Theory of shell structure and of the “magic” effect in spherical nuclei

V.G. Nosov† and A.M. Kamchatnov‡

†Russian Research Center Kurchatov Institute, pl. Kurchatova 1, Moscow, 123182 Russia
‡Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow Region, 142190 Russia

November 12, 2018

Abstract

A consistent theory is developed of the volume energy oscillations of spherical nuclei due to sharpness of the Fermi distribution boundary for quasiparticles. The lowest value of the oscillating part of the energy corresponds to a magic nucleus. A formula is obtained for the corresponding limiting momentum of a quasiparticle and it is shown that we have here an isolated point of a temperatureless second-order phase transition. An expression for the discontinuity of the derivative of the energy of the body with respect to the number of particles is obtained in the case of a sharp (step-like) Fermi distribution limit. Comparison with experimental nuclear-mass data permits some conclusions to be drawn regarding the true structure of the boundary layer of the Fermi distribution and regarding its variation with increasing nuclear size. In the region of magic nuclei actually accessible up to the present time, apparently no signs are observed of any appreciably expressed residual phenomenon, such as the Cooper phenomenon, which would result in instability of the energy spectrum of infinite nuclear matter with an absolutely sharp Fermi limit for quasiparticles.

1 Introduction. Macroscopic treatment of magic nuclei

The study of the nucleus considered as a macroscopic body originated with the well known work of von Weizsäcker [1]. Recognition of the distinction between volume and surface contributions to the binding energy was an important step in understanding the saturation properties of nuclear forces and served as the basis for current ideas regarding uniform nuclear matter (see, for example, Landau and Lifshitz [2]). The subsequent inclusion of the electrostatic energy and addition of the symmetry term taking into account the difference in the numbers of protons and neutrons [1] gave these ideas a rather high degree of refinement which permitted the total binding energies of a very large number of nuclei to be described

*Zh. Eksp. Teor. Fiz. 61, 1303–1318 (1971) [Sov. Pys. JETP 34, No. 4, 694-701 (1972)]
with high relative accuracy. This, however, only deepened interest in possible deviations from the Weizsäcker formula, and the question of these deviations has arisen repeatedly in one form or another during the past thirty-five years. The most easily perceived cause is the quantum-mechanical discreteness of elementary particles, i.e., simply the obvious fact that protons and neutrons can be added to a nucleus only in integral numbers. This, naturally has stimulated the consideration of other similar deviations as having a more or less clearly expressed quantum nature.

However, the question of which deviations from the Weizsäcker formula have a macroscopic origin lies essentially in a different plane. At the present time we have no serious basis for rejecting such a possibility. On the opposite, developments in recent years indicate that macroscopic quantum phenomena are rather typical for nuclei which are not too light. In the first place, the simplest model of a uniform body of this type with limited size—the independent-particle model with a constant general potential in the internal region—permits one to make rigorous calculation of several important characteristics. The instability demonstrated by Nosov [3] for a spherical configuration of this model has an explicitly macroscopic nature. It is true that determination of the true stable equilibrium shape of the body encounters serious difficulty that the problem has no small parameter. The attempts to ignore this fact, with resort to direct numerical calculations, are difficult to analyze and we will not set for ourselves this goal. However, as often happens in similar situations, experimental data come to our assistance. The “collective” macroscopic order of magnitude of quadrupole moments of non-spherical nuclei is well known; an individual quasiparticle could not produce a quadrupole moment of this order. Closely connected with this fact is the usually smooth behavior of the deformation, i.e., the fact that this macroscopic characteristic of an non-spherical nucleus is practically independent of the individual quantum state of the last nucleon (quasiparticle) of the Fermi distribution.

Also of great significance is the study, intensely carried out during the last fifteen years, of the rotation of the nucleus as a whole, and also of oscillations of the nuclear deformation. Satisfaction of the laws of quantum mechanics does not diminish, of course, the macroscopic nature of this type of motion. It is remarkable that, even from calculations based on a simple model [3], it can be clearly seen how the characteristics of the corresponding collective degree of freedom (for example, rigidity of the spherical configuration with respect to deformation) “develop” with increase of the number of particles in the nucleus. The macroscopic properties of a body should lose their meaning and physical content in the transition to too small number of particles.

The undoubted existence of spherical nuclei is not compatible with the primitive model of ref. [3], and the real situation in a nucleus must be more complex. The most important reason for that is probably the residual interaction between the quasiparticles, which is unavoidable in a body of finite size. The loss of equilibrium non-sphericity is difficult to imagine without some qualitative change in the nuclear structure. However, as was shown by the theory of the corresponding phase transition developed by Nosov [4], this complication of the physical picture only increases the role of macroscopic quantum effects. Actually, our attention is primarily attracted not only by the singularities of thermodynamic quantities (as occurs for ordinary temperature-dependent second-order phase transitions but also by the singularities of the macroscopic-body ground-state wave function (which depends parametrically on the
deformation), observed at the Curie point (see, for example, Eq. (28) in ref. [4])\(^1\).

It is possible that the significance of macroscopic quantum effects in a nucleus is still somewhat underestimated. In any case, against the background of the progress described above, the widely held opinion that the so-called magic numbers are clearly of non-macroscopic origin [6] appears to be more a dogmatic assertion than a fact following directly from experiment. It is natural to relate a theoretical study of the macroscopic properties of a medium with the experimentally observed singularities of the thermodynamic variables. This facilitates observation and detailed investigation of characteristic phenomena such as phase transitions. A specific feature of a nucleus is the direct accessibility of absolute zero temperature (the ground state), and the most important thermodynamic variable turns out to be the corresponding energy, i.e., the nuclear mass. As far as can be judged from the experimental data shown schematically in Fig. 1, the singularities under discussion are apparently breaks, i.e., discontinuities in the derivative of the energy with respect to the number of particles. Where the curve becomes sluggish, almost horizontal, on one side of the singularity, we are entering the region of non-spherical nuclei, and the Curie point corresponds to the phase transition discussed by Nosov [4], a consequence of which, in particular, is a change in the equilibrium shape of the nucleus. In addition, in Fig. 1 we can clearly see the magic cusps, i.e., downward spikes at whose vertices are located the corresponding magic nuclei. We emphasize the difference of this singularity from the ordinary Curie point. A qualitative difference between the phases—different values of the chemical potential—arises only near an isolated transition point. Away from this point it is not possible to point to a quality which would be possessed, say, by one of the phases while the other would not have it. The actual state of the body apparently does not undergo a discontinuity (with macroscopic accuracy, of course; see the following section), so that in other respects we appear to be dealing with a second-order transition.

In opposition to the impression created by Fig. 1, the widely used explanation of magic numbers [6] appeals directly to the pattern of filling by fermions of \((2j + 1)\)-fold degenerate single-particle levels in the field of some spherically symmetric potential. After a shell is filled, the next nucleon approaches the lower edge of the region of continuum states and the nucleon binding energy \(\varepsilon\) (the chemical potential taken with a reversed sign) correspondingly drops. The weak point of this type of interpretation is that a similar situation should arise also after the filling of each level individually, and not only of an entire definite group of levels (a shell). In comparison with the gaps separating neighboring shells, the distances between the levels inside each shell cannot always be small; there is no way in which such a small parameter could be obtained in this case. Specific calculations of single-nucleon level schemes confirm the validity of this reasoning (see, for example, the neutron level scheme from the monograph by Hodgson [7]). As a rule, the gap between shells is only two or three times greater than the typical distance between levels, and we would have to find a whole series of closely spaced cusps corresponding to the filling of each of the levels.

\(^1\)For ordinary condensed matter we can also give a physical example of a temperatureless second-order phase transition. When a single-domain ferromagnetic particle grows in size, beginning at some critical size, a smooth change occurs in the spin directions, which gradually destroys the uniformity of magnetization over the volume. The theory given by Frei et al. [5] permits wave functions of the phases to be determined near a transition point. It is easy to see that their properties are consistent with the semi-phenomenological reasoning developed by Nosov [4] for the case of a nucleus.
In reality, for not too light nuclei, beyond the magic number 28, only the cusps shown in Fig. 1 are observed, which correspond to the much less frequently encountered “true” magic numbers. It is symptomatic that even a small, far from qualitative, excess of the gaps between shells over the level spacing inside the shells is achieved by selection of a rather substantial number of parameters. The gaps following shells 2 and 8 turn out to be large for practically any reasonable potential [6], but for the magic numbers 28, 50, 82, and 126 it is already impossible to make this statement. The fact that even the average field acting on the nucleon is determined here by no less than four parameters (the potential-well radius and depth, the width of the transition layer at the surface, and the intensity of the spin-orbit interaction within its boundaries) naturally provides additional cause for skepticism. In final analysis, we can attempt to interpret almost any phenomenon as the result of appropriate selection of fitting parameters; however, we have a right to expect more from the theory. Therefore, the widespread explanation of magic numbers produces seems to be somewhat artificial.

The key to understanding the macroscopic nature of the magic cusps and the nature of the phenomenon itself, which does not depend on specific numerical values of the nuclear parameters (equilibrium density of nuclear matter, structure of the transition surface layer, value of spin-orbit coupling, and the like), lies in a well-known general property of Fermi systems. The thermodynamic variables of these systems (for example, the total magnetic moment, the energy, or number of particles \( N \)) usually reduce to sums over a large number of fermion-filled states characterized by definite sets of quantum numbers. The simple replacement of summation over quantum numbers by integration is a crude treatment which leads to a result depending smoothly on such variables as the limiting momentum \( k_f \) of the Fermi distribution or the intensity of the applied magnetic field. However, a rigorous calculation of the sum by means of Poisson’s formula [8]

\[
\sum_{n=0}^{\infty} \varphi(n) = \frac{1}{2} \varphi(0) + \int_0^\infty \varphi(n) dn + \sum_{\nu=1}^{\infty} \int_0^\infty \left( e^{i2\pi\nu n} + e^{-i2\pi\nu n} \right) \varphi(n) dn
\]

shows that the thermodynamic variables, generally speaking, undergo oscillations as a result of the third term in (1). Here the main contribution is from the quasiparticles closest to the Fermi surface. Actually, the oscillating integral which occurs inside the summation over \( \nu \) would be extremely small if \( \varphi(n) \) were a sufficiently smooth function. The latter, however, contains as a factor the statistical distribution of quasiparticles, which changes sharply in the vicinity of the Fermi surface. An increase in temperature smooths the \( \varphi(n) \) function, as a result of which the oscillating effect falls off exponentially. A well-known specific example of this phenomenon is the de Haas-van Alphen effect [9], i.e., quantum oscillations of the magnetic susceptibility of metals at low temperatures.

Since we have in mind first of all nuclear applications, it is particularly important to emphasize that, in addition to the sharpness of the Fermi distribution, there is another equally necessary condition. An oscillation clearly does not arise with only a single summation according to Eq. (1), i.e., if \( n \) is the only quantum number of the particles being

\(^2\)Here and subsequently we will refrain from making any far reaching parallels with the shell structure of an atom. The principal distinction from nuclear matter is due to the Coulomb field of the nucleus at the center, as a result of which the atom has a sharply expressed spatial non-uniformity.
discussed (in the general case, of quasiparticles). An elementary calculation shows that in
the one-dimensional case the last term in (1) describes only the aforementioned trivial fact
of addition of particles one at a time; physically this corresponds to the absence of a macro-
scopic effect\footnote{A similar situation occurs also in a three-dimensional potential well of sufficiently irregular shape so that
the particle energy is its only quantum number.}. An important role is therefore played by the fact that the quasiparticle in the
spherical nuclei discussed below has an orbital angular momentum $l$. From the calculations
of the next section it is evident that there are enough quantum numbers in a spherical nu-
cleus for occurrence of oscillations of a macroscopic scale. However, upon formal application
of relation (1), there can arise also terms which are not macroscopic in nature, and which
must be discarded. In making this distinction the decisive criterion is

$$\rho_f = k_f R \gg 1$$

($R$ is the nuclear radius); for brevity we will also refer to this dimensionless parameter as
the limiting momentum of the Fermi distribution.

To avoid misunderstanding, we note that the uses of Eq. (1) in solid-state physics and
in nuclear physics have somewhat different aims. In the study of metals by means of the de
Haasvan Alphen effect, problems of sharpness of the Fermi surface essentially do not arise,
and the problem is to determine the shape of the Fermi surface in momentum space (more
accurately, in quasi-momentum space) \cite{9}. On the other hand, in the spherical nuclei of
interest to us, the obvious isotropy removes the question of the “shape” of the Fermi limit,
but its detailed structure is nowhere near as clear, owing to the residual interaction (see
above). Furthermore, it is apparently only because of the residual interaction that spherical
nuclei in general exist—we noted above that in a model without the interaction \cite{3} a sphere
is unstable. However, the effect of this circumstance on the energy of the body as a whole
and on the structure of its quantum state in the region of rapid fall-off of the quasi-particle
distribution function, and also the limiting behavior in accordance with which the residual
interaction may disappear with increasing nuclear radius, represent a field which is still little
studied. Therefore, in the calculations which follow, we will take tentatively the ordinary
Fermi distribution function unperturbed by the residual interaction. In the current state of
the problem, only experiment can answer the question as to how closely we approach the
ideal limit of a step-shaped distribution for the nuclear sizes achievable at the present day.
Sections 3 and 4 of the present article are devoted to questions bearing on this point.

For what follows it is very important to comment on the various characteristics of the
quasiparticle and the possible relation between them. The point is that in comparison with
the primitive model of a Fermi gas in an external field, a real Fermi liquid (i.e., a bound
system of fermions of finite size) has some qualitative differences in this respect. We have
attempted to compare these situations schematically in Figs. 2a and 2b, respectively. In
both cases we can speak of an energy, if we reckon it from the zero of the kinetic energy
of an external free nucleon. At the limit of the Fermi distribution this quantity reduces to
the chemical potential $\varepsilon_f = -\varepsilon$, where $\varepsilon$ is the reversible work function of the particle for
removal from the nucleus (the nucleon binding energy). In addition, in the case corresponding
to Fig. 2a, there exists also an energy $\varepsilon'$ relative to the bottom of the potential well. It
determines the limiting momentum $\rho_f \propto \sqrt{\varepsilon' / f}$. 
Turning to a nuclear Fermi liquid (see Fig. 2b), we encounter the, strictly speaking, inadequate nature of the concept of the “bottom” of the potential well. Actually, a situation with noninteracting quasiparticles can exist only in the immediate vicinity of the Fermi limit. Even if we have in some sense complete data on the energy spectrum of the nucleus (we assume that the energy $E\{n_k\}$ of the body is known as a functional of the occupation numbers $n_k$), it is not possible to give a reasonable definition of the quasiparticle energy $\varepsilon'$ relative to the “bottom.” Nevertheless, the idea of a limiting momentum still makes sense. In principle we could deduce the value of $\rho_f$, say, from the form of the wave function of the last quasiparticle.

However, if the “bottom,” strictly speaking, does not exist, and the quasiparticle energy $\varepsilon'$ calculated with respect to it is not an adequate quantitative notion, then what physically determines the limiting momentum $\rho_f$? The answer to this question is given by the major assumption on which the theory developed in the next section is based.

2 Theory of the shell structure of a spherical nucleus

As a starting point for what follows we will assume that the value of $\rho_f$ is completely determined by the total number of particles $N$. It is assumed that the function $N(\rho_f)$ does not undergo oscillations$^4$. In a purely formal sense, only differentiability of this function is required (see below, the transition from Eq. (22) to Eq. (24)). However, in connection with criterion (2), it is natural to be interested in its asymptotic representation for large $\rho_f$. In that case the corresponding expansion should be terminated with a finite number of terms:

$$N(\rho_f) = \frac{4}{9\pi} \rho_f^3 - s \rho_f^2 + q \rho_f. \quad (3)$$

Actually the fifth term of the expansion, which is $\sim \rho_f^{-1}$, would give physically meaningless fractional additions to the number of particles. In a systematically macroscopic treatment it is obviously required to discard also the fourth term as describing the single-particle effect (see the discussion of this point in the Introduction). In what follows we will also drop all similar non-macroscopic terms of the type $\rho_f^0 \sim 1^5$.

The assumptions described above have a great similarity to the system of assumptions of the theory of an unbounded Fermi liquid [10,11]. In particular, the coefficient in the first term of the right-hand side of (3) corresponds (if the additional spin doubling is taken into account) to the volume contribution to the number of cells of phase space, that is, it is equal to the corresponding expression for an ideal Fermi gas. However, we have no basis for assuming that the remaining terms are also independent, to the same degree, of the law of interaction between particles. On the contrary, the surface term $-s \rho_f^2$, and also the

$^4$For the model of an ideal gas located in an externally applied potential well, the oscillations would be given by Eq. (16).

$^5$The correctness of the third term of Eq. (3) also could turn out to be questionable, since $2l + 1 \sim \rho_f$ particles fill a single level in a spherically symmetric field. However, the unavoidable zero-point oscillations of the deformation have a scale $\Delta \alpha \sim \rho_f^{-2}$, and the corresponding shift in particle energy is of the same order of magnitude. The degeneracy is as a result lifted to a sufficient degree, while, on the other hand, such small deformations do not yet violate the conservation of the integral of motion $l$ (see ref. [3]). Thus, the averaging of the function $N(\rho_f)$ implied in (3) is achieved automatically in a real situation.
curvature term \( q \rho_f \), take into account the structure of the transition layer on the nuclear surface, spin-orbit coupling, and so forth. Numerical values of the coefficients \( s \) and \( q \) must be determined experimentally (see the following section). We represent the ground-state energy of a spherical nucleus in the form of the sum

\[
E = E_0 + E_1
\]

of a smooth part \( E_0 \) and an oscillating part \( E_1 \). In the calculation of the latter, it is convenient to express it initially in terms of the variable \( \rho_f \). The coupling noted in the Introduction between the oscillations and quasi-particles approaching the Fermi limit permits the problem to be reduced to the model [3] of a gas in a well with a constant potential inside it (the last fact corresponds physically to uniformity of the spatial distribution of matter in the internal region of the nucleus). Subsequent use of Eq. (1) to carry out the summation over the quantum numbers \( l \) and \( n \) will lead to integrals of two substantially different types. Those of them which are due to practically the entire region \( 0 < \rho = kR < \rho_f \) of values of the particle wave number do not permit generalization to a real Fermi liquid. However, they depend smoothly on \( \rho_f \) and are not of interest here—the problem of explicit calculation of the function \( E_0(\rho_f) \) does not arise here. The integrals which have an oscillating dependence on \( \rho_f \) converge rapidly at \( \rho \simeq \rho_f \), and the generalization of their contribution to the case of a Fermi liquid is obvious. This fact even allows us to limit ourselves to calculation of the number of particles

\[
\tilde{N} = \tilde{N}_0 + \tilde{N}_1
\]

in this model. The point is that, in the terms which determine \( \tilde{N}_1 \), the energy of a single particle (subsequently a quasi-particle) would anyway be taken outside the integral sign as a slowly varying function. Equation (5) corresponds to the quantity

\[
\varphi(l, n) = (2l + 1)w_f(l, n),
\]

which must be summed over \( l \) and \( n \). The Fermi distribution

\[
w_f(l, n) = \begin{cases} 
1 & \text{for } \rho_n < \rho_f, \\
0 & \text{for } \rho_n > \rho_f,
\end{cases}
\]

depends on these same quantum numbers\(^6\) through the eigenvalues \( \rho = \rho_n \). The Bohr-Sommerfeld quantization rule [2] serves to determine the eigenvalues,

\[
\int_a^R k_l(r)dr = \pi(n + \gamma),
\]

where the internal turning point \( r = a \) is due to the centrifugal barrier, and \( \gamma < 1 \) defines an additional phase shift which depends on the nature of the boundary conditions. It is

\(^6\)In view of the macroscopic nature of the effect being studied, the existence of spin in the nucleon will be taken into account easily by subsequent doubling of the result. We note that in problems of this type it is more natural to begin the enumeration of the principal quantum number \( n \) not from unit but from zero. For example, the 1s state is assigned to \( n = 0 \). In particular, this provides the possibility of formally symmetric application of Eq. (1) to summation over the two quantum numbers (see Eq. (11) below).
not necessary to calculate integral (8) from the beginning, since in this case both the wave functions themselves (spherical Bessel functions) and their quasi-classical asymptotic forms are well known. Using a notation close to that of ref. [3], we have

\[ \rho (\sin \beta - \beta \cos \beta) = \pi (n + 3/4), \]

\[ \beta = \arccos \frac{l + 1/2}{\rho} = \arcsin \sqrt{1 - \frac{(l + 1/2)^2}{\rho^2}}. \]

The Jacobian of the transformation to the new variables also was determined in ref. [3]:

\[ dndl = \frac{1}{\pi \rho d\rho \sin^2 \beta d\beta}. \]

Two-fold summation of the function (6) according to Eq. (1) gives

\[ \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \varphi(l, n) = \frac{1}{4} \varphi(0, 0) + \iint_{0}^{\infty} \varphi(l, n) dldn \]

\[ + \sum_{\nu=1}^{\infty} \int_{0}^{\infty} \varphi(0, n) dndn + \sum_{\lambda=1}^{\infty} \int_{0}^{\infty} (e^{i2\pi \lambda l} + e^{-i2\pi \lambda l}) \varphi(l, n) dldn \]

\[ + \frac{1}{2} \left\{ \int_{0}^{\infty} \varphi(0, n) dndn + \sum_{\nu=1}^{\infty} \int_{0}^{\infty} (e^{i2\pi \nu n} + e^{-i2\pi \nu n}) \varphi(0, n) dndn \right\} \]

\[ + \frac{1}{2} \left\{ \int_{0}^{\infty} \varphi(l, 0) dldl + \sum_{\lambda=1}^{\infty} \int_{0}^{\infty} (e^{i2\pi \lambda l} + e^{-i2\pi \lambda l}) \varphi(l, 0) dldl \right\} \]

\[ + \sum_{\nu=1}^{\infty} \sum_{\lambda=1}^{\infty} \int_{0}^{\infty} \left[ e^{i2\pi (\lambda l + \nu n)} + e^{-i2\pi (\lambda l + \nu n)} + e^{i2\pi (\lambda l - \nu n)} + e^{-i2\pi (\lambda l - \nu n)} \right] \varphi(l, n) dldn. \]

All terms in the right-hand side of (11) permit analysis and classification on the basis of the criteria mentioned above. The non-macroscopic nature of the first of these terms is obvious. The non-oscillatory behavior of the second term follows directly from its form. After carrying out the integration, we can verify that the third term also provides no macroscopic contribution. As the result of integration on the basis of the same formulas (9) and (10) and subsequent summation over \( \lambda \), we find that the fourth term is \(-\rho_f/6\pi\). It depends smoothly on the limiting momentum. The same can be said of the two pairs of following terms, which are enclosed in curly brackets. In both cases the sum which adds to the integral actually describes its increase as the result of those levels which, with further advance of the Fermi limit, appear separately for \( \rho < \rho_f \).\(^7\)

The oscillations are described by the double sum over \( \lambda \) and \( \nu \) (the last term in Eq. (11)). Before we begin calculation of this sum, we will make one remark of a less formal nature. In addition to the Fermi limit \( \rho = \rho_f \) (see Eq. (7)) the distribution of particles along the \( l \) (or \( \beta \)) axis is also cut off—there are no negative orbital angular momenta. An intuitive

\(^7\)This rather formal fact has already been mentioned in the Introduction and commented on in footnote 5.
interpretation of this quantum phenomenon must lie in the fact that the shell oscillations depend on the relative position of these two limits. As will be seen from Eq. (19) below, a magic nucleus arises when the two limits coincide. In view of this role of the lower limit of the angular momentum scale, where $\beta \approx \pi/2$, it is convenient to introduce an additional angle

$$\tilde{\beta} = \pi/2 - \beta.$$  

(12)

Then it is easy to see that the integral under the summation sign, generally speaking, has the same structure as in the second term of the right-hand part of Eq. (11), i.e., it is non-macroscopic. However, a saddle point arises for a definite ratio between $\lambda$ and $\nu$ at the lower limit of the angular momentum axis, and this provides a macroscopic contribution.

If we take into account Eqs. (9) and (12), we can write the expansion of the argument of the exponential in powers of $\tilde{\beta}$ up to and including quadratic terms as follows:

$$2\pi(\lambda l + \nu n) \approx -\pi\lambda - \frac{3}{2}\pi\nu + 2\nu\rho + \pi(2\lambda - \nu)\rho\tilde{\beta} + \nu\rho\tilde{\beta}^2.$$  

(13)

Vanishing of the linear term (the condition for existence of a saddle point at $\tilde{\beta} = 0$) requires that

$$\nu = 2\lambda.$$  

(14)

Since the phase-space element is given by Eq. (10), we obtain from Eqs. (6), (7), (9), and (12)

$$\int\int e^{i2\pi(\lambda l + \nu n)} \varphi(l, n) dldn \approx \frac{2}{\pi} \int \rho_f e^{i4\lambda\rho} \int_0 e^{i2\lambda\rho\tilde{\beta}^2} \tilde{\beta} d\tilde{\beta} = \frac{\rho_f e^{i4\lambda\rho_f}}{8\pi \lambda^2}.$$  

(15)

Addition of the complex conjugate of the expression and summation over the single remaining free index leads to

$$\tilde{N}_1 = \frac{\rho_f}{4\pi} \sum_{\nu=1}^{\infty} \frac{\cos 4\nu\rho_f}{\nu^2}$$  

(16)

according to Eqs. (5) and (6). For conversion to the oscillating part of the energy of the nucleus $E_1$ it is necessary to take into account the nucleon spin by doubling, and also to multiply Eq. (16) by the energy $\varepsilon_f = -\varepsilon$ ($\varepsilon$ is the nucleon binding energy) of a single quasiparticle:

$$E_1 = -\varepsilon \frac{\rho_f}{2\pi} \mathcal{M}(\rho_f).$$  

(17)

Thus, for an absolutely sharp step-shaped Fermi limit for the quasiparticles, the shell effects in a spherical nucleus are described by a certain universal periodic function

$$\mathcal{M}(\rho_f) = \sum_{\nu=1}^{\infty} \frac{\cos 4\nu\rho_f}{\nu^2}.$$  

(18)

---

8This pertains to the first two exponential terms under the integral sign. Some other terms of the double sum have saddle points at intermediate angular-momentum values, which do not affect the result. It is interesting to note that in the preceding work devoted to calculation of the rigidity of the spherical configuration of the simplest model [3] these same points played the role of poles of the integrand, and incidentally gave likewise contribution.
whose plot is shown in Fig. 3. Its derivative has discontinuities at values of the argument

\[ k_f R = \frac{\pi}{2} p, \quad p = 2, 3, 4, \ldots, \]  

which correspond to the magic cusps (see Eq. (17)). In other words, Eq. (19) is a unique quantization rule for magic values of the parameter \( \rho_f = k_f R \).

We emphasize that the theory being developed is an expansion in inverse powers of the integer “number” of the magic nucleus \( p \) (see also Eq. (2)). It cannot pretend to give a quantitative description of the case of extremely small values, especially since it is then evidently impossible in general to make any reasonable separation of “smooth” and “oscillating” effects. However, the number of nodes of the radial wave function of the nucleon is such a stable characteristic that we can hope to trace it, at least qualitatively, to the lightest nuclei. Since \( \rho_f = \pi \) already corresponds to a 1s state (the doubly magic nucleus \(^2\text{He}^4_2\) corresponds to this physically), the region of possible values of \( p \) should begin with \( 2^9 \).

It is easy to verify that the right-hand part of Eq. (18) is a Fourier series for an elementary function which we will write out explicitly in a form valid for the two periods adjacent to the magic number \( p \):

\[ \mathcal{M}(\rho_f) = \frac{\pi^2}{6} - 2\pi \left| \rho_f - \frac{\pi}{2} p \right| + 4 \left( \rho_f - \frac{\pi}{2} p \right)^2, \quad \frac{\pi}{2} (p-1) < \rho_f < \frac{\pi}{2} (p+1). \]  

(20)

The absolute-value sign reflects the non-analyticity of the function at the magic cusp. Using the indices + and – to distinguish the values of the discontinuous function to the right and left respectively, we have

\[ \frac{d \mathcal{M}}{d \rho_f} \bigg|_{\pm} = \mp 2\pi. \]  

(21)

Now, returning to (17), it is not hard to obtain with the required accuracy an expression for the discontinuity in the derivative of the oscillating part of the energy of the nucleus:

\[ \Delta \left( \frac{d E_1}{d \rho_f} \right) = \rho_f(\varepsilon_+ + \varepsilon_-) = 2\rho_f \bar{\varepsilon}. \]  

(22)

In order to convert from the limiting momentum to the true number of particles (3), it is necessary to multiply both sides by \( d\rho_f/dN \). At the same time we recognize that the smooth component \( E_0 \) does not have a singularity at the cusp, so that Eq. (22) actually gives the discontinuity in the derivative of the entire energy \( E \):

\[ \frac{d \rho_f}{dN} \Delta \left( \frac{d E}{d \rho_f} \right) = 2\rho_f \frac{d \rho_f}{dN} \bar{\varepsilon}. \]  

(23)

\(^9\)The definition of the effective radius \( R \) of the nucleus implied in (19) concerns the internal structure of the nucleus exclusively. Since we have reduced the problem to a model with an impenetrable wall, we must represent the wall as constructed where the wave function of the corresponding quasiparticle extrapolated from the internal region approaches zero. In other words, this effective boundary of the nucleus can always be disposed so that the additional phase shift from the Bohr-Sommerfeld rule (8), in accordance with (9), will take on the value \( \gamma = 3/4 \) for the quasiparticles playing the principal role. In close connection with this fact, the equations expressing the shell oscillations in terms of \( \rho_f \) are universal; they do not depend on the spin-orbit interaction or on the structure of the surface layer where. After transformation to the \( N \)-scale this universality is lost (see also Eq. (3) and the explanation for it).
This relation for the discontinuity in the chemical potential can be given a more compact form:

$$\Delta \left( \frac{dE}{dN} \right) = \frac{\bar{\varepsilon}}{dN/{d(k_f R)^2}}.$$  \hspace{1cm} (24)

This can also be considered as a formula for the discontinuity in nucleon binding energy

$$\varepsilon = -\frac{dE}{dN}$$ \hspace{1cm} (25)

in the vicinity of a magic nucleus. Then, obviously, we must assume $\Delta \varepsilon \equiv \Delta (dE/dN) = \varepsilon_- - \varepsilon_+.$

### 3 Comparison with experiment

The most direct physical meaning is attached to the number-of-particles scale, as the most closely connected with experiment. We will discuss this after we have determined for the nuclear Fermi liquid, from experimental data, the numerical values of the coefficients $s$ and $q$ entering into Eq. (3). If we assume that, of the magic numbers found experimentally up to the present time, the most important in this connection are 82 and 126, then according to (19) and (3) these are sufficient to determine the two parameters. We finally obtain

$$s = 1.1, \hspace{1cm} q = 6.8.$$ \hspace{1cm} (26)

It is interesting to note that the surface term exceeds by only a factor of about two the value $\bar{s} = 1/2$ characteristic of an ideal Fermi gas adjacent to an impenetrable wall [12]. With the values in (26), Eqs. (3) and (19) for the number of particles in a magic nucleus take the form

$$N = 0.548p^3 - 2.79p^2 + 10.7p.$$ \hspace{1cm} (27)

The results of a calculation on the basis of Eq. (27) are compared with the known magic numbers in Table I. Down to $N = 28$ inclusive, the agreement must be considered satisfactory. For the lightest magic nuclei there is not even qualitative agreement.

If we take into account the two-component nature of nuclear matter, the oscillating term is given by the sum of expressions (17) for neutron and proton quasiparticles

$$E_1(N, Z) = -\varepsilon_N \frac{\rho_f^N}{2\pi} \mathfrak{M}(\rho_f^N) - \varepsilon_Z \frac{\rho_f^Z}{2\pi} \mathfrak{M}(\rho_f^Z).$$ \hspace{1cm} (28)

We note in this connection that the agreement observed so far of the corresponding magic numbers evidently indicates practically identical values of the parameters $s$ and $q$ for the two components. We may suppose that this is due to the relative smallness of the effects.

10The frequently encountered separation of a single $1f_{7/2}$ level in an individual shell has always been problematical. The reasoning and formulas of the preceding section create the impression of rejecting the magic number 20 which arises here. It is necessary, however, to make the reservation that magic phenomenon can in any case not be regarded as macroscopic when it comes to the lightest nuclei.
Table I

| p | N  | N_{theor} |
|---|----|-----------|
| 2 | 2  | 15        |
| 3 | 8  | 22        |
| 4 | 28 | 33        |
| 5 | 50 | 52        |
| 6 | 82 | 82        |
| 7 | 126| 126       |
| 8 | 184| 187       |
| 9 | 270|           |
| 10| 376|           |

distinguishing protons and neutrons in the nucleus, such as, for example, the Coulomb curve (the radial dependence of electrostatic potential in the internal region of the nucleus) ¹¹.

Clarification of the nature of the singularity in the energy $E(N, Z)$ at the point of occurrence of a doubly magic nucleus presents substantial theoretical interest. If we return to expression (20) and neglect in it the last quadratic term, we see that, according to (28), the surface $E_1(N, Z)$ has here the form of a pyramid of rhombic cross section with its axis directed vertically downward. As far as we can judge from the experimental data, the shape of the intersection of the mass surface with the plane $E_1 = \text{const}$ is actually close to a rhombus near a doubly magic nucleus; see, for example, ref. [13].

Incidentally, the separation of the oscillating part $E_1$ of the mass, from a purely practical point of view, suffers from a certain ambiguity. Therefore our attention is drawn to the relation (24), which does not depend on this procedure, for the discontinuity in binding energy of a nucleon of the corresponding type in a singly magic nucleus. Comparison with mass data (see, for example, ref. [14]) has shown that the theory based on the step-shaped distribution (7) does not agree with experiment for the magic numbers found up to the present time. Since the oscillations are due to the sharpness of the Fermi distribution, it is necessary to have in mind that the jump in quasiparticle occupation numbers from unity to zero is the maximum permissible by the Pauli principle. Consequently the oscillations calculated according to Eq. (7) are exaggerated, and the value $(\Delta \varepsilon)_0$ calculated from Eq. (24) actually exceeds everywhere the really observed binding-energy jump $\Delta \varepsilon$. It is natural to characterize this discrepancy by the quantity

$$\omega = \frac{(\Delta \varepsilon)_0}{\Delta \varepsilon} - 1,$$

which would approach zero in the ideal case (7) of absence of residual interaction between quasiparticles. Values of $\omega$ for 52 magic nuclei are listed in Table II ¹².

¹¹These remarks have pertained to the total number (3) of nucleons of a given kind in the nucleus. However, in regard to the more detailed properties of the residual interaction of quasiparticles close to the Fermi limit, the neutron and proton components may be far from identical; see below.

¹²The well known even-odd oscillations of nuclear masses are not related to the phenomenon being discussed. However, the widely used methods of calculating the corresponding correction (see, for example, ref. [15]) are purely empirical and can hardly be considered reliable. We therefore selected only those cases in which there are data on the binding energy of two nucleons. On removal of two nucleons of the same kind, the type of nucleus does not change, and the even-odd correction to the mass drops out of the result.
Each magic number is associated with several data differing in the number of nucleons of different kinds. Although some systematic behavior is apparently observed in the dependence on the latter, we will assume tentatively in each case that these are deviations of an accidental and uncorrelated nature. The corresponding average values of $\omega$ are shown in Fig. 4, together with the corresponding variances. The rapid decrease of $\omega$ in the transition to heavy magic nuclei reflects the naturally expected drop in strength of the residual interaction with increasing nuclear size. The electrically charged protons are less affected by the residual interaction from the very start, and at the end of the periodic table it shows a sharper drop than in the case of neutrons. We will dwell briefly on the attempts to provide some simple empirical description of the behavior of the points plotted in Fig. 4. From the number of curves that asymptotically approach $\omega = 0$, the possibility $\omega = C/p^3$ is suggested. For neutrons this gives $C = 336 \pm 12$; according to the criterion of likelihood [16] of the law $\omega \propto 1/p^3$, the probability of $\chi^2$ greater than the value observed in the present case is 20%. However, in the case of protons the corresponding probability of a similar law drops to 0.5%. Another possibility is that the proton curve $\omega(p)$ intersects the axis of abscissas, and we will discuss this in the next section.
4 Discussion

The problem of the energy spectrum of a quantum liquid consisting of fermions is rather complex in itself. In application to such a peculiar object as a nucleus it becomes particularly difficult and many-faceted. The accuracy of the description of its excitations in the model of an ideal gas of quasiparticles is limited by the residual interaction between them. It is natural to suppose that it is created only by the finite size of the system, and that in the transition to unbounded nuclear matter we would obtain the simplest variety of Fermi-liquid spectrum [10,11]. Another variant of the energy spectrum takes into account the possibility that, even in an infinite quantum liquid, residual phenomena such as the Cooper phenomenon [11] are preserved. We must suppose that the deviation shown in Fig. 4 from the asymptotic value $\omega = 0$ is not accidental. In spherical nuclei, which owe their very existence to the residual interaction, the latter must of course smear in some way the boundary of the Fermi distribution, and in so doing suppress the oscillations. As a result of this special role and, apparently, of the relatively large magnitude of the effect, it will probably be possible to clear up the question of the residual interaction, which is finally and with difficulty yielding to analysis.

The monotonic drop observed so far (Fig. 4) in the function $\omega(p)$ already permits some preliminary conclusions to be drawn. The point is that the shell oscillations calculated in the present article are an extremely fine instrument for analysis of the quasiparticle distribution near the limit $\rho \approx \rho_f$, and with increasing nuclear size the accuracy of this method is increased. In fact, according to (1), (9), (11), and (15), the oscillations penetrate below the Fermi limit by a depth $\Delta \rho \sim 1$, i.e., the relative thickness of the layer of the Fermi distribution occupied by them is $\sim 1/\rho_f \sim 1/R$. On the other hand, in the Cooper phenomenon the width of the zone of smearing of the distribution of initial quasiparticles does not depend on the size of the system. It can be seen from this how greatly the oscillations would be weakened in the presence of such a phenomenon. The drop in the $\omega(p)$ curve would be delayed and, furthermore, it evidently would have the reverse behavior. If still heavier magic nuclei do not exhibit similar features and the monotonic nature of the $\omega(p)$ function is further confirmed, it will be necessary to give a negative answer to the question of the Cooper phenomenon (or any other similar instability of an absolutely sharp Fermi limit of quasiparticles in infinite nuclear matter).

In speaking of the residual interaction, it is necessary to recall that not all conceivable varieties of this interaction are, so to speak, physically real. At least some variants of the interaction may be excluded by a canonical transformation to new quasiparticles without loss of sharpness in the Fermi limit of their statistical distribution. The well-known case of repulsive forces of zero radius between fermions [11] serves as an example of this. This tendency of a repulsive interaction to be “renormalized” may turn out to be important in regard to the proton component of nuclear matter. Actually, the points referring to protons in Fig. 4 may reflect a competition between the nuclear and Coulomb interactions. If the latter become dominant with increasing nuclear size, this may be expressed in the intersection of the corresponding $\omega(p)$ curve with the abscissa. This intersection would be a termination point for the function $\omega(p)$, beyond which the quasiparticles would satisfy the ordinary Fermi distribution (7). On the other hand, according to the results of ref. [3], disappearance of the residual interaction between proton quasiparticles would not, apparently, favor the
stable equilibrium nature of a spherical configuration. Even in the already studied region of nuclei beyond the doubly-magic lead, the data on the phase transition [4] appear rather symptomatic in this respect. Although the entire period from 82 to 126 contains 44 protons, addition to lead of only five of them turns out to be sufficient to remove the stability of the spherical nuclear shape. We may suppose that beyond the terminal point of the proton $\omega(p)$ curve the regions of existence of spherical nuclei narrow more rapidly or even will not exist at all.

We express our thanks to M.Ya. Amusya, A.I. Baz’, B.L. Birbrair, I.I. Gurevich, M.V. Kazarnovskii, L.P. Kudrin, I.M. Pavlichenkov, G.A. Pik-Pichak, V.P. Smilga, V.V. Sudakov, and O.B. Firsov for discussion of the results of this work. We also express our indebtedness to I.M. Lifshitz for pointing out to one of the authors (V.N.) the mathematical apparatus which apparently turns out to be most convenient for discussion of problems of this nature.

References

[1] C.F. Weizsacker, Z. Physik 96, 431 (1935).
[2] L.D. Landau and E.M. Lifshits, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963.
[3] V.G. Nosov, Zh. Eksp. Teor. Fiz. 57, 1765 (1969) [Sov. Phys.-JETP 30, 954 (1970)].
[4] V.G. Nosov, Zh. Eksp. Teor. Fiz. 53, 579 (1967) [Sov. Phys.-JETP 26, 375 (1968)].
[5] E.H. Frei, S. Shtrikman, and D. Treves, Phys. Rev. 106, 446 (1957).
[6] M. Goeppert Mayer and J. Jensen, Elementary Theory of Nuclear Shell Structure, New York, Wiley, 1955.
[7] P.E. Hodgson, The Optical Model of Elastic Scattering, Oxford, Clarendon Press, 1963.
[8] R. Courant and D. Hilbert, Methods of Mathematical Physics, New York, Interscience, 1953 (English translation).
[9] I.M. Lifshitz and A.M. Kosevich, DAN SSSR 96, 963 (1954); Zh. Eksp. Teor. Fiz. 29, 730 (1955) [Sov. Phys.-JETP 2, 636 (1956)].
[10] L.D. Landau, Zh. Eksp. Teor. Fiz. 30, 1058 (1966) [Sov. Phys.-JETP 3, 920 (1957)].
[11] L.D. Landau and E.M. Lifshitz, Statisticheskaya fizika (Statistical Physics), Fizmatgiz, 1964.
[12] D.L. Hill and J.A. Wheeler, Phys. Rev. 89, 1102 (1953).
[13] W.D. Myers and W.J. Swiatecki, Nucl. Phys. 81, 1 (1966).
[14] V.A. Kravtsov, Massy atomov i energii svyazi yader (Atomic Masses and Nuclear Binding Energies), Atomizdat, Moscow, 1965.
Figures captions

Fig. 1. The smooth part of the mass, described by the Weizsäcker formula, does not have singularities; it is taken as the reference zero of the “shell” effect pictured here. A more detailed and accurate plot would contain a whole set of curves corresponding to the different chemical elements (see, for example, the review of Myers and Swiatecki [13]). As a function of the number of protons $Z$ the behavior of the mass reveals no less sharply expressed features of a similar nature; see also Sections 3 and 4 of the present article.

Fig. 2.

Fig. 3.

Fig. 4. Values of the quantity $\omega$: $\circ$ — neutron magic numbers, $\bullet$ — proton magic numbers.
This figure "fig1.gif" is available in "gif" format from:

http://arxiv.org/ps/nucl-th/0310068v1
This figure "fig2.gif" is available in "gif" format from:

http://arxiv.org/ps/nucl-th/0310068v1
This figure "fig3.gif" is available in "gif" format from:

http://arxiv.org/ps/nucl-th/0310068v1
This figure "fig4.gif" is available in "gif" format from:

http://arxiv.org/ps/nucl-th/0310068v1