

# Odd-even mass difference and isospin dependent pairing interaction

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The neutron and proton odd-even mass differences are studied with Hartree-Fock+BCS (HFBCS) calculations with Skyrme interactions and an isospin dependent contact pairing interaction, which is recently derived from a microscopic nucleon-nucleon interaction. To this end, we perform HFBCS calculations for even and odd semi-magic Tin and Lead isotopes together with even and odd Z isotones with  $N=50$  and  $82$ . The filling approximation is applied to the last unoccupied particle in odd nuclei. Comparisons with the experimental data show a clear manifestation of the isospin dependent pairing correlations in both proton and neutron pairing gaps.

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It has been known that pairing correlations play an important role in finite and also infinite nuclear systems [1–3]. Recently, the theory of nuclear masses or binding energies has attracted renewed interest with the advent of self-consistent mean field theories, and also density functional theories (DFT) [4, 5]. A global feature of the nuclear binding energies is the odd-even mass staggering (OES) phenomenon. Several theoretical studies have been made to attribute this phenomenon to the BCS superfluidity in the nuclear ground states. It has been pointed out that other effects also contribute the OES effect [6, 7].

Recently, global calculations of nuclear masses became feasible by using modern computational resources. A goal of these global calculations is to improve the reliability of theories and to establish universal energy density functionals for nuclear masses. In this respect, the pairing correlations should be carefully examined by using microscopic methods such as Hartree-Fock(HF)+BCS or Hartree-Fock-Bogoliubov (HFB) theories. Indeed, first studies in this direction have been carried out and a possible isospin dependence of the effective pairing interaction has been discussed in the literature [8, 9].

The nuclear interaction may conserve the isospin at a fundamental level, but core polarization can induce isospin dependence when the core has a neutron excess. Another contribution may come from the Coulomb interaction. Recently, an effective isospin dependent pairing interaction was proposed from the study of nuclear matter pairing gaps calculated by realistic nucleon-nucleon interactions. In ref. [8], the density-dependent pairing interaction was defined by

$$V_{pair}(1,2) = V_0 g_\tau[\rho, \beta\tau_z] \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (1)$$

where  $\rho = \rho_n + \rho_p$  is the nuclear density and  $\beta$  is the asymmetry parameter  $\beta = (\rho_n - \rho_p)/\rho$ . The isovector dependence is introduced through the density-dependent term  $g_\tau$ . The function  $g_\tau$  is determined by the pairing gaps in nuclear matter and its functional form is given

by

$$g_\tau[\rho, \beta\tau_z] = 1 - f_s(\beta\tau_z)\eta_s \left(\frac{\rho}{\rho_0}\right)^{\alpha_s} - f_n(\beta\tau_z)\eta_n \left(\frac{\rho}{\rho_0}\right)^{\alpha_n}, \quad (2)$$

where  $\rho_0=0.16 \text{ fm}^{-3}$  is the saturation density of symmetric nuclear matter. We choose  $f_s(\beta\tau_z) = 1 - f_n(\beta\tau_z)$  and  $f_n(\beta\tau_z) = \beta\tau_z = [\rho_n(\mathbf{r}) - \rho_p(\mathbf{r})] \tau_z / \rho(\mathbf{r})$ . The parameters for  $g_\tau$  are obtained from the fit to the pairing gaps in symmetric and neutron matter obtained by the microscopic nucleon-nucleon interaction. The pairing strength  $V_0$  will be adjusted to give the best fit to odd-even staggering of nuclear masses.

interaction	$V_0$ (MeV)	$\rho_0 \text{ fm}^{-3}$	$\eta_s$	$\alpha_s$	$\eta_n$	$\alpha_n$
$g_\tau$	824	0.16 fm	0.677	0.365	0.931	0.378
$g_s$	1400	0.16 fm	1.	1.	—	—

TABLE I: Parameters for the density-dependent function  $g_\tau$  defined in Eq. (1) (first row) and  $g_s$  in Eq. (3). The parameters for  $g_\tau$  are obtained from the fit to the pairing gaps in symmetric and neutron matter obtained by the microscopic nucleon-nucleon interaction. The pairing strength  $V_0$  is adjusted to give the best fit to odd-even staggering of nuclear masses. The parameters for  $g_s$  correspond to a surface peaked pairing interaction with no isospin dependence. The parameters in this case are adjusted to a best global fit of nuclear masses [11].

In the the original EV8 code [10], a pure contact interaction was used without the isospin dependence. In our notation, this amounts replacing the isospin dependent function  $g_\tau$  in Eq. (1) by the isoscalar function

$$g_s = 1 - \eta_s \left(\frac{\rho}{\rho_0}\right)^{\alpha_s}. \quad (3)$$

The parameters in this case were adjusted to a best global fit of nuclear masses [11]. They correspond to a surface

peaked pairing interaction. Table I shows the parameters for  $g_\tau$  and  $g_s$  used in the present work.

In several previous publications [7–9], the OES was not obtained from the differences of calculated binding energies, but rather inferred from the average HFB gap parameters. It should be mentioned that the average HFB gaps are sometimes substantially different from the calculated odd-even mass differences. In this work, we compare directly the calculated OES with the experimental ones. There are several prescriptions to obtain the OES such as 3-point, 4-point, and 5-point formulas. We adopt the 3-point formula  $\Delta^{(3)}$  centered at odd nucleus, i.e., odd- $N$  nucleus for neutron gap and odd- $Z$  nucleus for proton gap [2]:

$$\Delta^{(3)}(N, Z) \equiv -\frac{\pi_N}{2} \left[ B(N-1, Z) - 2B(N, Z) + B(N+1, Z) \right], \quad (4)$$

where  $B(N, Z)$  is the binding energy of  $(N, Z)$  nucleus and  $\pi_N = (-)^N$  is the number parity. For even nuclei, the OES is known to be sensitive not only to the pairing gap, but also to mean field effects, i.e., shell effects and deformations [6, 7]. Therefore, the comparison of a theoretical pairing gap with OES should be done with caution. One advantage of  $\Delta_o^{(3)}$  ( $N = \text{odd}$  in eq. (5)) is the suppression of the contributions from the mean field to the gap. At a shell closure, the OES (5) does not go to zero as expected, but it increases substantially. This large gap is an artifact due to the shell effect, which is totally independent of the pairing gap itself.

We use the code EV8 [10] to carry out the HF+BCS calculations with Skyrme interactions. The pairing interaction (2) adopted is a contact interaction and can be used in a properly truncated configuration space. In the present study, the energy window is taken as 10 MeV around the Fermi level as is ref. [10]. This is a limitation of the EV8 code, which solves the HF+BCS equations via a discretization of the individual wavefunctions on a three-dimensional Cartesian mesh, while this program allows a flexibility in the determination of the nuclear shape. For a global study of OES, it is important to allow the flexibility of triaxial shapes.

First, the HF+BCS calculations are performed for even-even nuclei. The variables in the theory are the orbital wave functions  $\phi_i$  and the BCS amplitudes  $v_i$  and  $u_i = \sqrt{1 - v_i^2}$ . By solving the BCS equations for the amplitudes, one obtains the pairing energy from

$$E_{pair} = \sum_{i \neq j} V_{ij} u_i v_i u_j v_j + \sum_i V_{ii} v_i^2 \quad (5)$$

where  $V_{ij}$  are the matrix elements of the pairing interaction, Eq. (1), namely

$$V_{ij} = V_0 \int d^3r |\phi_i(\mathbf{r})|^2 |\phi_j(\mathbf{r})|^2 g_\tau[\rho(\mathbf{r}), \beta(\mathbf{r}) \tau_z],$$

where  $\rho(\mathbf{r}) = \sum_i v_i^2 |\phi_i(\mathbf{r})|^2$ .

In the present study, we take sub-closed shell nuclei only so that the HF minimum appears essentially around the spherical configurations. After determining the single-particle energies of even-even nuclei, the odd- $A$  nuclei are calculated with the so-called filling approximation for the odd particle starting from the HF+BCS solutions of neighboring even-even nuclei: one selects an orbital  $i$  to be blocked, and changes the BCS parameters  $v_i^2$  and  $u_i v_i$  for that orbital. The change is to set  $v_i^2 = u_i^2 = 1/2$  in Eq. (5) for the pairing energy at an orbital near the Fermi energy. Note that the filling approximation gives equal occupation numbers to both time-reversed partners, and does not account for the effects of time-odd fields. More details of the procedure are presented in ref. [11].

The HF+BCS calculations are performed by using SLy4 and SkP Skyrme interactions. The iteration procedure used in EV8 achieves an accuracy of about 100 keV, or less, in 500 iterations. For the pairing channels we take the surface-type contact interaction, Eq. (3), and the isospin dependent interaction, Eq. (2). The density dependence of the latter one is essentially the mixed-type interaction between the surface and the volume types. The pairing strength  $V_0$  depends on the energy window adopted for BCS calculations. The odd nucleus is treated in the filling approximation, by blocking one of the orbitals. The blocking candidates are chosen within an energy window of 10 MeV around the Fermi energy. This energy window is rather small, but it is the maximum allowed by the program EV8. It is shown that the EV8 model gives almost equivalent results to the HF+Bogoliubov model with a larger energy window, except unstable nuclei very close to the neutron drip line [11].

The calculated results are shown in Figs. 1-3. The HF+BCS results are compared with the experimental data and also the phenomenological parameterization

$$\bar{\Delta} = c/A^\alpha \quad (6)$$

with  $c = 4.66(4.31)$  MeV for neutrons (protons) and  $\alpha = 0.31$  which gives the rms residual of 0.25 MeV [11].

Figure 1 shows the OES  $\Delta_n^{(3)}$  for Sn and Pb isotopes. The calculations are performed with the SkP interaction. The overall agreement with the IS+IV pairing interaction (2) gives quite satisfactory results. Compared with the results with IS pairing (3), the difference is clearly seen in neutron-rich isotopes while the difference is rather small in neutron deficient isotopes. The difference of the two results in larger isospin nuclei is induced by the isospin dependence in Eq. (2) which weakens the pairing strength effectively in neutron-rich nuclei. The experimental OES  $\Delta_n^{(3)}$  for Sn isotopes is rather constant around 1.2 MeV until  $N=80$  and decrease below 1 MeV above  $N=82$ . This trend is well reproduced by the IS+IV pairing. On the other hand, the calculated results increase gradually as a function of  $N$  and reach up to 2 MeV in heavier Sn isotopes. This feature certainly does not agree with the

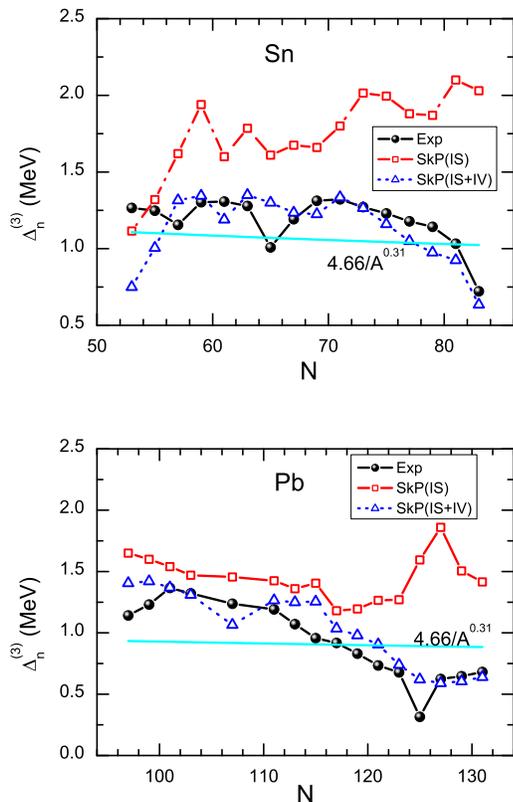


FIG. 1: (Color online) Odd-even mass staggering  $\Delta_n^{(3)}$  calculated by Eq. (5) for the semi-magic Sn and Pb isotopes. The SkP interaction is adopted together with the IS pairing (3) or the IS+IV pairing (2) in HF+BCS model. The filling approximation is applied to the last unoccupied particle in odd nuclei. See the text for details.

experimental one. The experimental  $\Delta_n^{(3)}$  for Pb isotopes is about 1.4 MeV in neutron-deficient Pb isotopes and go down to 0.7 MeV in neutron-rich isotopes. This trend is again well accounted by the IS+IV pairing while the IS pairing fails to reproduce this trend in neutron-rich isotopes. The phenomenological gap formula (6) gives good account of overall OES in medium-heavy and heavy nuclei. The average values of  $\Delta_n^{(3)}$  for Sn and Pb isotopes are also well reproduced by this formula, but the isospin dependence is relatively weak compared to the experiments and also the IS+IV results, especially in Pb isotopes. In Pb isotopes, the formula gives 0.93 MeV and 0.90 MeV for  $N=99$  and  $121$  isotopes, respectively, while the experimental values are 1.23 MeV and 0.73 MeV for the corresponding isotopes.

In Fig. 2, the calculated proton OES  $\Delta_p^{(3)}$  are shown together with the experimental data of  $N=50$  and  $N=82$  isotones. The IS+IV pairing gives again better agreement with the experimental data than the IS one. Notice that the IS+IV pairing strength becomes larger effectively for smaller  $Z$  isotones because of the isospin factor  $\tau_z = -1$  for protons in the interaction (2). Quantitatively, the IS pairing gives only about the half of the experimental values, even less than half for  $N=82$  isotones.

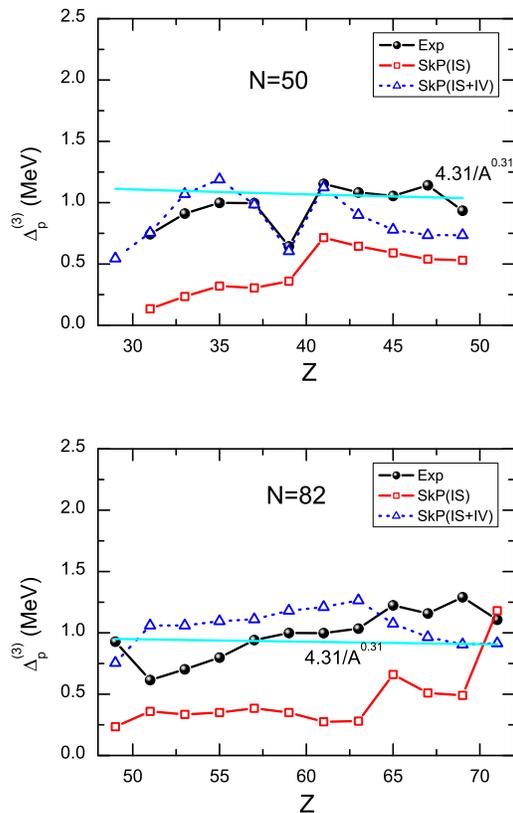


FIG. 2: (Color online) Odd-even mass staggering  $\Delta_p^{(3)}$  calculated with Eq. (5) for the  $N=50$  and  $N=82$  isotones. The SkP interaction is adopted together with the IS pairing (3) or the IS+IV pairing (2) in HF+BCS model. See the caption to Fig. 1 and the text for details.

On the other hand, the IS+IV pairing provides proper amount of the OES in both  $N=50$  and  $N=82$  isotones because of larger pairing strength for protons in proton deficient isotones. The kink at  $Z=39$  in the Fig. 1 for  $N=50$  isotones is due to the subshell structure at  $Z=40$  which is also appeared in the curve of isospin dependent pairing (the white triangles). The formula (6) gives the proton OES to be 1.10 and 1.04 MeV for  $Z=31$  and  $Z=47$  of  $N=50$  isotones respectively, while the experimental values are 0.74 and 1.14 MeV for  $Z=31$  and  $Z=47$  isotones, respectively. We should remind that the Coulomb interaction might play a role for proton OES which is discarded in the present calculations. Some renormalization of the effective pairing strength  $V_0$  might be needed to study the proton OES under the effect of the Coulomb interaction.

In Fig. 3, the IS+IV pairing is tested against another interaction SLy4 for Sn and Pb isotopes. The general features for SLy4 are quite similar to those of SkP except very neutron deficient isotopes. This might be due to the small energy window of EV8, but not real physical effect due to the different interactions. Thus the IS+IV pairing works well for OES irrespective of the Skyrme interactions SkP and SLy4.

In summary, we studied the neutron OES of Sn and

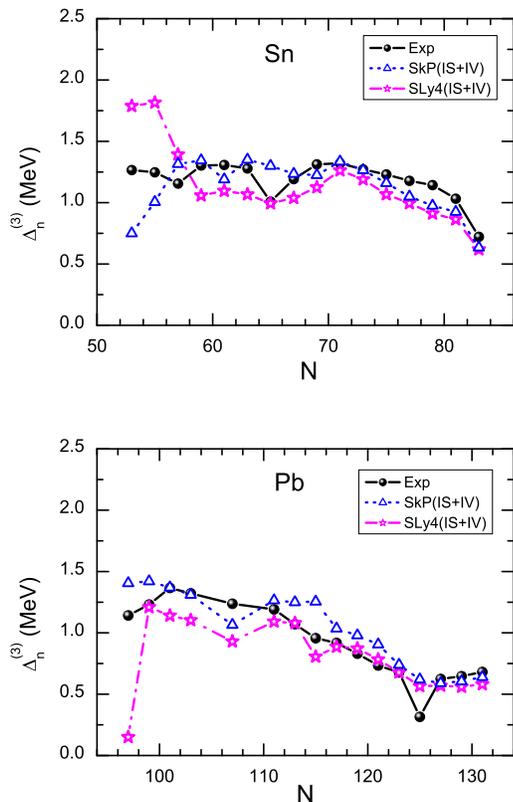


FIG. 3: (Color online) Odd-even mass staggering  $\Delta_n^{(3)}$  calculated with Eq. (5) for the  $N=50$  and  $N=82$  isotones. The SLy4 interaction is adopted together with the IS pairing (3) or the IS+IV pairing (2) in HF+BCS model. See the caption to Fig. 1 and the text for details.

Pb isotopes and also the proton OES of  $N=50$  and  $N=82$  isotones by using HF+BCS model with SkP and SLy4 in-

teractions together with the isospin dependence pairing (IS+IV pairing) and IS pairing interactions. The calculations are performed with the EV8 code for even-even nuclei and also even-odd nuclei using the filling approximation. For the neutron pairing gaps, the IS+IV pairing strength decreases gradually as a function of the asymmetry parameter  $(\rho_n(r) - \rho_p(r))/\rho(r)$ . On the other hand, the strength for protons is increasing for larger values of the asymmetry parameter because of the isospin factor in Eq. (2). The isotope dependence of the neutron OES  $\Delta_n^{(3)}$  is well reproduced by the present calculations with the isospin dependent pairing compared with the IS pairing. We can also see the good agreement between the experimental proton OES and the calculations with the isospin dependent pairing for  $N=50$  and  $N=82$  isotones.

We tested the IS+IV pairing for the Skyrme interaction SkP and found almost the same quantitative agreement as with SLy4, i.e., the results reproduces well the experimental data of the isotopes. Thus, we confirm the clear manifestation of the isospin dependence of the pairing interaction in the OES in comparison with the experimental data both for protons and neutrons. More comprehensive study of OES in the entire mass region is planned as a future work.

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