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USING LIPKIN-NOGAMI AND BCS PAIRING WITHIN MACROSCOPIC-MICROSCOPIC METHOD

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Abstract. The Lipkin-Nogami and BCS pairing theory used to calculate microscopic pairing corrections are compared for ^{240}Pu and ^{286}Cn using the spheroidal harmonic oscillator shell model and for ^{258}Fm with two-center shell model.

Key words: macroscopic-microscopic method, pairing corrections, Lipkin-Nogami method, shell corrections, superheavy nuclei.

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1. INTRODUCTION

Among the short-range residual interactions to be considered in nuclear theory, the pairing interaction is the most important [1–5]. There is much experimental evidence of pairing correlations in nuclei: the energy gap found in the excitation energy spectra of even-even deformed nuclei; the even-odd effect in nuclear masses; low-lying vibrational 2^+ states of even-even nuclei in the vicinity of closed shells; the spin zero of even-even nuclei and the spin determined by the last unpaired nucleon of odd-A nuclei; the existence of other spherical nuclei around the magic ones, *etc*.

A. Bohr *et al.* [6] suggested the analogy with electron correlations in the theory of superconductivity, developed by Bardeen, Cooper and Schriefer (BCS) [4]. Second quantization is usually used. The Bogoliubov-Valatin transformation allows to work with independent quasiparticles instead of interacting particles. BCS pairing corrections have been introduced by Strutinsky [7] in the same time with shell corrections. Alternatively, the residual pairing interactions can be treated within Lipkin-Nogami (LN) model [8–11].

As stated by Lipkin [8] in many-particle system theory there are many exam-

ples where the used wave functions are disregarding the existence of some conservation laws, *e.g.* Nilsson wave functions are not eigenfunctions of the total angular momentum and BCS [4] wave functions used to treat superconductors and pairing in nuclei do not conserve the number of particles. The Bogoliubov-Valatin transformation is not commutable with the nucleon-number operator [9] hence the wave function does not correspond to a system with a definite number of nucleons. Nevertheless, such wave functions have been used with great success to predict or explain experimental results. In the approach used by Lipkin to overcome this difficulty the independent particle wave function are not considered to be the true wave functions but "model wave functions" not including the effects of correlations. This effect on the energy eigenvalues may be eliminated by using a model Hamiltonian instead of the original Hamiltonian. Lipkin, Nogami and co-workers [8, 9, 12] proposed to minimize the expectation value of the model Hamiltonian

$$\hat{\mathcal{H}} = \hat{H} - \lambda_1 \hat{N} - \lambda_2 \hat{N}^2 \tag{1}$$

by determining λ_1 and λ_2 using certain conditions. $\hat{H}$ is the pairing Hamiltonian and $\hat{N}$ is the particle number operator. Minimization of the expectation value of $\hat{H} - \lambda_1 \hat{N}$ leads to the usual BCS model, with λ_1 determined from the particle number condition. Thus λ_1 is a Lagrange multiplier but the particle number fluctuation constant λ_2 is not.

There is also a practical reason for trying to find an alternative to BCS theory – the collapse happening whenever the spacing between single particle levels at the Fermi energy is too large (*e.g.* at magic numbers or for deformed actinide nuclei with neutron numbers 142 and 152 [11]): there may be a critical value of the pairing-force strength below which the BCS system of two nonlinear equations have no non-trivial solutions.

Following input quantities [10] are defined: pairing strength parameter G; the smooth effective-interaction pairing-gap Δ_G (not to be confused with the average pairing-gap $\bar{\Delta}$ – directly compared to experimental pairing gap). Calculated quantities are: the pairing gap Δ; Fermi energy λ; number-fluctuation constant λ_2; occupation probabilities v_k^2, and shifted-particle energies ϵ_k.

We have frequently used the macroscopic-microscopic method [13,14] to study heavy and superheavy nuclei [15–17], as well as the atomic clusters deposited on a surface [18–21] by employing up to now only BCS pairing corrections. In the present work we would like to compare the LN and BCS pairing corrections for two nuclei ^{240}Pu and ^{286}Cn using the spheroidal harmonic oscillator shell model and for ^{258}Fm with two-center shell model [22] at symmetry. Before illustrating the results we shall briefly present the spheroidal harmonic oscillator, the Strutinsky shell correction method, the BCS and LN pairing models.

2. SPHEROIDAL HARMONIC OSCILLATOR ENERGY LEVELS

The spheroidal harmonic oscillator has been used in various branches of Physics. The famous single-particle Nilsson model is very successful in Nuclear Physics. Its variants [23, 24] are of particular interest for atomic clusters [25].

2.1. NILSSON PARAMETRIZATION FOR A SPHEROIDAL NUCLEUS

For spheroidal shapes, generated by a potential with cylindrical symmetry

$$V = \frac{MR_0^2}{2}(\omega_\perp^2\rho^2 + \omega_z^2 z^2) \tag{2}$$

S. G. Nilsson [26] introduced the deformation ε by expressing the two deformation dependent frequencies by

$$\omega_\perp = \omega_0(\varepsilon)\left(1+\frac{\varepsilon}{3}\right) \qquad \omega_z = \omega_0(\varepsilon)\left(1-\frac{2\varepsilon}{3}\right). \tag{3}$$

The volume conservation, $\omega_\perp^2\omega_z = (\omega_0^0)^3$ allows to determine the dependence of $\omega_0(\varepsilon)$:

$$(\omega_0)^3\left(1+\frac{\varepsilon}{3}\right)\left(1-\frac{2\varepsilon}{3}\right) = (\omega_0^0)^3\ ;\ \omega_0 = \frac{\omega_0^0}{\left[1-\varepsilon^2\left(\frac{1}{3}+\frac{2\varepsilon}{27}\right)\right]^{1/3}}, \tag{4}$$

where for a nucleus with mass number A one takes $\hbar\omega_0^0 = 41A^{1/3}$ MeV and $\hbar^2/M = 41.5$ MeV·fm^2.

The shape of a spheroid with semiaxes a, c (c is the semiaxis along the symmetry) expressed in units of the spherical radius $R_0 = r_0A^{1/3}$ may be determined by a single deformation coordinate which can be the quadrupolar deformation [26] $\varepsilon = 3(c-a)/(2c+a)$. The eigenvalues [27] in units of $\hbar\omega_0^0$ are given by

$$\epsilon_i = [N+3/2+\varepsilon(n_\perp - 2N/3)][1-\varepsilon^2(1/3+2\varepsilon/27)]^{-1/3} \tag{5}$$

in which the quantum numbers $n_\perp$ and n_z are nonnegative integers. Their summation gives the main quantum number $N = n_\perp + n_z$. We have

$$E = \hbar\omega_z(n_z+1/2) + \hbar\omega_\perp(n_\perp+1). \tag{6}$$

A large degeneracy occurs when $\omega_\perp/\omega_z = n_c/n_a$, hence $\varepsilon = 3(n_c-n_a)/(n_a+2n_c)$. For example, at $n_c = n_a$ we get $\varepsilon = 0$ (sphere), with magic numbers 2, 8, 20, 40, 70, 112, 168, 240, 330, ... At $n_c = 2$, $n_a = 1$ one has $\varepsilon = 0.6$ and the magic numbers are 2, 4, 10, 16, 28, 40, 60, 80, 110, 140, 182, 224, 280, 336, ... At $n_c = 1$, $n_a = 2$ (oblate shape $\varepsilon = -0.75$) the magic numbers are 2, 6, 14, 26, 44, 68, 100, 140, 190, ... These magic numbers are changed if we include a spin-orbit interaction into the Hamiltonian. In units of $\hbar\omega_0^0$ one has a linear variation of the energy levels in

function of deformation ε. Due to the Pauli principle, each energy level ϵ_i, with quantum numbers $n_\perp$ and N, can accommodate $g = 2n_\perp + 2$ nucleons. One has a number of $(N+1)(N+2)$ nucleons in a completely occupied shell characterized by the main quantum number N, and the total number of states for the lowest $N+1$ shells is $\sum_{N=0}^{N}(N+1)(N+2) = (N+1)(N+2)(N+3)/3$ leading to the magic numbers mentioned above for a spherical shape, $\varepsilon = 0$ in the absence of the spin-orbit coupling (see Fig. 1).

In a system of cylindrical coordinates (ρ, φ, z) the wave function [28, 29] can be written as a product of the eigenfunctions

$$\psi_{n_r}^m(\rho) = \frac{\sqrt{2}}{\alpha_\perp} N_{n_r}^m \eta^{\frac{|m|}{2}} e^{-\frac{\eta}{2}} L_{n_r}^{|m|}(\eta) = \frac{\sqrt{2}}{\alpha_\perp} \psi_{n_r}^m(\eta), \tag{7}$$

$$\psi_{n_z}(z) = \frac{1}{\sqrt{\alpha_z}} N_{n_z} e^{-\frac{\xi^2}{2}} H_{n_z}(\xi) = \frac{1}{\sqrt{\alpha_z}} \psi_{n_z}(\xi), \tag{8}$$

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \tag{9}$$

where $L_{n_r}^{|m|}$ are the associated (or generalized) Laguerre polynomials and H_{n_z} are the Hermite polynomials. The variables η and ξ are defined by $\eta = \rho^2/\alpha_\perp^2$, $\xi = z/\alpha_z$, where $\alpha_\perp = \sqrt{\hbar/M\omega_\perp} \approx A^{1/6}\sqrt{\omega_0^0/\omega_\perp}$, $\alpha_z = \sqrt{\hbar/M\omega_z} \approx A^{1/6}\sqrt{\omega_0^0/\omega_z}$. The normalization constants

$$(N_{n_r}^m)^2 = \frac{n_r!}{(n_r + |m|)!} \ ; \ (N_{n_z})^2 = \frac{1}{\sqrt{\pi} 2^{n_z} n_z!} \tag{10}$$

are obtained from the orthonormalization conditions.

With increasing prolate deformation, ε, an energy level with $n_\perp = 0$ will decrease in energy

$$\epsilon(n_\perp = 0) = \left(n + \frac{3}{2} - \varepsilon\frac{2n}{3}\right)\left[1 - \varepsilon^2\left(\frac{1}{3} + \frac{2\varepsilon}{27}\right)\right]^{-1/3} \tag{11}$$

and the level with $n_\perp = n$ will increase in energy

$$\epsilon(n_\perp = n) = \left(n + \frac{3}{2} + \varepsilon\frac{n}{3}\right)\left[1 - \varepsilon^2\left(\frac{1}{3} + \frac{2\varepsilon}{27}\right)\right]^{-1/3}. \tag{12}$$

In this way, for a given prolate deformation and a maximum energy ϵ_m, there are n_{min} closed shells and other levels for high-order shells up to n_{max}:

$$n_{min} = \left\{\epsilon_m\left[1 - \varepsilon^2\left(\frac{1}{3} + \frac{2\varepsilon}{27}\right)\right]^{1/3} - \frac{3}{2}\right\}\frac{1}{1 + \varepsilon/3}, \tag{13}$$

$$n_{max} = \left\{\epsilon_m\left[1 - \varepsilon^2\left(\frac{1}{3} + \frac{2\varepsilon}{27}\right)\right]^{1/3} - \frac{3}{2}\right\}\frac{1}{1 - 2\varepsilon/3}. \tag{14}$$

In the corresponding computer program the levels are arranged in order of increasing energy and each level corresponds to $n_\perp + 1$ doubly degenerate states.

2.2. CLEMENGER PARAMETRIZATION FOR A SPHEROIDAL ATOMIC CLUSTER

This time the dimensionless semiaxes of the spheroid are given by

$$a = \left(\frac{2-\delta}{2+\delta}\right)^{1/3} \; ; \; c = \left(\frac{2+\delta}{2-\delta}\right)^{2/3} \; ; \; \frac{a}{c} = \frac{2-\delta}{2+\delta} = a^3 \; ; \; c = \frac{1}{a^2} \tag{15}$$

and the harmonic oscillator part of the potential [24] is given by

$$V = \frac{M\omega_0^2 R_0^2}{2}\left[\rho^2\left(\frac{2+\delta}{2-\delta}\right)^{2/3} + z^2\left(\frac{2-\delta}{2+\delta}\right)^{4/3}\right], \tag{16}$$

where ω_0 is a constant which for an atomic cluster may be estimated by the equation

$$\hbar\omega_0(N) = \frac{49 \text{ eV bohr}^2}{r_s^2 N^{1/3}}\left[1 + \frac{t}{r_s N^{1/3}}\right]^{-2} = \frac{13.72 \text{ eV Å}^2}{r_s R_0}\left[1 + \frac{t}{r_s N^{1/3}}\right]^{-2} \tag{17}$$

which is $3.0625N^{-1/3}$ for $N \gg 0.046$ in case of Na clusters. Since we consider solely monovalent elements, N in this eq. is the number of atoms for the family of clusters $\mathrm{M}_N^{Z\pm}$, r_s is the Wigner-Seitz radius expressed in atomic units, and t denotes the electronic spillout for the neutral cluster. In units of $\hbar\omega_0$ the eigenvalues are given by

$$\epsilon = \frac{2}{(2-\delta)^{1/3}(2+\delta)^{2/3}}\left[n + \frac{3}{2} + \delta\left(n_\perp - \frac{n}{2} + \frac{1}{4}\right)\right]. \tag{18}$$

The low lying energy levels for the six shells (main quantum number $n = 0, 1, 2, 3, 4, 5$) can be seen in Fig. 1. Besides the important degeneracy at a spherical shape ($\delta = 0$), one also have degeneracies at some superdeformed shapes, *e.g.* for prolate shapes at the ratio $c/a = (2+\delta)/(2-\delta) = 2$ *i.e.* $\delta = 2/3$.

3. SHELL CORRECTIONS

We split each single-particle degenerate level so that we use double-degenerate states (spin up and spin down) at input of shell, δU, and pairing corrections, δP, arranged in order of increasing energy. The total shell correction for protons and neutrons is given by

$$\delta U_p = \sum_{\nu=1}^{n} 2E_\nu - \tilde{U} \; ; \; \delta U_p + \delta U_n = \delta U \; ; \; \delta E = \delta U + \delta P. \tag{19}$$

Calculations for neutrons are similar with those for protons, hence we shall consider only protons in the following. We have infinite-depth potential wells, hence the level

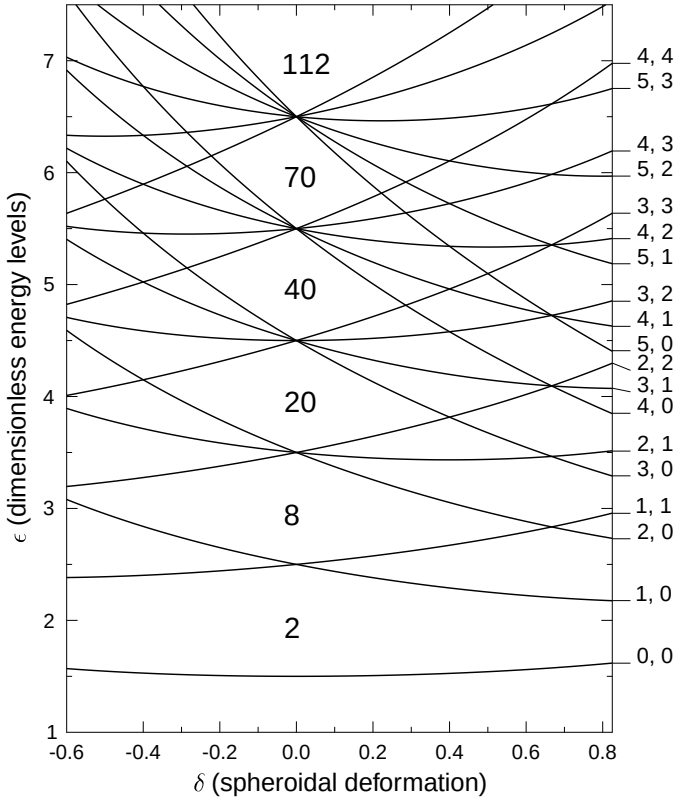

Fig. 1 – Harmonic oscillator energy levels in units of $\hbar\omega_0$ *versus* deformation δ. The quantum numbers $n, n_\perp$ are given for each level at the right-hand side of the figure. $\varepsilon = 6\delta/(6+\delta)$.

spectrum $\{\epsilon_i\}$ is discrete, and the level density g may be represented as a sum of delta functions. The smooth component $g_0(\epsilon)$ describing the average behavior of the level distribution and the oscillating component $\delta g(\epsilon)$ has a period of about $\hbar\omega_0^0$. The smoothed-level distribution density may be obtained by averaging the actual distribution over a finite energy interval $\Gamma \simeq \hbar\omega_0^0$

$$\tilde{g}(\epsilon) = \int_{-\infty}^{+\infty} \zeta\left(\frac{\epsilon-\epsilon'}{\gamma}\right) g(\epsilon')\,\mathrm{d}\epsilon' = \frac{1}{\gamma}\sum_{i=1}^{\infty}\left(\frac{\epsilon-\epsilon'}{\gamma}\right), \tag{20}$$

where $\gamma = \Gamma/\hbar\omega_0^0$.

At a given γ, all states producing a finite contribution to $\tilde{g}$, for $\epsilon \leq \tilde{\lambda}$, where $\tilde{\lambda} = E_F/\hbar\omega_0^0$ represents the Fermi energy, must be included. The level density fluctuations of faraway occupied levels could affect the level density $\tilde{g}$ and, consequently, the uniform level distribution energy $\tilde{U}$. This fact is of great importance for calculation of the shell correction obtained as a small difference of two large quantities.

In case of $m = 3$, frequently used in practice, the level density of the continuous level distribution is expressed as

$$\tilde{g}(\epsilon) = \left\{ \sum_{i=1}^{n_m} [2.1875 + y_i(y_i(1.75 - y_i/6) - 4.375)] e^{-y_i} \right\} (1.77245385\gamma)^{-1}. \quad (21)$$

The summation is performed up to the level n_m fulfilling the condition $|x_i| \geq 3$.

The Fermi energy $\tilde{\lambda}$ of a smoothed level distribution may be obtained from

$$N_p = \sum_{i=1}^{\infty} \left[1 + \mathrm{erf}(x_{iF}) + \frac{e^{-x_{iF}^2}}{\sqrt{\pi}} P_m(x_{iF}) \right], \quad (22)$$

where $P_0 = 0$; $P_1 = x_{iF}$; $P_2 = -x_{iF}(0.5y_{iF} - 1.75)$; $P_3 = x_{iF}[y_{iF}(y_{iF} - 8) + 14.25]/6$; $y_{iF} = x_{iF}^2 = (\tilde{\lambda} - \epsilon_i)^2/\gamma^2$.

This nonlinear equation, with $\tilde{\lambda}$ as unknown, can be solved numerically by using an iteration scheme (Newton-Raphson), which refines an initial guess $\tilde{\lambda}_0 = (\epsilon_n + \epsilon_{n+1})/2$ with $n = N_p/2$. For levels far away from the Fermi energy, satisfying the relationship $|x_{iF}| \geq 3$, we can approximate $N_p = \sum_i 1$, if $\epsilon < \tilde{\lambda}$ and $N_p = 0$, if $\epsilon > \tilde{\lambda}$.

If $\tilde{g_s}$ is the density of states at Fermi energy, $\tilde{\lambda}$, obtained from the shell correction calculation $\tilde{g_s} = \mathrm{d}Z/\mathrm{d}\epsilon$, (which is expressed in number of levels per $\hbar\omega_0^0$ spacing when the energy levels are expressed in units of $\hbar\omega_0^0$) the level density is half of this quantity:

$$\tilde{g_n} = \tilde{g_s}/2 = \frac{1}{2} \frac{\mathrm{d}Z}{\mathrm{d}\epsilon}. \quad (23)$$

The total energy of the uniform level distribution, $\tilde{U}$, reproduces the average behavior of the total energy but not its local fluctuations. It can be obtained from the relationship

$$\tilde{u} = \sum_{i=1} \left\{ \epsilon_i \left[1 + \mathrm{erf}(x_{iF}) + \frac{e^{-x_{iF}^2}}{\sqrt{\pi}} P_m(x_{iF}) \right] + \frac{\gamma e^{-x_{iF}^2}}{\sqrt{\pi}} Q_m(x_{iF}) \right\}, \quad (24)$$

where

$$Q_m = 1 + \sum_{k=1}^{m} a_{2k}(H_{2k} + 4kH_{2k-2}) = -a_{2m}H_{2m} \quad (25)$$

and $Q_0 = -1$; $Q_1 = y_{iF} - 0.5$; $Q_2 = y_{iF}(1.5 - 0.5y_{iF}) - 0.375$; $Q_3 = \{y_{iF}[11.25 + y_{iF}(y_{iF} - 7.5)] - 1.875\}/6$.

4. BCS PAIRING CORRECTIONS

We consider, like in the preceding section, a set of doubly degenerate levels $\{\epsilon_i\}$ expressed in units of $\hbar\omega_0^0$. In the absence of pairing field, the first $Z/2$ levels

are occupied, from a total number of n_t levels available. Only few levels below (n) and above (n') the Fermi energy are contributing to the pairing correlations. Usually $n' = n$. For proton levels the order of the Fermi level is $Z/2$ and the order of the lowest level taken into account in pairing calculations is $N_1 = Z/2 - n + 1$. The order of the corresponding highest level is $N_2 = Z/2 + n'$. If $\tilde{g}_s$ is the density of states at Fermi energy obtained from the shell correction calculation $\tilde{g}_s = \mathrm{d}Z/\mathrm{d}\epsilon$, expressed in number of levels per $\hbar\omega_0^0$ spacing, the level density is half of this quantity: $\tilde{g_n} = \tilde{g}_s/2$.

We can choose as computing parameter, the cut-off energy (in units of $\hbar\omega_0^0$), $\Omega \simeq 1 \gg \tilde{\Delta}$. Let us take the integer part of the following expression

$$\Omega\tilde{g}_s/2 = n = n'. \tag{26}$$

When from calculation we get $n > Z/2$ we shall take $n = Z/2$ and similarly if $n' > n_t - Z/2$ we consider $n' = n_t - Z/2$.

The gap parameter $\Delta = |G| \sum_k u_k v_k$ and the Fermi energy with pairing corellations λ (both in units of $\hbar\omega_0^0$) are obtained as solutions of a nonlinear system of two BCS equations

$$n' - n = \sum_{k=k_i}^{k_f} \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}, \tag{27}$$

$$\frac{2}{G} = \sum_{k=k_i}^{k_f} \frac{1}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}, \tag{28}$$

where $k_i = Z/2 - n + 1$; $k_f = Z/2 + n'$.

The pairing interaction G is calculated from a continuous distribution of levels

$$\frac{2}{G} = \int_{\tilde{\lambda}-\Omega}^{\tilde{\lambda}+\Omega} \frac{\tilde{g}(\epsilon)\,\mathrm{d}\epsilon}{\sqrt{(\epsilon - \tilde{\lambda})^2 + \tilde{\Delta}^2}}, \tag{29}$$

where $\tilde{\lambda}$ is the Fermi energy deduced from the shell correction calculations and $\tilde{\Delta}$ is the gap parameter, obtained from a fit to experimental data, usually taken as $\tilde{\Delta} = 12/\sqrt{A}\hbar\omega_0^0$.

Real positive solutions of BCS equations are allowed if

$$\frac{G}{2} \sum_k \frac{1}{|\epsilon_k - \lambda|} > 1, \tag{30}$$

i.e. for a pairing force (G-parameter) large enough at a given distribution of levels. The system can be solved numerically by Newton-Raphson method refining an initial guess

$$\begin{aligned} \lambda_0 &= (n_s\epsilon_d + n_d\epsilon_s)/(n_s + n_d) + G(n_s - n_d)/2, \\ \Delta_0^2 &= n_s n_d G^2 - (\epsilon_d - \epsilon_s)/4, \end{aligned} \tag{31}$$

where ϵ_s, n_s are the energy and degeneracy of the last occupied level and ϵ_d, n_d are the same quantities for the next level. Solutions around magic numbers, when $\Delta \to 0$, have been derived by Kumar *et al.* [30].

As a consequence of the pairing correlation, the levels situated below the Fermi energy are only partially filled, while those above the Fermi energy are partially empty; there is a given probability for each level to be occupied by a quasiparticle

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}\right] \tag{32}$$

or a hole

$$u_k^2 = 1 - v_k^2. \tag{33}$$

Only the levels in the near vicinity of the Fermi energy (in a range of the order of Δ around it) are influenced by the pairing correlations. For this reason, it is sufficient for the value of the cut-off parameter to exceed a given limit $\Omega \gg \tilde{\Delta}$, the value in itself having no significance.

At a given deformation, the pairing correction to the deformation energy is calculated by using the relationship $\delta p = p - \tilde{p}$, representing the difference between the pairing correlation energies for the discrete level distribution

$$p = \sum_{k=k_i}^{k_f} 2v_k^2\epsilon_k - 2\sum_{k=k_i}^{Z/2}\epsilon_k - \frac{\Delta^2}{G} \tag{34}$$

and for the continuous level distribution

$$\tilde{p} = -(\tilde{g}\tilde{\Delta}^2)/2 = -(\tilde{g}_s\tilde{\Delta}^2)/4. \tag{35}$$

A term $G(\sum_{k_i}^{k_f} v_k^4 - \sum_{k_i}^{Z/2} 1)$ is supposed to be negligibly small.

Compared to shell correction, the pairing correction is out of phase and smaller.

5. LIPKIN-NOGAMI PAIRING CORRECTIONS

In the following we shall follow the Ref. [10] for even-even nuclei. The effective interaction pairing gap *expression*, Δ_G, is different from the *model* average pairing gap, $\bar{\Delta}$, which may be compared with experimental odd-even mass differences. Instead of conventional $\Delta_G = 12/\sqrt{A}$, we use

$$\Delta_{Gn} = \frac{3.3B_s}{N^{1/3}} \;\; ; \quad \Delta_{Gp} = \frac{3.3B_s}{Z^{1/3}} \tag{36}$$

with the deformation-dependent surface term $B_s = 1$, as for spherical nuclei.

From Strutinsky shell corrections the average level density of doubly degene-

rate levels at Fermi energy $\tilde{\lambda}$ is given by eq. (23) or with notations from [10]

$$\tilde{\rho} = \frac{1}{2}\tilde{g}(\tilde{\lambda}), \tag{37}$$

where $\tilde{g}$ is the smooth level density in Strutinsky's shell correction method and $\tilde{\lambda}$ is the Fermi energy of the smoothed single-particle energy. In the LN case the shifted single-particle energies ϵ_k are assumed to be equally spaced; they are related to single-particle energies e_k by

$$\epsilon_k = e_k + (4\lambda_2 - G)v_k^2 \ , \ k = N_1, N_1+1, ..., N_2. \tag{38}$$

Since $v_k^2 \simeq 1$ far below Fermi surface and $v_k^2 \simeq 0$ far above, the corresponding single-particle energy distribution is approximately uniform far above and far below the Fermi surface but spread apart by the amount $4\lambda_2 - G$ close to the Fermi surface. The increased stability associated with gs configurations is due to the low level densities near Fermi surface.

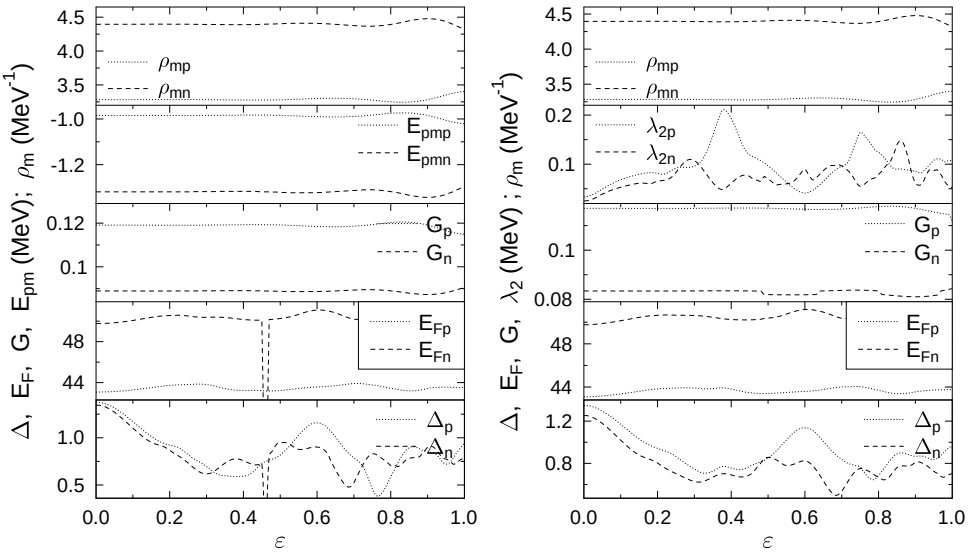

Fig. 2 – Some quantities of BCS (left) and Lipkin-Nogami (right) pairing calculations for ^{240}Pu using the energy levels of spheroidal harmonic oscillator. ρ_{mp} and ρ_{mn} are the densities of states at Fermi energy, eq. (37) for protons and neutrons. E_{pmp} and E_{pmn} are $\tilde{p} \times \hbar\omega_0^0$ for protons and neutrons. The solutions of BCS and Lipkin-Nogami set of equations are Fermi energies E_{Fp} and E_{Fn}, the gaps Δ_p and Δ_n, and λ_{2p} and λ_{2n}.

The dependence of pairing strength, G, on the effective interaction pairing gap, Δ_G, is obtained by assuming a constant level density for the average nucleus in the

vicinity of Fermi surface. In this way we may replace the sums by integrals:

$$\frac{1}{G}=\frac{\tilde{\rho}}{2}\int_{y1}^{y2}\frac{dx}{\sqrt{x^2+\Delta_G^2}}=\frac{\tilde{\rho}}{2}\left[\ln\left(\sqrt{y_2^2+\Delta_G^2}+y_2\right)-\ln\left(\sqrt{y_1^2+\Delta_G^2}+y_1\right)\right], \quad (39)$$

where

$$y_1=\frac{-Z/2+N_1-1}{\tilde{\rho}}=\frac{-n}{\tilde{\rho}}\ ;\ y_2=\frac{-Z/2+N_2}{\tilde{\rho}}=\frac{n'}{\tilde{\rho}}. \quad (40)$$

Pairing gap, Δ, Fermi energy, λ, number fluctuation constant, λ_2, occupation probability, v_k^2, shifted single-particle energies, ϵ_k, are determined by solving a system of $2(N_2-N_1)+5=2(n+n')-2+5=2(n+n')+3$ coupled nonlinear equations

$$N_{tot}=Z=2\sum_{N1}^{N2}v_k^2+2(N_1-1), \quad (41)$$

$$\frac{2}{G}=\sum_{N1}^{N2}\frac{1}{\sqrt{(\epsilon_k-\lambda)^2+\Delta^2}}, \quad (42)$$

$$v_k^2=\frac{1}{2}\left[1-\frac{\epsilon_k-\lambda}{\sqrt{(\epsilon_k-\lambda)^2+\Delta^2}}\right]\ ,\ k=N_1,N_1+1,...,N_2, \quad (43)$$

$$u_k^2=1-v_k^2\ ,\ k=N_1,N_1+1,...,N_2, \quad (44)$$

$$\epsilon_k=e_k+(4\lambda_2-G)v_k^2\ ,\ k=N_1,N_1+1,...,N_2, \quad (45)$$

$$\lambda_2=\frac{G}{4}\left[\frac{\left(\sum_{N1}^{N2}u_k^3v_k\right)\left(\sum_{N1}^{N2}u_kv_k^3\right)-\sum_{N1}^{N2}u_k^4v_k^4}{\left(\sum_{N1}^{N2}u_k^2v_k^2\right)^2-\sum_{N1}^{N2}u_k^4v_k^4}\right]. \quad (46)$$

This set of equations can be solved numerically by using the steepest descent method with Jacobian determinant.

The quasi-particle energy of the odd nucleon in an odd-A nucleus

$$E_k=\sqrt{(\epsilon_k-\lambda)^2+\Delta^2}+\lambda_2\ ,\ k=N_1,N_1+1,...,N_2. \quad (47)$$

In the LN model the quantity $\Delta+\lambda_2$ is identified with odd-even mass differences.

For even-even nuclei the pairing correlation energy plus quasi-particle energy is

$$E_{pc}=\sum_{N1}^{N2}2v_k^2e_k-\frac{\Delta^2}{G}-\frac{G}{2}\sum_{N1}^{N2}2v_k^4-4\lambda_2\sum_{N1}^{N2}u_k^2v_k^2. \quad (48)$$

For the average pairing correlation energy plus quasi-particle energy of an even-even nucleus we have

$$\tilde{E}_{pc} = \frac{\tilde{\rho}}{2}\left[(y_2 - G)\left(y_2 - \sqrt{y_2^2 + \Delta_G^2}\right) + (y_1 - G)\left(y_1 + \sqrt{y_1^2 + \Delta_G^2}\right)\right] + \frac{(G - 4\tilde{\lambda_2})\tilde{\rho}\Delta_G}{4}\left[\arctan\left(\frac{y_2}{\Delta_G}\right) - \arctan\left(\frac{y_1}{\Delta_G}\right)\right], \tag{49}$$

where

$$\tilde{\lambda}_2 = \left(\frac{A - C}{B - C}\right) \tag{50}$$

with

$$A = \left(\frac{\tilde{\rho}\Delta_G}{4}\right)^2 \left\{\left(\frac{2}{G\tilde{\rho}}\right)^2 - \left[\ln\left(\frac{\sqrt{y_2^2 + \Delta_G^2}}{\sqrt{y_1^2 + \Delta_G^2}}\right)\right]^2\right\}, \tag{51}$$

$$B = \left(\frac{\tilde{\rho}\Delta_G}{4}\right)^2 \left[\arctan\left(\frac{y_2}{\Delta_G}\right) - \arctan\left(\frac{y_1}{\Delta_G}\right)\right]^2, \tag{52}$$

$$C = \frac{\tilde{\rho}\Delta_G}{32}\left[\Delta_G\left(\frac{y_2}{y_2^2 + \Delta_G^2} - \frac{y_1}{y_1^2 + \Delta_G^2}\right) + \arctan\left(\frac{y_2}{\Delta_G}\right) - \arctan\left(\frac{y_1}{\Delta_G}\right)\right], \tag{53}$$

Pairing correction

$$\delta P = E_{pc} - \tilde{E}_{pc}. \tag{54}$$

As in BCS model, compared to shell correction, the pairing correction is out of phase and smaller.

6. RESULTS

We give in Fig. 2 some quantities of BCS (left) and Lipkin-Nogami (right) pairing calculations for ^{240}Pu using the energy levels of spheroidal harmonic oscillator. In this case $\Delta_{Gp} = 0.72578$ MeV and $\Delta_{Gn} = 0.62670$. For neutron energy levels at $\varepsilon = 0.460$ the BCS pair collapses which is seen in Fig. 2 as discontinuities for trivial solutions $\Delta_n = E_{Fn} = 0$ MeV. A remarkable fact is the absence of such a collapse for LN theory.

The famous double-hump variation of the total shell plus pairing correction energy $\delta E = \delta U + \delta P$ is shown in Fig. 3 for ^{240}Pu. The smoothing effect of pairing is evident. The total correction energy δE in case of LN is slightly shifted to larger values compared to BCS.

In a similar way behaves δE of the superheavy nucleus ^{286}Cn shown in Fig. 4. This time there is a relatively large range of values of deformation $\varepsilon = (0, 0.130)$ for BCS and $(0, 0.120)$ for LN where both kinds of pairing corrections for proton

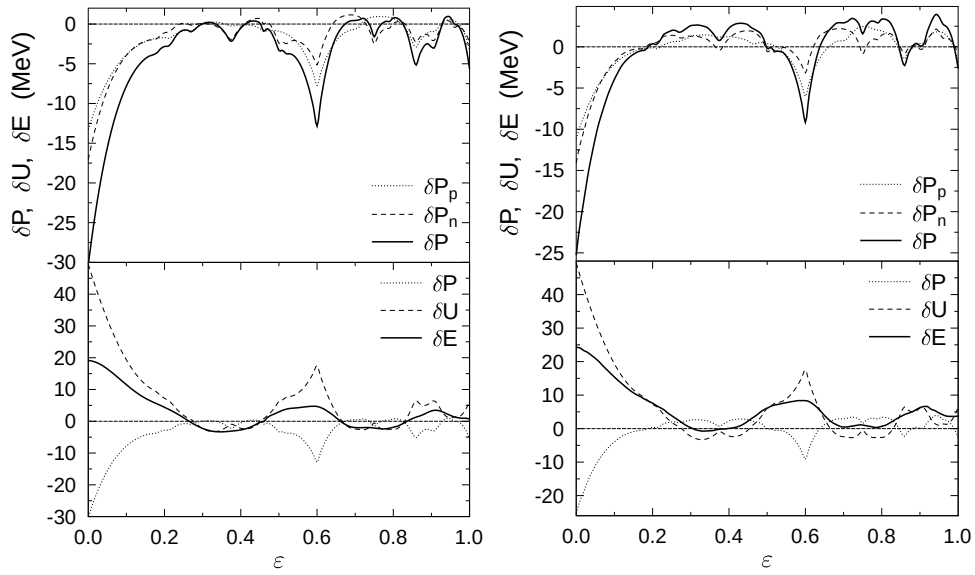

Fig. 3 – Microscopic pairing corrections (top) and shell plus pairing corrections (bottom) for ^{240}Pu using harmonic oscillator energy levels. BCS (left) and LN (right) calculations.

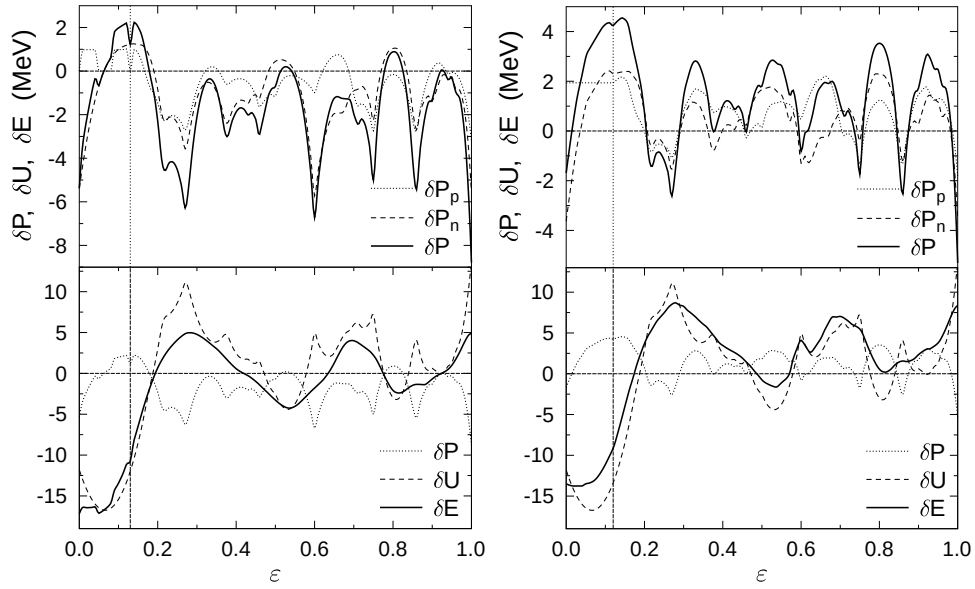

Fig. 4 – Microscopic pairing corrections (top) and shell plus pairing corrections (bottom) for ^{286}Cn using harmonic oscillator energy levels. BCS (left) and LN (right) calculations.

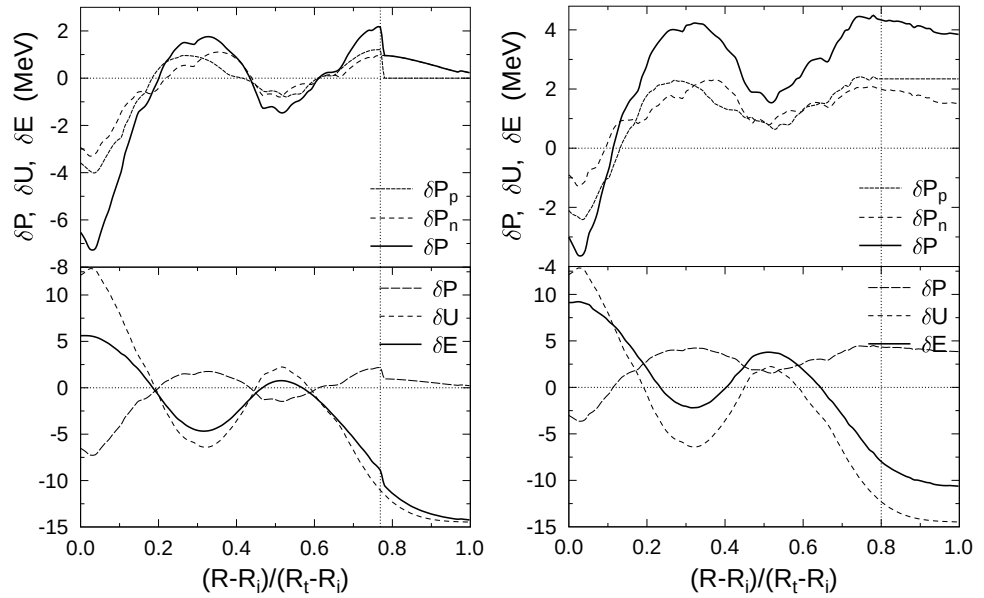

Fig. 5 – Microscopic pairing corrections (top) and shell plus pairing corrections (bottom) for ^{258}Fm at the mass asymmetry $\eta = 0$. The two center shell model energy levels are used.

energy levels are in collapse due to the proximity of a magic number of protons (near $Z = 112$). $\Delta_{Gp} = 0.68461$ MeV and $\Delta_{Gn} = 0.59110$.

As a last example we consider in Fig. 5 the microscopic pairing corrections and shell plus pairing corrections for ^{258}Fm at the mass asymmetry $\eta = 0$ calculated by using the most advanced two-center shell model [22]. R_i is the initial value of the separation distance between fragment centers and R_t is the separation distance at the touching point. Now the high density of levels for which both kinds of pairing collapses occurs not far from the touching point configurations, where the identical fragments posses a magic number of protons $Z_1 = Z_2 = 50$. The range corresponds to $x = (R - R_i)/(R_t - R_i) = (0.769, 1.0)$ for BCS and $(0.800, 1.0)$ for LN. $\Delta_{Gp} = 0.71096$ MeV and $\Delta_{Gn} = 0.61042$. Despite the almost simultaneous collapse of BCS and LN pairing, the net result of shell plus pairing corrections looks better for LN pairing theory in both Figs 5 and 3.

In conclusion the Lipkin-Nogami pairing theory offers some advantages compared to BCS from principial as well as practical point of view.

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