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IS IT NECESSARY TO READJUST THE PAIRING FORCE CONSTANT DUE TO PARTICLE NUMBER PROJECTION?

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Abstract. The difference between the results of the conventional fixed particle number pairing theory with a pairing force strength taken from the BCS approximation (FBCS) and the results of a fixed particle number theory with a pairing strength constant calculated directly from the odd–even mass differences (FPT) is studied. To date the FPT has been applied along the so called [1] "ground state valley" of the Potential Energy Surface (PES) for ^{240}Pu. The results show fluctuations of the difference between the FBCS and the FPT energies along this path up to 1.64 MeV.

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1. Introduction

In our previous papers [1] the differences between the results of the BCS theory and those of a theory with conserved particle number as a function of deformation, in the special case of the Potential Energy Surface (PES) of ^{240}Pu, have been studied. The use of particle number projection before variation (FBCS) produces noticeable fluctuations of the BCS pairing energy with respect to the FBCS energy over the whole PES. Therein and in the common realizations of the FBCS theory (especially in the case of heavy nuclei) it is tacitly assumed that the value of the pairing force strength G can be taken from the BCS theory. In the BCS framework the best way to estimate this constant consists in calculating first the "experimental" value of the pairing gap parameter Δ using experimental binding energies together with the well known odd–even mass-difference formula [2, 3] and second, pinning down the pairing force strength G from the BCS-equations such as to produce the same Δ. It is a priori not clear why the BCS solutions should be valid and relevant for the FBCS case.

For example, it was found [4] that the value of the pairing gap parameter Δ depends on how the particle number uncertainty has been treated (in the case of the Lipkin–Nogami Approximation (LN)). Similar conclusions have been reached in [5]. In [6] it was stressed that the errors due to particle number nonconservation do not depend much upon the special type of forces but mainly on the relative strength of the attractive short range part of the force compared to the average level spacing around the Fermi level.

Obviously a problem connected to the proper estimation of the value of the pairing strength parameter in elaborate pairing theories arises. In the usual FBCS instead of the value of the pairing gap parameter Δ one calculates [4] the quantity D measuring the "diffuseness" of the Fermi surface implied by various eigenfunctions. This is due to the fact that in the case of a projected theory, we can no longer use the parameter Δ as a measure for how strong the pairing correlations are. Nevertheless having the binding energies from an exact particle number projected theory one can calculate the gap parameter Δ and compare it to its experimental value [4].

The purpose of the present work is to add further insight into this problem by comparing the results of the fixed particle number pairing theory with a pairing force strength taken from the BCS approximation (FBCS) to the results of a fixed particle number theory (FPT) where the strength of the pairing force is "properly" estimated. The "proper" estimation consists in calculating the pairing gap parameter Δ as a function of the pairing strength G by using directly the particle number projected binding energies via the odd-even mass differences formula. Then the proper value of G is obtained in such a way that the value of the pairing gap parameter Δ calculated directly from the equations for the projected energy to be equal to its "experimental" value (i. e. to its value calculated with the experimental binding energies). To date this has been done for the "ground state valley" of ^{240}Pu.

The PES (ground state valley) is calculated by applying the Shell-Correction Method (SCM) based on a deformed Woods-Saxon potential. Some brief information about the SCM, the BCS-approximation and the particle-number projected binding energies is given in Sec. 2. The results for ^{240}Pu and the discussion follow in Sec. 3.

2. The Fixed Particle Number Theory Within the Shell Correction Method

The "standard" fixed particle number theory (FBCS) implies determining the parameters v_k of the BCS wave function

$$|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^+ a_{\bar{k}}^-)|0\rangle \tag{1}$$

$$u_k^2 + v_k^2 = 1 \tag{2}$$

by directly minimizing the projected energy [1]:

$$E_{\mathrm{PROJ}} = 2\Bigg(\sum_{\substack{k>0,\\ k\neq \mathrm{odd}}} \varepsilon_k v_k^2 P^{(k)}_{(A/2-1)} - G \sum_{\substack{k>k'>0,\\ k,k_l\neq \mathrm{odd}}} u_k v_k u_{k'} v_{k'} P^{(k,k')}_{(A/2-1)} \Bigg) / P_{A/2} + \varepsilon_{\mathrm{odd}} \tag{3}$$

where G is the ground state value of the pairing force strength, $\bar{\varepsilon}_k = \varepsilon_k - G/2$ are the modified single particle energies, and $P_N^{(r)}, P_N^{(r,r')}$ are the coefficients of the polynomials (in x) $\prod_{k>0,k\neq r}(u_k^2 + xv_k^2)$ and $\prod_{k>0,k\neq r,r'}(u_k^2 + xv_k^2)$, respectively. For more details of the employed projection technique one can consult Ref. [1]. As usual in the case of heavy nuclei the energies (3) are calculated for protons and neutrons separately.

Obviously this is the best that can be done, given the BCS ansatz (1) for the many-body wave function. In order to solve the FBCS equations (3) one needs in addition the values of the pairing strength constants $G_{Z,N}$ for protons and neutrons, respectively. As already mentioned, they are usually taken from the BCS approximation, i. e. by solving the BCS equation with a pairing gap parameter values $\Delta_{Z,N}$ extracted from the "experimental" odd-even mass-difference formula [2]

$$\Delta_Z = \frac{1}{4}(B(Z-2,N) - 3B(Z-1,N) + 3B(Z,N) - B(Z+1,N)) \tag{4}$$

with Δ_Z — the pairing gap parameter for protons and $B(Z,N)$ — the corresponding experimental binding energies. Analogous formula holds also for neutrons.

What we have done is to express the binding energies necessary to calculate the pairing gap parameter $\Delta_{Z,N}$ (4) as a function of the pairing strength parameter $G_{Z,N}$ by using directly the particle number projected energy (3). Requiring the so calculated value of $\Delta_{Z,N}$ to be equal to the "experimental" one, one deduces the proper pairing strength value, which corresponds to the projected binding energies.

The binding energies themselves are calculated by using the Strutinsky expression

$$E_{\text{TOTAL}} = E_{\text{LDM}} + \delta E_{\text{SHELL}} + \delta E_{\text{PAIR}} \tag{5}$$

where E_{LDM}, δE_{SHELL} and δE_{PAIR} denote the liquid drop, the Strutinsky shell correction and the pairing correction energies, respectively. The shell correction and the liquid drop energies are calculated by standard prescriptions and formulae [7, 8].

The SCM used is based on a deformed Woods-Saxon potential with a shape parametrization described in [6, 7]. This deformed Woods-Saxon potential involves three free parameters c, h and α, where c describes the elongation of the shapes, h — the neck parameter (chosen in a such way that $h = \alpha = 0$ describes approximately the family of threshold shapes) and α corresponds to the left-right asymmetry of the fissioning nuclei, with $\alpha = 0$ describing symmetric shapes. Small values of $h(\alpha = 0)$ coincide with the so called "liquid drop valley".

3. Results and Discussion

In the present work all binding energies needed for the calculation of the gap parameter $\Delta_{Z,N}$ (4) for ^{240}Pu have been represented as functions of the pairing strength constant $G_{Z,N}$. The latter have been renormalized for the different isotopes and nuclei needed, according to the phenomenological estimates $G \approx \text{const}/A$, i. e. $G(A_2) = G(A_1) * A_1/A_2$ (e. g. [9]). Here A denotes the corresponding mass numbers.

The fit of the calculated to the "experimental" pairing gap value Δ requires the pairing strength value G to be renormalized. We find in general that in the exact particle number projected case one needs a stronger pairing force compared to the BCS case in order to reproduce the experimental odd-even mass difference. In the case of $^{240}_{94}$Pu the value of the pairing strength increases with 6 % for neutrons and with 3 % for protons.

The PES of the nucleus $^{240}_{94}$Pu has been calculated according to the standard FBCS and to the FPT methods described above. The present calculation of the PES as well as the discussion in [1] suggest that the significant deformation points for this nucleus are localized as follows: the ground state at values of the deformation parameters of about $c = 1.2$, $h = -0.145$, $\alpha = 0.0$; the first saddle point at $c = 1.24$, $h = 0.15$, $\alpha = 0.0$; the isomer minimum at $c = 1.41$, $h = 0.0$, $\alpha = 0.0$; and the second saddle point at $c = 1.66$, $h = -0.075$. The energy of the outer barrier can be lowered significantly, however, by parity violating, left-right asymmetric shapes. As mentioned above, small values of h, or more precisely the deformation points $c = 1.0$–1.8, $h = 0.0$, $\alpha = 0.0$, describe the so called "liquid drop valley". The values of the PES along the set of values $c = 1.0$- 1.8, $h = -0.145$, $\alpha = 0.0$ we call the "ground state valley".

The difference between the energies obtained from FPT and the standard FBCS approaches along the ground state valley are shown in Fig. 1. First of all one can see an expected decrease of the total SCM energy due to the stronger pairing force. For $^{240}_{94}$Pu its average value is about -1.2 MeV. This decrease, however, has but a minor influence on the dynamics of the system at hand. Much more important are the changes in the PES, connected with the height and structure of the fission barriers. The difference itself has fluctuations between 0.74 and 1.64 MeV. Minimal difference is obtained in the vicinity of the ground state ($c = 1.21$, $h = -0.15$). These preliminary results are obtained assuming a deformation independent pairing strength.

The fluctuations of the energy obtained in the present work do recommend the renormalization of the pairing strength when using the exact particle-number projection technique.

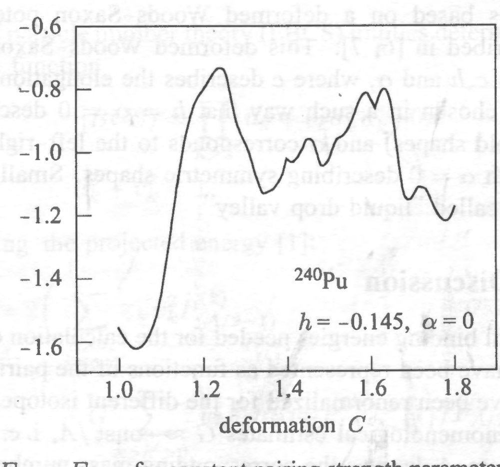

Fig. 1. The difference $E_{\text{FPT}} - E_{\text{FBCS}}$ for constant pairing strength parameters along the ground-state valley, as explained in text

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