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The Odd Atomic Nuclei Described by Macroscopic–Microscopic Method

Opis nieparzystych jąder atomowych metodą makroskopowo–mikroskopową

1. INTRODUCTION

There are many experimental data concerning the mean square radii (MSR) and electric quadrupole moments (Q_2) of odd nuclei [1, 2]. They show interesting systematics like odd–even staggering effect in MSR isotopic shifts, kink effect when crossing the magic neutron numbers or larger Q_2 of odd nuclei.

The theoretical description of the odd system demands the information about the features of the even core and quantum numbers of the possible state occupied by the odd particle. The odd–odd nuclei are specially difficult to investigate, because of the coupling between the two odd neutron and proton systems. The first estimates with Nilsson single particle potential of the potential energies of odd nuclei showed [3] that the state with the experimental values of angular momentum Ω^π occupied by the external particle is not always closest to the Fermi surface. It means that the parameters of the single particle hamiltonian should be revised in future calculation, or we should put the odd nucleon in the state corresponding to the proper experimental angular momentum and parity of even–odd nuclei.

2. THEORY

The potential energy of a nucleus by the macroscopic–microscopic method is

$$E = E_{\rm LD} + \delta E_{\rm micr} . \tag{1}$$

It consits of the liquid drop or droplet macroscopic term [4] and the microscopic correction $\delta E_{\rm micr}$ which contains the shell $\delta E_{\rm shell}$ and pairing $\delta E_{\rm pair}$ corrections for protons and neutrons

$$\delta E_{\rm micr} = (\delta E_{\rm shell} + \delta E_{\rm pair})_p + (\delta E_{\rm shell} + \delta E_{\rm pair})_n . \tag{2}$$

The shell correction is equal to the difference between the sum of single particle energies and the energy of the smoothed level scheme of the even core [5]

$$\delta E_{\rm shell} = 2\sum_{\nu>0}^{\nu_F} e_\nu - \int_{-\infty}^{e_F} \bar{\rho}(e) e \, de . \tag{3}$$

The single particle energies e_ν and wave functions $|\nu\rangle$ are obtained by the solution of the eigenproblem of hamiltonian with the average single particle potential. It is the Nilsson–Seo deformed harmonic oscillator potential [6] in our case

$$\hat{H}_0|\nu\rangle = e_\nu|\nu\rangle . \tag{4}$$

The quantum numbers describing single particle states are $|\nu\rangle = |Nn_z\Lambda\Omega\rangle$, $|-\nu\rangle = |Nn_z\Lambda-\Omega\rangle$. They are the quantum numbers of the oscillator asymptotic base: N — harmonic oscillator number; n_z — bosons number in z direction; Λ — orbital angular momentum; Ω — the z component of the total angular momentum.

The smoothed level scheme is obtained with the average density $\bar{\rho}(e)$ calculated with the weight function $j(e,e')$

$$\bar{\rho}(e) = \int_{-\infty}^{+\infty} \rho(e') j(e,e') de' . \tag{5}$$

The Fermi level e_F is evaluated from the nucleon number conservation

$$\int_{-\infty}^{e_F} \rho(e) de = \begin{cases} N^{\rm EVEN} \\ N^{\rm ODD} - 1 \end{cases} . \tag{6}$$

The shell correction namely is calculated for the even core only, because the external (odd particle) single particle energy does not take part in the process of the Strutinski's energy averaging. The pairing correction is the difference between the sum of all the occupied single particle levels and BCS energy E_{BCS} of the system, and the average pairing energy included already in the macroscopic part of energy

$$\delta E_{\mathrm{pair}} = E_{\mathrm{BCS}} - \sum_{\nu}^{\nu_F} e_\nu - \langle E_{\mathrm{pair}} \rangle \,, \tag{7}$$

where the summation goes over all the single particle states occupied by the nucleons (with even and odd time reversal parity). It is the same as in the formula (3) for the even system, but increased by the energy $e_{\nu'}$ of the level $|\nu'\rangle$ occupied by the odd particle for the odd system of protons or neutrons.

The BCS energy for odd system of N protons or neutrons is (for details see Appendix)

$$\begin{aligned} E_{\mathrm{BCS}}^{\mathrm{ODD}} &= 2 \sum_{\nu>0,\nu\neq\nu'} (e_\nu - GV_\nu^2)V_\nu^2 + (e_{\nu'} - GV_{\nu'}^2) - \frac{\Delta_{\nu'}^2}{G} \\ &\quad + G(U_{\nu'}V_{\nu'})^2 + G\sum_{\nu>0} V_\nu^4 \,. \end{aligned} \tag{8}$$

The occupation BCS factors U_ν, V_ν for $\nu \neq \nu'$ and blocked energy gap $\Delta_{\nu'}$ fulfill the BCS equations set

$$U_\nu^2 = \frac{1}{2}\left(1 + \frac{e_\nu - \lambda - GV_\nu^2}{\sqrt{(e_\nu - \lambda - GV_\nu^2)^2 + \Delta_{\nu'}^2}}\right) \qquad V_\nu^2 = 1 - U_\nu^2 \,; \tag{9}$$

$$\sum_{\nu>0,\nu\neq\nu'} \left(1 - \frac{e_\nu - \lambda - GV_\nu^2}{\sqrt{(e_\nu - \lambda - GV_\nu^2)^2 + \Delta_{\nu'}^2}}\right) = N - 1 \,. \tag{10}$$

The Fermi energy λ is found from the equation

$$\Delta_{\nu'} = G \sum_{\nu>0,\nu\neq\nu'} U_\nu V_\nu \,, \tag{11}$$

$$\frac{2}{G} = \sum_{\nu>0,\nu\neq\nu'} \frac{1}{\sqrt{(e_\nu - \lambda - GV_\nu^2)^2 + \Delta_{\nu'}^2}} \tag{12}$$

G is the pairing stregth [7].

The average pairing energy is [7]

$$\langle E_{\mathrm{pair}} \rangle = \frac{1}{2}\bar{\rho}\bar{\Delta}^2 \,, \tag{13}$$

where $\bar{\rho}$ is the average single particle level density (5) and $\bar{\Delta}$ denotes average energy gap of even core and is evaluated using the following equation:

$$G \approx \frac{1}{\bar{\rho} \ln \frac{2\varepsilon}{\bar{\Delta}}}, \tag{14}$$

2ε is the width of the energy "window" above and below Fermi surface, where the pairing interaction acts. The microscopic correction to the potential energy of the odd system is then

$$\begin{aligned} \delta E_{\text{micr}}^{\text{ODD}} &= 2 \sum_{\nu>0,\nu\neq\nu'}^{\nu_F} e_\nu - \int_{-\infty}^{e_F} \bar{\rho}(e) e \, de - \frac{1}{2}\bar{\rho}\,\bar{\Delta}^2 + G \sum_{\nu>0} V_\nu^4 \\ &+2 \sum_{\nu>0,\nu\neq\nu'} (e_\nu - G V_\nu^2)\, V_\nu^2 + e_{\nu'} - G V_{\nu'}^2 - \frac{\Delta_{\nu'}^2}{G} + G(U_{\nu'}V_{\nu'})^2 - \sum_{\nu}^{\nu_F} e_\nu \,. \end{aligned} \tag{15}$$

The first term of this formula together with $e_{\nu'}$ single particle energy of odd particle equals the sum of all the single particle states in the odd system so the microscopic correction for protons or neutrons for the odd system stays

$$\begin{aligned} \delta E_{\text{micr}}^{\text{ODD}} &= 2 \sum_{\nu>0,\nu\neq\nu'} e_\nu V_\nu^2 - G \sum_{\nu>0,\nu\neq\nu'} V_\nu^4 - G V_{\nu'}^2 + G V_{\nu'}^4 - \frac{\Delta_{\nu'}^2}{G} + G(U_{\nu'}V_{\nu'})^2 \\ &- \frac{1}{2}\bar{\rho}\bar{\Delta}^2 - \int_{-\infty}^{e_F} \bar{\rho}(e) e \, de \,. \end{aligned} \tag{16}$$

For the even system of one kind nucleons it is

$$\delta E_{\text{micr}}^{\text{EVEN}} = 2 \sum_{\nu>0} e_\nu V_\nu^2 - G \sum_{\nu>0} V_\nu^4 - \frac{\Delta^2}{G} - \frac{1}{2}\bar{\rho}\bar{\Delta}^2 - \int_{-\infty}^{e_F} \bar{\rho}(e) e \, de \,, \tag{17}$$

where

$$\Delta = G \sum_{\nu>0} U_\nu V_\nu \,. \tag{18}$$

After minimizing the potential energy of a whole nucleus versus the collective deformation parameters we get the equilibrium shape in which the average values Q_λ of the multipole operators is calculated

$$\hat{Q}_0 = r^2 \,, \tag{19}$$

$$\hat{Q}_2 = 2r^2 P_2(\cos\vartheta) \,. \tag{20}$$

using the formula

$$Q_\lambda = \langle \nu' | \widehat{Q}_\lambda | \nu' \rangle + 2 \sum_{\nu>0, \nu \neq \nu'} \langle \nu | \widehat{Q}_\lambda | \nu \rangle V_\nu^2 . \tag{21}$$

In eq. (20) P_2 is the Legendre polynomial.

The diagonal matrix element $\langle \nu' | \widehat{Q}_\lambda | \nu' \rangle$ is added only for the odd system. The electric moments are calculated for proton system only. Adding the correction for proton nonpoint distribution [8] we can get from eq. (21) the MSR value

$$\langle r^2 \rangle = \frac{Q_0}{Z} + 0.64 \text{ fm}^2 \tag{22}$$

which one can compare with the experimental data [1, 2].

3. RESULTS

The calculation was done for the rare earth nuclei with the average mass $A = 165$ on the two dimensional deformation grid of Nilsson quadrupole $\varepsilon = -0.6$ to 0.6 and hexadecapole $\varepsilon_4 = -0.12$ to 0.12 parameters.

The Seo–Nilsson single particle potential [6] was used and the pairing strength $G = 0.275\ \hbar\omega_0$ [7] for protons and neutrons was taken. The potential energy was calculated with liquid drop macroscpic part [9] and the unblocked (A27) version of pairing energy for odd system was used. The surfaces of potential energies and multipole moments were found and after energy minimization the equilibrium deformations were established. In these points the static multipole moments were calculated.

As an example of final results of our calculation we show the charge mean square radii of Nd isotopes.

In Figure 1 the charge MSR is compared with several sets of experimental data. One can see that the so–called model independent [2] values of the experimental MSR values (exp V1), (exp V2) and (exp V3) differ from each other up to 1.5 MeV. Their averaging done in Ref. [10] is denoted by diamonds. In fact only the MSR value of ^{142}Nd was measured the other data were obtained by adding their experimental isotopic shifts [1] (ISMSR)

$$\delta \langle r^2 \rangle = \langle r^2 \rangle^A - \langle r^2 \rangle^{A'} . \tag{23}$$

In Figure 2 these ISMSR values are drawn for $A' = 142$.

The general slope of the microscopic curve is reproduced, but the odd–even staggering effect demands the inclusion of blocking effect and the dynamical calculation like in Ref. [11].

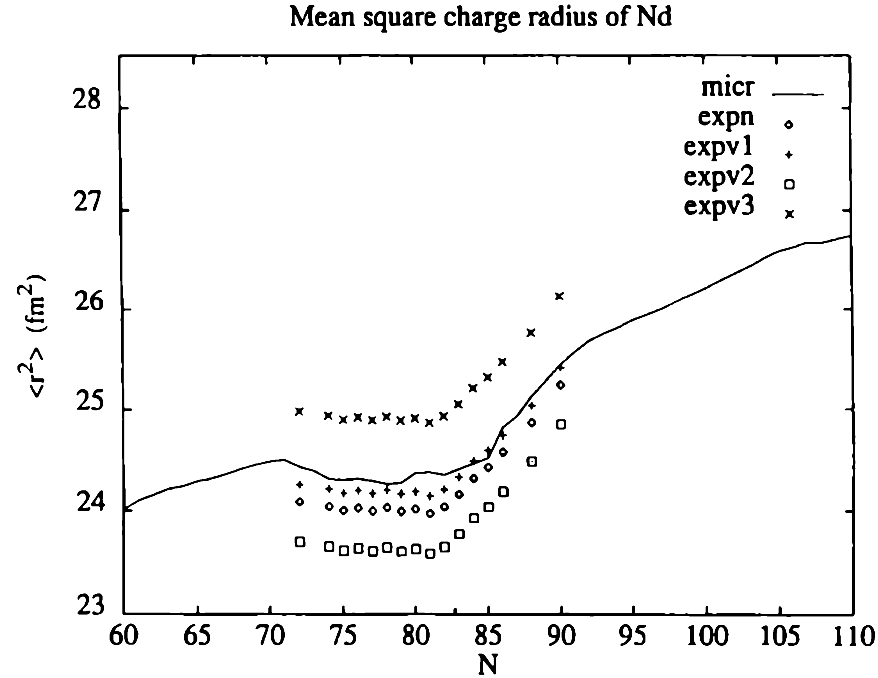

Fig. 1. The microscopic charge mean square radii in fm^2 of Nd isotopes (solid line) compared with the experimental data taken from ref. [2], obtained by: three parameter Fermi model (exp V_1), two parameter Fermi model (exp V_2), three parameter Gauss model (exp V_3) and from ref. [10]

Mikroskopowe średnie promienie kwadratowe ładunku w fm^2 w izotopach Nd (linia ciągła) porównane z danymi doświadczalnymi z artykułu [2], otrzymanymi w 3-parametrowym modelu Fermiego (exp V_1), dwuparametrowym modelu Fermiego (exp V_2), 3-parametrowym modelu Gaussa (exp V_3) i z artykułu [10] (exp n)

4. APPENDIX. THE BCS ENERGY OF ODD NUCLEONS SYSTEM

The BCS function $\Phi_{\rm BCS}$ is the ground state of the even system of nucleons. A ground state of the odd system of nucleons is described by the function

$$\Phi^{\rm ODD} = \alpha_{\nu'}^{+}\Phi_{\rm BCS}\,, \tag{A1}$$

where

$$\Phi_{\rm BCS} = \prod_{\nu>0}(U_\nu + V_\nu a_\nu^+ a_{-\nu}^+)|0\rangle \tag{A2}$$

$|0\rangle$ is the particle vacuum state

$$a_\nu|0\rangle = 0\,; \qquad \langle 0|a_\nu^+ = 0\,. \tag{A3}$$

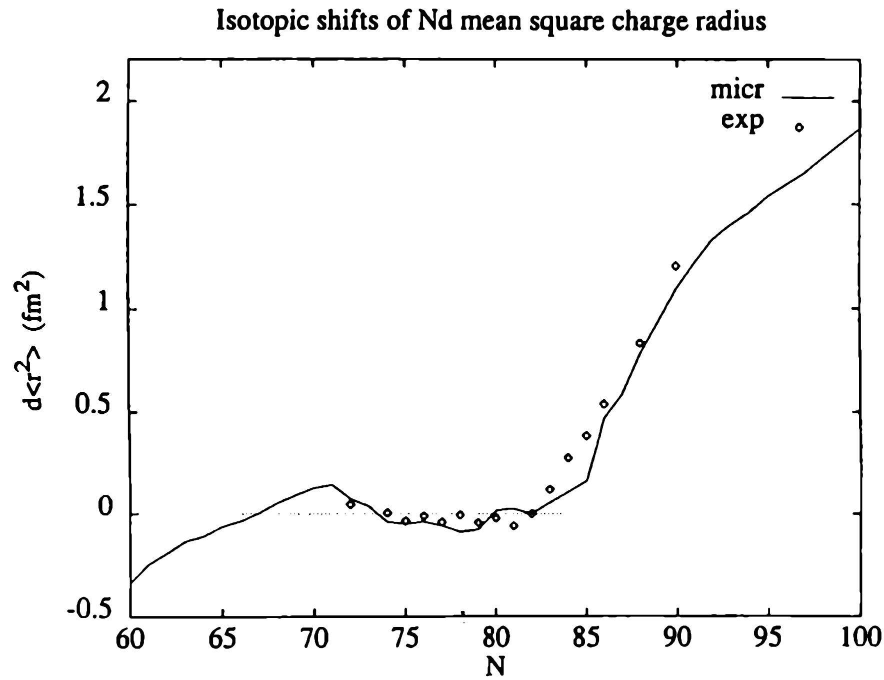

Fig. 2. The microscopic isotopic shifts of the electric charge mean square radii in fm^2 for Nd isotopes (solid line) compared with the experimental data [1] — diamonds
Mikroskopowe przesunięcia izotopowe elektrycznego średniego promienia kwadratowego ładunku w fm^2 dla izotopów Nd (linia ciągła) porównana z danymi doświadczalnymi [1] — romby

The $a_\nu, a^+_{-\nu}$ are the fermion annihilation and creation operators fulfilling the anticommutations rules:

$$\{a_\nu, a_\mu\} = \{a^+_\nu, a^+_\mu\} = 0 \, ; \qquad \{a^+_\nu, a_\mu\} = \delta_{\nu\mu} \, . \tag{A4}$$

The α_ν, α^+_ν are the quasiparticle annihilation and creation operators fulfilling the same anticommutation rules:

$$\{\alpha_\nu, \alpha\_mu\} = \{\alpha^+_\nu, \alpha^+_\mu\} = 0 \, ; \quad \{\alpha^+_\nu, \alpha_\mu\} = \delta_{\nu\mu} \, . \tag{A5}$$

and ensuring the conditions

$$\alpha_\nu|\Phi_{\rm BCS}\rangle = 0 \, ; \qquad \langle\Phi_{\rm BCS}|\alpha^+_\nu = 0 \, . \tag{A6}$$

The Bogolubov–Valatine transformation between the particle and quasiparticle operators is

$$
\begin{aligned}
\alpha_\nu^+ &= U_\nu a_\nu^+ - V_\nu a_{-\nu}\,; \\
\alpha_{-\nu}^+ &= U_\nu a_{-\nu}^+ + V_\nu a_\nu\,.
\end{aligned}
\tag{A7}
$$

The odd system function can be then written

$$
\Phi^{\mathrm{ODD}} = \alpha_{\nu'}^+ \prod_{\nu>0} (U_\nu + V_\nu a_\nu^+ a_{-\nu}^+)|0\rangle\,, \tag{A8}
$$

where the $|\nu'\rangle$ single particle state is for sure occupied by the odd particle, i.e. blocked in BCS theory.

The nuclear hamiltonian with pairing interaction is

$$
\widehat{H} = \sum_\nu e_\nu a_\nu^+ a_\nu - G \sum_{\nu>0,\mu>0} a_\nu^+ a_{-\nu}^+ a_{-\mu} a_\mu\,. \tag{A9}
$$

It can be easily expressed in quasiparticle space

$$
\begin{aligned}
\widehat{H} =& 2\sum_{\nu>0}(e_\nu - GV_\nu^2)V_\nu^2 - G\left(\sum_{\nu>0} U_\nu V_\nu\right)^2 + G\sum_{\nu>0} V_\nu^4 \\
&+ \sum_{\nu>0}\left\{(e_\nu - GV_\nu^2)(U_\nu^2 - V_\nu^2) + 2G\left(\sum_{\mu>0} U_\mu V_\mu\right) U_\nu V_\nu\right\}(\alpha_\nu^+\alpha_\nu + \alpha_{-\nu}^+\alpha_{-\nu}) \\
&+ 2\sum_{\nu>0}\left\{(e_\nu - GV_\nu^2)U_\nu V_\nu - G\left(\sum_{\mu>0} U_\mu V_\mu\right)(U_\nu^2 - V_\nu^2)\right\}(\alpha_\nu^+\alpha_{-\nu}^+ + \alpha_{-\nu}\alpha_\nu)\,.
\end{aligned}
\tag{A10}
$$

The terms responsible for the quasiparticle interaction are omitted here.

Denoting by $\widehat{H}_{ij}$ the hamiltonian terms containing i operators of quasiparticle creation and j operators of quasiparticle annihilation we can write eq. (A10) in the following way

$$
\widehat{H} = \widehat{H}_{00} + \widehat{H}_{11} + \widehat{H}_{20} + \widehat{H}_{02} + \ldots \tag{A11}
$$

Minimizing the energy of Φ^{ODD} state versus V_ν or U_ν parameters, except ν' state, with the particle conservation condition

$$
\langle \Phi^{\mathrm{ODD}} | \widehat{H} - \lambda \widehat{N} | \Phi^{\mathrm{ODD}} \rangle = \text{minimum}\,, \tag{A12}
$$

where $\hat{N}$ is the particle number operator:

$$\hat{N} = \sum_{\nu} a_{\nu}^{+} a_{\nu} \,, \tag{A13}$$

we get blocked set of the BCS equations:

$$V_{\nu}^{2} = \frac{1}{2}\left(1 - \frac{e_{\nu} - \lambda - GV_{\nu}^{2}}{\sqrt{(e_{\nu} - \lambda - GV_{\nu}^{2})^{2} + \Delta_{\nu'}^{2}}}\right) ; \qquad U_{\nu}^{2} = 1 - V_{\nu}^{2} ; \quad \text{(A14, A15)}$$

$$N - 1 = 2 \sum_{\nu>0,\nu\neq\nu'} V_{\nu}^{2} ; \qquad \Delta_{\nu'} = G \sum_{\nu>0,\nu\neq\nu'} U_{\nu} V_{\nu} \,. \quad (A16, A17)$$

The BCS energy can be written now

$$E_{\mathrm{BCS}}^{\mathrm{ODD}} = E_{0} + E_{\nu'} \,, \tag{A18}$$

where

$$E_{0} = 2 \sum_{\nu>0} (e_{\nu} - GV_{\nu}^{2}) V_{\nu}^{2} - G (\sum_{\nu>0} U_{\nu} V_{\nu})^{2} + G \sum_{\nu>0} V_{\nu}^{4} \tag{A19}$$

and

$$E_{\nu'} = (e_{\nu'} - GV_{\nu'}^{2})(U_{\nu'}^{2} - V_{\nu'}^{2}) + 2G (\sum_{\mu>0} U_{\mu} V_{\mu}) U_{\nu'} V_{\nu'} \,. \tag{A20}$$

The energy E^{ODD} can be also expressed in another way in the "blocked" or "quasiparticle" BCS form.

Putting

$$U_{\nu}^{2} - V_{\nu'}^{2} = 1 - 2V_{\nu'}^{2} \tag{A21}$$

and

$$\sum_{\nu>0} U_{\nu} V_{\nu} = \sum_{\nu>0,\nu\neq\nu'} U_{\nu} V_{\nu} + U_{\nu'} V_{\nu'} \tag{A22}$$

we get

$$E_{\mathrm{BCS}}^{\mathrm{ODD}} = 2 \sum_{\nu>0,\nu\neq\nu'} (e_{\nu} - GV_{\nu}^{2}) V_{\nu}^{2} + (e_{\nu'} - GV_{\nu'}^{2}) + G \sum_{\nu>0} V_{\nu}^{4} - \frac{\Delta_{\nu'}^{2}}{G} + GU_{\nu'}^{2} V_{\nu'}^{2} \,. \tag{A23}$$

Introducing

$$\tilde{e}_\nu \equiv e_\nu - \lambda - GV_\nu^2 \qquad \text{and} \qquad \Delta \equiv G \sum_{\nu>0} U_\nu V_\nu$$

we have

$$E_{\rm BCS}^{\rm ODD} = 2 \sum_{\nu>0,\nu\neq\nu'} \tilde{e}_\nu V_\nu^2 + \tilde{e}_{\nu'} + G \sum_{\nu>0} V_\nu^4 - \frac{\Delta_{\nu'}^2}{G} + \frac{G\Delta_{\nu'}^2}{4(\tilde{e}_{\nu'}^2 + \Delta_{\nu'}^2)} + N\lambda \tag{A24}$$

or

$$E_{\rm BCS}^{\rm ODD} = 2 \sum_{\nu>0} \tilde{e}_\nu V_\nu^2 + G \sum_{\nu>0} V_\nu^4 - \frac{\Delta^2}{G} + \sqrt{\tilde{e}_{\nu'}^2 + \Delta_{\nu'}^2} + \frac{G\Delta_{\nu'}^2}{2(\tilde{e}_{\nu'}^2 + \Delta_{\nu'}^2)} + N\lambda\,. \tag{A25}$$

All the (A18), (A23) and (A24) formulas for $E_{\rm BCS}^{\rm ODD}$ are equivalent and correct.

One can also omit the blocking effect in BCS equations, i.e. not exlude the ν' state in the sums but keep the particle number condition in a proper, blocked way. Then we get the formula

$$E_{\rm UNBLOCK}^{\rm ODD} \approx 2 \sum_{\nu>0,\nu\neq\nu'} \tilde{e}_\nu V_\nu^2 + \tilde{e}_{\nu'} + G \sum_{\nu>0} V_\nu^4 - \frac{\Delta^2}{G} + \frac{G\Delta^2}{4(\tilde{e}_{\nu'}^2 + \Delta^2)} + N\lambda \tag{A26}$$

or

$$E_{\rm UNBLOCK}^{\rm ODD} \approx 2 \sum_{\nu>0} \tilde{e}_\nu V_\nu^2 + G \sum_{\nu>0} V_\nu^4 - \frac{\Delta^2}{G} + \sqrt{\tilde{e}_{\nu'}^2 + \Delta^2} + N\lambda\,. \tag{A27}$$

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STRESZCZENIE

W niniejszym artykule podajemy metodę rachunku energii potencjalnych i statycznych średnich promieni kwadratowych jąder nieparzystych. Do makroskopowej energii kroplowej dodaje się poprawkę powłokową Strutinskiego. Efekty łączenia nukleonów w pary uwzględniono metodą nadprzewodnictwa BCS.