of particular interest in this paper is the equation with $(k,s)=(1,1)$. This is the simplest member of the set (3.1) that has not been considered previously. Let us rewrite this equation as

$$M(N,Z)=M_0+h_1(N)+h_2(Z)+h_3(A)+h_4(E), \tag{3.2}$$

where, for convenience, the notation has been slightly changed.

Since the variables N, Z, A, and E are not independent the fitting of Eq. (3.2) to the known masses is not unique. The values of $M(N,Z)$ are unchanged if the h_i in Eq. (3.2) are replaced by H_i, where

$$H_1(N)=h_1(N)+a_1+a_2N+a_3N^2 , \tag{3.3a}$$

$$H_2(Z)=h_2(Z)+a_4+a_5Z+a_3Z^2 , \tag{3.3b}$$

$$H_3(A)=h_3(A)+a_6-\tfrac{1}{2}(a_5+a_2)A-\tfrac{1}{2}a_3A^2+a_7(-1)^A , \tag{3.3c}$$

$$H_4(E)=h_4(E)-(a_1+a_4+a_6)+\tfrac{1}{2}(a_5-a_2)E -\tfrac{1}{2}a_3E^2-a_7(-1)^E . \tag{3.3d}$$

The coefficients $a_i, i=1,\ldots,7$, are arbitrary. In the fitting this arbitrariness must be removed by imposing on the solution a sufficient number of independent conditions in terms of initial values or shapes of the point functions. A convenient method for the introduction of appropriate conditions is described in the Appendix.

Since Eq. (3.2) is invariant under the transformation (3.3), the choice of the coefficients a_i is a matter of convenience. However, it is reasonable to inquire whether these constants can be chosen in some meaningful way. For example, except for small Coulomb contributions, the charge symmetry of nuclear forces implies that the n-p interaction energy is unchanged if N and Z are interchanged, i.e.,

$$(E_Z-1)(E_N-1)M(N,Z)=(E_Z-1)(E_N-1)M(Z,N) . \tag{3.4}$$

The mass equation (3.2) satisfies this equation provided that

$$h_4(E)=h_4(-E) . \tag{3.5}$$

To exhibit this symmetry, to the extent that it exists, the constants a_i in Eqs. (3.3) must be chosen appropriately. From Eq. (3.3d) we have

$$h_4(0)=0=H_4(0)+(a_1+a_4+a_6+a_7) ,$$

$$h_4(E)-h_4(-E)=0 =H_4(E)-H_4(-E)-(a_5-a_2)E ,$$

$$E\neq 0 .$$

Thus conditions (3.5) are satisfied if, for all nonzero values of E, $[H_4(E)-H_4(-E)]/E$ is independent of E. The H_i are the solutions for arbitrary boundary conditions.

Obviously a symmetry, such as Eq. (3.5), is an intrinsic property of a given mass equation fitted to the known masses. The choice of boundary conditions can only make an existing property manifest. As will be shown in Sec. IV, boundary conditions can be chosen such that the mass equation

(3.2) satisfies conditions (3.5) to a very good approximation. A practical consequence is that the domain of definition of Eq. (3.2) is extended to large negative values of E and this allows a prediction of the excesses of proton-rich nuclei.

It is not clear that the higher-order equations in the set (3.1) will exhibit further symmetries or other desirable features. However, it is not unreasonable to expect that the individual point functions in these higher-order equations may have a more nearly independent physical meaning. As discussed in Sec. V, these are just the properties that improve the reliability of a mass equation when it is used as an extrapolation formula.

IV. COMPARISON OF MASS EQUATIONS

This section contains a comparison of the results obtained from a least-squares fit to the known mass excesses of the following equations:

$$M(N,Z)=M_0+g_1(N)+g_2(Z)+g_3(E)\,, \tag{4.1}$$

$$M(N,Z)=M_0+f_1(N)+f_2(Z)+f_3(A)\,, \tag{4.2}$$

$$M(N,Z)=M_0+h_1(N)+h_2(Z)+h_3(A)+h_4(E)\,, \tag{4.3}$$

$$M(N,Z)=M_0+q_1(N)+q_2(Z)+q_3(E)/A\,, \tag{4.4}$$

$$M(N,Z)=M_0+p_1(N)+p_2(Z)+p_3(A)+p_4(E)/A\,. \tag{4.5}$$

The first three of the above equations are the first three members of the set of equations (3.1) ordered according to the value of (k,s). Equations (4.4) and (4.5) are variations suggested by the form of the symmetry-energy term in the Weizsacker mass formula.[5]

Values of the parameters that occur in these equations were determined by the condition that they minimize the quantity

$$Q^2=\sum \lambda(N,Z)[m(N,Z)-M(N,Z)]^2\,, \tag{4.6}$$

where $m(N,Z)$ is a measured excess, $M(N,Z)$ is the function defined by one of the equations (4.1)–(4.5), $\lambda(N,Z)$ is the weight associated with the measured excess $m(N,Z)$, and the sum is over the known masses. Each point function at each value of its argument is considered as a separate parameter in the fitting procedure.

Values of the excesses $m(N,Z)$ were taken from the 1975 Wapstra-Bos[6] compilation. All excesses for nuclei with $8\leq Z\leq 100$ and $8\leq N\leq 154$ that are listed with an error less than 200 keV were included in the sum in Eq. (4.6). However, for reasons that are well understood, odd-odd $N=Z$ nuclei were not included, and, in the case of Eq. (4.2), nuclei with $N<Z$ were also excluded. For the results given below, $\lambda(N,Z)$ was set equal to unity for all excesses considered.

Three quantities were computed to measure the accuracy of the least-squares fit. These are

$$\sigma_1=\left[\sum[m(N,Z)-M(N,Z)]^2/n\right]^{1/2}, \tag{4.7a}$$

$$\sigma_2=\sum|m(N,Z)-M(N,Z)|/n\,, \tag{4.7b}$$

$$\sigma_3=\left[\sum[m(N,Z)-M(N,Z)]^2/(n-t)\right]^{1/2}, \tag{4.7c}$$

where n is the number of terms in the sum and t is the number of free parameters in the mass equation $M(N,Z)$. Values of these quantities are listed in Table I for the mass equations (4.1) through (4.5). Equation (4.4) fits the known excesses considerably better than does Eq. (4.1); however, the more accurate equations (4.2), (4.3), and (4.5) yield the same quality of fit according to these measures.

Except for Eq. (4.2) boundary conditions were chosen such that the functions of E are as symmetric as possible about $E=0$. As discussed in Sec. III, this symmetry is an intrinsic property of the fitted equation and the choice of boundary condi-

TABLE I. A comparison of the fits of Eqs. (4.1)–(4.5) to the known excesses. The quantities σ_1, σ_2, and σ_3 are defined by Eqs. (4.7); n is the number of measured excesses included in the fit and t is the number of parameters in the given mass equation.

	n	t	σ_1 (MeV)	σ_2 (MeV)	σ_3 (MeV)
Eq. (4.1):	1251	300	0.573	0.312	0.658
Eq. (4.2):	1199	476	0.139	0.102	0.180
Eq. (4.3):	1251	535	0.141	0.099	0.187
Eq. (4.4):	1251	300	0.323	0.221	0.371
Eq. (4.5):	1251	535	0.140	0.100	0.186

TABLE II. The fitted values in MeV of the function of $E=N-Z$ that occur in each of Eqs. (4.1), (4.3), (4.4), and (4.5). The symmetry condition (3.5), $-4\leq E\leq 4$, was imposed on each solution. Note that the functions $q_3(E)$ and $p_4(E)$ appear in the mass equations (4.4) and (4.5), respectively, divided by the mass number A.

E	Eq. (4.1) $g_3(E)$	Eq. (4.3) $h_4(E)$	Eq. (4.4) $q_3(E)$	Eq. (4.5) $p_4(E)$
0	0	0	0	0
1	2.800	40.899	66.0	2737.8
−1	2.379	40.800	62.3	2737.7
2	5.652	3.044	148.1	−73.1
−2	5.697	3.008	140.0	−73.4
3	9.920	44.416	277.2	2507.7
−3	9.963	44.410	263.6	2507.7
4	14.537	7.082	421.5	−459.4
−4	14.790	7.128	405.9	−458.5

TABLE III. Values of the point functions obtained by fitting Eq. (4.5) to the known excesses. The excess, in MeV, of a nucleus with $N \geq 8$, $Z \geq 8$, $A \geq 16$, and $-4 \leq E = N - Z \leq 58$ is obtained from the equation

$$M(N,Z) = -4.7370 + P_1(N) + P_2(Z) + P_3(A) + 100P_4(E)/A .$$

Excesses for nuclei with $E < -4$ can be obtained by replacing $P_4(E)$ by $P_4(|E|)$ in this equation.

N	$P_1(N)$	N	$P_1(N)$	N	$P_1(N)$	N	$P_1(N)$	N	$P_1(N)$
8	0.000	38	−1850.501	68	−505.904	98	2574.059	128	6 863.165
9	−157.042	39	−1842.183	69	−426.039	99	2700.717	129	7 023.199
10	−308.191	40	−1833.783	70	−346.804	100	2827.289	130	7 182.494
11	−445.114	41	−1819.306	71	−263.364	101	2956.504	131	7 344.047
12	−576.695	42	−1804.969	72	−180.616	102	3085.707	132	7 504.698
13	−695.726	43	−1784.802	73	−93.685	103	3217.509	133	7 667.603
14	−810.543	44	−1764.929	74	−7.528	104	3349.218	134	7 829.784
15	−913.701	45	−1739.410	75	82.629	105	3483.546	135	7 994.057
16	−1012.002	46	−1714.149	76	172.085	106	3617.778	136	8 157.745
17	−1100.756	47	−1683.600	77	265.358	107	3754.367	137	8 323.497
18	−1185.899	48	−1653.168	78	358.031	108	3890.887	138	8 488.527
19	−1262.291	49	−1617.606	79	454.380	109	4030.089	139	8 655.759
20	−1336.120	50	−1582.062	80	550.151	110	4169.094	140	8 822.222
21	−1400.332	51	−1540.052	81	649.443	111	4310.662	141	8 990.705
22	−1462.558	52	−1497.240	82	748.505	112	4451.838	142	9 158.706
23	−1516.932	53	−1450.480	83	852.801	113	4595.764	143	9 328.648
24	−1569.778	54	−1403.177	84	956.787	114	4739.180	144	9 498.098
25	−1615.123	55	−1351.855	85	1063.954	115	4885.334	145	9 669.413
26	−1658.680	56	−1300.040	86	1171.017	116	5030.839	146	9 840.287
27	−1695.484	57	−1243.940	87	1281.263	117	5178.991	147	10 012.958
28	−1730.801	58	−1187.763	88	1391.209	118	5326.568	148	10 185.106
29	−1758.613	59	−1127.337	89	1504.462	119	5476.676	149	10 358.967
30	−1784.248	60	−1067.271	90	1616.731	120	5626.159	150	10 532.519
31	−1803.832	61	−1002.720	91	1732.450	121	5778.111	151	10 707.829
32	−1822.057	62	−938.695	92	1847.553	122	5929.477	152	10 882.726
33	−1834.094	63	−870.173	93	1965.966	123	6083.187	153	11 059.606
34	−1845.175	64	−802.131	94	2084.131	124	6236.346	154	11 236.123
35	−1849.983	65	−729.759	95	2205.397	125	6391.478		
36	−1854.519	66	−657.755	96	2326.330	126	6546.594		
37	−1852.517	67	−581.523	97	2450.323	127	6705.176		
Z	$P_2(Z)$	Z	$Z_2(Z)$	Z	$P_2(Z)$	Z	$P_2(Z)$	Z	$P_2(Z)$
8	−0.000	27	−1586.320	46	−1395.850	65	−135.263	84	1 908.367
9	−154.431	28	−1612.966	47	−1351.952	66	−46.619	85	2 035.462
10	−302.183	29	−1631.612	48	−1307.927	67	46.201	86	2 162.198
11	−435.403	30	−1648.073	49	−1258.544	68	139.250	87	2 292.010
12	−562.912	31	−1658.122	50	−1209.192	69	236.179	88	2 421.331
13	−677.556	32	−1666.491	51	−1153.292	70	333.467	89	2 553.837
14	−787.698	33	−1668.216	52	−1096.918	71	434.540	90	2 685.971
15	−885.747	34	−1668.984	53	−1036.073	72	535.967	91	2 821.129
16	−978.797	35	−1663.308	54	−974.847	73	640.744	92	2 955.894
17	−1062.016	36	−1656.836	55	−909.053	74	745.721	93	3 093.659
18	−1141.446	37	−1644.143	56	−843.081	75	854.332	94	3 231.206
19	−1211.800	38	−1630.634	57	−772.508	76	963.204	95	3 371.457
20	−1279.038	39	−1611.022	58	−701.908	77	1076.024	96	3 511.498
21	−1336.586	40	−1590.453	59	−626.675	78	1188.621	97	3 654.289
22	−1392.068	41	−1564.009	60	−551.495	79	1304.662	98	3 796.900
23	−1439.321	42	−1537.243	61	−471.799	80	1420.630	99	3 942.264
24	−1484.622	43	−1504.945	62	−392.055	81	1540.245	100	4 087.463
25	−1522.390	44	−1472.400	63	−307.929	82	1659.923		
26	−1558.042	45	−1434.270	64	−223.755	83	1784.199		
A	$P_3(A)$	A	$P_3(A)$	A	$P_3(A)$	A	$P_3(A)$	A	$P_3(A)$
16	0.000	64	3439.137	112	2110.902	160	−1905.339	208	−7 841.182
17	−0.000	65	3406.659	113	2026.899	161	−2028.181	209	−7 993.585
18	316.263	66	3455.931	114	1989.601	162	−2118.302	210	−8 120.841

TABLE III. (*Continued*)

A	$P_3(A)$	A	$P_3(A)$	A	$P_3(A)$	A	$P_3(A)$	A	$P_3(A)$
19	321.395	67	3421.067	115	1903.755	163	−2242.594	211	−8 274.003
20	608.043	68	3465.414	116	1863.847	164	−2334.452	212	−8 402.323
21	615.995	69	3428.041	117	1776.292	165	−2460.139	213	−8 556.389
22	878.928	70	3467.655	118	1733.727	166	−2553.899	214	−8 685.964
23	888.198	71	3427.934	119	1644.305	167	−2681.067	215	−8 840.933
24	1130.492	72	3462.861	120	1599.236	168	−2776.642	216	−8 971.743
25	1140.666	73	3420.695	121	1508.023	169	−2905.055	217	−9 127.693
26	1364.741	74	3450.943	122	1460.372	170	−3002.368	218	−9 259.709
27	1374.093	75	3406.237	123	1367.253	171	−3132.220	219	−9 416.580
28	1581.311	76	3432.269	124	1317.237	172	−3231.261	220	−9 549.804
29	1589.910	77	3385.195	125	1222.492	173	−3362.473	221	−9 707.705
30	1782.747	78	3407.294	126	1169.949	174	−3463.272	222	−9 842.037
31	1789.682	79	3358.070	127	1073.582	175	−3595.706	223	−10 000.872
32	1968.957	80	3376.030	128	1018.798	176	−3698.027	224	−10 136.328
33	1974.562	81	3324.550	129	920.841	177	−3831.770	225	−10 296.113
34	2141.785	82	3338.516	130	863.836	178	−3935.837	226	−10 432.729
35	2145.510	83	3284.947	131	764.342	179	−4070.906	227	−10 593.436
36	2301.788	84	3295.125	132	705.108	180	−4176.671	228	−10 731.169
37	2303.610	85	3239.112	133	603.940	181	−4313.021	229	−10 892.792
38	2449.532	86	3245.297	134	542.665	182	−4420.353	230	−11 031.652
39	2448.856	87	3186.910	135	439.970	183	−4558.050	231	−11 194.169
40	2585.090	88	3189.491	136	376.435	184	−4666.944	232	−11 334.040
41	2582.200	89	3128.833	137	272.301	185	−4805.754	233	−11 497.478
42	2709.391	90	3127.897	138	206.524	186	−4916.377	234	−11 638.361
43	2703.993	91	3065.321	139	100.826	187	−5056.499	235	−11 802.542
44	2822.207	92	3061.089	140	32.959	188	−5168.771	236	−11 944.359
45	2814.184	93	2996.425	141	−74.568	189	−5310.102	237	−12 109.487
46	2924.328	94	2988.829	142	−144.584	190	−5424.032	238	−12 252.291
47	2913.624	95	2922.054	143	−253.647	191	−5566.872	239	−12 418.191
48	3016.280	96	2911.396	144	−325.842	192	−5682.377	240	−12 561.937
49	3003.458	97	2842.396	145	−436.451	193	−5826.421	241	−12 728.535
50	3099.359	98	2828.583	146	−510.769	194	−5943.536	242	−12 873.174
51	3084.102	99	2757.976	147	−622.959	195	−6088.768	243	−13 040.496
52	3173.417	100	2740.631	148	−699.340	196	−6207.318	244	−13 186.140
53	3155.672	101	2668.027	149	−813.005	197	−6353.815	245	−13 354.235
54	3238.471	102	2647.675	150	−891.407	198	−6473.684	246	−13 500.862
55	3218.100	103	2572.922	151	−1006.707	199	−6621.291	247	−13 669.757
56	3294.807	104	2549.694	152	−1087.272	200	−6742.558	248	−13 817.353
57	3272.133	105	2473.067	153	−1204.216	201	−6891.086	249	−13 987.039
58	3342.815	106	2446.980	154	−1286.725	202	−7013.611	250	−14 135.514
59	3317.724	107	2368.520	155	−1405.186	203	−7163.316	251	−14 306.030
60	3382.920	108	2339.518	156	−1489.624	204	−7287.285	252	−14 455.548
61	3355.303	109	2259.277	157	−1609.548	205	−7438.061	253	−14 626.749
62	3414.856	110	2227.543	158	−1695.884	206	−7563.259	254	−14 777.111
63	3384.859	111	2145.473	159	−1817.138	207	−7714.961		
E	$P_4(E)$	E	$P_4(E)$	E	$P_4(E)$	E	$P_4(E)$	E	$P_4(E)$
−4	−4.585	9	−0.960	22	−189.962	35	−474.720	48	−939.012
−3	25.077	10	−35.597	23	−181.416	36	−531.529	49	−949.395
−2	−0.734	11	−16.461	24	−228.077	37	−535.206	50	−1 014.222
−1	27.377	12	−52.707	25	−221.375	38	−593.414	51	−1 025.515
0	0.000	13	−35.236	26	−269.845	39	−598.522	52	−1 091.371
1	27.378	14	−73.149	27	−264.961	40	−658.165	53	−1 103.637
2	−0.731	15	−57.453	28	−315.286	41	−664.496	54	−1 170.531
3	25.077	16	−97.141	29	−312.220	42	−725.363	55	−1 183.797
4	−4.594	17	−83.147	30	−364.409	43	−732.966	56	−1 251.688
5	19.614	18	−124.543	31	−363.156	44	−794.793	57	−1 266.388
6	−11.573	19	−112.366	32	−417.044	45	−803.193	58	−1 335.919
7	11.021	20	−155.493	33	−417.391	46	− 865.827		
8	−21.840	21	−145.076	34	−472.781	47	− 875.313		

tions will exhibit this symmetry only to the extent that it actually exists. Values of the functions of E that were obtained for the above equations are listed in Table II for $-4 \leq E \leq 4$.

It is obvious from these results that Eqs. (4.3) and (4.5) satisfy the symmetry conditions (3.5) to a very good approximation whereas Eqs. (4.1) and (4.4) do not. It seems reasonable to assume, particularly in the case of Eq. (4.5), that this symmetry extends to more negative values of E. With the terms $p_4(E)/A$ replaced by $p_4(|E|)/A$, Eq. (4.5) gives predictions for the excesses of proton-rich nuclei. Values of the point functions p_i that occur in Eq. (4.5) are given in Table III.

Equations (4.4) and (4.5) are in a class different than the other mass equations considered here in that they are not solutions of homogeneous difference equations. However, the same independent-particle model with fourfold degenerate single-particle levels that has been used to justify the Garvey-Kelson equations can be invoked to show that the symmetry effect yields a contribution of the form $p(|E|)/A$ to the ground-state energy of a nucleus. This is, in fact, one reason for the introduction of Eqs. (4.4) and (4.5) into the present discussion.

A mass table based on a fit of Eq. (4.2) to the 1975 tabulation has been published.[7] Although tabulations of the point functions obtained by fitting Eqs. (4.3) and (4.4) to the known excesses have not been published, only the results for Eq. (4.5) are given here. The reason is that we believe Eq. (4.5) to be the most useful of the mass equations considered. Values of the point functions in the remaining equations can be made available on request.

V. DISCUSSION

The reliability of mass equations of the type considered here has been questioned by several authors, most recently by Comay and Kelson.[8] The use of Eq. (4.3), for example, to predict excesses far from the region of known nuclei is based on the assumption that this mass equation gives an accurate representation of the functional dependence of the excesses not only for the known nuclei but also for nuclei in the region of extrapolation. As mentioned above, all of the mass equations in the set (3.1) probably fit the known excesses with about the same accuracy so that additional criteria are necessary to judge their relative reliability as extrapolation formulas. The possibility of introducing additional physical conditions, such as charge symmetry in Eq. (4.3), provides one such criterion.

As shown in Table II, Eq. (4.3) satisfies the symmetry condition (3.5) significantly better than does Eq. (4.1). As a consequence it is reasonable to expect that spurious correlations between the fitted values of the point functions are reduced in Eq. (4.3) compared with Eq. (4.1). All else being equal, it then follows that Eq. (4.3) is a more nearly accurate extrapolation formula than is Eq. (4.1). It remains to be determined whether the higher-order equations of the set (3.1) exhibit similar behavior. The fitting of these equations to the known masses is limited to rather small values of k and s since the number of adjustable parameters increases rapidly for successive values of (k, s). However, an investigation of the $(2,1)$ and $(2,2)$ equations seems reasonable.

Mass equations of the form

$$M'(N,Z) = M^*(N,Z) + M(N,Z)\,, \tag{5.1}$$

where M^* represents some theoretical expression for the excess and M is the general solution of a homogeneous difference equation, have been considered by Jänecke and co-workers.[4,5] The inhomogeneous term M^*, which accounts to first order for Coulomb, pairing, etc., energies, is introduced in an attempt to reduce spurious correlations between the point functions that define M. There is, however, a question whether this goal can be achieved with a few-parameter expression for M^*.

Equations (4.4) and (4.5) are of the form of Eq. (5.1). For Eq. (4.5), e.g., $M^*(N,Z) = p_4(N-Z)/(N+Z)$ and $M(N,Z)$ is the solution of the $(1,0)$ member of the set (3.1). The results given in Table II show that Eq. (4.5) satisfies the symmetry condition (3.5) significantly better than does Eq. (4.3). By the argument given above in the comparison of Eqs. (4.1) and (4.3), it is reasonable to expect that false correlations between the point functions are further reduced in going from Eq. (4.3) to (4.5). Although the inhomogeneous term M^* in Eq. (4.5) depends on many parameters, this equation retains the simplicity of application that characterize mass equations which are obtained as solutions of homogeneous difference equations.

APPENDIX

A convenient method for the specification of boundary conditions in the minimization problems (4.6) is described below.

Consider Eq. (4.6) rewritten as

$$Q^2 = \sum_{i=1}^{n} \lambda_i^2 \left(m_i - \sum_{j=1}^{t} a_{ij} h_j \right)^2 , \tag{A1}$$

where m_i is a measured excess and h_j represents a point function at a given value of its argument. The h_j that minimize Q^2 are the solutions of the

set of equations

$$\sum_{l=1}^{t}\sum_{i=1}^{n} a_{ik}\lambda_i^2 a_{il} h_l = \sum_{i=1}^{n} a_{ik}\lambda_i^2 m_i\,, \qquad (A2)$$

$$k = 1, \ldots, t\,,$$

which we rewrite as

$$bh = y\,, \qquad (A3)$$

where b is a symmetric $t \times t$ matrix with elements

$$b_{kl} = \sum_{i=1}^{n} a_{ik}\lambda_i^2 a_{il}\,, \qquad (A4)$$

and y is a t-dimensional column vector with components

$$y_k = \sum_{i=1}^{n} a_{ik}\lambda_i^2 m_i\,. \qquad (A5)$$

The λ_i^2 are the weights associated with the measured excesses m_i. The solution of Eq. (A3) is

$$h = b^{-1}y\,, \qquad (A6)$$

provided that the inverse of the matrix b exists.

As discussed in Sec. III, the variables N, Z, A, and E are not independent and, as a consequence, the matrix b is singular. In order to solve Eq. (A3) it is necessary to specify a number of independent boundary conditions sufficient to account for the rank deficiency of this matrix.

In an actual computation it is convenient to generate the symmetric $t \times t$ matrix b directly without first specifying the $n \times t$ matrix a since only about a quarter of the computer storage that would be required for the matrix a is taken up by the symmetric matrix b. In order to proceed in this fashion, however, it is necessary to impose boundary conditions directly on Eqs. (A3).

Typical boundary conditions are the specification of the values of particular h_l or as conditions on the shapes or symmetries of these point functions. Boundary conditions of these kinds can be written as

$$\sum_{j=1}^{t} a_{n+1,\,j} h_j = c_{n+1}\,,$$
$$\sum_{j=1}^{t} a_{n+q,\,j} h_j = c_{n+q} \qquad (A7)$$

If these boundary conditions are considered simply as additional mass equations, then, instead of Q^2, the quantity to be minimized is

$$Q'^2 = \sum_{i=1}^{n+q} \lambda_i^2 \left(m_i - \sum_{j=1}^{t} a_{ij} h_j\right)^2\,, \qquad (A8)$$

where, for $i > n$, $m_i = c_i$ and λ_i^2 is conveniently set equal to unity. The h_j that minimize Q'^2 are the solutions of the set of equations

$$\sum_{l=1}^{t}\left\{b_{kl} + \sum_{i=n+1}^{n+q} a_{ik}a_{il}\right\} h_l = y_k + \sum_{i=n+1}^{n+q} a_{ik}c_i\,, \qquad (A9)$$

$$k = 1, \ldots t\,.$$

It is shown below that the solution of Eq. (A9) is the solution of Eq. (A3) with boundary conditions given by Eqs. (A7).

In the case of boundary conditions of the form $h_{l_0} = 0$ the parameters in Eq. (A7) are $a_{n+1,\,j} = \delta_{jl_0}$ and $c_{n+1} = 0$ and Eqs. (A9) become

$$\sum_{l=1}^{t}\{b_{kl} + \delta_{kl_0}\delta_{ll_0}\}h_l = y_k\,. \qquad (A10)$$

Thus it is necessary only to add unity to the element $b_{l_0 l_0}$ of the matrix b in Eq. (A3) to take this boundary condition into account. Similarly conditions of the form

$$\sum h_4(E) = 0\,, \qquad (A11)$$

where the sum is over some subset of values of E, are taken into account by adding unity to all elements b_{kl} of the matrix b in Eq. (A3) where both h_k and h_l are included in the sum (A11).

That these simple modifications of the matrix b actually yield the solution of Eqs. (A3) with the desired boundary conditions is easily demonstrated. In Eqs. (A3) b is a symmetric $t \times t$ matrix of rank $r = t - q$; h and y are t-dimensional column vectors. Let b, h, and y be partitioned as

$$b = \begin{bmatrix} B_0 & B' \\ \tilde{B}' & B \end{bmatrix}\,, \quad h = \begin{bmatrix} H_0 \\ H \end{bmatrix}\,, \quad y = \begin{bmatrix} Y_0 \\ Y \end{bmatrix}\,, \qquad (A12)$$

where B is a symmetric $r \times r$ matrix of rank r, B' is a $q \times r$ matrix, $\tilde{B}'$ is the transpose of B', B_0 is a $q \times q$ matrix, H_0 and Y_0 are column vectors of dimension q, and H and Y are column vectors of dimension r. The partition (A12) is always possible since b is symmetric and of rank r. Equations (A3) can now be written as

$$B_0 H_0 + B'H = Y_0\,,$$
$$\tilde{B}'H_0 + BH = Y$$

or

$$H = B^{-1}(Y - \tilde{B}'H_0) \qquad (A13a)$$

$$(B_0 - B'B^{-1}\tilde{B}')H_0 = Y_0 - B'B^{-1}Y\,. \qquad (A13b)$$

Here $(B_0 - B'B^{-1}\tilde{B}')$ is a $q \times q$ matrix of rank zero, i.e.,

$$B_0 - B'B^{-1}\tilde{B}' = 0\,;$$

otherwise, Eqs. (A13b) would determine at least one component of H_0 in terms of the remaining

components in contradiction to the original assumption that the matrix b is of rank r. The solution of Eqs. (A3) is thus

$$h = \begin{bmatrix} H_0 \\ B^{-1}(Y - \tilde{B}'H_0) \end{bmatrix}, \tag{A14}$$

where the q components of H_0 are to be specified as boundary conditions.

Let these boundary conditions be given as

$$\Lambda H_0 = E, \tag{A15}$$

where Λ is a $q \times q$ matrix with elements

$$\Lambda_{kl} = \sum_{i=n+1}^{n+q} a_{ik} a_{il}, \quad k,l = 1, \ldots, q \tag{A16}$$

and E is a column vector of dimension q with components

$$E_k = \sum_{i=n+1}^{n+q} a_{ik} c_i, \quad k = 1, \ldots, q. \tag{A17}$$

Since these conditions are independent, Λ is nonsingular. Consider now the matrix equation

$$b'h = y', \tag{A18}$$

where

$$b' = \begin{bmatrix} B_0 + \Lambda & B' \\ \tilde{B}' & B \end{bmatrix}, \quad y' = \begin{bmatrix} Y_0 + E \\ Y \end{bmatrix}. \tag{A19}$$

Equation (A18) is just Eq. (A9) rewritten in matrix notation. The solution of Eq. (A18), obtained by a calculation identical with that given above for Eq. (A3), is

$$h = \begin{bmatrix} \Lambda^{-1}E \\ B^{-1}(Y - \tilde{B}'\Lambda^{-1}E) \end{bmatrix}, \tag{A20}$$

which is obviously the solution (A14) with the boundary conditions specified by Eqs. (A15).

For boundary conditions (A7) of the form $h_{l_0} = h_{l_1} = \cdots = h_{l_q} = 0$, it follows from Eqs. (A16) that $\Lambda = I$, where I is the unit $q \times q$ matrix, and from Eqs. (A17) that $E = 0$. According to Eq. (A19), to take these boundary conditions into account, the matrix b is modified by adding unity to the elements $b_{l_0 l_0}, b_{l_1 l_1}, \ldots, b_{l_q l_q}$ and the vector y remains unchanged.

The boundary conditions (A15) involve linear combinations of at most q point functions h_l whereas conditions (A11) may involve more than q functions. However, for any independent set of boundary conditions there exists an orthogonal transformation O such that in the partition of the vector Oh, which appears in the transformed equation (A3), the components of the vector H_0 are the appropriate linear combinations of the point functions. To show that the above simple modifications in the matrix b also account for boundary conditions (A11) is straightforward but somewhat more tedious and the details will not be given here.

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