A Note on the Thomas-Fermi Statistical Method

E. FEENBERG
Institute for Advanced Study, Princeton, New Jersey
(Received July 16, 1937)

The accuracy with which binding energies can be computed using the statistical approximation is shown to depend strongly on the symmetry character of the wave function when the forces are of the short range saturation type met with in nuclear theory. Recent calculations on the relation between the neutron excess in heavy nuclei and the saturation properties of nuclear forces are reinterpreted in the light of this result.

THE Thomas-Fermi statistical method has been applied to fix upper bounds on the magnitude of nuclear forces[1] and to obtain necessary conditions for the occurrence of saturation in heavy nuclei.[2] These applications are legitimate because the method consists essentially in the calculation of an expectation value of the Hamiltonian operator with an especially simple wave function. Since an expectation value cannot lie below the true normal state eigenvalue, all forms of the interaction operator which yield too much binding energy in the statistical approximation must be rejected.

Recently the statistical approximation has been used to study the relation between the neutron excess, $A-2Z$, in heavy nuclei and the exchange properties of the nuclear forces.[3] In the statistical approximation a nucleus can be characterized qualitatively by the statement that it consists of a collection of "4" groups and "2" groups.[4] Two neutrons and two protons in one space orbit constitute a "4" group while two neutrons with opposed spins in a single space orbit form a "2" group. The wave function has a definite symmetry character[5] described by the partition quantum number $(4+4+\cdots+4+2+2+\cdots 2)$ with $\frac{1}{2}Z$ "fours" and $\frac{1}{2}(A-2Z)$ "twos." (Actually the symmetry character has little significance for heavy nuclei. The mixing effect of the spin exchange and Coulomb forces produces a state which is a linear combination of many different partitions.) For a fixed A, the value of $A-2Z$ which makes the energy as low as possible is determined by the conflict between the Coulomb interactions tending to increase the neutron excess and the saturation properties of the nuclear forces which tend to associate stability with a high degree of symmetry. Clearly the question of how the degree of accuracy of the statistical approximation depends on the symmetry character of the wave function must be answered before much significance can be attached to calculations of neutron excess in heavy nuclei.

To examine this question consider a generalized nuclear system with the Hamiltonian operator[6]

$$H=-\tfrac{1}{2}\sum\Delta_l-\sum_{i<j}J(r_{ij})(nP_{ij}+1)/(n+1) \quad (1)$$

subject to the condition that no more than n particles can occupy the same orbit. The physical possibilities include $n=2$ and $n=4$. Under these conditions the normal state binding energy plotted against the total mass will show an "n" group structure which gradually merges into a straight line for heavy nuclei. It is reasonable to suppose that the total binding energy of a collection of "n" groups will be somewhat greater than that of the separated n particle systems.

The binding energy of a single n particle system can be computed approximately by using the Gaussian wave function

$$\psi_n=C_n\exp\left[-(\nu/2)\sum_{i<j}r_{ij}^2\right]. \quad (2)$$

The expectation value of the energy is given by

[1] E. Majorana, Zeits. f. Physik **82**, 137 (1933); W. Heisenberg, *Rapport du Septieme Congres Solvay* (Paris, 1934); G. C. Wick, Nuovo Cimento **11**, 227 (1934); K. Nakabayasi, Zeits. f. Physik **97**, 211 (1935); C. F. v. Weizsacker, Zeits. f. Physik **96**, 431 (1935); H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8**, 82 (1936).

[2] G. Breit and E. Feenberg, Phys. Rev. **50**, 850 (1936).

[3] H. Volz, Zeits. f. Physik **105**, 537 (1937).

[4] The discussion is limited to systems containing even numbers of neutrons and protons.

[5] E. Wigner, Phys. Rev. **51**, 106 (1937).

[6] P_{ij} is the Majorana exchange operator; the spin exchange operator Q_{ij} appears in Eq. (12).

$$\epsilon_n = 3n(n-1)\nu/4 - \tfrac{1}{2}n(n-1)(4/\pi^{\frac{1}{2}})\int_0^\infty J(r/(\tfrac{1}{2}n\nu)^{\frac{1}{2}})e^{-r^2}r^2dr. \quad (3)$$

Now we proceed to calculate the energy of a collection of "n" groups by means of the statistical method. Let N (an integral multiple of n) designate the number of particles in the system and $E(n, N)$ the energy value given by the statistical method. By comparing ϵ_n and $n/N\cdot E(n, N)$ something can be learned about the way in which the degree of accuracy of $E(n, N)$ depends on n. In the statistical model the radius R of the nucleus and the maximum momentum of the particles in the nucleus are connected by the relation $(RP)^3 = 9\pi N/2n$. The energy has the form

$$E(n, N) = 0.3NP^2 - n(n-1)/8 \cdot \int\cdots\int J(q-q')(q|\rho|q')^2 d\tau d\tau' \quad (4)$$

with[1]

$$(q-\xi/2|\rho|q+\xi/2) = (\sin \xi P/\xi - P\cos \xi P)/(\pi\xi)^2, \quad |q| \leqq R, \quad (5)$$
$$= 0, \quad |q| > R.$$

From Eqs. (4) and (5) we obtain the energy per "n" group

$$n/N\cdot E(n, N) = 0.3nP^2 - \tfrac{1}{2}n(n-1)(6/\pi) \cdot \int_0^\infty J(r/P)(\sin r - r\cos r)^2/r^4\cdot dr. \quad (6)$$

A great simplification is made possible by the fact that the function $1/9\cdot r^2 \exp[-\lambda r^2]$ $(\lambda^{3/2} = 1/6\pi^{\frac{1}{2}})$ approximates very closely to $(\sin r - r\cos r)^2/r^4$ up to the first maximum of the latter function. The constant λ is determined by the condition

$$1/9\cdot\int_0^\infty r^2 \exp[-\lambda r^2]dr = \int_0^\infty (\sin r - r\cos r)^2/r^4\cdot dr = \pi/6. \quad (7)$$

If $J(r)$ is an error function or a linear combination of error functions with positive coefficients, the potential energy in Eq. (6) is increased by the substitution of $1/9\cdot r^2\exp[-\lambda r^2]$ for $(\sin r - r\cos r)^2/r^4$. Thus, for a reasonably general form of potential function, we obtain a lower limit to $E(n, N)$ defined by the equation

$$n/N\cdot E'(n, N) = 0.3nP^2 - \tfrac{1}{2}n(n-1)(4/\pi^{\frac{1}{2}}) \cdot \int_0^\infty J(r/P\lambda^{\frac{1}{2}})\exp[-r^2]r^2dr. \quad (8)$$

The substitution $3n(n-1)\nu/4 = 0.3nP^2$ transforms Eqs. (3) into

$$\epsilon_n = 0.3nP^2 - \tfrac{1}{2}n(n-1)(4/\pi^{\frac{1}{2}}) \cdot \int_0^\infty J(r/P(n/5(n-1))^{\frac{1}{2}})\exp[-r^2]r^2dr. \quad (9)$$

The general assumption about the form of $J(r)$ made in the preceding paragraph and the inequality $n/5(n-1) > \lambda = 0.2068$ which is satisfied for $n < 31$ imply the relation

$$\epsilon_n < n/N\cdot E'(n, N) < n/N\cdot E(n, N). \quad (10)$$

Eq. (10) is still valid if E, E', and ϵ_n are replaced by the minimum values of the three functions defined by the Eqs. (6), (8) and (9), respectively. It is known that the Gaussian wave function for an n particle system is increasingly unsatisfactory as n is decreased.[7] In actual nuclear calculations the Gaussian wave function is very bad for $n=2$, but already surprisingly good for $n=4$. Thus ϵ_n is an increasingly bad upper limit on the true n particle eigenvalue as n is decreased.

The quantity

$$\theta(n) = (n/5\lambda(n-1))^{\frac{1}{2}} \quad (11)$$

is a monatonic decreasing function of n and greater than unity for $n < 31$. This quantity can be interpreted as the ratio of the effective ranges of the intranuclear forces in the n particle calculation and in the statistical calculation. More than half of the drop to the asymptotic value $(5\lambda)^{-\frac{1}{2}}$ occurs in passing from $n=2$ to $n=4$. The relation $\theta(n) > 1$ means that the statistical calculation yields no binding energy for a collection of "n" groups. This result must be ascribed to the inadequacy of the method.

From Volz's form of the Hamiltonian operator,

$$H = -\tfrac{1}{2}\sum\Delta_i - \sum_{i<j} V(r_{ij})(-5 + 14P_{ij} - 7P_{ij}Q_{ij} + 10Q_{ij})/12, \quad (12)$$

[7] E. Feenberg, Phys. Rev. **47**, 850 (1935).

we obtain the energy equation

$$E(4, N)=0.3NP^2 -(9/8)\int\cdots\int V(q-q')(q|\rho|q')^2 d\tau d\tau', \quad (13)$$

when the system contains equal numbers of neutrons and protons and

$$E(2, N)=0.3NP^2 -(1/8)\int\cdots\int V(q-q')(q|\rho|q')^2 d\tau d\tau', \quad (14)$$

when the system contains only neutrons. These equations are identical with Eq. (4) if for $n=4$ we take $J(r)=3/4\cdot V(r)$ and for $n=2$, $J(r)=\frac{1}{2}V(r)$. The same correspondences hold also for the four and two particle systems. Since the statistical approximation gives no binding energy between "2" groups and also none between "4" groups there is little likelihood that it is adequate for the calculation of the interactions within a mixed system containing both "2" and "4" groups.

Evidently the statistical method yields decidedly less accurate results for $n=2$ than for $n=4$. Although the problem considered here is not identical with that of determining the neutron excess in heavy nuclei, there is enough similarity to suggest that the values of $A-2Z$ given by the statistical approximation are too small by a large factor.[8] In view of this possibility the argument given by Volz for his special form of the symmetrical interaction operator must be considered inconclusive. Moreover the interaction operator proposed by Volz contains such large spin exchange terms[9] as to preclude the existence of a partition quantum number for even the lightest nuclei (with the single exception of the deuteron) and thus comes into conflict with the evidence presented by Wigner[10] for the usefulness of the partition quantum number in ordering the empirical material on the stability of isobars up to $A\sim 50$. Actually the simple theory without spin exchange forces discussed by Wigner begins to make $A-2Z$ too large in the neighborhood of $A\sim 50$. According to the calculations of Volz any discrepancy, with Wigner's choice of interaction operator, should be in the direction of making $A-2Z$ too small. However, for the comparison of isobars, Wigner's calculations are unquestionably much better than those based on the statistical approximation. One may conclude that the evidence available at present does not support the contention that very large spin exchange forces are required to account for the large neutron excess in heavy nuclei.

[8] In a letter to the writer Dr. Volz states that a calculation which will test this point is in progress.

[9] The sum of the Heisenberg and pure spin exchange operators is small, but each separately is large.

[10] E. Wigner, Phys. Rev. **51**, 947 (1937).