BOUNDARY ENERGY OF A FERMI GAS IN A POTENTIAL WELL

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The relation between the Fermi energy and number of particles is extended to the case of a gas in a potential well with a diffuse edge. The results are employed to calculate the boundary Fermi energy of neutrons in heavy nuclei accurate to ~ 1 MeV. The mean distance between the levels and the nuclear surface energy are calculated, using the optical-model potential, for the last elements of the periodic table.

1. INTRODUCTION

THE boundary energy ϵ_0 of a Fermi gas in a potential well can be connected with the number of its particles N. In order to obtain this dependence for a spherically-symmetrical potential in the form

$$U = U_0/[1 + e^{-\alpha(r-R)}], \tag{1.1}$$

we shall derive in Sec. 2 a quasiclassical condition for quantization and use it in Sec. 3 to obtain the first two terms of the expansion of $N(\epsilon_0)$ in the dimensions of the system for this potential.

It can be shown [1)] that the coefficient preceding the value of the surface S in the second term of the expansion of $N(\epsilon_0)$ is connected with the surface energy and does not depend on the form of the system, provided the curvature is proportional to $V^{-1/3}$ or to $S^{-1/2}$, where V is the volume of the system. The method presented makes it possible to carry out similar calculations for any potential well with a diffuse edge.

Specific calculations of the neutron Fermi energy for heavy nuclei are given in Sec. 4. The corrections obtained to the fundamental formula

$$\varepsilon_\infty = (\hbar^2/2M)(3\pi^2 N/V)^{2/3} \tag{1.2}$$

increase the energy of the Fermi boundary of the nuclei by 25% and decrease by 10% the average distance between the nucleon levels of the nuclei at the end of the periodic table, in agreement with experiment.

An expansion of $N(\epsilon_0)$ was obtained previously [1] for a well with infinite walls, and our formula (3.8) goes over into this expansion as $\alpha \to \infty$ and $U_0 \to \infty$.

2. EFFECTIVE BOUNDARY CONDITION

We shall seek the quantization condition in the potential (1.2) for $\alpha R \gg 1$. In the region

$$1/\alpha \ll R - r \ll R \tag{2.1}$$

the quasiclassical radial functions of free motion should coincide with the asymptotic expression for the exact solution near the discontinuity of the potential.

We neglect the variation of the centrifugal potential in the radial Schrödinger equation, (introducing thereby a relative error ~ (R − r)/R):

$$\left\{\frac{d^2}{dr^2} + k_l^2 - \frac{p^2}{1 + e^{-\alpha(r-R)}}\right\}\chi^{(1)}(r) = 0. \tag{2.2}$$

Here

$$k_l^2 = 2M\varepsilon - l(l+1)/R^2 \cong 2M\varepsilon - \lambda^2/R^2, \qquad \lambda = l + 1/2.$$

Its solution is (see, for example, [2]),

$$\chi^{(1)}(r) = Ae^{-\varkappa(r-R)} F\left(\frac{\varkappa + ik_l}{\alpha}, \frac{\varkappa - ik_l}{\alpha}, 1 + \frac{2\varkappa}{\alpha}, -e^{-\alpha(r-R)}\right), \tag{2.3}$$

where $\kappa = \sqrt{p^2 + k_l^2}$, and has an asymptotic value

$$\chi^{(1)}(r) \to B \sin[k_l(r - R) + \varphi(\lambda)], \tag{2.4}$$

$$\varphi(\lambda) = -\arcsin\frac{k_l}{p} + 2\arg\Pi\left(\frac{\varkappa + ik_l}{\alpha}\right) - \arg\Pi\left(\frac{2ik_l}{\alpha}\right)$$

$$\Pi(z) = \Gamma(z + 1). \tag{2.5}$$

On the other hand, the quasiclassical solution is

$$\chi^{(2)}(r) = \frac{C}{k_l}\sin\left(\int_{r_0}^{r}\sqrt{2M\varepsilon - \frac{\lambda^2}{r^2}}\,dr + \frac{\pi}{4}\right), \tag{2.6}$$

$$R - r \gg \frac{1}{\alpha},$$

[1)] We are grateful to Academician Ya. B. Zel'dovich for supplying us with this unpublished result.

$r_0 = \lambda/\sqrt{2M\epsilon}$. Writing in (2.6)

$$\int_{r_0}^{r} \sqrt{2M\varepsilon - \lambda^2/r^2}\, dr \cong \int_{r_0}^{R} \sqrt{2M\varepsilon - \lambda^2/r^2}\, dr + (r - R)\, k_l \tag{2.7}$$

and comparing (2.5) with (2.6) we get

$$\sqrt{z_{n\lambda}^2 - \lambda^2} - \lambda \arccos(\lambda/z_{n\lambda}) = \pi(n - \tfrac{1}{4}) + \varphi(\lambda), \tag{2.8}$$

where

$$z_{n\lambda} = k_{n\lambda} R = R\sqrt{2M\varepsilon_{n\lambda}}, \qquad n = 1, 2, \ldots,$$
$$\lambda = {}^1/_2, {}^3/_2, {}^5/_2, \ldots$$

As will be shown below, the inaccuracy of condition (2.8) does not affect the corrections of interest to us.

3. CALCULATION OF $\epsilon_0(N)$ AND OF THE SURFACE ENERGY

With the aid of the obtained quantization condition we now determine the number of states with energy below the Fermi boundary

$$N = 2\sum_{n,\lambda} 2\lambda = 2\sum_{\lambda={}^1/_2}^{\lambda=\lambda_{max}} 2\lambda n(\lambda), \qquad z_{n\lambda} \leqslant z_0 \equiv k_0 R. \tag{3.1}$$

Here $n(\lambda)$ is the number of levels with given λ; in our notation $n(\lambda)$ is the number of the last level below the Fermi boundary.

Taking into account the monotonicity of the left half of (2.8) with respect to $z_{n\lambda}$, we find that $n(\lambda) = E[x(\lambda)]$ —the integer part of $x(\lambda)$, determined by the expression

$$\pi[x(\lambda) - \tfrac{1}{4}] = \sqrt{z_0^2 - \lambda^2} - \lambda \arccos(\lambda/z_0) - \varphi(\lambda). \tag{3.2}$$

The same equation determines also the inverse function $\lambda(x)$.

The summation in (3.1) is carried out up to a λ_{max} such that there still exists one level below the Fermi boundary, i.e., $n(\lambda_{max}) = 1$. Obviously,

$$\lambda_{max} = \lambda(1) + O(1). \tag{3.3}$$

In calculating the sum (3.1) by the Euler-Maclaurin formula (see [3])

$$\sum_{k=0}^{m} f(k) = \int_0^m f(t)\, dt + \tfrac{1}{2}[f(m) + f(0)] + \ldots, \tag{3.4}$$

which in this case gives series in powers of z_0^{-1}, it is sufficient to confine oneself to the integral

$$N = \int_{1/2}^{\lambda_{max}} 4\lambda E[x(\lambda)]\, d\lambda. \tag{3.5}$$

To calculate the integral in (3.5) we make use of a formula that can be derived by induction:

$$\int_0^x \psi(t) E(t)\, dt = E(x)\int_0^x \psi(t)\, dt - \sum_{n=1}^{E(x)} \int_0^n \psi(t)\, dt. \tag{3.6}$$

Then (3.6) transforms to

$$N = \sum_{m=1}^{m=E[x(0)]} 2\lambda^2(m), \tag{3.7}$$

and using (3.2), (3.3), and (3.4) we obtain for the number of particles

$$N = \frac{k_0^3 V}{3\pi^2} - \frac{k_0^2 S}{8\pi} + \frac{k_0^2 S}{2\pi^2}\int_0^1 \left(\frac{\lambda}{z_0}\right)^2 \frac{d\varphi}{d(\lambda/z_0)}\, d\left(\frac{\lambda}{z_0}\right). \tag{3.8}$$

(Formula (3.8) can be obtained in a different manner, by noting in (3.5) that $x - E(x)$ oscillates rapidly with an average value $\frac{1}{2}$, and replacing $E(x)$ by $x - \frac{1}{2}$. Integration by parts again yields (3.8).)

It is seen from (3.8) that to obtain the "surface" corrections it is sufficient to know $\varphi(\lambda)$ in the zeroth approximation in $1/z_0$. We can now estimate the influence of the errors in the quantization condition. We begin with the error of the quasiclassical approximation:

$$\delta N \leqslant \int_0^{\lambda(1)} \left(\frac{d\lambda_{n\lambda}}{dr}\right)_{r=R} \lambda d\lambda \sim \int_0^{\lambda(1)} \frac{\lambda^3 d\lambda}{(z_0^2 - \lambda^2)^{3/2}} \sim z_0^{4/3}. \tag{3.9}$$

Here $\lambda_{n\lambda}$ is the de Broglie wavelength and $\lambda(1)$ is determined from (3.2) with $x = 1$ in the form

$$\lambda(1) = z_0 - \tfrac{1}{2}(9\pi/4)^{2/3} z_0^{1/3} + \ldots \tag{3.10}$$

Expanding in (2.2) the centrifugal potential to the next term, and introducing the corresponding corrections in condition (2.8), we see that in the optimal case, when the "joining together" is in the region $R - r \sim \alpha^{-1} \ln \alpha R$, the error in the number of particles is smaller in order of magnitude than $z_0^{3/4}$. The same can be said concerning the errors due to the use of the asymptotic expression (2.5) and due to the next terms in the expansion (2.7). Thus, the next term in the expansion (3.8) has an order of magnitude not higher than $z_0^{4/3}$.

From (3.8) with $\varphi(\lambda)$ from (2.5) we obtain for the boundary energy ϵ_0 and for the total kinetic energy E the asymptotic formulas

$$\frac{\varepsilon_0}{\varepsilon_\infty} = 1 + \frac{S}{k_\infty V}\left(\frac{\pi}{4} - \frac{p^2}{k_\infty^2}\right.$$
$$\left. \times \int_0^{\arcsin(k_\infty/p)} \left(t + \arg \frac{\Pi(2ip\sin t/\alpha)}{\Pi^2(pe^{it}/\alpha)}\right)\sin 2t\, dt\right), \tag{3.11}$$

$$E = \frac{\hbar^2}{2M}\int_0^{k_0} k^2 \frac{dN}{dk}\, dk = \frac{3}{5}\varepsilon_\infty N + \sigma S, \tag{3.12}$$

where

$$\sigma = \frac{\varepsilon_\infty k_\infty^2}{16\pi^2}\left\{1 + 16\int_0^1 (x^3 - x)\left[\arcsin\frac{k_\infty x}{p}\right.\right.$$
$$\left.\left. + \arg \frac{\Pi(2ik_\infty x/\alpha)}{\Pi^2(p\alpha^{-1}\exp\{i\arcsin(k_\infty x/p)\})}\right] dx\right\}.$$

The distance between the levels $d\epsilon_0/dN$ is expressed directly in terms of the phase $\varphi(k_0)$ in the form ($\gamma \equiv k_\infty/p$).

$$\frac{d\varepsilon_0}{dN} = \frac{2\pi^2\varepsilon_0}{k_0^3 V}\left[1 + \frac{S}{k_\infty V}\left(\frac{\pi}{4}\arcsin\gamma + \arg\frac{\Pi^2(\delta e^{i\arcsin\gamma})}{\Pi(2i\delta\gamma)}\right)\right]. \tag{3.13}$$

The integrals in (3.11) and (3.12) can be calculated in the limiting cases of large and small $\delta \equiv p/\alpha$, using the known expansion (see [4]). The first of these expansions (the Stirling formula) yields even for $\delta \sim 1$ a relative error $\sim 0.1\%$ in (3.14). We obtain here

$$\frac{\varepsilon_0}{\varepsilon_\infty} = 1 + \frac{4S}{3\pi V}\left\{\frac{1}{\gamma^2} - \ln(2\gamma) - \frac{(1-\gamma^2)^{3/2}}{\gamma^3}\arcsin\gamma\right\} + \frac{\alpha S(3-4\gamma^2)}{36k_0^2 V}, \tag{3.14}$$

$$\sigma = \frac{4\varepsilon_\infty k_\infty^2}{15\pi^2}\left[\frac{\delta(1-\gamma^2)^{5/2}\arcsin\gamma}{\gamma^4} - \gamma\ln(2\gamma) - \frac{\gamma}{12\delta} + \frac{5}{48\delta\gamma} + \frac{7\delta}{3\gamma} - \frac{\delta}{\gamma^3}\right].$$

Formulas (3.14) and (3.15) do not hold for a rectangular well.

Going to the limit in (3.11) and (3.12) as $\alpha \to \infty$, we then get

$$\frac{\varepsilon_0}{\varepsilon_\infty} = 1 + \frac{S}{k_\infty V}\left[\frac{\pi}{4} - \left(1 - \frac{1}{2\gamma^2}\right)\arcsin\gamma - \frac{\sqrt{1-\gamma^2}}{2\gamma}\right],$$

$$\sigma = \varepsilon_\infty k_\infty^2 \frac{3\gamma(1-2\gamma^2)\sqrt{1-\gamma^2} - (8\gamma^4 - 8\gamma^2 + 3)\arcsin\gamma + 2\pi\gamma^4}{32\pi^2\gamma^4}. \tag{3.15}$$

4. CONCLUSION

Regarding nucleons as a Fermi gas in a potential (1.1), we can apply the results obtained to the calculation of the energy of the Fermi boundary of nuclei. The universality indicated in the introduction enables us to compare with experiment the Fermi energy and the average distance between levels also for deformed nuclei.

The formula (3.14) for the Fermi energy can be represented in the form (we assume $U_0 = (80-56)N/A$ MeV and $\alpha = 1.55 \times 10^{13}$ cm^{-1}[5])

$$\varepsilon_0/\varepsilon_\infty = 1 + A^{-1/3} f(N/A), \tag{4.1}$$

where f(x) is given by the following table:

$x =$	0.50	0.52	0.54	0.56	0.58	0.60	0.62
$f(x) =$	1.74	1.71	1.51	1.50	1.40	1.34	1.20
$x =$	0.64	0.66	0.68				
$f(x) =$	1.13	1.00	0.90				

For the end of the periodic table the distance between levels $d\epsilon_0/dN$ is of the order of 0.17 MeV, which is 10% smaller than the distance between the levels in the infinite system. The Nilsson scheme gives $d\epsilon_0/dN \cong 0.13$ MeV. The surface tension as obtained from (3.14) is $\sigma S/N \cong 6$ MeV for a per-unit "volume" energy $E_{vol}/N = \frac{3}{5}\epsilon_\infty \cong 21$ MeV.

For $A \gtrsim 200$ the error of (4.1) can be assumed to be 1—2 MeV. Within the limits of such accuracy, the order of magnitude of $E_b(N,A) = U_0(N,A) - \epsilon(N,A)$ for the chosen type of $U_0(N,A)$, as given by (4.1), agrees with experiment. For example, for $N/A \sim 0.6$ and $A \approx 200$ we obtain from (4.1) $E_b \sim 4$ MeV, whereas the experimental value is ~ 5—6 MeV.

[1] D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1102 (1953).

[2] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Gostekhizdat, 1948, p. 96. [Transl. Pergamon, 1958].

[3] E. Madelung, Mathematical Tools for the Physicist, Dover, 1944.

[4] I. S. Gradshteĭn and I. M. Ryzhik, Tablitsy integralov, summ, ryadov i proizvedeniĭ (Tables of Integrals, Sums, Series, and Products), Fizmatgiz, 1962, pp. 953-4.

[5] P. É. Nemirovskiĭ, Sovremennye modeli atomnogo yadra (Modern Models of the Atomic Nucleus), Atomizdat, 1960.

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