# Shape dependence of pairing gap energies and the structure of Hg and Pb isotopes

Satoshi Yoshida and Noboru Takigawa

Department of Physics, Faculty of Science, Tohoku University, 980-77 Sendai, Japan

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The ground states of Hg and Pb isotopes are studied in the framework of deformed relativistic mean field theory with pairing interactions in the BCS theory. We show that the neutron and proton gap parameters strongly depend on deformation, and demonstrate that it is crucially important to solve the gap equations for each deformation in order to discuss the shape and the charge radius of these isotopes. The oblate shape and the charge radius of neutron deficient Hg isotopes are well reproduced. Our calculations suggest that the atomic number 82 stays a magic number for all the Pb isotopes we studied, and well reproduce the isotope shifts of Pb isotopes. [S0556-2813(97)06303-6]

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#### I. INTRODUCTION

The change of nuclear structure, e.g., of the nuclear shape, over a broad range of isotopes of various elements is one of the fundamental interests in nuclear physics. The advent of radioactive nuclear beams makes such study one of the most popular current subjects. From theoretical points of view, one interesting question in this connection is to clarify whether the relativistic mean field (RMF) theory, which is getting very popular in the past decades, can reproduce the existing data and is reliable to predict the structure of nuclei further away from the stability line. This paper addresses this question by choosing Hg and Pb isotopes as testing grounds.

It is well known that the oblate and the prolate states coexist in low energy region in Hg isotopes and that the ground state is oblate for all the known neutron deficient Hg isotopes [1–8]. Our previous calculations [9,10] within the framework of the relativistic mean field theory treating the pairing interaction in the BCS theory in the constant  $\Delta$  approximation with the average proton and neutron gap parameters have failed to reproduce the oblate shape for some isotopes such as <sup>184</sup>Hg. As a consequence, the experimentally discovered smooth isotope dependence of the charge radius [2] has also not been reproduced.

As for Pb isotopes, there exists a debate concerning whether Z=82 is a stable magic number or not [11–13]. Our calculations mentioned above predict that some of the lead isotopes are deformed suggesting that Z=82 loses magicity for those isotopes. However, similarly to the case of Hg isotopes, our RMF calculations in the constant  $\Delta$  approximation using the average neutron and proton gap parameters are not consistent with the smooth variation of the experimental charge radius of the lead isotopes [14–16]. Many of the old non relativistic Hartree-Fock calculations share a similar problem, i.e., they predict a prolate deformation for the ground state of some of the Hg isotopes. On the other hand, Nazarewicz [17] and Möller *et al.* [18] have recently shown that the macroscopic-microscopic approach can correctly reproduce the oblate shape for the known neutron deficient Hg isotopes. Tajima *et al.* [19] also have shown that nonrelativistic Skyrme Hartree-Fock calculations can reproduce the correct shape of Hg isotopes. A common feature of these calculations is that they solve the gap equations instead of assuming constant gap parameters independent of the deformation. The nonrelativistic Hartree-Fock-Bogoliubov calculations of Delaroche *et al.* [20] also reproduce the oblate shape of the ground states of neutron deficient Hg isotopes.

In our previous paper [21], we pointed out that the results of the RMF calculations strongly depend on the choice of pairing gap parameters. In this paper, we solve the gap equations for each deformation, i.e., we take a constant G approximation, instead of assuming constant gap parameters. We thus show that it is crucial indeed to solve the gap equations for each deformation, and that the relativistic mean field theory can then reproduce the correct shape of the ground state of all the neutron deficient Hg isotopes, as well as the smooth isotope variation of the charge radii of Hg and Pb isotopes.

The paper is organized as follows. In Sec. II, we briefly describe our formalism. In Sec. III, we apply our formalism to Hg and Pb isotopes. We show that the neutron and proton gap parameters strongly depend on deformation. The summary is given in Sec. IV.

#### **II. THEORETICAL FRAMEWORK**

We assume the following relativistic Lagrangian density  $(\mathcal{L})$  [22–26] for the interacting many-body system consisting of nucleons, scalar ( $\sigma$ ) and vector ( $\omega, \vec{\rho}$ ) mesons, and photons:

$$\mathcal{L} = \overline{\psi}_i \{ i \gamma^{\mu} \partial_{\mu} \} \psi_i + \frac{1}{2} \partial^{\mu} \sigma \partial_{\mu} \sigma - U(\sigma) - g_{\sigma} \overline{\psi}_i \psi_i \sigma - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} m_{\omega}^2 \omega^{\mu} \omega_{\mu} - g_{\omega} \overline{\psi}_i \gamma^{\mu} \psi_i \omega_{\mu} - \frac{1}{4} \vec{B}^{\mu\nu} \vec{B}_{\mu\nu} + \frac{1}{2} m_{\rho}^2 \vec{\rho}^{\mu} \vec{\rho}_{\mu} - g_{\rho} \overline{\psi}_i \gamma^{\mu} \vec{\tau} \psi_i \vec{\rho}_{\mu} - \frac{1}{4} F^{\mu\nu} F_{\mu\nu} - e \overline{\psi}_i \gamma^{\mu} \frac{(1 - \tau_{3i})}{2} \psi_i A_{\mu},$$
(1)

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where  $\psi_i$  are the Dirac spinors for nucleons, and  $\sigma$ ,  $\omega$ , and  $\vec{\rho}$  are the field operators of mesons, and  $A_{\mu}$  those for photons. The scalar meson potential  $U(\sigma)$  is assumed to be non-linear [27]

$$U(\sigma) = \frac{1}{2}m_{\sigma}^{2}\sigma^{2} + \frac{1}{3}g_{2}\sigma^{3} + \frac{1}{4}g_{3}\sigma^{4}.$$
 (2)

The  $g_{\sigma}, g_{\omega}$ , and  $g_{\rho}$  are the coupling constants between the nucleons and the  $\sigma, \omega$ , and  $\rho$  mesons, respectively, while  $e^2/4\pi = 1/137$  that for photons. The  $g_2$  and  $g_3$  are parameters of the nonlinear potential for  $\sigma$  mesons. The  $m_{\sigma}, m_{\omega}, m_{\rho}$ , and M are the masses of  $\sigma, \omega, \rho$  mesons and of nucleons, respectively. The  $\Omega^{\mu\nu}, \vec{B}^{\mu\nu}$ , and  $F^{\mu\nu}$  are the field tensors for the  $\omega^{\mu}, \vec{\rho}^{\mu}$  and the photon fields, respectively.

We introduce the mean field approximation in solving the Euler-Lagrange equations for mesons and nucleons. We then determine the wave functions and single particle energies by expanding the upper and lower components of Dirac spinors and the meson fields in a deformed harmonic oscillator basis [25]. The maximum oscillator quanta  $N_{\text{max}}$  is taken to be 12 for spherical and normal deformations, and 20 for superdeformed states. These coupled equations are solved by self-consistent iteration. We constraint by the value of the total quadrupole moment in order to study the energy surface as a function of deformation. We choose the so-called NL1 set [24] in this paper.

The central issue of this paper is to discuss the effects of pairing interaction. We treat them in the BCS theory, where the gap equation is given by

$$\frac{2}{G} = \sum_{k=0}^{k_{\max}} \frac{1}{\sqrt{(e_k - \lambda)^2 + \Delta^2}}.$$
(3)

We choose  $k_{\text{max}}$  such that the corresponding energy is given by  $e_{k_{\text{max}}} = \lambda + 2\hbar\omega$ . Assuming a constant level density for the average nucleus in the vicinity of the Fermi surface, we rewrite this equation as [18]

$$\frac{2}{G_n} = \rho_n \int_{y_1}^{y_2} \frac{d\epsilon}{\sqrt{\epsilon^2 + \overline{\Delta}_n^2}}$$
(4)

for neutrons, where the level density  $\rho_n$  is taken to be

$$\rho_n = \left(\frac{2}{3\pi^2}\right)^{1/3} \frac{mr_0^2}{\hbar^2} A^{2/3} N^{1/3} \tag{5}$$

following the Thomas-Fermi approximation. Similar equations hold for protons. The upper and lower limits of the integration in Eq. (4) are

$$y_2 = 2\hbar\omega,$$
  
$$y_1 = -N/(2\rho_n).$$
 (6)

In our calculations, we use the average gap parameters [18]

$$\overline{\Delta}_n = 4.8/N^{1/3},$$
  
 $\overline{\Delta}_p = 4.8/Z^{1/3}$  (7)

in Eq. (4) and the corresponding equation for protons, and determine the strengths of the pairing interactions  $G_n$  and  $G_p$ , which are independent of deformation. We then use these values in the gap equation (3) for neutrons and for protons and solve it to determine the gap parameters  $\Delta_n$  and  $\Delta_p$  for each deformation. Notice that the single particle energies  $e_k$  depend on deformation.

The quadrupole moments of the protons and neutrons are calculated with the resultant single particle wave functions. The deformation parameter  $\beta$  is then estimated by

$$Q = Q_n + Q_p = \sqrt{\frac{9}{5\pi}} A R^2 \beta, \qquad (8)$$

where  $R = 1.2A^{1/3}$ . We also calculate the mean square radius of protons  $\langle R_p^2 \rangle$ , and obtain the charge radius as  $R_c = \sqrt{\langle R_p^2 \rangle + 0.64}$  fm by taking the finite size of protons into account.

## **III. RESULTS AND DISCUSSIONS**

In this section, we discuss the results of our calculations. Figure 1 shows the binding energy of <sup>184</sup>Hg as a function of the deformation parameter. Contrary to our previous calculations in the constant  $\Delta$  approximation using the average gap parameters, the oblate shape of the ground state is well reproduced. The calculations also reproduce the experimental discovery that the oblate and the prolate states coexist very closely to each other.

Figure 2 shows the calculated splitting of the intrinsic energies for the oblate and the prolate states for a wide range of Hg isotopes (the filled circles). It agrees very well with the experimental data (the filled triangles) [3,4]. Our calculations predict that there exits only oblate state for Hg isotopes beyond A = 190. This is consistent with the results in Ref. [17], though Ref. [17] predicts no prolate state already for A = 190. Figure 3 shows the variation of the charge radius of Hg isotopes. The charge radii of the oblate and the prolate shapes are shown by the filled and the open circles, respectively, while the experimental radius is given by the filled triangle [2]. Since our present calculations well reproduce the experimental data.

The key of these successes is a proper treatment of the pairing interaction. In Fig. 4, we show the neutron and pro-



FIG. 1. Energy surface of  $^{184}$ Hg as a function of the quadrupole deformation parameter  $\beta$ .



FIG. 2. The difference of the intrinsic energies of the oblate and the prolate states for various Hg isotopes. The results of the relativistic mean field calculations (the filled circles) are compared with the experimental data (the filled triangles) [3,4].

ton gap parameters obtained by solving the gap equations for each deformation (filled circles). The figure clearly shows a very strong dependence of the gap parameters on deformation. For comparison, the figure includes the average gap parameters by Madland-Nix [28] (the dashed line), by Möller et al. [18] (the solid line), and by a standard  $12/\sqrt{A}$  formula [29] (the dot-dashed line). An important observation is that the proton gap parameter is zero for certain range of deformation parameter including the oblate deformation corresponding to the ground state,  $\beta_{exp} \sim -0.13$ . On the other hand, the neutron gap parameter corresponding to the ground state deformation is more than 50% larger than the average gap parameter. Notice also that the proton and the neutron gap parameters for the superdeformed configuration are significantly different from the average values. The origin why the proton gap parameter becomes zero can be understood if we examine the single particle levels shown in Fig. 5. We find a clear energy gap between the 80th and the next levels for certain deformation including the oblate deformation for the ground state of <sup>184</sup>Hg. This situation is common to all neutron deficient Hg isotopes. In passing we should like to remark that the zero pairing gap in Fig. 4 will become a small finite gap if one properly treats the problem of number fluctuation in the BCS theory [18].

We now discuss the results of our calculations for Pb isotopes. Our calculations predict that all the Pb isotopes we studied, i.e.,  $190 \le A \le 214$ , are spherical. In that sense,



FIG. 3. Isotope dependence of the charge radius of Hg isotopes. The experimental data (the filled triangles) [2] are compared with the charge radii calculated for the oblate states corresponding to the ground states (the filled circles). The charge radii of the excited prolate configurations are also shown (the open circles).



FIG. 4. Neutron and proton gap parameters as functions of deformation (the filled circles). The dashed, the solid, and the dotdashed lines correspond to the average gap parameters of Madland-Nix [28], Möller *et al.* [18], and to a standard  $12/\sqrt{A}$  formula [29].

Z=82 stays a magic number in this mass region. Figure 6 compares the calculated charge radius with the experimental data [14–16] for various Pb isotopes. Since our calculations predict spherical shape for all the isotopes, the experimental charge radius is well reproduced. In Fig. 7, we compare the theoretical calculations and the experimental data [14–16] of the scaled isotope shifts, where  $\Delta R_c^2$  is the squared charge radius relative to that for <sup>208</sup>Pb, while  $\Delta R_{LD}^2$  is the squared charge radius relative to that for <sup>208</sup>Pb in the liquid drop model, i.e.,  $R_{LD} = \frac{3}{5} \times 1.2A^{1/3}$ . We see that our calculations almost perfectly reproduce the experimental data including the kink at <sup>208</sup>Pb (see [30] for an explanation of the kink).

# **IV. SUMMARY**

We studied the shape and the charge radius of Hg and Pb isotopes in the framework of the relativistic mean field theory. We have shown that our calculations very well reproduce the existing data. The lesson of this study is that it is crucially important to properly treat the pairing interaction. By solving the gap equations, we have shown that both proton and neutron gap parameters strongly depend on deformation. A striking fact is that the proton gap parameter is almost zero for certain values of deformation including the oblate ground state deformation for Hg isotopes. This is a



FIG. 5. Single particle levels of protons for  $^{184}$ Hg as functions of the quadrupole deformation parameter  $\beta$ .



FIG. 6. Isotope dependence of the charge radius of Pb isotopes. The filled triangles are the experimental data [14–16]. The filled and open circles were calculated by the relativistic mean field theory. They correspond to the spherical ground state, and to an excited oblate state, respectively.

consequence of "Z=80 magic number." This offers a simple solution for the long standing problem of the failure of Hartree-Fock calculations in reproducing the experimentally discovered oblate shape. Our results will be independent of the choice of the parameter set NL1 and the average gap parameters given by Eq. (7).

This is the first attempt in the relativistic mean field calculations, where the pairing interaction in the BCS theory is treated in constant G approximation instead of constant  $\Delta$ approximation. It would now be very interesting to explore the change of structure such as the shape of nuclei much far away from the beta stability line by using the relativistic mean field theory with a proper treatment of the pairing interaction, i.e., in the constant G approximation. In this connection, one should mention that there exists an alternative method to treat the pairing interaction, i.e., the relativistic



FIG. 7. Scaled isotope shifts of Pb isotopes. The experimental data [14-16] and the results of the relativistic mean field calculations are shown by the filled triangles and circles, respectively.

Hartree-Bogoliubov theory [31]. This approach is superior to the BCS theory in the sense that it can be applied to more exotic nuclei, where the average gap parameters cannot be easily obtained. So far, however, such studies are limited to calculations for spherical shape.

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