# ACCESSING PAIRING CORRELATION FROM AVERAGE PARING GAPS ALONG POTENTIAL ENERGY SURFACES

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## Abstract

In this work, the paring correlation along the energy surfaces for some light nuclei has been investigated. To this end, constrained Hartree-Fock+BCS method with Skyrme interaction is employed. Variation of average paring gaps along with the Nilsson single- particle levels at each constrained nuclear shapes shows the relation between nuclear shapes, paring correlation and nature of single particle levels. The calculated results indicate that the effect of paring depends on the level density in the vicinity of highest occupied level.

**Keywords**: Skyrme Hartree-Fock + BCS method

## Introduction

Pairing correlations, which play not only a crucial role in superconducting solids but also contribute an important complement of nuclear shell structure (Bardeen, J., L. N. Cooper, and J. R. Schrieffer, 1957). The key feature of pairing correlations is the occurrence of an energy gap in the excitation spectrum.This gap manifests itself in two different kinds of energetic observables: first, there is a gap in the excitation spectra of even-even nuclei, which does not appear in the spectra of odd-mass number or odd-odd nuclei, and second, there occurs a shift between the interpolation curves of the ground-state binding energies of even-even as compared to odd-mass nuclei, which is called the odd-even mass staggering (Bender, M. et al, 2000). For light and medium-mass nuclei, the staggering has two components. The first one originates from pairing while the second, comparable in magnitude, has its roots in the deformed mean-field (Satula, W., J. Dobaczewski and W. Nazarewicz, 1998). Most often, pairing correlations are described within the Hartree-Fock framework by generalizing the mean-field concept to include a pairing field with the use of the BCS (Bardeen, Cooper, and Schrieffer) approximation by employing a self-consistent approach. We employ Skyrme interaction which can simplify the calculations with its zero-range form to successfully describe the masses, charge radii and excited states of finite nuclei. In this work, we will investigate the effects of pairing correlation in some selected even-even nuclei ($^{28}$Si, $^{22}$Ne, $^{36}$Mg) with the calculated potential energy surfaces by employing the Ev8 code (Ryssens, W. et al, 2014).

## Theoretical Framework

The full many-body Hamiltonian can be written as follows

$$H = \sum_{i=1}^{N} \hat{t}_i + \frac{1}{2}\sum_{i\neq j}^{N} \hat{V}(r_i, r_j) \qquad (1)$$

where the first term is the one-body kinetic energy, and the second term represents the two-body force with the Coulomb interaction. The simplified expression for the Hatree-Fock equation is obtained as

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$$\left(-\frac{\hbar^2}{2m}\nabla^2+\int d\mathbf{r}'\rho\ \mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\right)\varphi_i\ \mathbf{r}\ -\int d\mathbf{r}'\rho\ \mathbf{r},\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\varphi_i\ \mathbf{r}'\ =\varepsilon_i\varphi_i\ \mathbf{r}\ . \tag{2}$$

This equation is known as the Hartree-Fock equation which looks like the regular one-body Schrödinger equation, with the extra non-local term. The Skyrme interaction is one of the most widely used energy functional for nuclear structure calculations. In the Skyrme-Hartree-Fock approach, the total binding energy of the system is given by the sum of the kinetic and Coulomb energies as well as the Skyrme energy functional that models the effective interaction between nucleons is shown in the following equation (Bender, M., and P. H. Heenen, 2003),

$$\mathrm{E}=\mathrm{E}_{\mathrm{Coulomb}}+\mathrm{E}_{\mathrm{kin}}+\mathrm{E}_{\mathrm{Sk}}\,. \tag{3}$$

The Skyrme energy ( $E_{Sk}$ ), is derived by evaluating,

$$E_{Sk}=\frac{1}{2}\sum_{i,j}^{A}\int\phi_i^*\left(\mathbf{r}'\right)\phi_j^*\left(\mathbf{r}'\right)\hat{Y}_{sk}\left(\mathbf{r},\mathbf{r}'\right)\left(1-\hat{P}_M\hat{P}_\sigma\hat{P}_q\right)\phi_i\left(\mathbf{r}\right)\phi_j\left(\mathbf{r}\right)d\mathbf{r}\ d\mathbf{r}'\big|_{\mathbf{r}=\mathbf{r}'}\,. \tag{4}$$

The Hartree-Fock equations with Skyrme interaction is given by

$$\begin{aligned}E_{Sk}=\ & B_1\rho^2\ \mathbf{r}\ +B_2\sum_q\rho_q^2\ \mathbf{r}\ +B_3\ \rho\ \mathbf{r}\ \tau\ r\ -j^2\ \mathbf{r}\ \ +B_4\sum_q\ \rho_q\ \mathbf{r}\ \tau_q\ \mathbf{r}\ -j_q^2\ \mathbf{r}\\ &+B_5\rho\ \mathbf{r}\ \nabla^2\rho\ \mathbf{r}\ +B_6\sum_q\rho_q\ \mathbf{r}\ \nabla^2\rho_q\ \mathbf{r}\ +B_7\rho^\alpha\ \mathbf{r}\ \rho^2\ \mathbf{r}\ +B_8\rho^\alpha\ \mathbf{r}\ \sum_q\rho_q^2\ \mathbf{r}\\ &+B_9\left[\rho\ \mathbf{r}\ \nabla.J\ \mathbf{r}\ +S\ \mathbf{r}\ .\ \nabla\times j\ \mathbf{r}\ \ +\sum_q\ \rho_q\ \mathbf{r}\ \nabla.J_q\ \mathbf{r}\ +S_q\ \mathbf{r}\ .\ \nabla\times j_q\ \mathbf{r}\ \right]\\ &+B_{10}S^2\ \mathbf{r}\ +B_{11}\sum_q S_q^2\ \mathbf{r}\ +B_{12}S^2\ \mathbf{r}\ \rho^\alpha\ \mathbf{r}\ +B_{13}\rho^\alpha\ \mathbf{r}\ \sum_q S_q^2\ \mathbf{r}\ \rho_q^\alpha\ \mathbf{r}\\ &+B_{14}\ S\ \mathbf{r}\ .T\ \mathbf{r}\ -J^2\ \mathbf{r}\ \ +B_{15}\ S\ \mathbf{r}\ \nabla^2S\ \mathbf{r}\\ &+B_{16}\sum_q\ S_q\ \mathbf{r}\ .T_q\ \mathbf{r}\ -J_q^2\ \mathbf{r}\ \ \ +B_{17}\sum_q S_q\ \mathbf{r}\ \nabla^2S_q\ \mathbf{r}\ .\end{aligned} \tag{5}$$

The formulation of BCS theory and gap equation will be solved in pairing problems with the use of Hamiltonian that contains a single-particle part and residual interaction acting on the states k and –k. It has the form

$$\hat{H}=\sum_k\varepsilon_k^0\hat{a}_k^\dagger\hat{a}_k+\sum_{kk'>0}\left\langle k,-k\left|v\right|k',-k'\right\rangle\hat{a}_k^\dagger\ \hat{a}_{-k}^\dagger\hat{a}_{-k'}\hat{a}_{k'} \tag{6}$$

where $\hat{a}_k^\dagger\hat{a}_k$ is the creation operator of each pair. For the simple case, the matrix element $\left\langle k,-k\left|v\right|k',-k'\right\rangle$ is assumed to be independent of the state k and is given by a constant number, $-G$. The Hamiltonian then becomes

$$\hat{H}=\sum_k\varepsilon_k^0\hat{a}_k^\dagger\hat{a}_k-G\sum_{kk'>0}\hat{a}_k^\dagger\ \hat{a}_{-k}^\dagger\hat{a}_{-k'}\hat{a}_{k'}\,. \tag{7}$$

The approximate BCS ground state wave function of the Hamiltonian is

$$\left|BCS\right\rangle=\prod_{k>0}^{\infty}(u_k+v_k\,\hat{a}_k^\dagger\,\hat{a}_{-k}^\dagger)\left|0\right\rangle. \tag{8}$$

We have to use the variational principle with a constraint to the particle number.

$$\hat{H}' = \hat{H} - \lambda N \ . \tag{9}$$

The Lagrange multiplier $\lambda$ is determined by the condition that the expectation value of the particle number operator with respect to the BCS state must be the particle number N of the system,

$$\left\langle BCS \middle| \hat{N} \middle| BCS \right\rangle = 2\sum_{k>0} v_k^2 = N, \tag{10}$$

and the expectation value of the constrained Hamiltonian leads to

$$\left\langle BCS \middle| \hat{H} - \lambda \hat{N} \middle| BCS \right\rangle = 2\sum_{k>0} (\varepsilon_k^0 - \lambda) v_k^2 - G\left( \sum_{k>0} u_k v_k \right)^2 - G\sum_{k>0} v_k^4 \ . \tag{11}$$

The occupation probability of each paired state can be calculated by solving the gap equation iteratively.

This obtained

$$\begin{pmatrix} u_k^2 \\ v_k^2 \end{pmatrix} = \frac{1}{2}\left[ 1 \pm \frac{\varepsilon_k^0 - \lambda}{\sqrt{(\varepsilon_k^0 - \lambda)^2 + \Delta^2}} \right] \tag{12}$$

where, $v_k^2$ and $u_k^2$ are occupation and inoccupation probabilities of the single particle levels k or –k. The gap equation becomes

$$\Delta_k = \frac{G}{2}\sum_{k>0} \frac{\Delta_k}{\sqrt{\varepsilon_k^0 - \lambda\ ^2 + \Delta_k^2}}. \tag{13}$$

The energy of the system in equation (7) becomes

$$E = 2\sum_{k>0} v_k^2 \varepsilon_k^0 - \frac{\Delta^2}{G} \tag{14}$$

where, $\frac{\Delta^2}{G}$ is called the pairing energy.

These occupation probabilities $v_k^2$ are used in replacing all the sums over the occupied orbital by a sum over all orbital multiplied with the corresponding occupation probabilities:

$$\sum_{i=1}^{A} .... \Rightarrow \sum_{k} v_k^2 \ . \tag{15}$$

If the sum over k is unrestricted, the sums in equation (13) diverge. One has to introduce cut-off energy in these sums. Therefore, in the calculations including pairing interaction; an additional parameter such as the pairing cut-off or the size of the pairing window is needed.

## Results and Discussion

The occurrence of gaps or regions of the low single particle level density around the Fermi surface is correlated with the deformed ground state energies. Thus, it is necessary to calculate the potential energy surfaces to predict the shape of the nucleus whether it has stable or deformed nature. In this framework, the constrained quadrupole moment is added to the Hamiltonian to generate energy surfaces. We calculate the potential energy surfaces as a function of quadrupole deformation parameter using constrained Hartree-Fock method as follows

$$\langle H' \rangle = \langle H \rangle - \lambda \langle \hat{Q} \rangle, \tag{16}$$

The deformation parameter $\beta_{\ell m}$ is related to the total mass of the moment which can be seen as follows

$$\beta_{\ell m} = \frac{4\pi}{3R_0^{\ell} A} \langle \hat{Q}_{\ell m} \rangle \tag{17}$$

The connections between $q_i$ and the Cartesian quadrupole moments are given by the following equations

$$\langle \hat{Q}_x \rangle = -\frac{1}{2}\ q_1 - q_2 \tag{18}$$

$$\langle \hat{Q}_y \rangle = -\frac{1}{2}\ q_1 + \ 2q_2 \tag{19}$$

$$\langle \hat{Q}_z \rangle = \frac{1}{2}\ 2q_1 + \ q_2\ . \tag{20}$$

An alternate representation is given in terms of the deformation parameter ($q$) and the triaxiality angle ($\gamma$). Their relationship can be represented by

$$q_1 = q\cos\ \gamma\ - \frac{1}{\sqrt{3}} q \sin\ \gamma \tag{21}$$

$$q_2 = \frac{2}{\sqrt{3}}\ q\ \sin\ \gamma\ . \tag{22}$$

In this work, Ev8 code is used to solve the mean-field equations for the Skyrme energy density functional. The single particle wave functions are discretized on a 3-dimensional (3D) Cartesian mesh to solve the mean-field equations (Ryssens, W. et al, 2014). There are many sets of the Skyrme parameters which have been generated to reproduce the nuclear matter properties. In this work, the Sly4 and SGII parameter sets are chosen because they are powerful to investigate neutron-rich nuclei. The Sly4 parameter set provides more consistent binding energies with experimental data than the SGII parameter set as shown in Table 1.1. These experimental data are reported by the National Nuclear Data Center (https://www.nndc.bnl.gov/nudat2/). For this reason, Sly4 parameter set will be used in this work.

**Table 1.1 Comparison of ground state minimum energies for each parameter set and experimental data.**

| Nucleus | SGII | Sly4 | Experimental data |
|---|---|---|---|
| $^{28}$Si | 243.49 MeV | 234.56 MeV | 236.54 MeV |
| $^{22}$Ne | 187.91 MeV | 177.45 MeV | 177.77 MeV |
| $^{36}$Mg | 283.63 MeV | 263.08 MeV | 260.78 MeV |

The calculated potential energy surfaces (PES) are depicted in Fig. 1(a) for (i)$^{28}$Si, (ii)$^{22}$Ne and (iii)$^{36}$Mg. In general, the nuclei having minimum energy located at the positive deformation parameter describes the prolate shape whereas the minimum energy with negative deformation parameter stands for the oblate shape. The energy surface for $^{28}$Si shows a deep oblate minimum, while that for $^{22}$Ne and $^{36}$Mg show prolate minimum. As can be seen in Fig 1, $^{28}$Si nucleus has energy minimum of oblate configuration which has the ground state energy of -234.56 MeV at $\beta_2$ = -0.32. Next to $^{28}$Si, the PES of $^{22}$Ne nucleus shows the prolate configuration with ground state energy (-177.45 MeV) and its quadrupole deformation is 0.42. The potential energy surface of $^{36}$Mg nucleus shows the prolate configuration ($\beta_2$ = 0.39) with the ground state minimum of nearly -263 MeV.

It is well known that pairing plays a decisive role in the open shell nuclei. The energy gap is a measure of the width of the transition between highly occupied states and unoccupied ones. The appropriate pairing strength (G) is considered to reproduce ground state binding energies. The paring strength $G = 410\,\mathrm{MeVfm}^3$ is used for both protons and neutrons in this calculation. A smooth pairing energy cut-off of 5 MeV around the Fermi level is also used to overcome the divergence case. The zero-range density-dependent pairing force is employed for the pairing interaction as follows

$$V(r_1, r_2) = -g\frac{1-\hat{P}_\sigma}{2}\left(1-\frac{\rho\ \bar{r}}{\rho_0}\right)\delta\ r_1 - r_2 \qquad (23)$$

where $\hat{P}_\sigma$ is the spin-exchange operator, $\rho_0 = 0.16\ \mathrm{fm}^{-3}$ and $r = \frac{r_1 - r_2}{2}$.

The corresponding average neutron pairing gaps as a function of quadruple deformation for $^{28}$Si, $^{22}$Ne and $^{36}$Mg are depicted in Fig. 1 (b). In $^{28}$Si and $^{22}$Ne, there is no pairing gap at the absolute minimum; it can be assumed that there is no pairing effect at these regions. It is predicted that the energy spacing between next unoccupied level and last occupied one is larger than the energy available from pairing of nucleons in the last occupied levels. For $^{36}$Mg nucleus, the effect of pairing correlation becomes weaker as the paring gap decreases near the deformed ground state.

The formation of deformed minima can be related to the occurrence of gaps or regions of low single particle level density around the highest occupied level. To illustrate the effect of pairing correlation and the level density, the neutron single-particle energy levels versus quadruple deformation for the selected nuclei are depicted in Fig. 1 (c). For deformed nuclei such as $^{28}$Si, $^{22}$Ne and $^{36}$Mg; the deformation removes the degeneracy of energy levels at spherical shape and energy levels split-up according to their angular momentum. Solid curves correspond

to levels with positive parity whereas short-dashed curves denote levels with negative parity. The red circles indicated the magic number. From these figures, it can be seen that the lower level density leads to smaller pairing gaps (or pairing correlation) near local minima, on the other hand, denser level density to larger pairing effects.

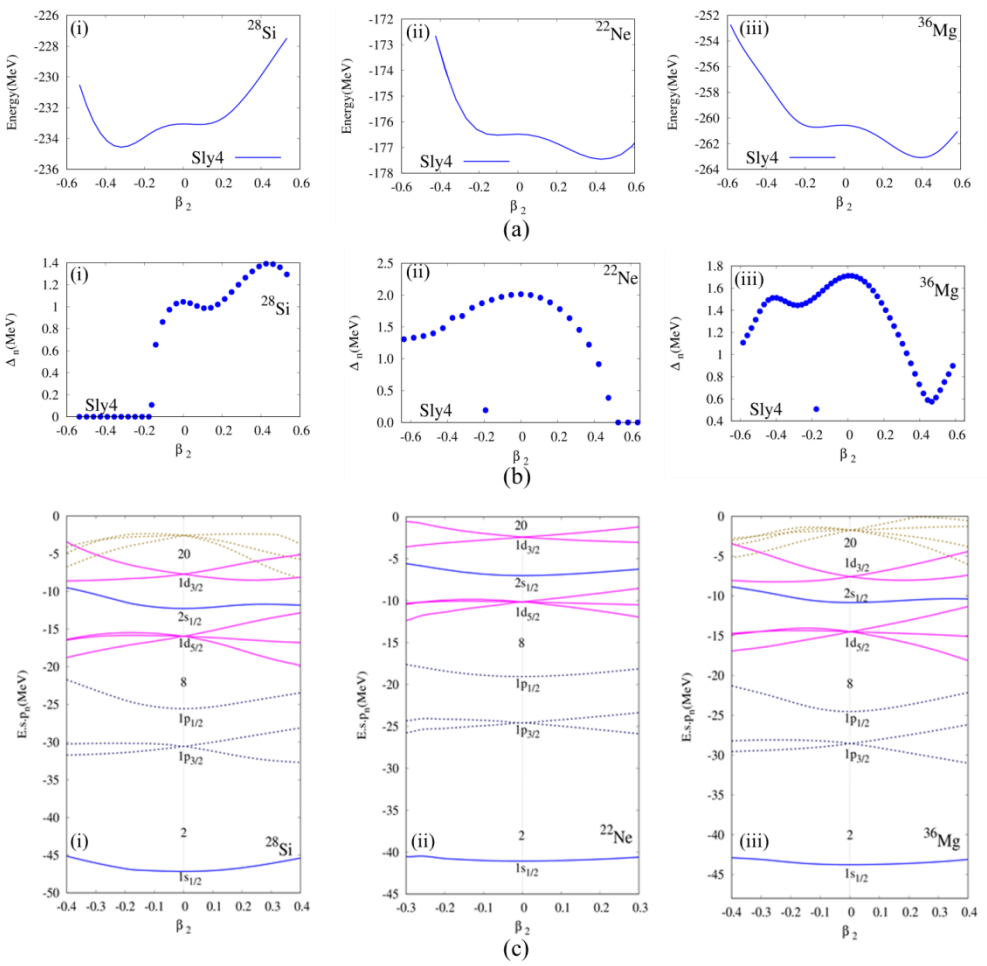


**Figure 1** (a) Potential energy surfaces (b) Average neutron pairing gaps $\Delta_n$ and (c) Neutron single-particle energy levels versus quadruple deformation $\beta_2$ for (i) $^{28}$Si, (ii) $^{22}$Ne and (iii) $^{36}$Mg obtained with Sly4 parameter set.

## Summary and Conclusion

In this work, we have compared the potential energy surfaces as a function of deformation parameters for some selected nuclei, namely, $^{28}$Si, $^{22}$Ne and $^{36}$Mg using the two Skyrme parameter sets (Sly4, SGII). From these results, the energy surface for $^{28}$Si shows a deep oblate minimum meanwhile $^{22}$Ne and $^{36}$Mg show prolate minimum. Then we calculate the corresponding average neutron pairing gaps and neutron single particle levels as a function of quadrupole deformation with the choice of the Sly4 parameter set to provide the fact that pairing plays an important role in determining the shapes of nuclei. It is found that the lower level density leads to smaller pairing gaps (or pairing correlation) near local minima, on the other hand, denser level density to larger pairing effects. At spherical shapes, pairing correlation

becomes strongest due to dense level density. It can be concluded that the effect of paring depends on the level density in the vicinity of the Fermi surface.

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