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THE CURVATURE CORRECTION IN THE NUCLEAR MASS FORMULA[†]

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ABSTRACT: The curvature correction to the nuclear binding energy is obtained by using an averaged level density appropriate to describe, up to curvature effects, the independent particle aspect of the nuclear many-body problem. The relation between the surface and curvature coefficients is seen to depend exclusively on the radius of the nucleus and the behaviour of the wave functions at the surface. Corresponding to a realistic surface term, the curvature correction is found to be such that it increases the binding energy, although the actual value is very sensitive to the parametrization of the nuclear radius in terms of the mass number.

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I. INTRODUCTION

In the search of a mass formula reliable for extrapolation away from the known nuclei, a number of corrections to the semi-empirical Bethe-Weizsäcker mass formula have been proposed[1]. Though small compared to the leading terms, i.e. volume, surface, symmetry and Coulomb energies, these corrections are important for a detailed adjustment to the nuclear data. Furthermore, they become critical in other problems as, for example, in the prediction of the existence of superheavy elements (a few MeV difference produces vast changes in the calculated lifetimes). These new terms in the mass formula are usually - but not always - inferred from theoretical models. Their numerical values are either estimated from the corresponding models or obtained from fits to the experimental data. The results do not always agree.

For the "curvature" correction, which in the extended formulas is the term proportional to $A^{1/3}$, there is disagreement even with respect to its sign. Yet, to quote R. W. Hasse[2], "... curvature has a major influence on the saddle point properties. Large values of the curvature correction coefficient favor the formation of a secondary minimum in the fission barrier of heavy elements. For superheavy elements this gives rise to the possibility of quasi-molecular states". The state of affairs characterizing the curvature term is the following. On the basis of the Thomas-Fermi model and of the droplet model, a small curvature correction that decreases the binding energy is predicted[3]. On the other hand, a curvature correction of the same order of magnitude but of opposite sign is found to be needed in order to obtain good agreement with the experimental Coulomb energies[4]. Earlier, a large curvature correction which increased the binding energy was predicted on a phenomenological shell model basis; and it was furthermore shown that such a term was able to produce deformation in the light and medium heavy nuclei, where the Coulomb repulsion would not[5]. It is clearly a confusing situation.

The present paper is an attempt to clarify the question by relying on general quantum mechanical characteristics of the nuclear many-body system. The point of view is the following. It is well known that in spite of the complexity of the nuclear aggregate the gross features of the nucleus seem to correspond to those of a system of particles moving independently in a common self consistent potential well. In agreement with the characteristics of the observed nuclear density, the nuclear potential is generally considered to be constant up to a certain range and to fall rapidly to zero afterwards. The single-particle wave functions are then quite close to free waves within the interior of the nucleus and only become distorted in the vicinity of the

surface where they have to go into an exponential decay[6]. In view of this circumstance one can expect, as suggested by R. Balian and C. Bloch[7], that the actual density distribution of single particle levels may be reproduced fairly well by that of the eigenvalues of the wave equation $(\nabla^2 + k^2)\,\varphi = 0$ in a finite domain of the same shape as the original potential, with an appropriate boundary condition. Furthermore, an even better agreement should be obtained between averaged level distributions, provided the width of the averaging function is large enough to wipe out the bunching of the energy levels. Insofar as Balian and Bloch[7] have solved the wave equation problem with arbitrary boundary conditions including up to curvature effects, we propose to use their general result to study the structure of the ground state energy of the many nucleon system.

The Hartree-Fock energy of the system is given by

$$E = \tfrac{1}{2} \sum_i \{ \epsilon_i + t_i \} \tag{1}$$

where ϵ_i and t_i are respectively the single particle energy and the kinetic energy of the i-th particle in the self consistent potential well. To calculate the total energy without solving exactly the nuclear problem, we substitute the summation by an integration with the smooth energy level distribution provided in ref. 7, where surface and curvature effects have been taken into account. We therefore evaluate:

$$E_\gamma = \tfrac{1}{2} \int_{-V_0}^{-\epsilon_F} \{ \epsilon + t(\epsilon) \}\, \rho_\gamma(\epsilon)\, d\epsilon \ , \tag{2}$$

where γ is the width of the spreading function used to smooth out the actual level density

$$\rho(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i) \ . \tag{3}$$

The integration in eq. (2) goes from the bottom of the potential well $-V_0$, up to the Fermi level, $-\epsilon_F$, which is determined - as a requirement for self-consistency- by the condition

$$A = \int_{-V_0}^{-\epsilon_F} \rho_\gamma(\epsilon)\, d\epsilon \ , \tag{4}$$

being A the total number of nucleons.

Let us point out that this procedure (eq. 2), is in fact Strutinsky's prescription [1, 8] to compute the smooth part in the nuclear binding energy, which is then subtracted from the sum over the discrete spectrum to obtain the shell contribution. While in Strutinsky's work a numerical evaluation is carried out, here we shall obtain an analytic expression for the binding energy in terms of the mass number

In section II we review briefly the work of Balian and Bloch on the level density distribution. In section III, the calculation of the binding energy is carried out. The analysis and discussion of the surface and curvature corrections in terms of the boundary conditions is done in section IV. It is found that for realistic values of the parameters involved, the curvature correction always increases the binding energy, although the magnitude is very sensitive to the parametrization of the nuclear radius.

II. THE ENERGY LEVEL DENSITY

The problem considered by Balian and Bloch [7] is that of the averaged distribution of eigenvalues of the wave equation

$$(\nabla^2 + k^2)\,\varphi = 0\ , \tag{5}$$

within a volume V of arbitrary shape and for the general boundary condition

$$\frac{\partial \varphi}{\partial n} - K\varphi = 0 \tag{6}$$

for the normal derivative on the surface S, assumed to be smooth. Limiting cases are the well known Dirichlet and Neumann problems, corresponding to the boundary conditions

$$\varphi = 0 \qquad \text{(Dirichlet)} \tag{6'a}$$

$$\frac{\partial \varphi}{\partial n} = 0\ . \qquad \text{(Neumann)} \tag{6'b}$$

The exact energy level density is given by

$$\rho(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i)$$

$$= \lim_{\eta \to 0} (1/2\pi i) \int d^3 r \, [G(r, r'; \epsilon + i\eta) - G(r, r'; \epsilon - i\eta)]_{r=r'} , \tag{7}$$

where $G(r, r'; z)$ is the time-independent Green's function satisfying the equation

$$(\nabla^2 + z)\, G(r, r'; z) = -\delta(r - r') , \tag{8}$$

with the same boundary condition (6) as above.

A smoothed energy density function $\rho_\gamma(\epsilon)$ is now generated by averaging $\rho(\epsilon)$ with a Lorentzian weighting function of width γ, i.e.:

$$\rho_\gamma(\epsilon) \equiv \frac{\gamma}{\pi} \int_{-\infty}^{\infty} \frac{\rho(\epsilon')\, d\epsilon'}{(\epsilon - \epsilon')^2 + \gamma^2} = \frac{1}{\pi} \int d^3 r \, [\mathrm{Im}\, G(r, r'; \epsilon + i\gamma)]_{r=r'} . \tag{9}$$

The width γ is chosen large enough to wipe out the fluctuations due to the bunching of the energy levels (shell effects). Expression (9) is evaluated by an iterative procedure, starting from the Green's function G_0 for the infinite space (free propagation). The presence of a boundary then gives rise to an expression which can be pictured as a multiple reflection expansion. The successive terms are evaluated and summed, first under the assumption of a locally flat surface, i.e. substituting at every point the actual surface by the tangent plane. This gives the "surface" contribution to the density. Afterwards the changes due to the fact that the surface is actually curved are computed and the curvature term is obtained.

Finally Balian and Bloch determine the minimum value of the spreading width for which the expansion converges. And they furthermore show that $\rho_\gamma\,(\gamma = \gamma_{\min})$ does not differ significantly from the extrapolated distribution function $\rho_\gamma(\gamma = 0) \equiv \rho_0$, the use of which will then yield results conveniently independent of γ. The expression for ρ_0 is:

$$\rho_0(\epsilon) = (1/4\pi^3) \left[Vk + \int_S d\sigma_\omega \, [(\pi/4) - \delta_\omega] + \right.$$

$$\left. + (1/k) \int_S (d\sigma_\omega / R_\omega)(\tfrac{1}{3} + \cos^2 \delta_\omega - \delta_\omega \cot \delta_\omega) + \dots \right] , \tag{10}$$

where $d\sigma_\omega$ is the surface element at a point ω of S and R_ω is the mean curvature radius at that point. The boundary condition K_ω (eq. 6) is contained in

$$\delta_\omega(k) \equiv \tan^{-1} \frac{K_\omega}{k} \ . \tag{11}$$

The range of δ_ω is $0 \leqslant \delta_\omega \leqslant \pi/2$, the lower and upper boundaries corresponding to the Neumann and Dirichlet cases respectively.

III. THE BINDING ENERGY

In this section, we proceed to evaluate the energy of the many nucleon system as given in eq. (2), subject to the self-consistent condition (4). The asymptotic expression for ρ_γ, eq. (10), is used. However, rather than determine from the start the appropriate boundary condition, that is, the value of K in (6), we shall leave it as an adjustable parameter, and see whether the value required to give reasonable results for the binding energy corresponds to the known behaviour of actual single particle wavefunctions at the edge of the potential well.

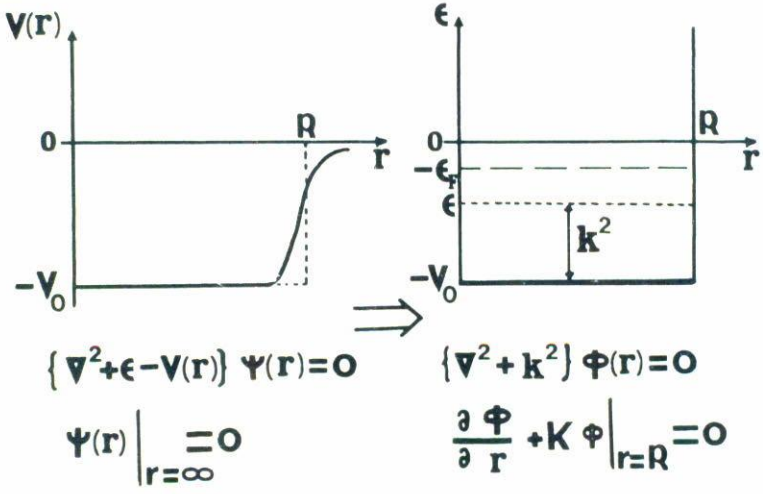

Fig. 1. The auxiliary problem

We shall limit ourselves to the case of a spherical nucleus. As the system is self bound by generating a potential of practically constant depth, the auxiliary problem consists then of a spherical region of radius R, where a constant potential $-V_0$ acts (see fig. 1). The single particle equation is then the wave equation (5). Assuming furthermore a uniform boundary condition $K_\omega = K$, the asymptotic averaged level distribution (10) is in this case:

$$\rho_0(\epsilon) = \frac{n}{4\pi^2}\left\{Vk + \left(\frac{\pi}{4} - \delta(k)\right)S + \frac{1}{R}f(\delta(k))\frac{S}{R}\right\}, \tag{12}$$

$$f(k) \equiv \tfrac{1}{3} + \cos^2\delta(k) - \delta(k)\cot\delta(k), \tag{13}$$

where $V = (4\pi/3)R^3$, $S = 4\pi R^2$, n is the spin-isospin degeneracy factor and

$$k^2 = V_0 + \epsilon; \tag{14}$$

units such that $(\hbar^2/2m) = 1$ are used.

The calculations are now straightforward, if we note that in the auxiliary problem, eq. (5), $t(\epsilon) = k^2$ and that from relation (14) $d\epsilon = 2kdk$. It follows that

$$A = \int_{-V_0}^{-\epsilon_F} \rho_0(\epsilon)\, d\epsilon = 2\int_0^{k_F} \rho_0(k)\, kdk$$

and

$$E = \tfrac{1}{2}\int_{-V_0}^{-\epsilon_F} \{\epsilon + t(\epsilon)\}\rho_0(\epsilon)\, d\epsilon = -\frac{V_0}{2}A + 2\int_0^{k_F} \rho_0(k)\, k^3 dk\ .$$

Using eq. (12), the results are:

$$A = \frac{n}{\pi}\left[\tfrac{2}{9}(kR)^3 + \left\{\frac{\pi}{4} - \delta + \tan\delta\left[\left(\frac{\pi}{2} - \delta\right)\tan\delta - 1\right]\right\}(kR)^2 + \right.$$

$$\left. + \left\{\tfrac{5}{3} - \delta\cot\delta - \left(\frac{\pi}{2} - \delta\right)\tan\delta\right\}(kR)\right]_{k=k_F} \tag{15}$$

and

$$E + \frac{V_0}{2} A = \frac{n}{\pi} k_F^2 \left\{ \frac{2}{15}(kR)^3 + \right.$$

$$+ \left\{ \frac{\pi}{4} - \delta - \tan\delta \left[\tfrac{1}{3} - \tan^2\delta + 4\left(\frac{\pi}{2} - \delta\right) \tan^3\delta \right] \right\} \frac{(kR)^2}{2} + \qquad (16)$$

$$\left. + \left\{ \frac{13}{9} - \delta \cot\delta + 3\tan^2\delta \left[\left(\frac{\pi}{2} - \delta\right) \tan\delta - 1 \right] \right\} \frac{kR}{2} \right\}_{k = k_F} .$$

The next step is to solve eq. (16) for the Fermi momentum and substitute in eq. (15) to obtain the desired result $E = E(A)$. From the structure of the equations, it is quite clear that only a numerical solution is possible.

In order to be able to proceed analytically however, we shall substitute $\delta(k)$ in eq. (12) by some average value $\bar{\delta}$, which becomes the parameter of the calculation involving the boundary condition. In this case we have

$$E = -\frac{V_0}{2} A +$$

$$+ \frac{n}{\pi} k_F^2 \left\{ \frac{2}{15}(k_F R)^2 + \left(\frac{\pi}{4} - \bar{\delta}\right) \frac{(k_F R)^2}{2} + \frac{2}{3} f(\bar{\delta})\, k_F R \right\} \qquad (17)$$

and

$$A = \frac{n}{\pi} \left\{ \frac{2}{9}(k_F R)^3 + \left(\frac{\pi}{4} - \bar{\delta}\right)(k_F R)^2 + 2 f(\bar{\delta})\, k_F R \right\} . \qquad (18)$$

Eq. (18) is now a simple algebraic equation in k_F which can be solved to give

$$k_F = (A^{1/3}/R)\left(\frac{9\pi}{2n}\right)^{1/3} \left\{ 1 - \left(\frac{2n}{9\pi}\right)^{1/3} \frac{3}{2} \left(\frac{\pi}{4} - \bar{\delta}\right) A^{-1/3} + \mathcal{O}(A^{-2/3}) + \ldots \right\} \qquad (19)$$

Substituting in eq. (17) we shall obtain an expression for the self consistent energy. We defer this to the next section, where the parametrization of R in terms of A is discussed.

We want to point out here that, upon taking in the approximate expressions (17), (18) and (19) the limiting values 0 and $\pi/2$ for δ, we recover the results that would follow from the exact expressions (15) and (16) in the corresponding cases, i.e., $K = 0$ and $K = \infty$. These results are

$$E = \frac{n}{\pi} k_F^2 \left\{ \frac{2}{15} (k_F R)^3 \pm \frac{\pi}{8} (k_F R)^2 + \frac{2}{9} k_F R \right\} \tag{20}$$

and

$$k_F = (A^{1/3}/R)\left(\frac{9\pi}{2n}\right)^{1/3} \left\{ 1 \mp \left(\frac{2n}{9\pi}\right)^{1/3} \frac{3}{2} \frac{\pi}{4} A^{-1/3} + \ldots \right\} , \tag{21}$$

where the upper and lower signs in the surface term correspond respectively to the Neumann ($K = 0 \Rightarrow \partial\varphi/\partial n = 0$) and Dirichlet ($K = \infty \Rightarrow \varphi = 0$) boundary conditions.

IV. THE CURVATURE CORRECTION

In accordance with the arguments given in sections I and III to justify the use of the auxiliary problem, the radius R of the domains is taken to be the same of the optical or shell model potential, that is:

$$R = r_0 A^{1/3} + c \ . \tag{22}$$

The constant c is not always included in shell model calculations. It is however needed in order to insure an A-independent central density[9]. We shall keep this constant and discuss our results in terms of it, as is done in a similar work[10] where the binding energy is calculated up to the surface correction term.

Using (22) and making power series expansions in $A^{1/3}$, expressions (17) and (19) yield for the binding energy of a symmetric nucleus ($N = Z$; $n = 4$), the following result:

$$B(A) = -E(A) = a_V A + a_S A^{2/3} + a_R A^{1/3} + \ldots \ , \tag{23}$$

where

$$a_V = + \frac{V_0}{2} - \frac{3}{5}\left(\frac{9\pi}{8}\right)^{2/3} \frac{\hbar^2}{2mr_0^2} \quad , \tag{24}$$

$$a_S = \frac{\hbar^2}{2mr_0^2}\left(\frac{9\pi}{8}\right)^{1/3}\left\{\frac{9}{4}\left(\frac{\pi}{4} - \bar{\delta}\right) + \frac{6}{5}\left(\frac{9\pi}{8}\right)^{1/3}\frac{c}{r_0}\right\} , \tag{25}$$

$$a_R = -\frac{\hbar^2}{2mr_0^2}\,3\left\{f(\bar{\delta}) + \frac{3}{2}\left(\frac{9\pi}{8}\right)^{1/3}\left(\frac{\pi}{4} - \bar{\delta}\right)\frac{c}{r_0} + \frac{3}{5}\left(\frac{9\pi}{8}\right)^{2/3}\left(\frac{c}{r_0}\right)^2\right\} . \tag{26}$$

Here we have introduced again the factor $(\hbar^2/2m)$ explicitly.

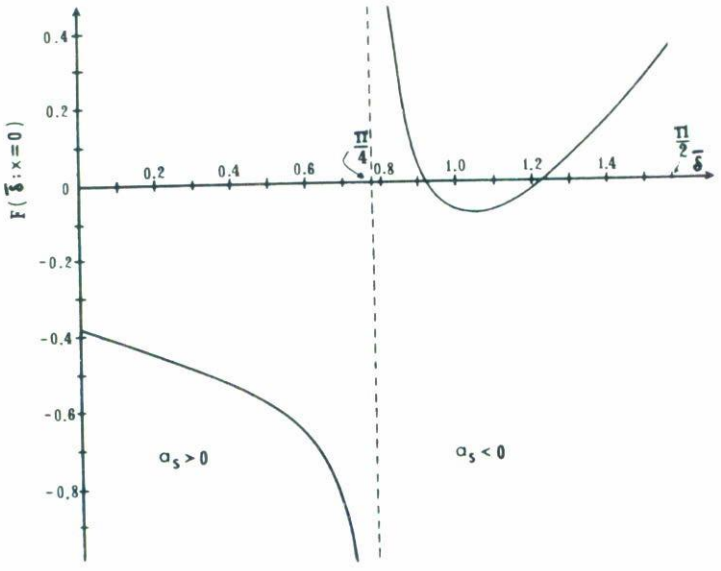

Fig. 2. a_R/a_S vs $\bar{\delta}$ for $x \equiv c/r_0 = 0$

The binding energy has been expressed as the sum of "volume", "surface" and "curvature" terms. The two last ones represent corrections due to the finite size of the nuclear system as can be seen by looking at $B(A)/A$ when A goes to infinity. Furthermore, the quotient

$$F(\bar{\delta}; x) \equiv \frac{a_R}{a_S}, \quad \left(x = \frac{c}{r_0}\right), \tag{27}$$

depends *exclusively* on the size parameters r_0 and c, eq. (22) and the boundary condition $\bar{\delta}$ which represents the behaviour of the wave functions at the surface. In figs. 2 and 3a, b, c, the function $F(\bar{\delta}; x)$ is plotted for different values of x. As r_0 is quite definitely determined to be between 1.0 and 1.5 Fermis, the variation of x reflects the dependence on c of a_S and a_R. The singularity corresponds to the value of $\bar{\delta}$ for which a_S changes sign, being positive to the left and negative to the right. The right side is the region of interest, as everyone agrees that the surface correction is negative, i.e., decreases the binding energy. This region corresponds to values of $\bar{\delta}$ larger than $\pi/4$, the lower bound increasing as c increases. So we are always on the side of the Dirichlet limit ($\bar{\delta} \to \pi/2$, $\varphi \to 0$ with $\partial\varphi/\partial n$ finite) which clearly represents the behaviour of bound state wave functions at the surface (the Neumann limit $\bar{\delta} \to 0$, $\partial\varphi/\partial n \to 0$ is rather to be related to resonant states). We therefore have agreement between a physical surface correction and realistic surface properties of the wave functions.

The function $F(\bar{\delta}; x)$ is very sensitive to the value of x; the terms in which it appears soon dominate the numerator, as can be seen from the reversal of the asymptotic behaviour at the singularity, for $x \approx 0.13$. From then on, the "physical" branch of F (i.e. the one for which $a_S < 0$) quickly ($x \approx 0.31$) becomes entirely negative up to $\bar{\delta} = \pi/2$. So that, for $x \geqslant 0.21$, the curvature correction has always the opposite sign to surface one, i.e., the curvature increases the binding energy (figs. 3b, c); also the relative magnitude increases rapidly with x. Only for very small values of x can one find a curvature term of the same sign as the surface term, depending on the value of $\bar{\delta}$, as can be seen from figs. 2 and 3a.

Finally we proceed to some numerical estimates of the curvature coefficient a_R, with two sets of parameters. From optical model analysis[11], we take $r_0 = 1.16$ F and $c = 0.6$ F as set I. This corresponds to $x = 0.517$ (fig. 3c). Also, if one puts $c = 0$, one should take a larger r_0, as pointed out in ref. 10 where the value $r_0 = 1.27$F is given; this is set II. In both cases we determine $\bar{\delta}$ by requiring $a_S = -18$ MeV, which is a firmly established value[12].

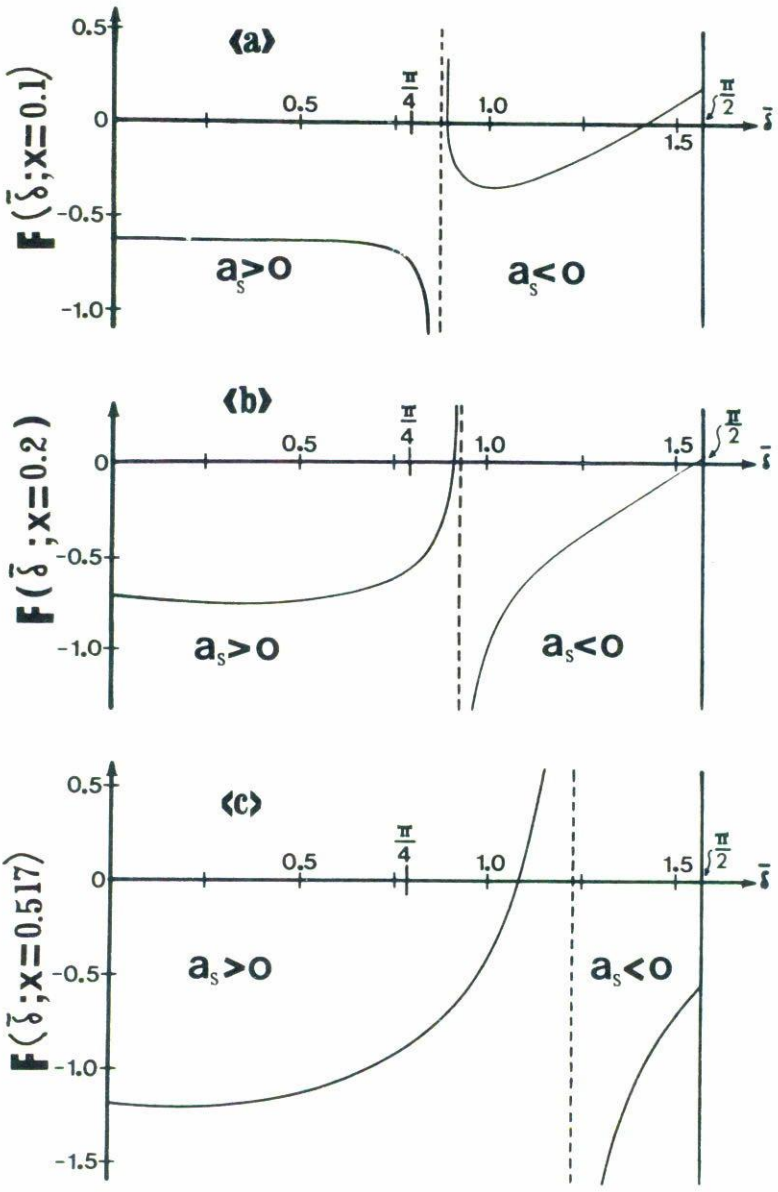

Fig. 3a, b, c a_R/a_S vs $\bar{\delta}$ for $x \neq 0$

We also consider the need of an effective mass m^* to reflect in some measure the non-locality of the self consistent nuclear field[+] and the value $m^* = 0.5m$ is taken. The results are given in Table I.

TABLE I

		$m^* = m$		$m^* = 0.5m$	
$a_S = -18$ MeV		$\bar{\delta}$	a_R (MeV)	$\bar{\delta}$	a_R (MeV)
I)	$r_0 = 1.27$F, $c = 0$	1.287	- 1.17	0.986	1.56
II)	$r_0 = 1.16$F, $c = 0.6$F	1.539	10.8	1.373	20.7

V. CONCLUSIONS

General quantum mechanical characteristics of the nuclear many-body problem have been used to establish the structure of the curvature correction in the semi-empirical nuclear mass formula. Such characteristics are independent single-particle motion in a self consistent potential well, which is practically constant up to the surface where it falls rapidly to zero. Under realistic conditions, that is, an effective mass $m^* < m$, arising from the non locality of the potential and a parametrization of the nuclear radius that insures an A-independent central density ($c \neq 0$), it is found that the curvature correction *increases* the binding energy. The numerical value is however very sensitive to the parametrization of the nuclear radius.

[+] This is discussed in ref. 5 where the modifications of the potential well depth due to non locality are also obtained. As these have not been taken into account here, a discussion of the volume term as given in eq. 24 is not meaningul: in fact no value of V_0 can reproduce both the phenomenological values of a_V and ϵ_F.

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REFERENCES

1. Myers, W.D. and Swiatecki, W. J., Nuc. Phys. 81 (1966) 1
   Strutinsky, V.M., Nuc. Phys. A95 (1967) 420; A122 (1969) 1
   Seeger, Ph. A., Proc. 2nd Int. Conf. on Nuclidic Masses (Vienna); Ed. W.H. Johnson, Springer-Verlag (1964)
2. Hasse, R.W., Ann. Phys., 68 (1971) 377
3. Myers, W.D. and Swiatecki, W. J., Ann. Phys. 55 (1969) 395
   Nemeth, J. and Gadioli, E., Phys. Lett. 34B (1971) 117
4. Truran, J.W., Cameron, A.G.W., Hilf, E., CERN-70-30, Vol. 1.275
5. Bauer, M. and Canuto V., Ark. f. Fys. 36 (1967) 393
   Bauer, M. and Canuto V., Proc. 3rd Int. Conf. on Atomic Masses (Winnipeg), Ed. R.C. Barber, Un. of Manitoba Press, p. 234 (1967)
6. Strayer, M.R. and Kerman, A.K., Prep. Orsay 1972
7. Balian, R. and Bloch, C., Ann. Phys. 60 (1970) 401
8. Strutinsky, V.M. and Tyapin, A.S., Sov. Phys. JETR 18 (1964) 664
   Badhuri, R.K. and Ross, C.K., Phys. Rev. Lett. 27 (1971) 606
9. Swiatecki, W.J., Proc. Phys. Soc., 44 (1951) 226
10. Siemens, Ph. and Sobiczewski, A., Phys. Lett. 41B (1972) 16
11. Hodgson, P.E., Ann. Rev. Nuc. Sci. 17 (1967) 1
12. Bethe, H., Ann. Rev. Nuc. Sci. 21 (1971) 93.

RESUMEN

Se obtiene la corrección por curvatura de la energía de ligadura nuclear, usando una densidad de niveles promedio apropiada para describir hasta efectos de curvatura, el aspecto de partículas independientes del problema nuclear de muchos cuerpos. La relación entre los coeficientes de superficie y curvatura depende exclusivamente del radio del núcleo y del comportamiento de las funciones de onda en la superficie. Correspondiendo a un término

realista de superficie, se encuentra que la corrección de la curvatura es tal que aumenta la energía de ligadura, aunque el valor real es muy sensible a la parametrización del radio nuclear en términos del número de masa.