Pseudospin symmetry in relativistic mean field theory

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Relating the pseudospin symmetry back to the Dirac equation through the framework of relativistic Hartree-Bogoliubov (RHB) theory, the pseudospin approximation in real nuclei is discussed. From the Dirac equation, the mechanism behind the pseudospin symmetry was studied and the pseudospin symmetry is shown to be connected with the competition between the centrifugal barrier (CB) and the pseudospin orbital potential (PSOP), which is mainly decided by the derivative of the difference between the scalar and vector potentials. With the scalar and vector potentials derived from a self-consistent relativistic Hartree-Bogoliubov calculation, the pseudospin symmetry and its energy dependence in real nuclei is discussed. [S0556-2813(98)50508-0]

The concept of pseudospin is that the single particle orbitals with $j=l+1/2$ and $j=(l+2)-1/2$ lie very close in energy and can therefore be labeled as pseudospin doublets with quantum number $\tilde{n}=n-1$, $\tilde{l}=l-1$, and $\tilde{s}=s=1/2$. This concept is originally found in spherical nuclei [1,2], but later proved to be a good approximation in deformed nuclei as well [3,4]. It is shown that pseudospin symmetry remains an important physical concept even in the case of triaxiality [5]. The origin of pseudospin is proved to be connected with the special ratio in the strength of the spin-orbit and orbit-orbit interactions [6,7] and the unitary operator performing a transformation from normal spin to pseudospin space have been discussed [6–8]. However, it is not explained why this special ratio is allowed in nuclei. The relation between the pseudospin symmetry and the relativistic mean field (RMF) theory [9] was first noted in Ref. [10], in which Bahri *et al.* found that the RMF explains approximately the strengths of spin-orbit and orbit-orbit interactions found by nonrelativistic calculations. More details have been given in Refs. [11, 12, in which it was suggested that the origin of pseudospin is related to the strength of the scalar and vector potentials. In a recent paper Ginocchio took a step further and revealed that pseudo-orbital angular momentum is nothing but the "orbital angular momentum" of the lower component of the Dirac wave function [13]. He also built the connection between the pseudospin symmetry and the equality in the scalar and vector potentials. Here in this paper, we will show that the quality of pseudospin symmetry is connected with the competition between the centrifugal barrier (CB) and the pseudospin orbital potential (PSOP), which is mainly decided by the derivative of the difference between the scalar and vector potentials. With the scalar and vector potentials derived from a self-consistent relativistic Hartree-Bogoliubov calculation, the pseudospin symmetry and its energy dependence in real nuclei is discussed.

As RMF is very successful in describing various quantities in the nuclear structure, e.g., [14], it is interesting to check how good the pseudospin symmetry is in RMF for real nuclei. Relating the pseudospin symmetry back to the Dirac equation through the framework of relativistic Hartree-

Bogoliubov (RHB) theory, the pseudospin symmetry approximation in real nuclei is *i*, discussed here in this paper. The recently suggested relativistic Hartree-Bogoliubov (RHB) theory in coordinate space [15] has been used for the present investigation. As this theory takes into account the proper isospin dependence of the spin-orbit term, it is able to provide a good description of global experimental data not only for stable nuclei but also for exotic nuclei throughout the nuclear chart [16]. Starting from the RHB, instead of assuming the equality in the magnitude of the scalar and vector potentials, we treated the equation exactly and obtained a general formalism leading to the pseudospin symmetry. We chose ^{88}Zr and ^{120}Zr to study the energy splitting of the pseudospin partners and its energy dependence as examples.

The Dirac equation for nucleons in RMF is as follows:

$$[\vec{\alpha}\cdot\vec{p}+V_V(\vec{r})+\beta(M+V_S(\vec{r}))]\psi(\vec{r})=\epsilon\psi(\vec{r}), \qquad (1)$$

which describes a Dirac spinor with mass M moving in a potential decided by the scalar potential $V_S(\vec{r})$ and vector potential $V_V(\vec{r})$. The wave function $\psi(\vec{r})$ consists of the upper component g and lower component f,

$$\psi(\vec{r})=\begin{pmatrix} g \\ f \end{pmatrix}=\begin{pmatrix} i\dfrac{G_i^{lj}(r)}{r}Y_{jm}^l(\theta,\phi) \\ \dfrac{F_i^{lj}(r)}{r}(\vec{\sigma}\cdot\hat{\vec{r}})Y_{jm}^l(\theta,\phi) \end{pmatrix} \qquad (2)$$

and the Dirac matrix α and β are as follows:

$$\vec{\alpha}=\begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \qquad \beta=\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \qquad (3)$$

With $\epsilon=M+E$, the potential $V=V_V(\vec{r})+V_S(\vec{r})$, which is around -50 MeV, and the effective mass $M^*=M+V_S(\vec{r})$, the relation between the upper and lower components of the wave function can be written as

$$g = \frac{1}{E-V}(\vec{\sigma}\cdot\vec{p})f,$$

$$f = \frac{1}{E+2M^*-V}(\vec{\sigma}\cdot\vec{p})g. \tag{4}$$

Then the coupled equations are reduced to uncoupled ones for the upper and lower components, respectively. Effectively we get the corresponding Schrödinger equation for both components:

$$(\vec{\sigma}\cdot\vec{p})\frac{1}{E+2M^*-V}(\vec{\sigma}\cdot\vec{p})g = (E-V)g,$$

$$(\vec{\sigma}\cdot\vec{p})\frac{1}{E-V}(\vec{\sigma}\cdot\vec{p})f = (E+2M^*-V)f. \tag{5}$$

In the spherical case, V depends only on the radius. We chose the phase convention of the vector spherical harmonics as

$$(\vec{\sigma}\cdot\vec{r})Y_{jm}^{l} = -Y_{jm}^{l'}, \tag{6}$$

where

$$l' = 2j - l = \begin{cases} l+1, & j = l+1/2 \\ j-1, & j = l-1/2. \end{cases} \tag{7}$$

Here l' is nothing but the pseudo-orbital angular momentum. After some tedious procedures, one gets the radial equation for the lower and upper components, respectively:

$$\left[\frac{d^2}{dr^2} + \frac{1}{E-V}\frac{dV}{dr}\frac{d}{dr}\right]F_i^{lj}(r)$$

$$+ \left[\frac{\kappa(1-\kappa)}{r^2} - \frac{1}{E-V}\frac{\kappa}{r}\frac{dV}{dr}\right]F_i^{lj}(r)$$

$$= -(E+2M^*-V)(E-V)F_i^{lj}(r), \tag{8}$$

$$\left[\frac{d^2}{dr^2} - \frac{1}{E+2M^*-V}\frac{d(2M^*-V)}{dr}\frac{d}{dr}\right]G_i^{lj}(r)$$

$$- \left[\frac{\kappa(1+\kappa)}{r^2} + \frac{1}{E+2M^*-V}\frac{\kappa}{r}\frac{d(2M^*-V)}{dr}\right]G_i^{lj}(r)$$

$$= -(E+2M^*-V)(E-V)G_i^{lj}(r), \tag{9}$$

where

$$\kappa = \begin{cases} -l-1, & j = l+1/2 \\ l, & j = l-1/2. \end{cases} \tag{10}$$

Then one can get

$$\kappa(\kappa-1) = l'(l'+1), \quad \kappa(\kappa+1) = l(l+1). \tag{11}$$

It is clear that one can use either Eq. (8) or equivalently Eq. (9) to get the eigenvalues E and the corresponding eigenfunctions. Normally Eq. (9) is used in the literature and the spin-orbital splitting is discussed in connection with the corresponding spin-orbital potential

$$\frac{1}{E+2M^*-V}\frac{\kappa}{r}\frac{d(2M^*-V)}{dr}.$$

If Eq. (8) is used instead and the pseudo spin-orbital potential (PSOP) term

$$\frac{1}{E-V}\frac{\kappa}{r}\frac{dV}{dr}$$

is neglected, then the eigenvalues E for the same l' will degenerate. This is the phenomenon of pseudospin symmetry observed in [1,2]. It means Eq. (4) is the transformation between the normal spin formalism and the pseudospin formalism.

In Eq. (8), the term that splits the pseudospin partners is simply the PSOP. The hidden symmetry for the pseudospin approximation is revealed as $dV/dr = 0$, which is more general and includes $V = 0$ discussed in [13] as a special case. Unfortunately, this condition is not satisfied in the nuclei and the pseudospin symmetry is an approximation. However, if

$$\frac{1}{E-V}\frac{\kappa}{r}\frac{dV}{dr} \ll \frac{\kappa(1-\kappa)}{r^2},$$

the pseudospin approximation will be good. Thus, the comparison of the relative magnitude of the centrifugal barrier (CB),

$$\frac{\kappa(1-\kappa)}{r^2},$$

and the PSOP can provide us with some information on the pseudospin symmetry. In the following we take ^{88}Zr and ^{120}Zr as examples and study how good the pseudospin symmetry is.

For this purpose, the relativistic Hartree-Bogoliubov (RHB) theory in coordinate space has been used [15]. We use here the nonlinear Lagrangian parameter set NLSH [17] which could provide a good description of all nuclei from oxygen to lead. As we study not only the closed shell nuclei, but also the open shell nuclei, the inclusion of the pairing is necessary. The pairing interaction is the same as Ref. [18]. As shown in Ref. [16], the particle levels for the bound states in the canonical basis are the same as those by solving the Dirac equation with the scalar and vector potentials from RHB. Therefore Eqs. (8) and (9) remain the same in the canonical basis even after the pairing interaction has been taken into account. The binding energy of $8.650A$ MeV for ^{88}Zr agrees well with the experimental values of $8.666A$ MeV. The neutron single particle energies for all four sets of pseudospin partners, i.e., $1d_{3/2}$ and $2s_{1/2}$, $1f_{5/2}$ and $2p_{3/2}$, $1g_{7/2}$ and $2d_{5/2}$, and $2d_{3/2}$ and $3s_{1/2}$ in ^{88}Zr and ^{120}Zr are given in Table I. As seen in Table I, the energy splitting between pseudospin partners decreases with the decreasing binding energy. The single particle energy splitting between $3s_{1/2}$ and its partner $2d_{3/2}$ in ^{120}Zr is 0.14 MeV. While that between $2s_{1/2}$ and $1d_{3/2}$ is 1.61 MeV, which is bigger than the former one by a factor of 10. Thus the pseudospin symmetry becomes better near the Fermi surface, which is in agreement with the experimental observation. The same conclusion has been obtained by solving the Dirac

TABLE I. The binding energies of pseudospin partners in ^{88}Zr and ^{120}Zr.

nlj	^{88}Zr	^{120}Zr	nlj	^{88}Zr	^{120}Zr
$2s_{1/2}$	-31.40	-31.62	$2p_{3/2}$	-16.36	-18.81
$1d_{3/2}$	-33.40	-33.23	$1f_{5/2}$	-18.85	-20.95
$3s_{1/2}$	-1.53	-6.00	$2d_{5/2}$	-3.73	-7.39
$2d_{3/2}$	-1.60	-5.86	$1g_{7/2}$	-4.54	-8.52

equation with spherical square potential well [13]. The pseudospin splitting in ^{88}Zr is similar to that of ^{120}Zr.

In order to see the energy dependence of the pseudospin orbital splitting more clearly, we plot

$$\Delta E_1 = \frac{E_{l'j=l'-1/2} - E_{l'j=l'+1/2}}{2l'+1} \quad \text{versus}$$

$$E_1 = \frac{E_{l'j=l'-1/2} + E_{l'j=l'+1/2}}{2}$$

in ^{88}Zr (filled squares) and ^{120}Zr (filled circles) in Fig. 1. The pseudospin splitting for $3s_{1/2}$ and $2d_{3/2}$ is more than 10 times smaller than that of the $2s_{1/2}$ and $1d_{3/2}$. It is seen that although there is some shift in the binding energy from ^{88}Zr to ^{120}Zr, the pattern is more or less the same, i.e., a monotonous decreasing behavior with a decreasing binding energy, which means that the pseudospin symmetry remains a good approximation for both stable and exotic nuclei. As a reference, the normal spin splitting
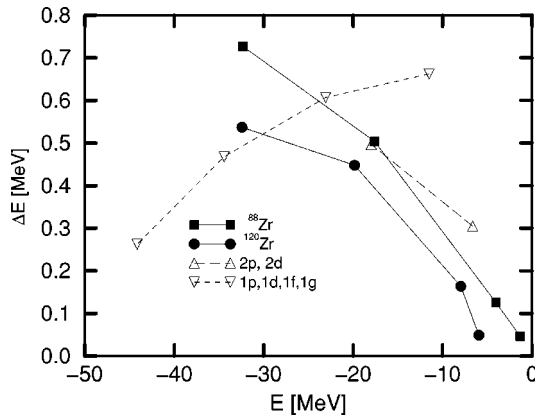

FIG. 1. The pseudospin orbit splitting $\Delta E_1 = (E_{l'j=l'-1/2} - E_{l'j=l'+1/2})/2l'+1$ versus the binding energy $E_1 = (E_{l'j=l'-1/2} + E_{l'j=l'+1/2})/2$ for ^{88}Zr (filled squares) and ^{120}Zr (filled circles). From left to right, the pseudospin partners correspond to $(1d_{3/2}, 2s_{1/2})$, $(1f_{5/2}, 2p_{3/2})$, $(1g_{7/2}, 2d_{5/2})$, and $(2d_{3/2}, 3s_{1/2})$, respectively. The spin-orbit splitting $\Delta E_2 = (E_{lj=l-1/2} - E_{lj=l+1/2})/2l+1$ versus the binding energy $E_2 = (E_{lj=l-1/2} + E_{lj=l+1/2})/2$ in ^{120}Zr are also given for $(1p_{3/2}, 1p_{1/2})$, $(1d_{5/2}, 1d_{3/2})$, $(1f_{7/2}, 1f_{5/2})$, $(1g_{9/2}, 1g_{7/2})$ (inverse triangle) and $(2p_{3/2}, 2p_{1/2})$, $(2d_{5/2}, 2d_{3/2})$ (triangle) from left to right, respectively. The $\Delta E(E)$ in the figure is either ΔE_1 or ΔE_2 (E_1 or E_2) here.
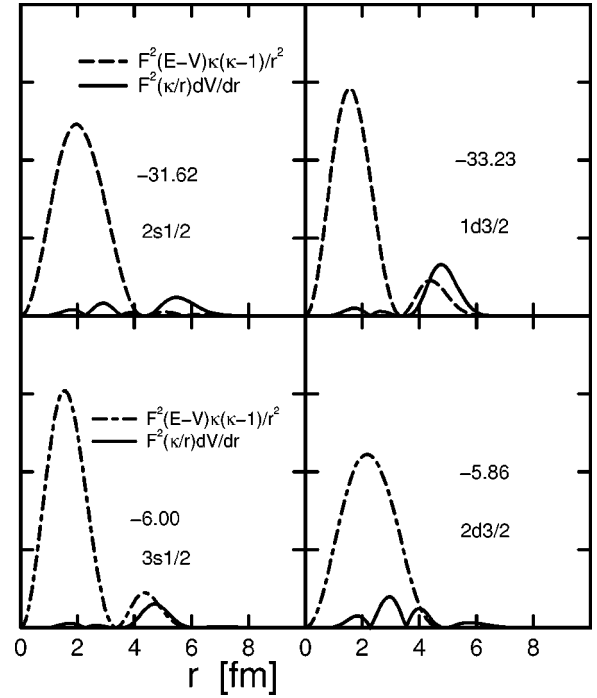

FIG. 2. The comparison of the effective centrifugal barrier (CB) $(E-V)[\kappa(\kappa-1)]/r^2$ (dashed lines and dot-dashed lines) and the effective pseudospin orbital potential (PSOP) $(\kappa/r)(dV/dr)$ (solid line) multiplied by the squares of the wave function F of the lower components in arbitrary scales for $d_{3/2}$ (upper) and $s_{1/2}$ (lower) in ^{120}Zr. The dashed lines are for $1d_{3/2}$ and $2s_{1/2}$, and the dot-dashed lines are for $2d_{3/2}$ and $3s_{1/2}$.

$$\Delta E_2 = \frac{E_{lj=l-1/2} - E_{lj=l+1/2}}{2l+1} \quad \text{versus}$$

$$E_2 = \frac{E_{lj=l-1/2} + E_{lj=l+1/2}}{2}$$

in ^{120}Zr are also given for $(1p_{3/2}, 1p_{1/2})$, $(1d_{5/2}, 1d_{3/2})$, $(1f_{7/2}, 1f_{5/2})$, $(1g_{9/2}, 1g_{7/2})$ (inverse triangle) and $(2p_{3/2}, 2p_{1/2})$, $(2d_{5/2}, 2d_{3/2})$ (triangle) from the left to the right, respectively. Compared to the pseudospin case, the normal spin splitting is less energy dependent, because the energy comes in the denominator in the form of $E + 2M^* - V$ in Eq. (9). The smallest spin-orbital splitting is nearly five times bigger than the smallest pseudospin splitting. It should be noticed that the normal splitting for the case of the quantum number $n=1$ increases with a decreasing binding energy and the opposite pattern occurs for the $n=2$, which may connect with the diffuseness of the potential in neutron rich nuclei [19].

To understand why the energy splitting of pseudospin partner changes with different binding energies and why the pseudospin approximation is good in RMF, the PSOP and CB should be examined carefully. Unfortunately, it is very hard to compare them clearly, as the PSOP has a singularity at $E \sim V$. As we are only interested in the relative magnitude of the CB and the PSOP, we introduce the effective CB, $(E-V)[\kappa(\kappa-1)]/r^2$, and the effective PSOP, $(\kappa/r)(dV/dr)$, for comparison. They correspond to the CB and the PSOP multiplied by a common factor $E-V$, respectively.

The effective PSOP does not depend on the binding energy of the single particle level, but on the angular momentum and parity. On the other hand the effective CB depends on the energy. By comparing these two effective potentials one could see the energy dependence of the pseudospin symmetry. In order to examine this problem carefully, we compare the effective CB (dashed lines or dot-dashed lines) and the effective PSOP (solid lines) multiplied by the squares of the lower component wave function $F(r)$, which are given in Fig. 2, for $2s_{1/2}$ (upper left), $3s_{1/2}$ (lower left), $1d_{3/2}$ (upper right), and $2d_{3/2}$ (lower right) of ^{120}Zr in arbitrary scales. The pseudospin approximation is much better for the less bound pseudospin partners, because the effective CB is smaller for the more deeply bound states. This is in agreement with the results shown in Fig. 1. The integrated values of the potentials in Fig. 2 with r are proportional to their contribution to the energy after some proper renormalization. It is clear that the contribution of the effective CB (dashed lines or dot-dashed lines) is much bigger than that of the effective PSOP (solid lines).

In conclusion, the pseudospin symmetry is examined in realistic calculation in the framework of relativistic Hartree-Bogoliubov theory. We have proved that if $dV/dr=0$ is satisfied, the pseudospin symmetry is exact. Further the new condition

$$\frac{1}{E-V}\frac{\kappa}{r}\frac{dV}{dr} \ll \frac{\kappa(1-\kappa)}{r^2}$$

is found under which the symmetry is preserved approximately. We have examined under this condition how good approximation the pseudospin symmetry is in RHB. For a given angular momentum and parity channel, the effective

CB, $(E-V)[\kappa(\kappa-1)]/r^2$, becomes stronger for the less bound level, so the pseudospin symmetry for the weakly bound state is better than that for the deeply bound state, which is in agreement with the experimental observation [1,2]. The pseudo spin symmetry is found to be a good approximation even for exotic nuclei. The above conclusion has been well supported by the examples of ^{88}Zr and ^{120}Zr. From the simple Dirac equation, it has been shown that there are two equivalent ways to solve the coupled Dirac equation for the upper and lower components, i.e., the normal spin formalism and pseudospin formalism. Both formalisms are equivalent as long as the energies and wavefunctions are concerned. Their relation is given by Eq. (4), which indicates that the unitary transformation from the conventional formalism to the pseudospin formalism has the ''p helicity'' [11,12,20]. After the completion of this manuscript, we found that Ginocchio and Madland had done a RMF calculation without pairing [21]. It is shown that the occurrence of approximate pseudospin symmetry in nuclei is connected with certain similarities in the relativistic single-nucleon wave functions of the corresponding pseudospin doublets. This is in agreement with the conclusion here, if the condition

$$\frac{1}{E-V}\frac{\kappa}{r}\frac{dV}{dr} \ll \frac{\kappa(1-\kappa)}{r^2}$$

is satisfied, the pseudospin symmetry is preserved approximately and similarities in the relativistic single-nucleon wave functions of the corresponding pseudospin doublets will occur.

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