Generalized Hugenholtz–Van Hove Theorem and a New Mass Relation for Finite Nuclei

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The usual Hugenholtz–Van Hove theorem for a Fermi system is extended to describe asymmetric nuclear matter. It has been further developed to describe finite nuclei. It is shown that this extended relation could be used as a basis for a new mass relation which has both the liquid-drop and single-particle features. Its success in predicting masses of exotic neutron-rich nuclei is demonstrated.

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The Hugenholtz–Van Hove (HVH) theorem[1] in general deals with the single-particle properties of a Fermi gas with interaction at the absolute zero of temperature. It states that for a system with number of particles A and total energy E,

$$\frac{E}{A} + \rho \left.\frac{\partial(E/A)}{\partial\rho}\right|_v = \left.\frac{\partial E}{\partial A}\right|_v , \tag{1}$$

where ρ is the number density. The derivatives are taken at constant volume v. It has been shown by Bethe[2] under Hartree-Fock approximation and also more rigorously by Hugenholtz and Van Hove[1] that $(\partial E/\partial A)_v$ is equal to the Fermi energy ϵ which is also the same as the separation energy with a negative sign. At equilibrium, i.e., at a density such that the pressure vanishes, one obtains as a special case

$$\epsilon = E/A. \tag{2}$$

This theorem, being valid for any Fermi system, is applicable to ^{3}He and especially to nuclear matter. In the past, this theorem has provided useful guidelines in the development of Brueckner theory.[3]

In this Letter, first we attempt to extend this theorem to the asymmetric Fermi system and in particular to asymmetric nuclear matter, an extension which we have not come across anywhere. Then, using this extended HVH theorem as a basis, we obtain a similar relation suitable for finite nuclei. It is needless to emphasize the usefulness of such a relation involving three observable quantities of a nucleus, namely, its binding energy, and neutron and proton separation energies. Further, we demonstrate that this relation has a great potentiality as a mass relation in general, and can be used reliably to predict masses far from the valley of stability.

Consider asymmetric nuclear matter with Z protons and N neutrons. Let ρ be the number density and E be the total ground-state energy. The total energy E can be considered as a function of (N, Z) or (A, β), where $A = N + Z$ and $\beta = (N-Z)/(N+Z)$, the asymmetry parameter. The neutron and proton Fermi energies are, respectively, $\epsilon_n = (\partial E/\partial N)_v$ and $\epsilon_p = (\partial E/\partial Z)_v$. Now

$$\left(\frac{\partial E}{\partial A}\right)_v = \left(\frac{\partial E}{\partial N}\right)_{v,Z}\left(\frac{\partial N}{\partial A}\right)_\beta + \left(\frac{\partial E}{\partial Z}\right)_{v,N}\left(\frac{\partial Z}{\partial A}\right)_\beta = \tfrac{1}{2}[(1+\beta)\epsilon_n + (1-\beta)\epsilon_p]. \tag{3}$$

Thus from Eqs. (1) and (3) we obtain

$$\frac{E}{A} + \rho \left.\frac{\partial(E/A)}{\partial\rho}\right|_v = \tfrac{1}{2}[(1+\beta)\epsilon_n + (1-\beta)\epsilon_p]. \tag{4}$$

For a symmetric system, i.e., $N = Z$ and also where one kind of particle is present, Eq. (4) reduces to the usual HVH equation (1). Thus Eq. (4) can be called the generalized HVH theorem. At equilibrium, i.e., for the ground state, the pressure vanishes and Eq. (4) reduces to

$$E/A = \tfrac{1}{2}[(1+\beta)\epsilon_n + (1-\beta)\epsilon_p]. \tag{5}$$

The above relation is strictly true for asymmetric nuclear matter. If we could incorporate the surface, the Coulomb, and the pairing effects into Eq. (5), we could hope to arrive at a relation applicable to finite nuclei. This is achieved in the following way.

The total energy appearing in Eq. (5) can be written as

$$E = E^F - a_s A^{2/3} - a_C Z^2/A^{1/3} + \delta(A, Z), \tag{6}$$

where E^F is the ground-state energy of the nucleus with N neutrons and Z protons. The superscript "F" denotes the finite nucleus, a_s and a_C are surface and Coulomb coefficients, and $\delta(A,$

Z) is the pairing term. Then, using Eq. (6), the Fermi energies can also be expressed in terms of their counterparts for the finite nuclei as

$$\epsilon_n = \epsilon_n{}^F - a_s[A^{2/3} - (A-1)^{2/3}] - a_C Z^2[A^{-1/3} - (A-1)^{-1/3}] + [\delta(A,Z) - \delta(A-1,Z)],$$
$$\epsilon_p = \epsilon_p{}^F - a_s[A^{2/3} - (A-1)^{2/3}] - a_C[Z^2/A^{1/3} - (Z-1)^2/(A-1)^{1/3}] + [\delta(A,Z) - \delta(A-1,Z-1)]. \quad (7)$$

Now with the help of Eqs. (6) and (7), the relation (5) reduces to

$$E^F/A - \tfrac{1}{2}[(1+\beta)\epsilon_n{}^F + (1-\beta)\epsilon_p{}^F] = S(A,Z), \quad (8)$$

where

$$S(A,Z) = a_s[A^{-1/3} - A^{2/3} + (A-1)^{2/3}] + a_C[Z^2(1-A)A^{-4/3} + \tfrac{1}{2}(A-1)^{-1/3}\{Z^2(1+\beta) + (Z-1)^2(1-\beta)\}]$$
$$+ \delta(A,Z)(1-A^{-1}) - \tfrac{1}{2}(1+\beta)\delta(A-1,Z) - \tfrac{1}{2}(1-\beta)\delta(A-1,Z-1).$$

It is worth mentioning here that the function $S(A,Z)$ arises solely as a result of the finiteness of the nucleus. For the pairing term, we have taken the standard function

$$\delta(A,Z) = \begin{cases} +\Delta A^{-3/4} & \text{for even-even nuclei,} \\ 0 & \text{for odd-}A\text{ nuclei,} \\ -\Delta A^{-3/4} & \text{for odd-odd nuclei,} \end{cases}$$

where Δ is a parameter.

Thus Eq. (8) contains three parameters namely a_s, a_C, and Δ. In order to see how well Eq. (8) describes reality we took the experimental[4] binding energies and neutron and proton separation energies of 277 nuclei ranging between $Z=10$ and $A=20$ to $Z=101$ and $A=253$ in the valley of stability and performed a least-squares fit with Eq. (8) to determine the three parameters. The values of the parameters so obtained are $a_s=26.679$ MeV, $a_C=0.827$ MeV, and $\Delta=34.549$ MeV which are close to the standard values. The root mean square deviation was found to be 0.39 MeV. Figure 1 shows a histogram of the deviation between the left-hand side and the right-hand side of Eq. (8) obtained in our fit. This shows that relation (8) is fulfilled quite well throughout the Periodic Table.

Equation (8) can be used as a mass relation if we express the Fermi energies $\epsilon_n{}^F$ and $\epsilon_p{}^F$ in terms of the binding energies of the neighboring nuclei. Then Eq. (8) would read as

$$E^F(N,Z)/A - \tfrac{1}{2}[(1+\beta)\{E^F(N,Z) - E^F(N-1,Z)\} + (1-\beta)\{E^F(N,Z) - E^F(N,Z-1)\}] = S(A,Z). \quad (9)$$

The above equation describes a relation among the masses of three neighboring nuclei with neutron and proton numbers (N,Z), $(N-1,Z)$, and $(N,Z-1)$ and hence can be considered as a mass relation. It must be noted here that the above mass relation is of hybrid nature having liquid-drop features, represented through the coefficients a_s, a_C, and Δ, and single-particle features like those of Garvey *et al.*,[5] represented through the mass differences. The hybridization of these two extreme models in nuclear physics is expected to describe the nuclear properties better. To verify this, we have confronted the model with a severe test of predicting the binding energies of nuclei far from the valley of stability. It has been mentioned earlier that we have used the data of 277 nuclei lying in the valley of stability in our least-squares fit. The fit represented through the histogram (Fig. 1) shows the quality of the results for mass prediction in that region. In general the error in the prediction should be similar to the deviation presented in Fig. 1. Now, using the same values of the parameters a_s, a_C, and Δ, we predict the masses of twenty neutron-rich nuclei in different regions away from the valley of stability. The results are presented in Table I. The data for low-mass nuclei have been taken from Jelley *et al.*[6] and for high-mass nuclei from the mass table compiled by Viola *et al.*[7] These nuclei have been classified into two groups: neutron rich and ultra neutron rich. For both of these groups, we have also presented the results of Garvey *et al.* from their 1969 mass table, and those of the droplet model[8] calculated by Myers.[9] Our mass relation uses two known masses and hence to make the comparison with the predictions of Garvey *et al.* more meaningful, we have chosen twelve cases, under the group "neutron rich," which are close to the boundary of the experimentally measured masses used by them in their table. For the prediction of masses of such nuclei through the mass relation of Garvey *et al.*,

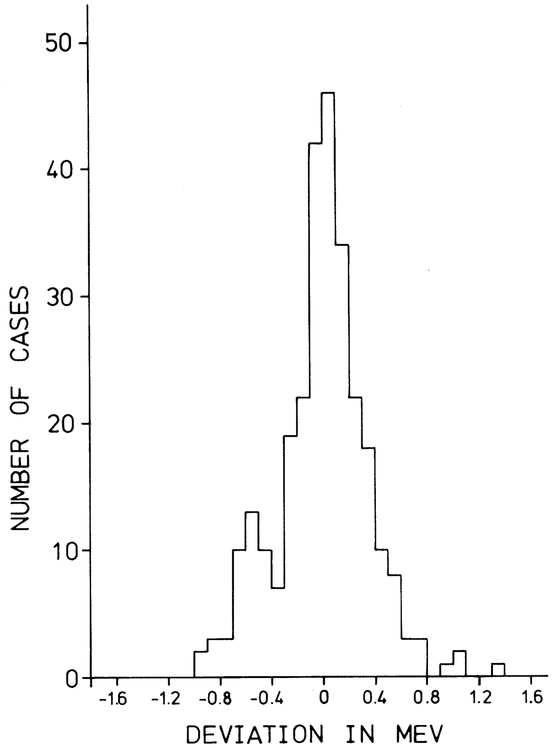

FIG. 1. Histogram of the differences between the left-hand side and the right-hand side of Eq. (8) vs the number of cases for 277 nuclei ranging from $Z = 10$ and $A = 20$ to $Z = 101$ and $A = 253$ in the valley of stability. For the values of the parameters, see the text.

at least two or more experimentally known masses are used.[5] In most cases our results are closer to experiment than are those of Garvey *et al.* We also find that our discrepancies are in general lower than those of the droplet model for these nuclei.

The group of eight nuclei presented under the category "ultra neutron rich" are quite far from the valley of stability. Our results are quite close to experiment, the worst case being ^{238}At which shows a discrepancy of 1.22 MeV. The predictions of Garvey *et al.* and also of the droplet model are off by several megaelectronvolts from experiment. In the case of the former, such large discrepancies may be due to the accumulated errors resulting from extrapolation to such far regions. However, in our case we do not have such errors due to accumulation. If we consider the fact that these two groups of nuclei are away from the valley of stability and have not been used in the least-squares fit, the agreement of the predicted masses with experiment is indeed impressive.

TABLE I. Predictions of binding energy for different categories of nuclei. Z, N, and A are respectively the proton, neutron, and mass number of the nucleus. Columns 3–5 give, respectively, the differences between the calculated and experimental binding energies due to the present model, Garvey *et al.* (Ref. 5) (GK), and the droplet model calculated by Myers (My). The last column gives the experimental binding energies.

		Binding Energy (MeV)			
Category	Nucleus $^{A}_{N}X_{Z}$	Calc.-Expt.	GK-Expt.	My-Expt.	Expt.
Neutron-	$^{29}_{17}\mathrm{Mg}_{12}$	0.69	1.96	-0.45	235.28
rich	$^{31}_{18}\mathrm{Al}_{13}$	-0.98	1.72	-0.19	256.06
	$^{64}_{37}\mathrm{Co}_{27}$	-0.87	-0.15	0.07	555.57
	$^{84}_{50}\mathrm{Se}_{34}$	0.65	0.74	1.96	727.34
	$^{104}_{62}\mathrm{Mo}_{42}$	-0.13	0.16	1.52	886.78
	$^{143}_{88}\mathrm{Cs}_{55}$	1.00	1.14	0.98	1178.43
	$^{165}_{101}\mathrm{Gd}_{64}$	0.03	0.96	0.34	1337.96
	$^{181}_{111}\mathrm{Yb}_{70}$	0.31	0.23	-0.38	1446.63
	$^{197}_{122}\mathrm{Re}_{75}$	-0.51	-0.53	0.48	1552.22
	$^{204}_{126}\mathrm{Pt}_{78}$	-0.22	0.63	0.61	1603.17
	$^{221}_{137}\mathrm{Po}_{84}$	0.54	-0.06	1.82	1698.08
	$^{236}_{147}\mathrm{Ac}_{89}$	0.30	-0.44	2.18	1783.66
Ultra	$^{143}_{89}\mathrm{Xe}_{54}$	0.84	2.39	2.16	1171.30
Neutron-rich	$^{161}_{101}\mathrm{Nd}_{60}$	0.35	3.91	3.93	1293.75
	$^{180}_{114}\mathrm{Dy}_{66}$	-0.21	-1.65	4.37	1418.46
	$^{201}_{130}\mathrm{Lu}_{71}$	1.50	-6.57	7.92	1536.68
	$^{223}_{144}\mathrm{Au}_{79}$	1.02	-8.66	6.83	1675.28
	$^{228}_{146}\mathrm{Pb}_{82}$	-0.67	-7.47	2.94	1719.22
	$^{238}_{153}\mathrm{At}_{85}$	1.22	-4.10	8.00	1769.21
	$^{258}_{166}\mathrm{U}_{92}$	-0.54	-	14.56	1879.83
N=Z	$^{30}_{15}\mathrm{P}_{15}$	-1.14	-	0.11	250.60
odd-odd	$^{34}_{17}\mathrm{Cl}_{17}$	-0.97	-	-2.07	285.58
and Z>N	$^{42}_{21}\mathrm{Sc}_{21}$	-0.57	-	-0.54	354.71
	$^{46}_{23}\mathrm{V}_{23}$	0.50	-	0.43	390.35
	$^{50}_{25}\mathrm{Mn}_{25}$	0.50	-	1.56	426.66
	$^{22}_{10}\mathrm{Mg}_{12}$	0.69	-	4.11	168.32
	$^{24}_{11}\mathrm{Al}_{13}$	-0.70	-	4.15	183.45
	$^{28}_{13}\mathrm{P}_{15}$	0.15	-	3.53	221.92
	$^{38}_{18}\mathrm{Ca}_{20}$	0.38	-	0.11	312.75
	$^{39}_{19}\mathrm{Ca}_{20}$	-0.19	-	-1.27	326.44
	$^{42}_{20}\mathrm{Ti}_{22}$	-0.18	-	1.67	345.16

We have also attempted to predict the masses of some nuclei with $N=Z$ odd and $Z>N$, which also were not included in our least-squares fit. For such nuclei, the mass relation of Garvey *et al.* does not work, and that is why we have compared our results only with those of the droplet model in Table I. For $N=Z$ odd-odd nuclei our results compare well with those of the predictions of the droplet model. However, for $Z>N$ nuclei our predictions are invariably closer to experiment in most cases. From the quality of the agreement with experiment it appears that our model may be suitable even for these classes of nuclei.

In conclusion we would like to emphasize that the extended HVH theorem (4) obtained here is quite general and useful. It has led to the interesting relation Eq. (8) which relates three important properties of finite nuclei, namely, the ground-state energy, and the neutron and proton separation energies. When treated as a mass relation, its success with only three adjustable parameters is somewhat surprising. Indeed it is more so as the parameters determined by fitting with normal nuclei work quite well for the exotic ones. The main cause of its success with a fewer number of parameters is that the "energy differences," which appear in Eq. (9), cancel the other less important effects like deformation, shell correction, etc., to a great extent. It has a unique feature that it combines the two main important aspects of nuclear dynamics, namely, the liquid-drop and single-particle aspects, and has its origin in the many-body theory. The present study is by no means complete; however, it is extensive enough to establish the relation (8) and show clearly that it has the potentiality of being used as a mass relation. However, more work is needed to construct a mass table on this basis, which will be taken up later.

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