Relativistic symmetry in deformed nuclei by similarity renormalization group

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The similarity renormalization group is used to transform a general Dirac Hamiltonian into diagonal form. The diagonal Dirac operator consists of the nonrelativistic term, the spin-orbit term, the dynamical term, and the relativistic modification of kinetic energy, which are very useful to explore the symmetries hidden in the Dirac Hamiltonian for any deformed system. As an example, the relativistic symmetries in an axially deformed nucleus are investigated by comparing the contributions of every term to the single particle energies and their correlations with the deformation. The result shows that the deformation considerably influences the spin-orbit interaction and dynamical effect, which play a critical role in the relativistic symmetries and its breaking.

It is well known that the spin and pseudospin symmetries play a critical role in the shell structure and its evolution. The introduction of the spin-orbit potential to the single-particle shell model can well explain the experimentally observed existence of magic numbers for nuclei close to the valley of β stability. To understand the near degeneracy between two single-particle states with the quantum numbers \((n - 1, l + 2, j = l + 3/2)\) and \((n, l, j = l + 1/2)\), the concept of pseudospin symmetry (PSS) was introduced by defining the \(\hat{n} = n - 1, \hat{l} = l + 1, \hat{j} = \hat{l} + 1/2\) as the pseudospin doublets. The doublets persist for deformed nuclei as well. The axially deformed single-particle orbits with the asymptotic Nilsson quantum numbers \((\Omega = \Lambda + 1/2[N, n_3, \Lambda])\) and \((\Omega = \Lambda + 3/2[N, n_3, \Lambda + 2])\) are quasidegenerate, and can be viewed as the pseudospin doublets \((\Omega = \Lambda + 1/2[N = N - 1, n_3 = n_3, \Lambda = \Lambda + 1])\). Since the PSS is suggested in atomic nuclei, there have been comprehensive efforts to understand its origin. In 1997, the PSS was shown to be a symmetry of the Dirac Hamiltonian. The pseudo-orbital angular momentum \(\hat{l}\) is nothing but the orbital angular momentum of the lower component of the Dirac spinor, and the equality in magnitude but difference in sign of the scalar potential \(S\) and vector potential \(V\) was suggested as the exact PSS limit. Soon afterwards, this condition was generalized to \(d(S + V)/dr = 0\). As there exist no bound nuclei in the PSS limit, much effort is devoted to the mechanism of pseudospin breaking. By transforming the Dirac equation into a Schrödinger-like one, the influence of every term on the pseudospin breaking was checked and the dynamical nature of PSS was suggested in real nuclei. In order to better understand the symmetry of the Dirac Hamiltonian, the spin symmetry in the anti-nucleon was studied with the same origin as PSS discovered. Further, the supersymmetric description of PSS was presented for the spherical and axially deformed nuclei. In combination with the perturbative theory, the non-perturbative nature of PSS was indicated. Moreover, this symmetry was also checked in the resonant states. More reviews on the PSS can be found in the literatures and the references therein.

Regardless of these pioneering studies, the origin of PSS has not been fully understood in the relativistic framework. Recently, we have applied the similarity renormalization group (SRG) to Dirac Hamiltonian for a spherical system, and obtained a diagonal Dirac operator, which consists of the nonrelativistic term, the spin-orbit term, the dynamical term, the relativistic modification of kinetic energy, and the other term. In the diagonal Dirac operator, every term mentioned above is Hermitian, and all the defects in the usual decoupling disappear, which is very useful to analyze the PSS hidden in the Dirac Hamiltonian. As pointed out by Liang and etc.\footnote{[10]}, the work in Ref.\footnote{[20]} fills the gap between perturbation calculations and the supersymmetry descriptions. They have applied the operator under the lowest-order approximation to research on the origin of PSS and its breaking mechanism by the supersymmetry quantum mechanics and perturbation theory.\footnote{[10]} By including the lowest-order spin-orbit term, they have further investigated the spin-orbit effect on the PSS breaking.\footnote{[21]} We have applied the operator to check the contributions of every term to the pseudospin splitting and their influences on the PSS in Refs.\footnote{[22],[23].}

Considering that most of the real nuclei are deformed, in this paper we apply SRG to a general Dirac Hamiltonian and transform it into a diagonal form while keeps every term Hermitian. Such a study is significant for not only nuclei. As pointed out in Ref.\footnote{[15]}, the cylindrical geometries are relevant to a number of problems, including electron channeling in crystals, structure of axially deformed nuclei, and quark confinement in spheroidal flux tubes. As an example, we check the relativistic symmetry for an axially deformed nucleus by comparing the contributions of every term to the single particle energies and their correlations with the deformation to disclose the origin of the PSS and its breaking mechanism in deformed nuclei.

For simplicity, we sketch our formalism with the following Dirac Hamiltonian:

\[
H = \beta M + \hat{\alpha} \cdot \hat{\mathbf{p}} + (\beta S + V),
\]

where \(S\) and \(V\) represent the scalar potential and vector potential, respectively. For transforming \(H\) into a diagonal form, Wegner’s formulation of the SRG is adopted. The initial Hamiltonian \(H\) is transformed by the unitary
operator $U(l)$ according to
\[ H(l) = U(l)H U^\dagger(l), \quad H(0) = H \] (2)
where $l$ is a flow parameter. Differentiation of Eq. (2) gives the flow equation as
\[ \frac{d}{dl} H(l) = [\eta(l), H(l)], \] (3)
with the generator
\[ \eta(l) = \frac{dU(l)}{dl} U^\dagger(l) = -\eta^\dagger(l). \] (4)
The generator $\eta(l)$ should be chosen in such a way, so that the off-diagonal matrix elements decay. A good choice is defined by $\eta(l) = [H_d(l), H(l)]$, where $H_d(l)$ is the diagonal part of $H(l)$ [24]. For the Dirac Hamiltonian (1), it is appropriate to choose $\eta(l) = [\beta M, H(l)]$ [24]. In the choice of $\eta(l)$, $H(l)$ can be evolved into a diagonal form in the limit $l \to \infty$. By using the technique in Ref. [24], we have obtained the diagonalized Dirac operator as
\[ H_D = \begin{pmatrix} H_P + M & 0 \\ 0 & -H_P C - M \end{pmatrix}, \] (5)
where
\[ H_P = \Sigma + \frac{p^2}{2M} - \frac{1}{2M^2} (Sp^2 - \nabla S \cdot \nabla) \]
\[ + \frac{1}{4M^2} \nabla \times \hat{p} \cdot \nabla \Delta \times \hat{p} \]
\[ + \frac{S}{2M^3} (Sp^2 - 2\nabla S \cdot \nabla) - \frac{S}{2M^3} \nabla \Delta \times \hat{p} \]
\[ - \frac{1}{16M^3} \left( (\nabla \Sigma)^2 - 2\nabla \Sigma \cdot \nabla \Delta + 4S\nabla^2 \Sigma \right) \]
\[ - \frac{p^4}{8M^3} + O \left( \frac{1}{M^4} \right), \] (6)
is an operator describing Dirac particle. Its charge-conjugation $H_P^C$ is an operator describing Dirac anti-particle. $\Sigma = V + S$ and $\Delta = V - S$ denote the combinations of the scalar potential $S$ and the vector potential $V$. Different from Ref. [24], $H_P$ here is applicable for any deformed system. From Eq. (6), we can see that the operators reflecting the spin-orbit interaction and the dynamic effect have been extracted explicitly from the original Dirac Hamiltonian.

To make it clear, we decompose $H_P$ into five terms: $\Sigma + \frac{p^2}{2M} - \frac{1}{2M^2} (Sp^2 - \nabla S \cdot \nabla) + \frac{S}{2M^3} (Sp^2 - 2\nabla S \cdot \nabla)\frac{1}{3M^2} \nabla \times \hat{p} \cdot \nabla \times \hat{p}$, $- \frac{S}{2M^3} \nabla \times \hat{p} \cdot \nabla \Delta \times \hat{p}$, $- \frac{4S}{3M^4} \nabla^2 \Sigma - \frac{1}{16M^3} \left( (\nabla \Sigma)^2 - 2\nabla \Sigma \cdot \nabla \Delta + 4S\nabla^2 \Sigma \right)$, which are respectively labeled as $O_1, O_2, \ldots, O_5$. In this decomposition, every term $O_i (i = 1, 2, \ldots, 5)$ is Hermitian. $O_1$ corresponds to the operator describing Dirac particle in the nonrelativistic limit. $O_2$ is related to the dynamical effect. The spin-orbit interaction is reflected in the $O_3$. $O_4$ is the relativistic modification of kinetic energy. As $O_4$ is Hermitian, we can calculate the contribution of every term to the single particle energies, which is helpful to disclose the origin of relativistic symmetries. Especially, we can explore the deformation driven effect of the spin-orbit interaction and dynamical term, which is interesting not only for nuclei, but also for quantum controls and materials designs.

As $H_P$ is appropriate for any deformed system. As an example, we apply it to an axially quadrupole-deformed nucleus. The corresponding potentials are adopted as [23]
\[ S (\vec{r}) = S_0 (r) + S_2 (r) P_2 (\theta), \]
\[ V (\vec{r}) = V_0 (r) + V_2 (r) P_2 (\theta), \] (7)
where $P_2 (\theta) = \frac{1}{2} (3 \cos^2 \theta - 1)$. The radial parts in Eq. (7) take the Woods-Saxon form,
\[ S_0 (r) = S_{WS} f(r), \quad S_2 (r) = -\beta_2 S_{WS} k(r), \]
\[ V_0 (r) = V_{WS} f(r), \quad V_2 (r) = -\beta_2 V_{WS} k(r), \] (8)
where \( \beta_2 \) is a parameter controlling the deformation. 

\[ \frac{d}{dl} (H(l) | \psi(l) \rangle) = [\eta(l), H(l) | \psi(l) \rangle] \]
(3)
with \( f(r) = \frac{1}{1 + \exp \left( \frac{-r}{\alpha} \right)} \), and \( k(r) = r \frac{df(r)}{dr} \). Here \( V_{\text{WS}} \) and \( S_{\text{WS}} \) are, respectively, the typical depths of the scalar and vector potentials in RMF chosen as 350 and -405 MeV, the diffuseness of the potential \( a \) is fixed as 0.67 fm, and \( \beta_2 \) is the axial deformation parameter of the potential. The radius \( R \equiv r_0 A^{1/3} \) with \( r_0 = 1.27 \text{ fm} \). \(^{154}\text{Dy}\) is chosen as an example. The energy spectra of \( H_F \) are calculated by expansion in harmonic oscillator basis. The contribution of \( O_i \) to the energy level \( E_k \) is calculated by the formula \( \langle k | O_i | k \rangle = \int \psi_k^* O_i \psi_k d^3r \), where \( k \) marks the single particle state considered.

In Fig. 1, we show the variations of the single particle energies from all the relativistic modifications with \( \beta_2 \) for a pair of spin doublet, which are labeled by the corresponding spherical states with \( \Omega = 1/2 \). The spin-orbit term and dynamical term play a dominant role in the relativistic modifications of the energies, while the influences from the other terms is minor. Furthermore, the relativistic modification contributed by the spin-orbit interaction is remarkably associated with \( \beta_2 \). The same case also appears in the dynamical term. Over the range of deformation considered, the energies contributed by the spin-orbit term are negative for the spin aligned states and positive for the spin unaligned states, while those by the dynamic term are always positive. The same conclusions can be obtained for all the states with \( l \neq 0 \) in the spherical notation.

Considering that the relativistic effect originates mainly from the spin-orbit interaction and dynamical effect, it is necessary to compare their dependencies on the deformation for the different angular momentum states. In Fig. 2, we display the energies contributed by the spin-orbit term and dynamical term varying with \( \beta_2 \) for the four pairs of spin doublets with \( \Omega = 1/2 \). The spin-orbit splittings at \( \beta_2 = 0 \) are almost the most remarkable. With the increasing of deformation toward the oblate or prolate direction, the spin-orbit splittings reduce. For all the doublets considered, the energies contributed by the spin-orbit term is negative for the spin aligned states and positive for the spin unaligned states, and the spin-orbit splittings increase with the increasing angular momentum. Different from the spin-orbit interaction, the energies contributed by the dynamical term first decrease, then increase with the evolution of deformation from oblate to prolate, and are more sensitive to the deformation for the states with higher angular momentum. Similar to that in Fig. 1, the energies by the dynamical term is always positive. The same conclusions can be obtained for the states with \( \Omega > 1/2 \).

As the deformation influences the spin-orbit interaction and dynamical effect, which play a critical role in the energy level structure, it is interesting to explore the PSS and its origin for deformed nuclei. In Figs. 3 and 4, we show the variations of the energy splitting from every term with \( \beta_2 \) for the four pairs of pseudospin doublets. The variation of total energy splitting with \( \beta_2 \) is dominated by the three parts: the nonrelativistic term, the spin-orbit term, and the dynamic term. The influences from the relativistic modification of kinetic energy and the other term are almost negligible. The conclusion is consistent with that for the spherical nuclei \(^{20}\text{Ca}\). Over the range of \( \beta_2 \) here, the energy splitting from the nonrelativistic term is the most remarkable. The relativistic PSS is significantly improved, which comes mainly from the spin-orbit interaction and dynamical effect. Compared with the dynamical effect, the spin-orbit interaction is more sensitive to \( \beta_2 \) in the oblate side. The PSS becoming worse with the increasing of \( |\beta_2| \) is mainly due to the weaker spin-orbit interaction. In the prolate side, the PSS becomes worse with the increasing of \( \beta_2 \) for the doublets \((1/2|202\rangle, 3/2|222 \rangle) \) and \((1/2|320\rangle, 3/2|332 \rangle) \), which is attributed to a combination of the weaker spin-orbit improvement and the stronger dynamical breaking (or the weaker dynamical improvement). However for the doublets \((5/2|402\rangle, 7/2|404 \rangle) \) and \((5/2|512\rangle, 7/2|514 \rangle) \), the spin-orbit improvement becomes stronger and the dynamical breaking becomes weaker (or the dynamical improvement becomes stronger) with \( \beta_2 \), which result in the PSS becoming better. These have explained the reason why the PSS becomes worse for the more bound energy levels and better for the energy levels closer to the continuum (to see Fig. 5) for most of the heavy nuclei holding prolate shape.

In order to better grasp the PSS in deformed nuclei, the single particle energies for all the pseudospin doublets are plotted against the deformation \( \beta_2 \) ranging from -0.3 to 0.5 in Fig. 5, where the pseudospin doublets are labeled with the asymptotic Nilsson quantum numbers \( \Omega[N, n_3, \Lambda] \). For zero deformation \( \beta_2 = 0 \), the orbits are indicated by the corresponding spherical states. The figure reveals the following: (i) The energy difference between the pseudospin unaligned and aligned states always remains positive over the range of deformation considered here. (ii) The energy splittings between the pseudospin partners are more sensitive to \( \beta_2 \) for the oblate side than that for the prolate side. (iii) The energy splitting between the pseudospin partners is smaller for the valence orbits and for the partners just below the Fermi surface. The systematics has been explained well in the preceding analysis.

In summary, we apply the similarity renormalization group to transform a general Dirac Hamiltonian into diagonal form. The diagonal Dirac operator consists of the nonrelativistic term, the spin-orbit term, the dynamic term, and the relativistic modification of kinetic energy, and the other term, which are very useful to explore the symmetries hidden in the Dirac Hamiltonian. As an example, we have checked the relativistic symmetries for an axially deformed nucleus by comparing the contributions of every term to the single particle energies and their correlations with the deformation. It is shown that the spin-orbit interaction and dynamical effect play the key roles in the PSS. Their contributions
to the pseudospin energy splitting are correlated with the deformation of the potential and the quantum numbers of the state. Over the range of the deformation considered here, the spin-orbit interaction always improves the PSS, while the dynamical effect relates to the deformation and the particular state. For the deeply bound energy levels, the contribution of the dynamical term is a breaking of the PSS, while for the energy levels near to the continuum, the contribution of dynamical term becomes an improvement to the PSS. Compared with the dynamical effect, the dependence of the spin-orbit interaction on the deformation is more sensitive, which dominates the change of PSS in the oblate side. In the prolate side, with the development of energies with deformation toward the continuum, that the PSS becomes better is due to the stronger spin-orbit improvement and the weaker dynamical breaking (or the stronger dynamical improvement). The cause of better PSS for the levels closer to the continuum has been disclosed and the systematics of PSS associated with the deformation has been clarified.

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FIG. 1: (Color online) Comparisons of the contributions of all the relativistic modifications to the single particle energies and their correlations with the deformation parameter $\beta_2$ for a pair of spin doublet, which are indicated by the corresponding spherical states with $\Omega = \frac{1}{2}$. The ‘dynamic, spinorb, relakin, and other’ denote the dynamical term, the spin-orbit term, the relativistic modification of kinetic energy, and the other term, respectively. For guiding eyes, a sum of all the relativistic modifications is marked as ‘totalre’.

FIG. 2: (Color online) The contributions of the spin-orbit term and the dynamical term to the single particle energies and their correlations with the deformation parameter $\beta_2$ for four pairs of spin doublets with $\Omega = \frac{1}{2}$. 
FIG. 3: (Color online) Comparisons of the contributions of all the terms in $H_P$ to the pseudospin energy splittings and their correlations with the deformation parameter $\beta_2$ for the doublets $(1/2[420], 3/2[422])$ and $(1/2[530], 3/2[532])$. The 'nonrel, dynamic, spinorb, relak', and other' denote the nonrelativistic part, the dynamical term, the spin-orbit term, the relativistic modification of kinetic energy, and the other term, respectively. For guiding eyes, the total pseudospin energy splitting is marked as 'total'.

FIG. 4: (Color online) The same as Fig.3, but for the doublets $(5/2[402], 7/2[404])$ and $(5/2[512], 7/2[514])$. 
FIG. 5: (Color online) The single particle levels for all the pseudospin doublets in the nucleus $^{154}$Dy as a function of the quadrupole deformation parameter $\beta_2$. 