

MASSES FROM INHOMOGENEOUS PARTIAL DIFFERENCE EQUATIONS*

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Procedures are described for obtaining mass predictions from the solutions of inhomogeneous partial difference equations. The inhomogeneous contributions result from the variation with nucleon number and neutron excess of the effective neutron-proton interaction. A simple liquid-drop-model expression has been used for these contributions to obtain the present predictions. The most general solutions of the difference equation have been subjected to a χ^2 -minimization procedure (boundary condition) based on the new atomic mass adjustment of Wapstra and Bos. The resulting solution can be viewed as a many-parameter mass equation with about 220 parameters. About 5000 mass values have been calculated for nuclei with $A \geq 65$. The standard deviation between calculated and experimental mass-excess values is $\sigma_m = 289$ keV.

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PARTIAL DIFFERENCE EQUATIONS

Many mass equations $M(N,Z)$ are obtained as analytic expressions from nuclear-structure considerations. While the underlying theory or model, such as the liquid-drop model or the shell model, establishes the analytic form of the equations, some of the parameters contained in the equations are generally not, or only poorly, predicted by the theory. These parameters are subsequently determined by minimizing the differences $M(N,Z) - M_{\text{exp}}(N,Z)$ for all known masses.

A different approach by means of inhomogeneous partial difference equations is described in the present contribution (see Refs. 1-3 for details). If $M_{\text{exact}}(N,Z)$ represents the exact masses of all known and unknown nuclei, the objective is to find a mass equation $M(N,Z)$ which satisfies

$$M(N,Z) = M_{\text{exact}}(N,Z), \quad (1)$$

[or more realistically, of course, $M(N,Z) \approx M_{\text{exact}}(N,Z)$]. If D represents a partial difference operator, then

$$D M(N,Z) = [D M(N,Z)]_{\text{exact}} \quad (2)$$

is also correct. We now invert the problem. If $[D M(N,Z)]_{\text{exact}}$ is assumed to be known from nuclear-structure theories and if the inhomogeneous partial difference Eq. (2) has a unique solution $M(N,Z)$, then $M(N,Z) = M_{\text{exact}}(N,Z)$. In order to obtain a unique solution over a range of N and Z values, it must be required (boundary condition) to reproduce all precisely known experimental masses $M_{\text{exp}}(N,Z)$. It is concluded that very limited information about $M_{\text{exact}}(N,Z)$ may be sufficient to derive an exact mass equation.

Solutions $M(N,Z)$ of the inhomogeneous partial difference equation

$$D M(N,Z) = [D M(N,Z)]_{\text{theor}} \quad (3)$$

based on *approximate* theories or assumptions for $[D M(N,Z)]_{\text{theor}}$ will describe the exact masses only approximately, $M(N,Z) \approx M_{\text{exact}}(N,Z)$. The earlier boundary condition has to be replaced by a χ^2 -minimization of the differences $M(N,Z) - M_{\text{exp}}(N,Z)$, and the range of validity is that for which Eq. (3) yields unique solutions.

Furthermore, if two independent operators D_T and D_L can be found with theoretical predictions

$[D_T M(N,Z)]_{\text{theor}}$ and $[D_L M(N,Z)]_{\text{theor}}$, then the resulting solutions $M_T(N,Z)$ and $M_L(N,Z)$ of the inhomogeneous partial difference equations

$$D_T M(N,Z) = [D_T M(N,Z)]_{\text{theor}} \quad (4)$$

and

$$D_L M(N,Z) = [D_L M(N,Z)]_{\text{theor}} \quad (5)$$

must satisfy $M_L(N,Z) - M_T(N,Z) \approx 0$ for all values of N and Z for which both solutions are unique. This is a necessary condition, and the degree to which it is violated, particularly for neutron-rich and proton-rich nuclei, makes it possible³ to judge the reliability of the underlying theoretical assumptions and with it the reliability of mass predictions.

Another possible approach² for treating the two Eqs. (4) and (5) consists of finding those solutions which satisfy both difference equations simultaneously with the original boundary condition again replaced by the χ^2 -minimization.

The theoretical contributions on the right-hand side of Eqs. (4) and (5) generally contain small errors. The solutions $M_T(N,Z)$ and $M_L(N,Z)$ may therefore include systematic errors which will become important for neutron-rich and proton-rich nuclei. Such systematic errors can be reduced² if the solutions are subjected to constraints which, for example, ensure that the solutions satisfy charge symmetry of nuclear forces or ensure reasonable predictions for the Coulomb energies.

Partial difference operators D_T and D_L have been constructed from operators ${}^{m,n}\Delta$ defined by

$${}^{m,n}\Delta f(N,Z) \equiv f(N,Z) - f(N-m, Z-n) \quad (6)$$

(this definition differs slightly from that used in Ref. 3). The quantity

$$I_{np}(N,Z) \equiv {}^{1,0}\Delta {}^{0,1}\Delta B(N,Z) = -{}^{1,0}\Delta {}^{0,1}\Delta M(N,Z) \quad (7)$$

$[B(N,Z) = \text{binding energy}]$ represents essentially the effective neutron-proton interaction¹⁻⁴ I_{np} . The effective interaction I_{np} is responsible for the symmetry energy term in mass equations. Additional small contributions to I_{np} result from the neutron-proton pairing energy, from the Coulomb energy (since the isotope-shift coefficient of the nuclear-charge radius is generally different from zero), and from collective effects. Partial difference equations in accord with the above general considera-

tions can now be obtained by considering the dependence on the neutron excess $N - Z = 2T_z$ and the nucleon number $N + Z = A$ of the quantity I_{np} . We therefore define the transverse and longitudinal partial difference operators

$$D_T \equiv -^{1,-1}\Delta^{1,0}\Delta^{0,1}\Delta \quad (8)$$

and

$$D_L \equiv -^{1,1}\Delta^{1,0}\Delta^{0,1}\Delta. \quad (9)$$

For the contributions which vary smoothly with N and Z (or A and T_z), Eqs. (7), (8), and (9) can be written approximately as

$$I_{np}(N,Z) \approx \frac{\partial^2}{\partial N \partial Z} M(N,Z) = -\left(\frac{\partial^2}{\partial A^2} - \frac{1}{4} \frac{\partial^2}{\partial T_z^2}\right) M(N,Z), \quad (10)$$

$$D_T \approx -\left(\frac{\partial}{\partial N} - \frac{\partial}{\partial Z}\right) \frac{\partial^2}{\partial N \partial Z} = -\frac{\partial}{\partial T_z} \left(\frac{\partial^2}{\partial A^2} - \frac{1}{4} \frac{\partial^2}{\partial T_z^2}\right), \quad (11)$$

$$D_L \approx -\left(\frac{\partial}{\partial N} + \frac{\partial}{\partial Z}\right) \frac{\partial^2}{\partial N \partial Z} = -2 \frac{\partial}{\partial A} \left(\frac{\partial^2}{\partial A^2} - \frac{1}{4} \frac{\partial^2}{\partial T_z^2}\right). \quad (12)$$

The inhomogeneous partial difference Eqs. (4) and (5) based on the operators of Eqs. (8) and (9) are sche-

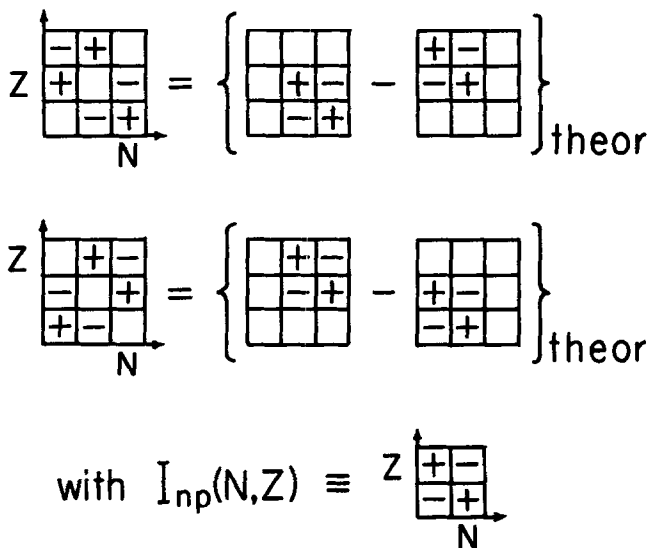


Fig. 1. Schematic representation of the transverse and longitudinal inhomogeneous partial difference Eqs. (4) and (5) based on the operators D_T and D_L of Eqs. (8) and (9). The boxes represent nuclei from the nuclidic chart with N horizontal and Z vertical. The presence of a plus or a minus sign in a box indicates that the mass value of the respective nucleus is to be added or subtracted

matically represented in Fig. 1. Included in the figure is the schematic representation of the definition for the effective neutron-proton interaction I_{np} from Eq. (7). The connection with the Garvey-Kelson nuclidic mass relations⁵ becomes quite apparent in this notation. The transverse and longitudinal Garvey-Kelson relations are represented by the *homogeneous* partial difference equations

$$D_T M(N,Z) = 0 \quad (13)$$

and

$$D_L M(N,Z) = 0. \quad (14)$$

Figure 2 shows about 500 values for I_{np} calculated from Eq. (7) and the experimental masses of Ref. 6. The data are plotted as a function of A separately for even- A and odd- A nuclei. The even- A -odd- A effect has been explained by de-Shalit⁴ who showed that I_{np} can be written in the form

$$I_{np} = I_0 + (-1)^A I'. \quad (15)$$

Here, I_0 represents an averaged interaction between a

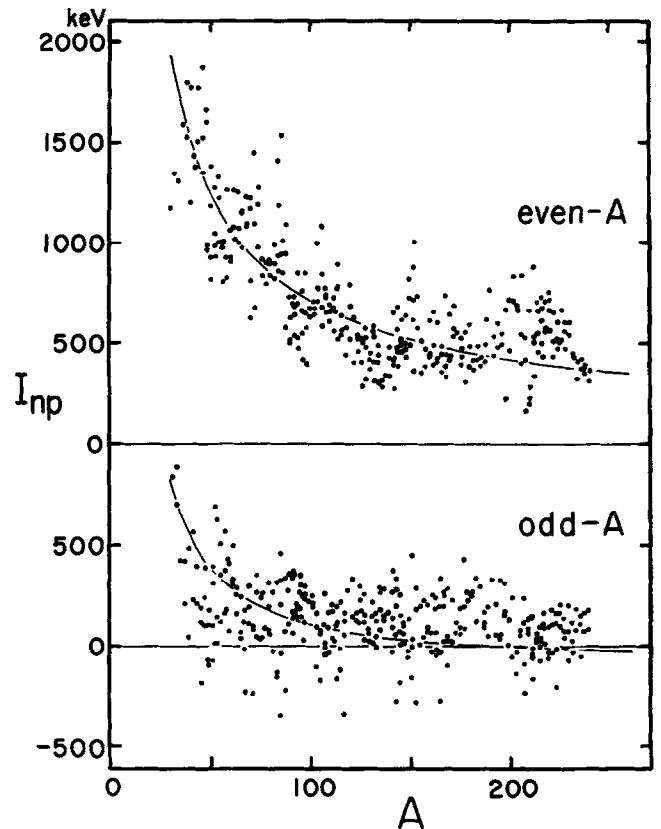


Fig. 2. Plot of the effective neutron-proton interaction I_{np} derived from the experimental masses as a function of A by means of Eq. (7). The lines are calculated from the Bethe-Weizsäcker liquid-drop-model equation for nuclei along the line of β -stability (figure taken from the first article in Ref. 1; B-W parameters used are listed there)

neutron and a proton in the outermost shells of an odd-odd nucleus while I' accounts for the increased binding (pairing energy) in the ground state. The overall behavior is quite well described even by simple mass equations. The two lines in Fig. 2 are calculated¹ for nuclei along the line of β -stability from the Bethe-Weizsäcker liquid-drop-model mass equation. The experimental evidence for the dependence on the *two* variables nucleon number and neutron excess is discussed in Ref. 1.

General solutions of the inhomogeneous third-order transverse and longitudinal partial difference equations

$$-{}^{1,-1}\Delta^{1,0}\Delta^{0,1}\Delta M(N,Z) = [{}^{1,-1}\Delta I_{np}(N,Z)]_{\text{theor}} \quad (16)$$

and

$$-{}^{1,1}\Delta^{1,0}\Delta^{0,1}\Delta M(N,Z) = [{}^{1,1}\Delta I_{np}(N,Z)]_{\text{theor}} \quad (17)$$

[Eqs. (4) and (5) with (8) and (9)] consist of a particular solution of the inhomogeneous equation and the most general solution of the homogeneous equation. Solutions can easily be obtained if certain simple *assumptions* are made about the A - and T_z -dependence of $I_{np}(N,Z) = I_{np}(A, T_z)$ which convert Eqs. (16) and (17) into *homogeneous* equations. If I_{np} is assumed to be independent of T_z or independent of A , then

$$M(N,Z) = g_1(N) + g_2(Z) + g_3(N+Z) \quad (18)$$

and

$$M(N,Z) = f_1(N) + f_2(Z) + f_3(N-Z) \quad (19)$$

are the most general solutions of the homogeneous transverse and longitudinal Eqs. (16) and (17), respectively. If I_{np} is assumed to be independent of T_z and A (separately for even- A and odd- A), then Eqs. (18) and (19) represent again the most general solutions, and the most general simultaneous solution is

$$M(N,Z) = h_1(N) + h_2(Z) + \eta_1(N-Z)^2 + \eta_2\delta_{oo} + \eta_3\delta_{ee} + \eta_4\delta_{eo} + \eta_5\delta_{oe}. \quad (20)$$

Here, $g_i(k)$, $f_i(k)$, and $h_i(k)$ are arbitrary functions, and the η_i are arbitrary constants. The quantity δ_{oo} is unity for $N = \text{odd}$, $Z = \text{odd}$ and is zero otherwise. The quantities δ_{ee} , δ_{eo} and δ_{oe} have similar meanings. The functions $h_1(N)$ and $h_2(Z)$ must contain nuclear and Coulomb energy contributions to satisfy charge symmetry of nuclear forces. Thus,

$$h_1(N) + h_2(Z) = h_{\text{nuc}}(N) + h_{\text{nuc}}(Z) + h_{\text{Coul}}(Z) \quad (21)$$

with

$$\begin{aligned} h_{\text{nuc}}(k) &= h_1(k), \\ h_{\text{Coul}}(k) &= h_2(k) - h_1(k). \end{aligned} \quad (22)$$

The same is the case for the functions $g_i(k)$ and $f_i(k)$ as well as for the functions $G_i(k)$, $F_i(k)$, and $H_i(k)$ introduced below. The functions $g_i(k)$, $f_i(k)$, and $h_i(k)$ can be determined from a χ^2 -minimization to the experimentally known masses. Equations (18) and (19) represent, of course, the transverse and longitudinal Garvey-Kelson mass equations.⁵ Since the above assumptions are strongly violated near $T = 0$, the solutions can be used only for nuclei with $N > Z$ (and $N = Z = \text{even}$).

Many theoretical expressions for the right-hand sides of the inhomogeneous partial difference Eqs. (16) and (17) are easily available. *Any* given mass equation $M_{\text{eq}}(N,Z)$ contains terms which describe the dependence on T_z and A of the effective interaction I_{np} . These terms, mostly contained in the expression for the symmetry energy, can be obtained by calculating the required differences. The underlying theoretical considerations for these contributions are, of course, those used in the derivation of the respective mass equation. The most general solutions of Eqs. (16) and (17) then become

$$M(N,Z) = M_{\text{eq}}(N,Z) + G_1(N) + G_2(Z) + G_3(N+Z) \quad (23)$$

and

$$M(N,Z) = M_{\text{eq}}(N,Z) + F_1(N) + F_2(Z) + F_3(N-Z). \quad (24)$$

The most general simultaneous solution is

$$M(N,Z) = M_{\text{eq}}(N,Z) + H_1(N) + H_2(Z) + \eta_1(N-Z)^2 + \eta_2\delta_{oo} + \eta_3\delta_{ee} + \eta_4\delta_{eo} + \eta_5\delta_{oe}. \quad (25)$$

Here, $G_i(k)$, $F_i(k)$, and $H_i(k)$ are arbitrary functions and the η_i are arbitrary constants. These can again be determined from a χ^2 -minimization of the differences between experimental and calculated masses for those regions of N , Z , $N+Z$, and $N-Z$ for which experimental masses are known. While the expression for $M_{\text{eq}}(N,Z)$ enters explicitly into the solutions (23), (24), and (25), the only quantities which these solutions and $M_{\text{eq}}(N,Z)$ have in common are certain third-order partial differences which are generally on the order of 10 keV (see Fig. 5 of Ref. 1).

CALCULATIONS AND COEFFICIENTS

Computer programs have been written by us which make it possible to obtain the functions $G_i(k)$, $F_i(k)$, and $H_i(k)$ as numerical values for each integer argument from systems of a few hundred linear equations in a few hundred unknowns. Since use is made of sparse matrix subroutines, the computing time is only about ten seconds for a given equation on the University

of Michigan AMDAHL 470V/6 computer and about twice as long on the compatible IBM 370/168.

Preliminary results for the transverse and longitudinal inhomogeneous equations according to Eqs. (23) and (24) have been obtained³ for several shell-model and liquid-drop-model expressions for I_{np} . The standard deviations σ_m between calculated and experimental mass-excess values are typically 110 keV and 200 keV, respectively. The consistency test mentioned earlier has been applied to a few cases.³ Detailed results are available for the simultaneous solutions according to Eq. (25). Solutions have been obtained² for 16 different assumptions and theories about $I_{np}(N,Z)$ including shell-model^{7,8} and liquid-drop-model⁹⁻¹¹ expressions. The standard deviations σ_m between calculated and experimental mass-excess values ($N \geq 20$ and $Z \geq 20$) are typically 250 keV. However, it was found that the standard deviations σ_c for reproducing the experimental Coulomb displacement energies were much bigger and ranged from about 650 to 1750 keV. The functions $H_{\text{nucl}}(k)$ and $H_{\text{Coul}}(k)$ display a divergent behavior. It was further observed that there exist strong correlations between the Coulomb energy and the symmetry energy terms. A misrepresentation of the former is always accompanied by a misrepresentation of the latter thus affecting mass predictions for very neutron-rich and proton-rich nuclei.

A similar situation exists for the transverse Garvey-Kelson mass-equation.⁵ The standard deviation σ_m for the differences between calculated and experimental mass-excess values is about 120 keV, but the calculated Coulomb displacement energies exhibit deviations with $\sigma_c \approx 2700$ keV.

Additional constraints were introduced in order to overcome this problem. Since the terms $H_1(N)$ and $H_2(Z)$ of Eq. (25) contain nuclear and Coulomb energy contributions, obvious constraints are $H_1(k) = H_2(k)$ or $\eta_1 = 0$ which eliminate any modifications of the Coulomb energy or symmetry energy terms of $M_{\text{eq}}(N,Z)$. Results were again obtained from χ^2 -minimizations for the various assumptions and theories about I_{np} . The functions $H_{\text{nucl}}(k) \equiv H_1(k)$ and $H_{\text{Coul}}(k) \equiv H_2(k) - H_1(k)$ are now well behaved. Figure 3 shows an example based on the constraint $\eta_1 = 0$. The dependence of $H_{\text{Coul}}(Z)$ on Z is smooth, and $H_{\text{nucl}}(N$ or $Z)$ displays pronounced shell and pairing effects as expected.

Of the many new mass equations obtained, one was chosen for presentation in this contribution (referred to as solution S-C in Ref. 2). It is the simultaneous solution Eq. (25) of the inhomogeneous equations derived under the constraint $\eta_1 = 0$ with the effective neutron-proton interaction I_{np} taken from the liquid-drop-model expression of Seeger.¹¹ It should be used only for $A \geq 65$. The dependence of the effective neu-

tron-proton interaction I_{np} on shell-model configurations becomes too important in light nuclei and cannot be neglected. The selection of the above solution is based on the standard deviations σ_m and σ_c in conjunction with their variation under constraints (see Ref. 2 for more details).

The functions $H_1(N)$ and $H_2(Z)$ were obtained from a slightly modified χ^2 -minimization procedure by solving a system of about 220 linear equations in about 220 unknowns. The new experimental mass values of Wapstra and Bos¹² were used as input data. By quadratically adding 100 keV to the experimental uncertainties, values with uncertainties less than 100 keV are thereby given essentially equal weight, and reduced weight is given to those with larger uncertainties.

Mass excesses $\Delta M(N,Z)$ are calculated from

$$\Delta M(N,Z) = \Delta M_{\text{eq}}(N,Z) + H_1(N) + H_2(Z) + \eta_1(N-Z)^2 + \eta_2\delta_{oo} + \eta_3\delta_{ee} + \eta_4\delta_{eo} + \eta_5\delta_{oe} \quad (26)$$

(the δ_{oo} etc. are again Kronecker symbols) with

$$\Delta M_{\text{eq}}(N,Z) = N\Delta M_n + Z\Delta M_H - B_{\text{eq}}(N,Z), \quad (27)$$

$$B_{\text{eq}}(N,Z) = \alpha A - \beta \frac{(N-Z)^2}{A} - \gamma A^{2/3} + \eta \frac{(N-Z)^2}{A^{4/3}} - 864 \frac{Z^2}{r_0 A^{1/3}} \left\{ 1 - \frac{0.76361}{Z^{2/3}} - \frac{2.453}{r_0^2 A^{2/3}} \right\} + 7000 \exp\left(-6 \frac{|N-Z|}{A}\right) + 14.33 \times 10^{-3} Z^{2.39}. \quad (28)$$

With the exception of the pairing energy term $\pm(9600 \text{ keV})A^{-1/2}$ which is replaced by contributions to

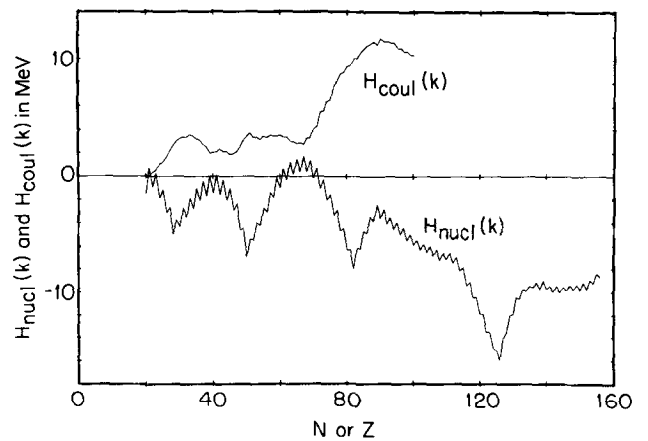


Fig. 3. Plot of the functions $H_{\text{nucl}}(k) \equiv H_1(k)$ and $H_{\text{Coul}}(k) \equiv H_2(k) - H_1(k)$ for the simultaneous solution, Eq. (26) with Eqs. (27) and (28), of the inhomogeneous partial difference Eqs. (4) and (5)

$H_1(N)$ and $H_2(Z)$. Eq. (28) is a binding energy expression of Seeger.¹¹ The small third-order differences in the

inhomogeneous partial difference Eqs. (16) and (17) depend essentially only on the symmetry energy terms with β and η . All quantities are in units of keV.

Values of Coefficients

$\Delta M_n =$	8071.43	keV, mass excess of the neutron
$\Delta M_H =$	7289.03	keV, mass excess of hydrogen
$\alpha =$	15971.3	keV, volume-energy coefficient
$\beta =$	30047	keV, first symmetry-energy coefficient
$\gamma =$	20806	keV, surface-energy coefficient
$\eta =$	45350	keV, second symmetry-energy coefficient
$r_0 =$	1.16552	fm, charge-radius constant
$\eta_1 =$	0	keV, symmetry-energy parameter
$\eta_2 = \eta_3 =$	-108.0	keV, pairing-energy parameters
$\eta_4 = \eta_5 =$	0	keV, pairing-energy parameters

The functions $H_1(N)$ and $H_2(Z)$ are given in the table. The functions $H_{\text{nucl}}(k) \equiv H_1(k)$ and $H_{\text{Coul}}(k) \equiv H_2(k) - H_1(k)$ are displayed in Fig. 3. The standard deviation for the differences between calculated and experimental mass-excess values ($N \geq 20$ and $Z \geq 20$) is $\sigma_m = 289$ keV, the standard deviation for the differences between calculated and experimental Coulomb displacement energies is $\sigma_c = 432$ keV. About 5000 predicted mass values for nuclei with $A \geq 65$ are included in the tabulation.

It should be pointed out that multiparameter mass equations like the present one must be considered with some caution. It has been shown² that χ^2 per degree of freedom (which characterizes the goodness of fit) *over the domain of measured mass values* generally decreases inversely with the number of parameters. However, very little can be inferred from a small value of σ_m alone about the expected reliability outside and particularly far away from the region of known masses. It is for this reason that other criteria² including consistency tests³ are important.

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TABLE. Functions $H_1(N)$ and $H_2(Z)$ in keV

$H_1(N)$										
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	20
712.4	-936.5	250.7	-1876.1	-1146.7	-3206.0	-2681.7	-5041.3	-3736.1	-1441.2	30
-2775.0	-3536.4	-1915.4	-2818.0	-988.3	-2127.0	-383.7	-1670.4	17.9	-4389.6	40
117.8	-1535.0	-274.5	-2090.6	-1006.1	-2958.9	-2353.4	-4658.3	-4484.3	-1378.7	50
-5420.1	-5484.4	-3956.1	-4208.0	-2718.5	-3100.7	-1341.0	-1751.8	-129.7	-6924.9	60
659.2	-314.1	1193.6	193.7	1460.1	408.6	1701.1	392.0	1353.9	-968.3	70
696.3	-1062.5	-283.0	-2657.2	-1471.1	-3363.4	-2857.3	-4711.9	-4493.0	-146.7	80
-6259.0	-9023.3	-6186.7	-6213.4	-4896.4	-4905.7	-3468.7	-3845.2	-2456.1	-6351.0	90
-2830.0	-4098.1	-3507.0	-4597.8	-3907.5	-5021.0	-4438.6	-5525.9	-4988.3	-3626.9	100
-5456.6	-6320.5	-5828.7	-6535.0	-5995.7	-6772.7	-6279.4	-7207.3	-6560.4	-5904.5	110
-6546.0	-7449.1	-6899.7	-8194.4	-7902.7	-9447.4	-9127.6	-10482.3	-10430.2	-7130.5	120
-11892.6	-13461.5	-13482.0	-14981.5	-15147.7	-15928.4	-14118.0	-13648.9	-12015.9	-11887.8	130
-10450.4	-10598.4	-9776.4	-9911.9	-9510.2	-9654.6	-9136.5	-9777.7	-9013.3	-11973.7	140
-9486.9	-10004.3	-9486.0	-10024.3	-9591.8	-9686.0	-9377.0	-9803.4	-9352.4	-9766.8	150
-9196.3	-9799.5	-9007.1	-9264.8	-8420.4	-8734.8	0.0	0.0	0.0	-9837.4	160
$H_2(Z)$										
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	20
750.5	-632.7	735.5	-852.5	88.0	-1625.3	-564.5	-2485.8	-788.7	-1203.5	30
519.1	-238.1	1615.1	582.7	2186.5	943.3	2299.9	800.2	1967.4	657.2	40
2161.7	750.6	1813.3	-7.3	829.3	-1033.9	-269.6	-2174.3	-1445.4	-3571.0	50
-1771.3	-2223.0	-620.6	-1096.0	704.6	170.2	2126.3	1657.3	3264.4	2515.1	60
2960.1	2997.7	4168.5	3139.9	4232.6	3280.8	4376.9	3633.9	4633.5	3968.0	70
5138.2	4476.0	5286.6	4389.0	5110.8	4330.5	5325.4	4079.7	4416.8	3024.8	80
3192.7	2089.6	3956.7	4372.6	6247.5	6323.1	7899.6	7711.4	8786.8	8198.0	90
8723.3	7511.5	7962.3	6865.4	7096.6	6016.8	6286.2	5216.3	5460.8	4502.9	100

The first line gives $H_1(1), H_1(2), \dots, H_1(10)$; the second line gives $H_1(11), H_1(12), \dots, H_1(20)$, etc.