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# Pairing Approximation in Spherical Nuclei - I.

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**Summary.** — The pairing theory (BCS-method) is applied to spherical nuclei in order to calculate some characteristic physical properties. The main points are: i) insertion of an effective (realistic) two-nucleon force in the pairing matrix elements; ii) definition of a phenomenological nuclear potential in order to determine the single-particle states. The effective two-nucleon interaction was obtained from the Hamada-Johnston expression by means of a Scott-Moszkowski procedure; the complete set of nuclear potentials (of Saxon-Woods type) contains 5 constants which were determined from specific nuclear properties (empirical determination of the self-consistent field occurring in a Hartree-Bogoliubov treatment). The gap equation was solved numerically taking into account all relevant single-particle states. The final results (separation energies and quasi-particle excitations) as well as the corresponding empirical data are plotted simultaneously as functions of the nucleon numbers (Fig. 4 and 5). There is a satisfactory agreement just within the spherical regions; in particular the correspondence between the typical irregularities at the magic numbers and between the characteristic variations of the quasi-particle levels and of the pairing energies should be emphasized.

## 1. – Introduction and survey.

From a systematic survey of nuclear data one obtains a large number of characteristic features which are intuitively understood from the general principles of shell structure [1-4]. As an example we have plotted the empirical

[1] N. ZELDES: *Nucl. Phys.*, **7**, 27 (1958); N. ZELDES, M. GRONAU and A. LEV: *Nucl. Phys.*, **63**, 1 (1965).

[2] M. BEINER and K. BLEULER: *Nucl. Phys.*, **22**, 589 (1961).

[3] M. BEINER: *Forschungsberichte des Landes Nordrhein-Westfalen* (1964), No. 1407 (to be obtained from our Institute).

[4] K. BLEULER, *et al.*: *Nuclear Separation Energies, Report of the Lysekil-Conference,* 1966.

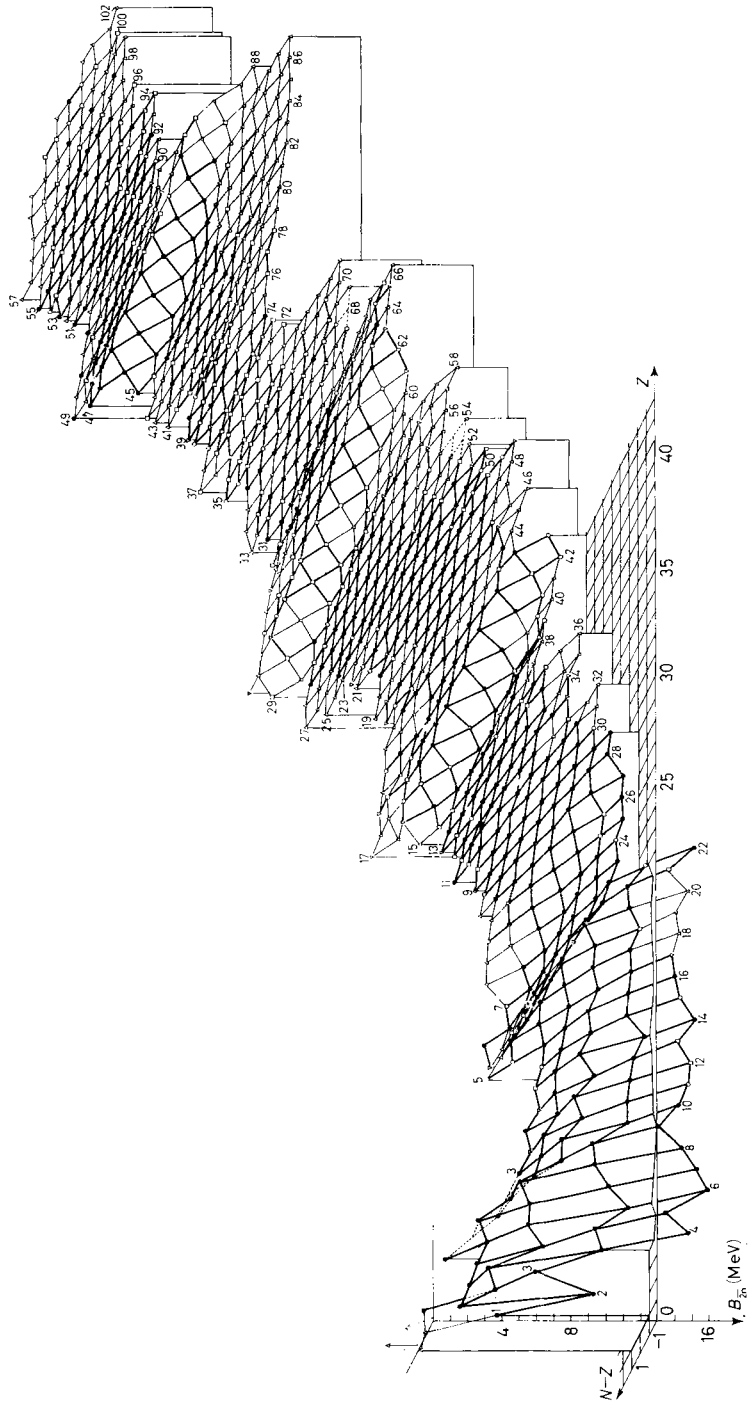


Fig. 1. – Mean separation energy of neutrons $B_{2n}$: $B_{2n}(Z,N)=\frac{1}{2}[B(Z,N+1)-B(Z,N-1)]$ 3-dimensional plot: horizontal co-ordinates $Z$ and $N-Z$, vertical co-ordinate (downwards) $B_{2n}$. • Error $\leqslant$ 0.020 MeV, ▫ error $\leqslant$ 0.050 MeV, ○ error $\leqslant$ 0.100 MeV, ▽ error $\leqslant$ 0.200 MeV, △ error $>$ 0.200 MeV.

« mean separation » energy of neutrons as a function of the nucleon numbers $Z$ and $N$ (see Fig. 1). This « mean separation » energy is defined by

$$B_{2n}(Z, N) \equiv \tfrac{1}{2}[B(Z, N+1) - B(Z, N-1)], \tag{1.1}$$

where $B(Z, N)$ represents the total nuclear binding energy which, in our case, was taken from the new tables of Mattauch *et al.* [5]; an analogous expression is used for the protons. The double step was introduced in order to eliminate the even-odd mass differences. We thus obtained a smooth surface which, however, is interrupted by characteristic steps at certain lines of constant $N$-values (magic numbers). This behaviour corresponds, of course, to the closing of spherical shells of independent particles. Similar properties continue to hold for the empirical « single particle » states, *i.e.* ground-states and low-lying excited states of odd nuclei within the spherical regions. If for each assignment the corresponding separation energies are plotted within the same diagram we obtain a characteristic system of restricted surfaces (« leaves ») which, again, is easily understood from this point of view (see Fig. 2). In this case the separation energies are naturally defined by

$$B_n^{J^\pm}(Z, N) \equiv B^{J^\pm}(Z, N) - B(Z, N-1), \quad (Z \text{ even}, N \text{ odd}), \tag{1.2}$$

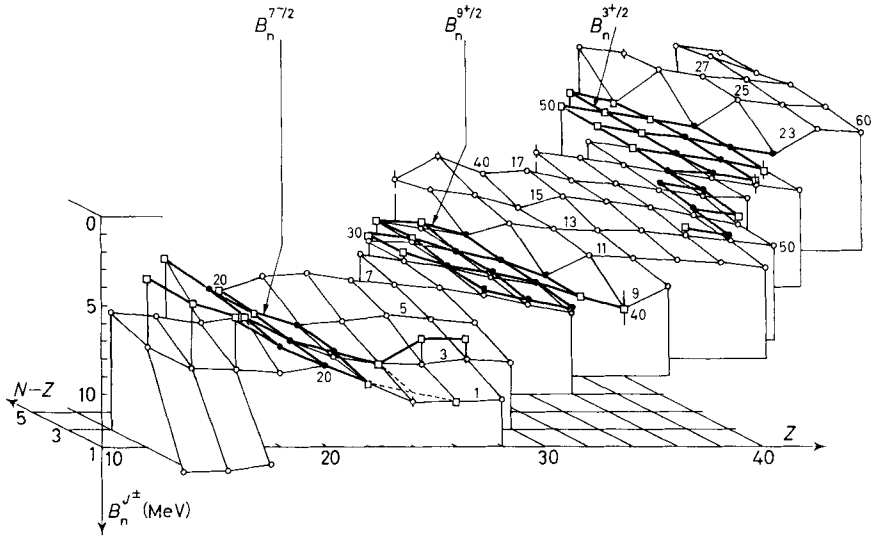


Fig. 2. – Neutron separation energies $B_n^{J^\pm}(Z, N)$ ($Z$ even, $N$ odd): $B_n^{J^\pm}(Z, N) = B^{J^\pm}(Z, N) - B(Z, N-1)$. Heavy lines connect ground and excited states of the same assignment $J^\pm$. • Spin certain, ▫ spin probable, ○ other spins, ground states.

[5] J. MATTAUCH, W. THIELE and A. H. WAPSTRA: *Nucl. Phys.*, **67**, 1 (1965).

where the excitation energy is incorporated in $B^{J^{\pm}}$ (*sc.* generalized separation energies). All points corresponding to the same assignment $J^{\pm}$ were then connected by a system of heavy lines thus representing a continuous variation of the independent particle levels with $Z$ and $N$.

It is, however, evident that the empirical data will not, by any means, be in quantitive agreement with an « ideal » structure, such as independent particles moving in a potential well. For instance, the average spacing of the empirical single-particle levels is much smaller than the « ideal » shell value, which is essentially determined by the nuclear radius. Moreover, no irregularities of the separation energies are observed at the subshell closures. This fact indicates that the sharp change of occupation probabilities occuring at the Fermi level in the naive picture may be the main reason for the disagreement.

On the other hand, the « ideal » structure corresponds very closely to a Hartree-Fock (HF) treatment of the $n$-body system. It is, therefore, obvious that we should look for a suitable generalization of this method. We therefore consider as a next step the Hartree-Bogoliubov (HB) or more precisely, the Valatin approximation ([6-9]) in which a smoothed Fermi limit is introduced from the outset. In addition, the nucleus is replaced within the framework of this method by a system of quasi-particles with a relatively weak interaction. This fact also corresponds exactly to the general empirical nuclear properties. For these reasons we introduce this approximation as a basis of our calculations. At present, however, it does not appear to be possible to use the full scheme —at least in the case of heavier nuclei—for a detailed numerical treatment.

We therefore introduce a rather drastic simplification. It may be seen that the HB-equation (as given by VALATIN ([7])) represents a coupled system consisting of a generalized HF-problem and a slightly enlarged pairing equation (*). Now, the corresponding generalized (nonlocal) nuclear potential, appearing as a quadratic expression of the unknown wave functions in these equations, is just replaced by a phenomenological local potential well of the Woods-Saxon type. In other words, the nuclear potential is determined directly from a series of typical empirical data. All details of the determination of this potential will be given in Sect. **2**; the main point was to use a form which gives a fair account of the single-particle levels, within a limited energy interval just around the Fermi level.

We thus remain with the numerical solution of a problem which has the well-known form of the pairing (BCS) approximation (see Sect. **4**). We have,

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([6]) N. N. BOGOLIUBOV: *Sov. Phys. Usp.*, **2**, 236 (1959).

([7]) J. G. VALATIN: *Phys. Rev.*, **122**, 1012 (1961).

([8]) M. BARANGER: *Phys. Rev.*, **122**, 992 (1961); **130**, 1244 (1963).

([9]) C. BLOCH and A. MESSIAH: *Nucl. Phys.*, **39**, 95 (1962).

(*) The separation of the Valatin system will be discussed in a subsequent paper. In order to check our method we have considered the limiting case of nuclear matter.

however, to bear in mind that the HB-scheme is applicable only if effective (finite) nuclear forces are introduced from the outset. Within the framework of our approximation we have therefore to use the same forces also for the BCS calculations. They were determined explicitly using a Scott-Moszkowski procedure and the well-known Hamada-Johnston expression for nuclear forces (see Sect. **3**).

Our calculations are thus based on the following principles which define, in fact, an intuitive « nuclear model »:

*a*) Introduction of a nuclear potential constructed from specific nuclear properties (Sect. **2**).

*b*) Determination of an effective (finite) two-nucleon interaction from the scattering data (Sect. **3**).

*c*) Insertion of these forces as an additional direct interaction which is treated within the framework of the pairing approximation (Sect. **4**).

There are, of course, many generalizations like nonlocality of the nuclear potential and deformation (*).

A formal advantage of this « pairing model » is the possibility of determination of nuclear properties as (« continuous ») functions of the nucleon numbers $N$ and $Z$. This enables us to make rather detailed comparisons with the empirical data which we have represented by « continuous » surfaces (compare Fig. 1 and 2).

The calculations following the above-mentioned prescriptions have been carried out within all « spherical » regions of the periodic table (the details of the calculations are given in Part II of this work). The results may be summarized as follows.

There is a fairly good agreement with the empirical data in relatively large regions; *i.e.* there is a good fit of the mean separation energies and pairing effects (see Fig. 4, Sect. **4**) and of the generalized separation energies (see Fig. 5, Sect. **4**). In particular, the characteristic steps at the end of the major shells are fairly well reproduced whereas some « expected » irregularities at the closures of the subshells are eliminated completely. In other words, the pairing effects are just strong enough to eliminate the subshell effects whereas they still leave some steps at the major shells. These steps are, however, strongly reduced with respect to the « ideal » values.

Finally, one should explain why such a simple model is already so close to reality, especially in view of the fact that only the pairing part of the direct interactions is taken into account and that the nuclear potential has a phenom-

(*) The spherical case however, has already a relatively large domain of validity and represents the simplest case for a complete mathematical treatment.

enological character. The following arguments might be considered in this connection:

1) Within the spherical regions the pairing plays the role of an overwhelming interaction, *i.e.*, it reduces substantially the effects of all other types of direct interactions because of the special structure of the total state (correlations) induced by the pairing forces (*).

2) The numerical values of our pairing matrix elements differ only slightly from the results of more detailed calculations (short-range correlations) in lighter nuclei ([10]).

3) Our local potential replaces the more general (nonlocal) HB expression as long as the relevant single-particle states in the neighborhood of the Fermi level are considered. The deviations found for heavier nuclei ($A > 90$) should be partly ascribed to the nonlocality of the potential.

A more detailed discussion of the average potential especially with respect to the spin-orbit splitting which so far was determined phenomenologically (Sect. **2**) will be given in a subsequent paper ([11]).

## 2. – The nuclear potential.

The numerical basis of our work is the determination of the nuclear potential in the domain of spherical structures. Within our scheme this potential should, in principle, be calculated from self-consistency (HB or, as a first approximation HF). In view of the length of these calculations for heavy nuclei, and a rather critical uncertainty of the 2-body interaction, we make the following assumptions: i) existence of a self-consistent potential; ii) possibility of an approximate determination of appropriate nuclear properties (average values) from this potential alone. If we assume, in addition, that a local expression of special analytical form may be used it becomes possible to determine our potential directly from the nuclear properties mentioned above. We have, therefore, introduced the following rules:

1) We assume a central symmetric form of the Woods-Saxon type

$$W^c(r) \equiv - W_0 \left(1 + \exp\left[\frac{r - r^0}{\alpha_5}\right]\right)^{-1}. \tag{2.1}$$

(*) This point will be discussed in a forthcoming paper by D. SCHÜTTE.

([10]) See for example: T. T. S. KUO and G. E. BROWN: *Nucl. Phys.*, **85**, 40 (1966), compare Table 10, p. 70.

([11]) Compare K. BLEULER: *Proc. S.I.F.*, Course **36** (New York ond Gordon, 1966), p. 464.

This expression contains three parameters: radius $r^0$, surface thickness $\alpha_5$ and depth $W_0$. $\alpha_5$ is assumed to be independent of $Z$ and $N$, whereas $r^0$ satisfies the usual radius law $r^0 = \alpha_4 A^{\frac{1}{3}}$. $W_0$ is different for protons and neutrons and has the following well-known $N$-, $Z$-dependence ($W_0^{(p)}$ for protons and $W_0^{(n)}$ for neutrons)

$$W_0^{(p)}_{(n)} \equiv \alpha_1 \pm \alpha_2 \frac{N-Z}{A} . \tag{2.2}$$

2) We add a phenomenological spin orbit coupling of the Thomas type

$$W^{ls}(r)\, \boldsymbol{l}\cdot\boldsymbol{s} \equiv -\alpha_3 \lambda\!\!\!^{-2}_{\pi} \frac{1}{r} \frac{\mathrm{d}W^c(r)}{\mathrm{d}r} \cdot \frac{\boldsymbol{l}\cdot\boldsymbol{s}}{\hbar^2} \tag{2.3}$$

where $\lambda\!\!\!^{-}_{\pi} = 1.41$ fm. $\alpha_3$ is a characteristic dimensionless constant and assumed to be independent of $N$ and $Z$. The same expression holds for protons and neutrons with the corresponding potential $W^c(r)$.

3) For the protons we add the Coulomb potential $W^{Cb}(r)$ which is calculated from the empirical charge distribution as measured by R. HOFSTADTER.

We are thus left with 5 constants (*i.e.* the parameters $\alpha_1$–$\alpha_5$) which determine the complete set of nuclear potentials for the spherical regions. We now use the following nuclear properties in order to determine their numerical values:

1) The empirical nuclear charge distributions within the spherical regions.

2) The mean separation energies of neutrons and protons as functions of $Z$ and $N$, *i.e.* our empirical surfaces $B_{2\bar{n}}$ and $B_{2\bar{p}}$. According to the HB-scheme they are directly related to the (regularized) Fermi energies of the unknown potential (see Fig. 4, dashed lines).

3) The empirical sequence of single-particle levels throughout the spherical regions of the periodic table and their relative distances. A graphical survey was given by different authors ([3,12]).

In order to use these conditions explicitly the single-particle eigenfunctions have to be determined for all relevant values of $N$ and $Z$ and for various sets of the parameter $\alpha_1$–$\alpha_5$. The nuclear properties mentioned above were then determined (and adjusted) explicitly from such a simplified single-particle model. The sequence of single-particle levels for the « best fit » is shown by the light lines in Fig. 4. It was interesting to realize that all three

([12]) P. KLINKENBERG: *Rev. Mod. Phys.*, **24**, 63 (1952); K. BLEULER and CH. TERREAUX: *Helv. Phys. Acta*, **30**, 183 (1957).

conditions could be satisfied simultaneously (with relatively small deviations) although there is a very large overdetermination: several unknown functions of the two variables $N$ and $Z$ against only 5 constants at our disposal. This fact assures us of a certain consistency of our method, especially in view of the constancy of the potential depth parameter $\alpha_1$. (Actually it may be seen from our subsequent calculations that the addition of direct interactions has only a small effect on the particular nuclear properties invoked here.)

Our consistent values for the 5 constants are (see ref. [3])

$$(2.4) \quad \alpha_1 = 55.5\,\text{MeV}, \quad \alpha_2 = 33.2\,\text{MeV}, \quad \alpha_3 = 0.36, \quad \alpha_4 = 1.21\,\text{fm}, \quad \alpha_5 = 0.68\,\text{fm}.$$

In addition, we have checked that the potential depth and the « symmetry energy » of a somewhat simplified nuclear matter model are in fair agreement with the corresponding parameters $\alpha_1$ and $\alpha_2$ [13]. Similar values have been obtained independently by P. C. SOOD [14]. $\alpha_3$ is to a large extent determined by condition 3) and it should be noted in this connection that our subsequent BCS-transformation does not alter appreciably the sequence (and even the relative distances) of the relevant levels although there is a rather large change of the absolute values; compare Fig. 4 and formula (4.10). The possibility of a theoretical determination of $\alpha_3$ from a generalized HF-scheme (parity mixing) has been discussed by one of us [11].

## 3. – The effective nuclear forces.

In a second stage we now have to construct the effective two-body forces using the nucleon-nucleon scattering data $(0 \div 300)$ MeV as well as the known properties of the deuteron (binding energy and quadrupole moment). In this paper we give just a short survey of the construction of this interaction, whereas the details will be contained in a special paper [15]. The two-body potentials proposed so far satisfying the scattering data up to 320 MeV contain always a repulsive core of considerable strength. They are, therefore, incompatible with a Hartree-Fock approximation or a pairing theory in conventional form. It has been shown [16] that even a soft-core chosen in order to reproduce the behaviour of the $S$-phase at high energies has still a prejudicial influence on the binding energy and the relevant pairing matrix elements. To avoid these difficulties we propose a potential suggested by the fundamental separation

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[13] K. ERKELENZ: private communication.

[14] P. C. SOOD: *Nucl. Phys.*, **89**, 553 (1966).

[15] M. BEINER, K. BLEULER and K. ERKELENZ: *Effective Nuclear Forces*, to be published in *Nuovo Cimento*.

[16] K. ERKELENZ: private communication.

method of Moszkowski and Scott ([17]). Starting from the fact that the repulsion produced by the hard-core is effectively canceled by the inner part of the attraction we define a cut-off radius for this region in such a way that the remaining long-range tail of the potential reproduces the free nucleon-nucleon scattering data. In other words, we determine the cut-off radius directly from the nucleon-nucleon scattering data.

Our effective potential is based upon the well-known Hamada-Johnston form, however, with free numerical parameters in the various analytical expressions. The cut-off radii which we now insert, are in general energy, spin and parity dependent. They were determined together with the free parameters by fitting the scattering phases and deuteron data. However, within the energy interval to be considered in nuclear structure we showed that it was even possible to choose energy-independent cut-off radii. This implies large simplifications in the subsequent calculations. It is important to observe in this connection that even the $S$-phases are in relatively good agreement within the relevant energy interval (see Fig. 3), although it is evident that the change in sign of the $S_0$-phase which takes place at about 240 MeV will not be reproduced.

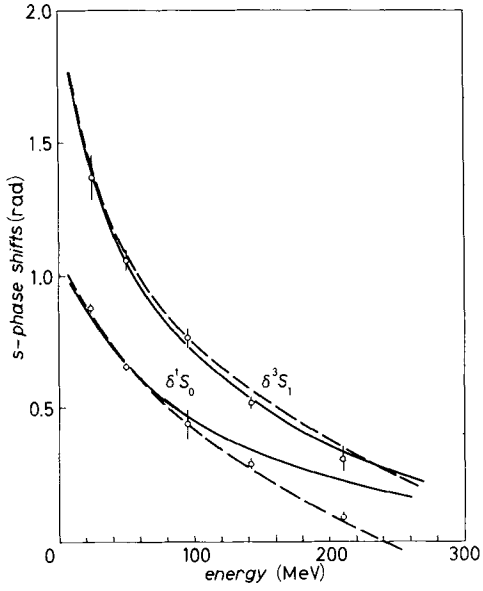


Fig. 3. – Energy dependence of experimental and calculated $S$-phase shifts: – – – Hamada-Johnston, ——— our effective potential, o experimental.

The following rather lengthy expression states our final result.

Our potential consists of four terms

$$V = V_C + V_T S_{12} + V_{LS} \boldsymbol{L}\cdot\boldsymbol{S} + V_{LL} L_{12}\,, \tag{3.1}$$

where $C$, $T$, $LS$ and $LL$ refer to central, tensor, linear $LS$ and quadratic $LS$ potential, respectively. The operators $S_{12}$ and $L_{12}$ are defined by

$$S_{12} = \frac{3(\boldsymbol{\sigma}_1\cdot\boldsymbol{r})(\boldsymbol{\sigma}_2\cdot\boldsymbol{r})}{\boldsymbol{r}^2} - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)$$

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([17]) S. Moszkowski and R. Scott: *Ann. of Phys.*, **11**, 65 (1960).

and

$$L_{12} = (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \boldsymbol{L}^2 - \tfrac{1}{2} \{(\boldsymbol{\sigma}_1 \cdot \boldsymbol{L})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{L}) + (\boldsymbol{\sigma}_2 \cdot \boldsymbol{L})(\boldsymbol{\sigma}_1 \cdot \boldsymbol{L})\} .$$

The $V_i$ ($i$ stands for $C$, $T$, $LS$, $LL$) are spin-parity dependent and given by

$$\text{(3.2)} \qquad \begin{cases} V_C = f^2 \dfrac{\mu}{3} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) Y (1 + a_C Y + b_C Y^2) , \\ V_T = f^2 \dfrac{\mu}{3} (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) Z (1 + a_T Y) , \\ V_{LS} = \mu G_{LS} Y^2 (1 + b_{LS} Y) , \\ V_{LL} = \mu G_{LL} x^{-2} Z (1 + a_{LL} Y + b_{LL} Y^2) , \end{cases}$$

where $\mu = 140$ MeV is the pion mass and $f^2 = 0.08$ the pion coupling constant. $Y$ and $Z$ represents the central and tensor functional form, respectively, of the one-pion exchange potential OPEP

$$\text{(3.2')} \qquad Y = \frac{e^{-x}}{x} , \qquad Z = Y \left(1 + \frac{3}{x} + \frac{3}{x^2}\right) ,$$

with $x = \mu_C r$ ($\mu_C$ = reciprocal Compton wave length of the pion measured in fm$^{-1}$). Hence, for sufficiently large $r$, the potentials $V_C$ and $V_T$ go over to the OPEP (with $f^2 = 0.08$). The additional terms with the coefficients $a$ and $b$ can be interpreted—within the model of the one-boson exchange potentials ([18])—as a contribution simulating the higher-boson exchanges. In the inner region, defined by the cut-off radius $d$, all four-potential terms in (3.1) vanish simultaneously. It must, however, be realized that this region is slightly

TABLE I. – *Numerical values of the parameters and cut-off radii d for the invariant subspaces of the two-body system.*

| Subspaces | Parameters and cut-off | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $d$ (fm) | $a_C$ | $b_C$ | $a_T$ | $G_{LL}$ | $a_{LL}$ | $b_{LL}$ | $G_{LS}$ | $b_{LS}$ |
| even-singlet (*) | 1.07 | 15 | 0 | 0 | −0.003 | −1 | 0 | 0 | 0 |
| even-triplet | 1.07 | 11.5 | 0 | 0 | 0.007 | 0 | 0 | −0.17 | 0 |
| odd-singlet | 0.80 | − 8 | 12 | 0 | −0.003 | 3 | 9 | 0 | 0 |
| odd-triplet | 0.80 | − 2 | 1 | −1 | 0 | 0 | 0 | 0.23 | −7 |

(*) Solution (II) of ref. ([15]).

([18]) R. BRYAN and B. SCOTT: *Phys. Rev.*, **135**, B 434 (1964); C. EFTIMIU and K. ERKELENZ: to be published in *Nuovo Cimento*.

different for the various terms according to their spin and parity indices. The various parameters which determine our effective potential are given in Table I. (The cut-off radii $d$ are measured in fm, the « deviation » parameters $a$, $b$ and the relative potential strength $G$ are dimensionless). Equations (3.1-2′) together with this Table define our potential. It will now be used in our subsequent pairing calculations.

## 4. – The pairing theory.

We now use the single-particle state functions and the corresponding eigenvalues of our nuclear potential $W$ as well as the effective nucleon-nucleon force $V$ in order to set up the Hamiltonian of our model. Leaving out the pairing forces between unlike particles (*) this « formal » Hamiltonian has the following structure:

$$H^{\text{total}} = H_{\text{n}} + H_{\text{p}} . \tag{4.1}$$

The two parts refer to protons (index p) and neutrons (index n) respectively. In both cases $H$ has the form (**)

$$H = \sum_{jm} (\varepsilon_j - \lambda) a^{\dagger}_{jm} a_{jm} + \tfrac{1}{2} \sum_{\substack{jm \\ j'm'}} \langle jm, j-m|V|j'm', j'-m'\rangle a^{\dagger}_{jm} a^{\dagger}_{j-m} a_{j'-m'} a_{j'm'} , \tag{4.2}$$

where $jm$ represents the usual abbreviation for the complete set of quantum numbers $nl\bar{j}m$ of our single-particle states (the total single-particle spin is now denoted by $\bar{j}$). We added the « chemical potential » because we shall have no longer sharp particle numbers within our approximation (***). We thus have two Lagrange-parameters $\lambda_{\text{n}}$ and $\lambda_{\text{p}}$ which shall be related to the two supplementary conditions fixing the average particle numbers for $N$ and $Z$. The exact signification of this formal shell-model Hamiltonian within the HB-approximation will be given in a forthcoming paper.

It contains the characteristic terms of the original Hamiltonian of the $n$-body system rewritten in a HF-basis. The additional term of the form $-\frac{1}{2}\overline{V}\sum_{jm} a^{\dagger}_{jm} a_{jm}$ ($\overline{V}$ represents the average HF potential energy per particle) has been dropped because its effect amounts to the subtraction of a constant $\overline{V}/2$ in all our $\varepsilon_i$- and $\lambda$-values. In the calculation of the separation energies, which

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(*) This point will be discussed in a forthcoming paper by D. SCHÜTTE and A. FRIEDERICH.

(**) In a slightly different connection (description of valence nucleons) this Hamiltonian had been proposed by J. R. SCHRIEFFER (*Nucl. Phys.*, **35**, 363 (1962)).

(***) *Note added in proofs.* - Calculations with sharp nucleon numbers have been done at our Institute by J. GARCIA: private communication.

are now given by

$$-\lambda-\frac{\overline{V}}{2}+\sum_{1}^{N}\frac{\partial(\varepsilon_j-\frac{1}{2}\overline{V})}{\partial N}$$

this constant ($\overline{V}/2$) practically cancels the terms containing the derivatives with respect to the particle number $N$. Within the restricted frame of our Hamiltonian (4.2) we therefore obtain the separation energies just from the resulting $\lambda$-values. The additional term, however, is needed if the total binding energies were considered.

We now perform the « classical » Bogoliubov-Valatin transformation

$$\xi^{\dagger}_{jm}=u_j a^{\dagger}_{jm}-(-)^{j-m}v_j a_{j-m}\,, \qquad u_j^2+v_j^2=1\,, \tag{4.3}$$

yielding

$$\begin{aligned} H=&\sum_{jm}[(\varepsilon_j-\lambda+\tfrac{1}{2}\delta\varepsilon_j)v_j^2+\tfrac{1}{2}\Delta_{jm}(-)^{j-m}v_j u_j]+\\ &+\sum_{jm}[(\varepsilon_j-\lambda+\delta\varepsilon_j)(u_j^2-v_j^2)-2\Delta_{jm}(-)^{j-m}v_j u_j]\xi^{\dagger}_{jm}\xi_{jm}+\\ &+\sum_{jm}[(\varepsilon_j-\lambda+\delta\varepsilon_j)(-)^{j-m}v_j u_j+\tfrac{1}{2}\Delta_{jm}(u_j^2-v_j^2)](\xi^{\dagger}_{jm}\xi^{\dagger}_{j-m}+\xi_{j-m}\xi_{jm})+\\ &+H_{\mathrm{int}}\equiv H_{00}+H_{11}+H_{20}+H_{\mathrm{int}}\,, \end{aligned} \tag{4.4}$$

with

$$\delta\varepsilon_j\equiv\langle jm,\, j-m|V|(jm,\, j-m)-(j-m,\, jm)\rangle v_j^2$$

and

$$\Delta_{jm}\equiv\sum_{j'm'}\langle j'm',\, j'-m'|V|jm,\, j-m\rangle(-)^{j'-m'}v_{j'}u_{j'}\,. \tag{4.5}$$

In view of the spherical symmetry of $V$ we have the following $m$-dependence of $\Delta_{jm}$:

$$\Delta_{jm}=\Delta_j(-)^{j-m}\,, \tag{4.6}$$

with

$$\Delta_j\equiv\sum_{j'm'}\langle j'm',\, j'-m'|V|jm,\, j-m\rangle(-)^{j+j'-m-m'}v_{j'}u_{j'}\,.$$

The usual condition $H_{20}=0$ yields, if we neglect the $\delta\varepsilon_j$ (*),

$$2(\varepsilon_j-\lambda)u_j v_j+\Delta_j(u_j^2-v_j^2)=0\,. \tag{4.7}$$

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(*) The $\delta\varepsilon_j$ lie between 0 and $G_{jj}$, where $G_{jj}$ represents the diagonal elements of the gap matrix. (This follows from (4.8) and $0<v_j^2<1$). They are therefore, in general small (see Part II, Tables 10 and 11 of Appendix B). On the other hand, within the HB-frame, matrix elements of this diagonal type contribute directly to the HB self-consistent potential (see ref. [7,8]), and the corresponding change of $\varepsilon_j$ is just given by $\delta\varepsilon_j$.

Introducing the « gap matrix » $G$ by

$$(4.8)\quad G_{jj'} \equiv -\frac{2}{(2\bar{j}+1)(2\bar{j}'+1)} \sum_{\substack{m \\ m'}} (-)^{\bar{j}+\bar{j}'-m-m'} \langle jm, j-m|-V|j'm', j'-m'\rangle ,$$

the solution of (4.7) (with (4.6)) follows from the well-known system of gap equations (this system corresponds—by a redefinition of the $\varepsilon_j$—to the « pairing part » of the HB-equations)

$$(4.9)\qquad \Delta_j = \frac{1}{2} \sum_{j'} (\bar{j}' + \tfrac{1}{2}) \frac{G_{jj'}}{E_{j'}} \Delta_{j'} ,$$

where

$$(4.10)\qquad E_j \equiv + \sqrt{(\varepsilon_j - \lambda)^2 + \Delta_j^2} ,$$

if we put

$$(4.11)\qquad v_j^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_j - \lambda}{E_j}\right), \quad u_j^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_j - \lambda}{E_j}\right), \qquad \left(u_j v_j = -\frac{1}{2}\Delta_j / E_j\right).$$

The ground states $|0\rangle$ are now determined from

$$(4.12)\qquad \xi_{jm}|0\rangle = 0 \qquad \text{for all } jm ,$$

and one obtains for the expectation value of the particle numbers

$$(4.13)\qquad \langle 0|\sum_{jm} a_{jm}^{\dagger} a_{jm}|0\rangle = \sum_{j} (2\bar{j}+1) v_j^2 .$$

Therefore, the supplementary conditions read

$$(4.14)\qquad \sum_{j} (2\bar{j}+1) v_j^2 = \begin{cases} Z \text{ for the proton system}, \\ N \text{ for the neutron system}. \end{cases}$$

Our « diagonalized » Hamiltonian now has the form (omitting the remaining interaction among the quasi-particles)

$$(4.15)\qquad H = \sum_{j} (\bar{j} + \tfrac{1}{2}) \left\{ (\varepsilon_j - \lambda)\left(1 - \frac{\varepsilon_j - \lambda}{E_j}\right) - \frac{1}{2}\frac{\Delta_j^2}{E_j} \right\} + \sum_{jm} E_j \xi_{jm}^{\dagger} \xi_{jm} .$$

Our system of equations ((4.8), (4.9), (4.10), (4.14)) has been solved numerically (computer) for all « ideal » nuclei $\left((Z, \bar{N}(Z)\right)$ and $\left(\bar{Z}(N), N\right))$ situated on the mid-

dle line $(N = \bar{N}(Z))$ of the flow of stable elements. In each case all relevant states $j$ which occur within the gap equation (4.9) were taken into account; the $G$'s were calculated explicitly from (4.8) and the expressions (3.1) and (3.2) for the nuclear forces using the Moshinsky method. All details are to be found in Part II of this work.

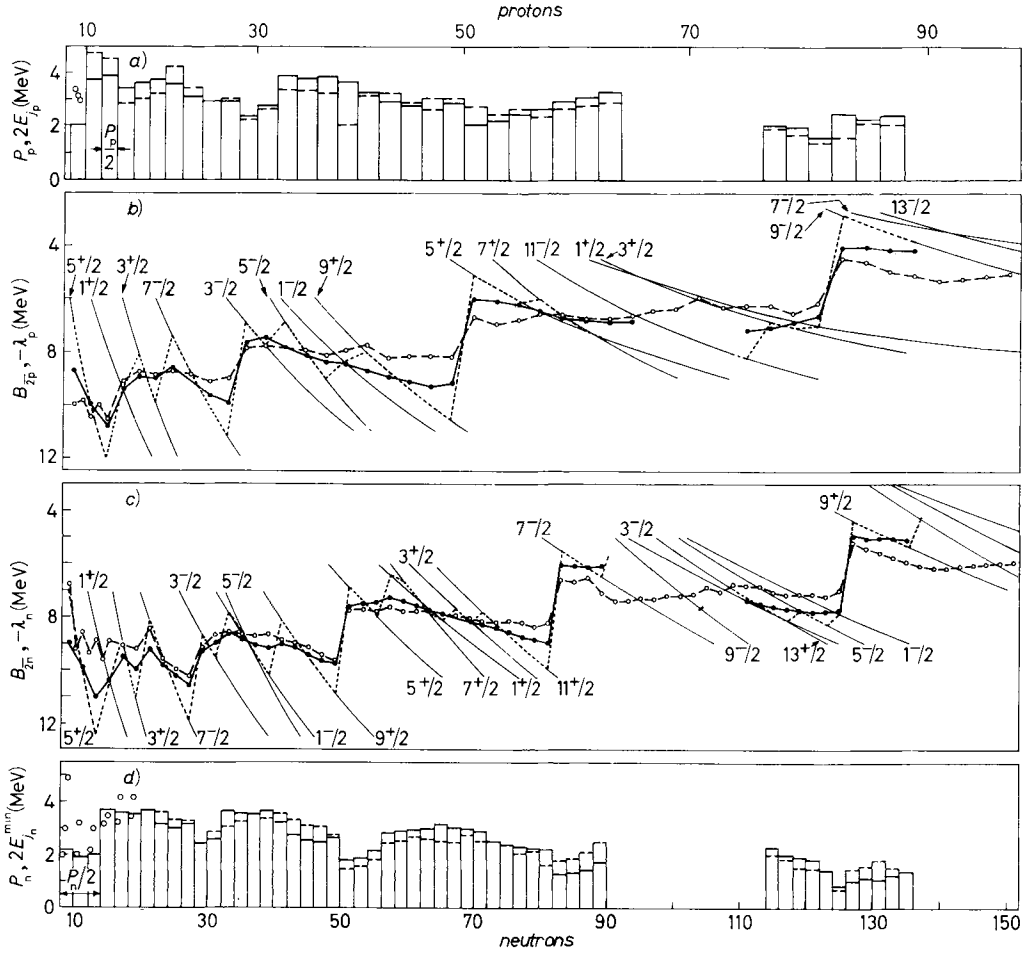


Fig. 4. – Comparison of separation and pairing energies: $2E^{min}_{j_p}$: theoretical pairing energy of protons, $P_p$: experimental pairing energy of protons, $-\lambda_p$: theoretical mean separation energy of protons, $B_{2\bar{p}}$: experimental mean separation energy of protons, $2E^{min}_{j_n}$: theoretical pairing energy of neutrons, $P_n$: experimental pairing energy of neutrons, $-\lambda_n$: theoretical mean separation energy of neutrons, $B_{2\bar{n}}$: experimental mean separation energy of neutrons. *a*) Full-line histogram: $2E^{min}_{j_p}$; broken histogram: $P_p$; *b*) ●——●——● $-\lambda_p$; ○— —○— —○ $B_{2\bar{p}}$; ——— $\varepsilon_{j_p}$; – – – original Fermi limits (without pairing); *c*) ●——●——● $-\lambda_n$; ○— —○— —○ $B_{2\bar{n}}$; ——— $\varepsilon_{j_n}$; – – – original Fermi limits; *d*) full-line histogram: $2E^{min}_{j_n}$; broken histogram: $P_n$.

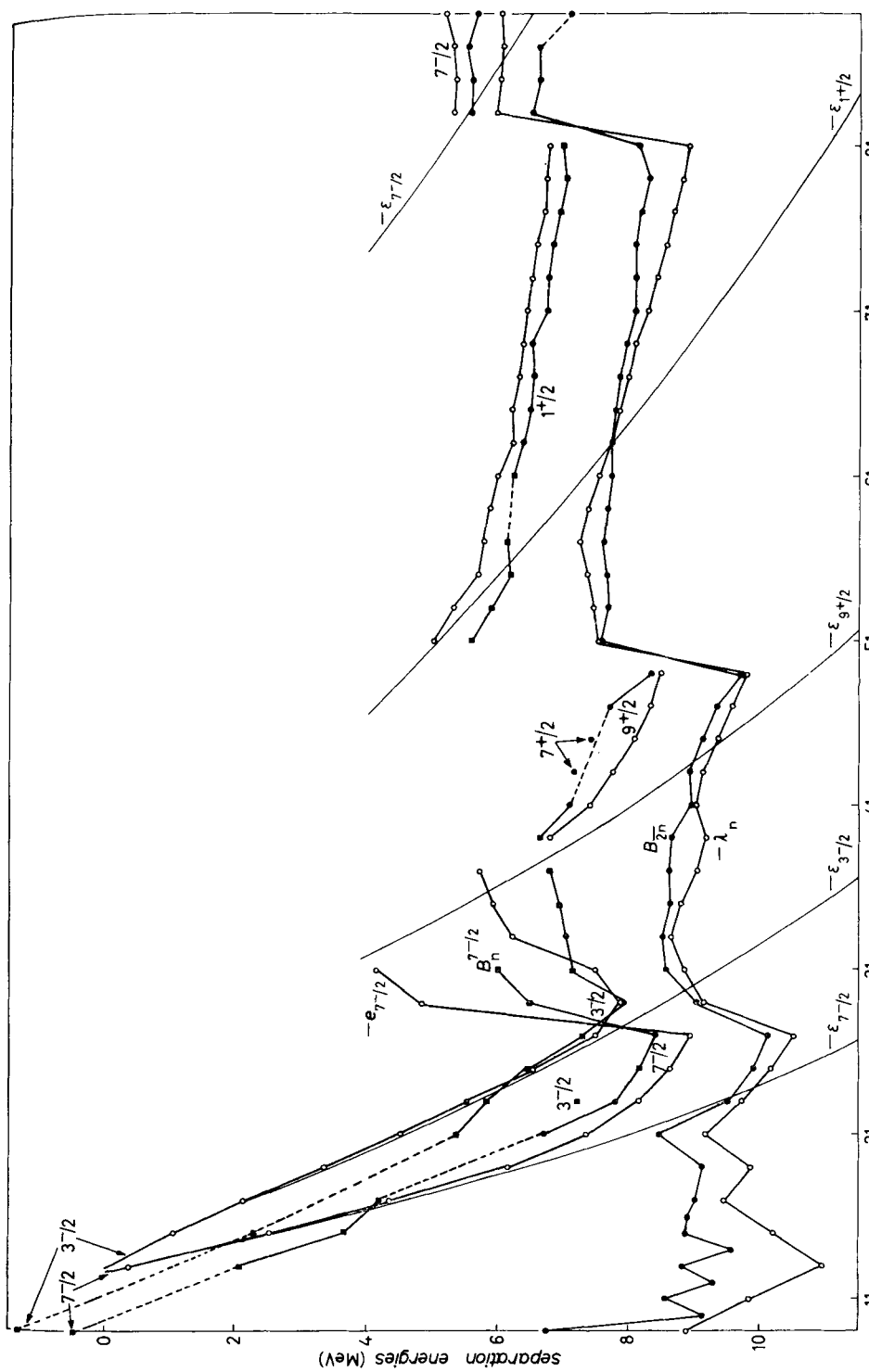


Fig. 5. – Comparison of neutron separation energies. Ground states of even nuclei: experimental values $B_{2n}(Z, N) = \frac{1}{2}[B(Z, N+1) - B(Z, N-1)]$, theoretical values $-\lambda_n$; single-particle states of odd-$N$ nuclei (5 selected subshells): experimental values $B_n^{J^\pi}(Z, N) = B^{J^\pi}(Z, N) - B(Z, N-1)$, theoretical values $-e_{j_n} = -(\lambda_n + E_{j_n})$;

The solutions yield the numerical values for our characteristic functions

$$(4.16) \qquad \lambda_p\big(Z, \bar{N}(Z)\big) = \lambda_p(Z)\,, \quad \lambda_n(N)\,; \quad E_{j_p}(Z) \quad \text{and} \quad E_{j_n}(N)\,,$$

which directly represent, within our restricted frame, the mean separation energies $B_{2\bar{p}}$ for protons and $B_{2\bar{n}}$ for neutrons as well as the excitation energies of the quasi-protons and quasi-neutrons. These « theoretical » functions can be directly compared to the corresponding empirical curves which were obtained by the « intersections » (through the middle line) of our energy surfaces (compare Fig. 1 and 2). We therefore plot theoretical and empirical curves just within the same diagram (Fig. 4 and 5) which thus contain our main results in a comprehensive form.

## 5. – Conclusions.

Our graphical representations give the possibility of a direct comparison between our calculated values and the empirical data. In Fig. 4 (middle parts) we have plotted empirical and theoretical mean separation energies, whereas some typical examples of generalized separation energies of odd-$N$ nuclei are shown in Fig. 5. The empirical and theoretical curves are in good agreement over all the spherical regions; the correspondence of the steps which occur at the magic numbers and the rather typical behaviour of the excited states should be noted. We have, however, a rather large energy scale in our representation; the absolute deviations for the separation energies are, therefore, quite appreciable although small compared to the total depth of the nuclear potential.

On the other hand, there is even a better agreement if we compare our theoretical values for the « gap » directly with the empirical data obtained from the even-odd mass differences. Such a comparison is shown in Fig. 4 (top and bottom parts). Theoretical values (full-line histogram) are calculated from formula (4.10), whereas the empirical data (broken histogram) are taken from the Mattauch tables. It should be pointed out that the absolute values as well as the typical variations with $Z$ or $N$ of the pairing effect are in good agreement. This is rather satisfactory because the gap values are perhaps the most characteristic results of our calculations.

In view of the general correspondence (especially with respect to the $N$-, $Z$-dependence of our results) it should be emphasized that only 5 constants ($\alpha_1$–$\alpha_5$) had to be adapted within our scheme, using to a large extent experimental data which are not directly related to the present ones (*e.g.* charge distributions, etc.). The remaining discrepancies within the region of heavier elements are perhaps due to the fact that we choose a nuclear potential of

local character, whereas the HF- or HB-potentials exhibit rather strong non-localities. (This fact may also be seen from the empirical energy location of the deep-seated single-particle states). Our next task, therefore, is (as a first stage) a numerical treatment of the HF-approximation using the same effective two-body forces (*). The present single-particle wave functions could then be introduced in a first step of the iteration process.

The complete numerical results and a more detailed discussion will be given in Part II of this work.

* * *

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(*) *Note added in proofs.* - Such HF calculations with the effective potential (3.1) are being done at the same institute (H. PETRY and D. SCHÜTTE: to be published).

## RIASSUNTO (*)

Si applica la teoria dell'accoppriamento (metodo di BCS) ai nuclei sferici allo scopo di calcolare alcune proprietà fisiche caratteristiche. I punti principali sono: i) inserzione di una effettiva (realistica) forza di due nucleoni negli elementi della matrice di accoppiamento; ii) definizione di un potenziale nucleare fenomenologico allo scopo di determinare gli stati di particella singola. Si è ottenuta l'interazione di due nucleoni effettiva dall'espressione di Hamada-Johnston per mezzo del procedimento di Scott-Moszkowski; il gruppo completo dei potenziali nucleari (del tipo di Saxon-Woods) contiene 5 costanti che sono state determinate dalle proprietà nucleari specifiche (determinazione empirica del campo auto-compatibile che interviene nel trattamento di Hartree-Bogoliubov). Si è risolta numericamente l'equazione del gap tenendo conto di tutti i più importanti stati di particella singola. Si riportano in diagramma i risultati finali (energie di separazione ed eccitazione di quasi particella) assieme ai corrispondenti dati empirici in funzione del numero di nucleoni (Figure 3 e 4). Si ha un accordo soddisfacente proprio entro le regioni sferiche; si deve mettere in rilievo in particolare la corrispondenza fra le irregolarità tipiche ai numeri magici e fra le variazioni caratteristiche dei livelli di quasi particelle e delle energie di accoppiamento.

(*) *Traduzione a cura della Redazione.*

**Приближение спаривания в сферических ядрах.** – I.

**Резюме** (*). — Теория спаривания (метод BCS) применяется к сферическим ядрам для вычисления некоторых характеристических физических свойств. Главными проблемами являются: 1) введение эффективной (реалистичной) двух-нуклонной силы в матричные элементы спаривания; 2) определение феноменологического ядерного потенциала для описания одночастичных состояний. Получается, что эффективное двух-нуклонное взаимодействие принимает вид выражения Хамада-Джонстона посредством процедуры Скотта-Моцковского; полная система ядерных потенциалов (типа Саксона-Вудса) содержит 5 констант, которые определяются из специфических ядерных свойств. (Эмпирическое определение самосогласованного поля, встречающегося в трактовке Хартри-Боголюбова.) Уравнение щели решается численно, принимая во внимание все относящиеся к делу одно-частичные состояния. Окончательные результаты (энергии отделения и квазичастичные возбуждения) и соответствующие эмпирические данные вычерчиваются одновременно как функции атомных номеров (рисунки 4 и 5). Существует удовлетворительное согласие лишь внутри сферических областей, в частности, следует отметить соответствие между типичными нерегулярностями при магических числах и между характреристическими изменениями квазичастичных уровней и энергий спаривания.

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(*) *Переведено редакцией.*