Probing the Symmetries of the Dirac Hamiltonian with Axially Deformed Scalar and Vector Potentials by Similarity Renormalization Group

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Symmetry is an important and basic topic in physics. The similarity renormalization group theory provides a novel view to study the symmetries hidden in the Dirac Hamiltonian, especially for the deformed system. Based on the similarity renormalization group theory, the contributions from the nonrelativistic term, the spin-orbit term, the dynamical term, the relativistic modification of kinetic energy, and the Darwin term are self-consistently extracted from a general Dirac Hamiltonian and, hence, we get an accurate description for their dependence on the deformation. Taking an axially deformed nucleus as an example, we find that the self-consistent description of the nonrelativistic term, spin-orbit term, and dynamical term is crucial for understanding the relativistic symmetries and their breaking in a deformed nuclear system.

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The symmetries of the Dirac Hamiltonian play a key role in the interpretation of many physical phenomena. Spin symmetry (SS) occurs in the spectrum of mesons with one heavy quark and it has been used to explain the absence of quark spin-orbit splitting (spin doublets) [1], which is observed in heavy-light quark mesons. Pseudospin symmetry (PSS) emerges in the single-nucleon spectrum. Two single-nucleon orbitals with quantum numbers ($n-1$, $l+2$, $j=l+3/2$) and (n, l, $j=l+1/2$) are near degenerate, and can be viewed as pseudospin doublets ($\tilde{n}=n-1$, $\tilde{l}=l+1$, $j=\tilde{l}\pm 1/2$) [2,3]. This symmetry is also present in deformed nuclei. The axially deformed single-particle orbits with asymptotic Nilsson quantum numbers ($\Omega=\Lambda+1/2[N,n_3,\Lambda]$) and ($\Omega=\Lambda+3/2$ $[N,n_3,\Lambda+2]$) are quasidegenerate [4]. In addition, spin and pseudospin symmetries are also concerned in atomic and molecular physics with particles trapped in some special atomic and molecular potentials [5,6].

For the above-mentioned reasons, there have been comprehensive efforts to understand the origin of spin and pseudospin symmetries. Based on the single-particle Hamiltonian of the oscillator shell model, the origin of PSS was connected with a special ratio in the strength of the spin-orbit and orbit-orbit interactions [7], and a pseudo state ($\tilde{l}$, $\tilde{s}$) can be mapped from a normal state (l, s) by a helicity unitary transformation [8]. A substantial progress was achieved in Ref. [9], where, PSS was shown to be a symmetry of the Dirac Hamiltonian with the pseudo-orbital angular momentum $\tilde{l}$ being nothing but the orbital angular momentum of the lower component of the Dirac spinor. The equality in magnitude but difference in sign of the scalar potential S and vector potential V was suggested as the exact PSS limit. This condition was extended to $d(S+V)/dr=0$ in Ref. [10], which can be approximately satisfied in exotic nuclei. To better grasp the symmetries, the SU(2) algebra was established in the Dirac Hamiltonian [11]. Further, in the (pseudo)spin symmetry limit, the Dirac Hamiltonian with special potentials was shown to possess U(3) symmetry [12] and chiral symmetry [13,14]. The supersymmetric description of the Dirac Hamiltonian was presented in Refs. [15–17]. The symmetries were also studied in resonant states [18,19], scattering states [20,21], and the antinucleon spectrum [22,23]. More research on the symmetries can be found in Refs. [24–26] and in the references therein.

As there are no bound states in the PSS limit, much effort has been devoted to the mechanism of pseudospin breaking. By transforming the Dirac equation into a Schrödinger-like equation, the influence of every component on pseudospin breaking was checked and the dynamical nature of PSS was suggested [23,27,28]. However, in these studies, one inevitably encounters a singularity in calculating the contribution of every component to the pseudospin splitting and the coupling between the operator and its eigenenergy in solving the Schrödinger-like equation for the lower component of the Dirac spinor. Recently, we have applied the similarity renormalization group (SRG) theory to the Dirac Hamiltonian for a spherical system, and obtained a diagonal Dirac operator [29], which is very useful in analyzing PSS hidden in the Dirac Hamiltonian [30,31], since all defects in the usual decoupling disappear. As pointed out in Ref. [25], the work in Ref. [29] fills the gap between perturbation calculations and supersymmetry descriptions. They have applied the operator under the lowest-order approximation to study the origin of PSS and its breaking mechanism by supersymmetry quantum mechanics and perturbation theory [25]. By including the lowest-order spin-orbit term, they have further investigated the spin-orbit effect on PSS breaking [32].

However, the operator obtained in Ref. [29] is only applicable for a spherical system. In this Letter we apply the

SRG theory to a general Dirac Hamiltonian and transform it into a diagonal form. The diagonal Dirac operator is applicable to explore the symmetries of the Dirac Hamiltonian for any deformed system, which is significant not only for nuclei. As pointed out in Ref. [16], the cylindrical geometries are relevant to a number of problems, including electron channeling in crystals, quark confinement in spheroidal flux tubes, etc. Furthermore, we have explicitly extracted these operators reflecting spin-orbit coupling and the dynamical effect with any deformed potential. These operators are useful in describing many physical phenomena in different fields of physics, as the spin-orbit interaction plays an important role in the spin Hall effect [33] and spin-orbit coupled Bose-Einstein condensates [34]. As an example, we apply the diagonal Dirac operator to explore the relativistic symmetries for an axially deformed nucleus, and investigate the deformed effect and dynamical nature of the relativistic symmetries in deformed nuclei.

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

$$H = \beta M + \vec{\alpha}\cdot\vec{p} + (\beta S + V), \tag{1}$$

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 theory is adopted [35]. The initial Hamiltonian H is transformed by the unitary operator $U(l)$ according to

$$H(l) = U(l) H U^{\dagger}(l), \qquad H(0) = H, \tag{2}$$

where l is a flow parameter. Differentiation of Eq. (2) gives the flow equation as

$$\frac{d}{dl}H(l) = [\eta(l), H(l)], \tag{3}$$

with the generator

$$\eta(l) = \frac{dU(l)}{dl}U^{\dagger}(l) = -\eta^{\dagger}(l). \tag{4}$$

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 $H(l)$ [35]. For the Dirac Hamiltonian (1), it is appropriate to choose $\eta(l) = [\beta M, H(l)]$ [29]. 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. [29], we have obtained the diagonalized Dirac operator as

$$H_D = \begin{pmatrix} H_P + M & 0 \\ 0 & -H_P^C - M \end{pmatrix}, \tag{5}$$

where H_P is an operator describing a Dirac particle, and its charge-conjugation H_P^C is an operator describing a Dirac antiparticle. The operator H_P consists of the five Hermitian components

$$H_P = H_n + H_d + H_c + H_k + H_w, \tag{6}$$

where

$$\begin{aligned} H_n &= \Sigma + \frac{p^2}{2M}, \\ H_d &= -\frac{1}{2M^2}(Sp^2 - \nabla S\cdot\nabla) + \frac{S}{2M^3}(Sp^2 - 2\nabla S\cdot\nabla), \\ H_c &= \frac{1}{4M^2}\left(1 - \frac{2S}{M}\right)\vec{\sigma}\cdot(\nabla\Delta\times\vec{p}), \\ H_k &= -\frac{p^4}{8M^3}, \\ H_w &= \frac{1}{16M^3}[2(M-2S)\nabla^2\Sigma + (\nabla\Sigma)^2 + 2\nabla\Sigma\cdot\nabla\Delta]. \end{aligned} \tag{7}$$

H_n corresponds to the operator describing a Dirac particle in the nonrelativistic limit. H_d is related to the dynamical effect. The spin-orbit interaction is reflected in H_c. H_k represents the relativistic modification of kinetic energy. H_w can be viewed as the Darwin term. $\Sigma = V + S$ and $\Delta = V - S$ denotes the combinations of the scalar potential S and the vector potential V. As H_n, H_d, H_c, H_k, and H_w are Hermitian, we can calculate the contribution of every term to the single-particle energies, which is helpful to disclose the origin of relativistic symmetries. For example, the contribution of H_n to the energy level E_k can be calculated by the formula $\langle k|H_n|k\rangle = \int \psi_k^* H_n \psi_k d^3\vec{r}$, where k marks the single particle state considered. Different from Ref. [29], H_P here is applicable for any deformed system, and can be used to 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 [36]

$$\begin{aligned} S(\vec{r}) &= S_0(r) + S_2(r)P_2(\theta), \\ V(\vec{r}) &= V_0(r) + V_2(r)P_2(\theta), \end{aligned} \tag{8}$$

where $P_2(\theta) = 1/2\,(3\cos^2\theta - 1)$. The radial parts of the potentials in Eq. (8) take the Woods-Saxon form

$$\begin{aligned} S_0(r) &= S_{\mathrm{WS}}f(r), \qquad S_2(r) = -\beta_2 S_{\mathrm{WS}}k(r), \\ V_0(r) &= V_{\mathrm{WS}}f(r), \qquad V_2(r) = -\beta_2 V_{\mathrm{WS}}k(r), \end{aligned} \tag{9}$$

with $f(r) = 1/(1+\exp((r-R)/a))$ and $k(r) = r(df(r)/dr)$. Here S_{WS} and V_{WS}, respectively the typical depths of the scalar and vector potentials in the relativistic mean field model, are chosen as -450 and 350 MeV, the diffuseness of the potential a is fixed as 0.67 fm, and β_2

is the axial deformation parameter of the potential. The radius $R \equiv r_0 A^{1/3}$ with $r_0 = 1.27$ fm. ^{154}Dy is chosen as an example. The energy spectra of H_P are calculated by expansion in the harmonic oscillator basis.

Figure 1 shows the contribution of every relativistic modification to the single particle energies and its evolution to β_2 for a pair of spin and pseudospin doublets, which are labeled with the asymptotic Nilsson quantum numbers $\Omega[N, n_3, \Lambda]$. For simplicity of understanding, the corresponding spherical notations are also marked there. Similarly, this labeling scheme is also adopted in the next figures. From Fig. 1, it can be seen that the total relativistic modification comes mainly from the contributions of the dynamical term H_d and the spin-orbit term H_c, while those from the relativistic modification of kinetic energy H_k and the Darwin term H_w are almost negligible. Furthermore, these relativistic modifications from the dynamical term and the spin-orbit term are, remarkably, associated with β_2. Over the range of deformation under consideration, the energies contributed by the spin-orbit term are negative for the spin aligned (pseudospin unaligned) states and positive for the spin unaligned (pseudospin aligned) states, whereas those contributed by the dynamical term are always positive. These play important roles in the relativistic symmetries.

Since these relativistic modifications are significant, it is necessary to explore their influences on the relativistic symmetries, which is helpful to disclose the origins of the relativistic symmetries and their breaking mechanisms. In Fig. 2, we demonstrate the variation of the energy splitting between the spin doublets (hereinafter referred to as "spin energy splitting") with β_2 for four pairs of spin doublets. From Fig. 2(a), one can see that the spin energy splitting comes almost entirely from the contribution of the spin-orbit term H_c on the prolate side. The contributions of the nonrelativistic term H_n and the dynamical term H_d to the spin energy splitting nearly cancel each other out, while those from the relativistic modification of kinetic energy H_k and the Darwin term H_w are negligible. In addition, the spin energy splitting increases with increasing deformation. The same case also appears in Figs. 2(b) and 2(d) for these doublets with $\Omega = j$, where Ω is the projection of total angular momentum j on the third axis. However, for these doublets with $\Omega < j$ [see Fig. 2(c)], there is a slight deviation between the spin energy splitting and that contributed by H_c. Nonetheless, spin symmetry breaking in deformed nuclei comes mainly from the spin-orbit term since the operator reflecting the spin-orbit interaction is almost completely separated from the Dirac Hamiltonian. On the oblate side, all of these terms including the nonrelativistic, the spin-orbit coupling, and the dynamical terms have important influences on the spin energy splitting. Especially for the nonrelativistic term and the spin-orbit term, their contributions to the spin energy splitting are sensitive to β_2. Significant deviations between the spin energy splitting and that contributed by H_c reflect the presence of non-negligible configuration mixing there.

Compared with spin symmetry, the origin of pseudospin symmetry is more complicated for deformed nuclei. In Fig. 3, we exhibit the variations of the energy splitting

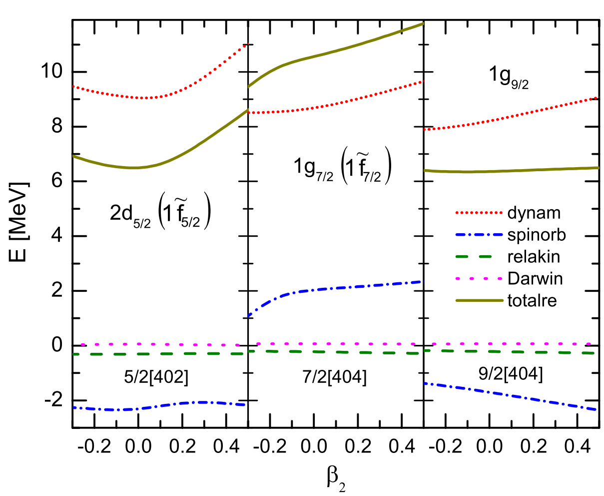

FIG. 1 (color online). Comparisons of the contributions of all the relativistic modifications to the single particle energies and their correlations with the deformation parameter β_2 for a pair of spin and pseudospin doublets, where "dynam," "spinorb," "relakin," and "Darwin" denote the dynamical term, the spin-orbit term, the relativistic modification of kinetic energy, and the Darwin term, respectively. As a guide to the eyes, a sum of all the relativistic modifications is marked "totalre."

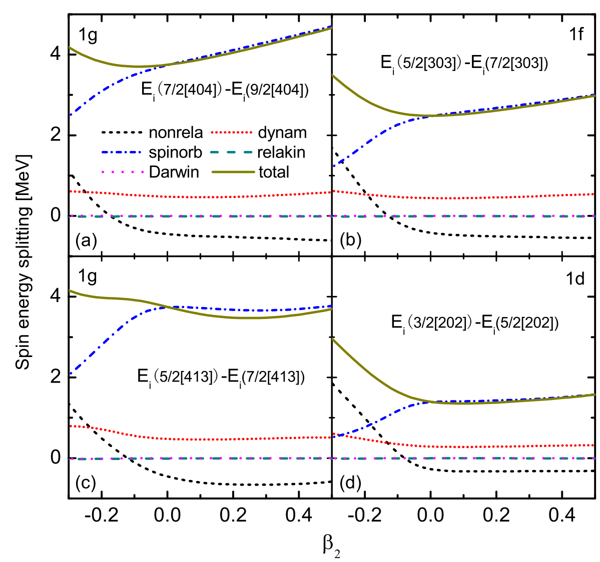

FIG. 2 (color online). Comparisons of the contributions of all the terms in H_P to the spin energy splitting and their correlations with the deformation parameter β_2 for four pairs of spin doublets. Here "nonrela," "dynam," "spinorb," "relakin," and "Darwin" denote the nonrelativistic part, the dynamical term, the spin-orbit term, the relativistic modification of kinetic energy, and the Darwin term, respectively. As a guide to the eyes, the total pseudospin energy splitting is marked as "total."

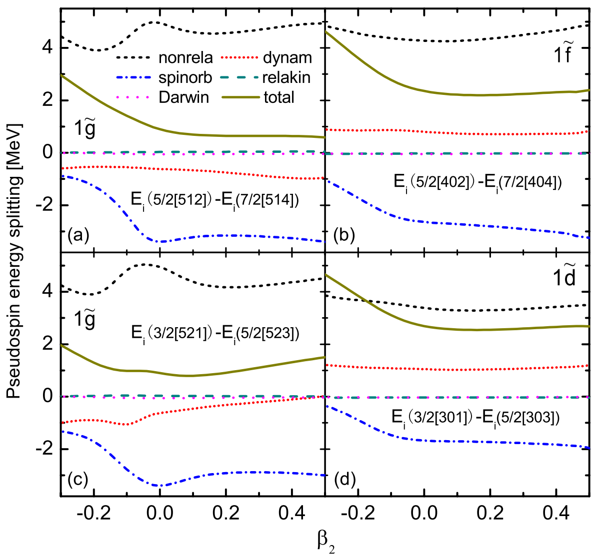

FIG. 3 (color online). Same as Fig. 2, but for pseudospin energy splitting.

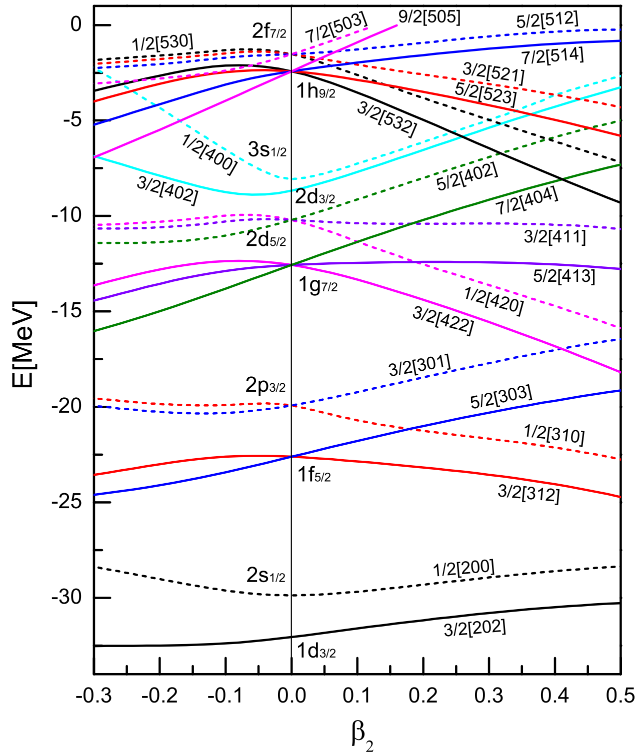

FIG. 4 (color online). Single particle levels for all pseudospin doublets in the nucleus [154]Dy as a function of the quadrupole deformation parameter β_2.

between pseudospin doublets with β_2 for four pairs of pseudospin doublets. The variation of the total energy splitting with β_2 is dominated by the three parts: the nonrelativistic term H_n, the spin-orbit term H_c, and the dynamical term H_d. The influences from the relativistic modification of kinetic energy H_k and the Darwin term H_w are fairly minor. Over the range of β_2 here, the energy splitting from the nonrelativistic term H_n is the most remarkable. The relativistic PSS is significantly improved, which comes mainly from the spin-orbit interaction and the dynamical effect. The spin-orbit interaction always improves PSS. Whether PSS is improved or destroyed by the dynamical term depends on the particular doublets and the deformation. For these doublets close to the continuum, the contribution of the dynamical term is an improvement to PSS [Fig. 3(a)], while for those far from the continuum, the contribution of the dynamical term becomes destructive to PSS [Figs. 3(b) and 3(d)]. For these doublets near the continuum developing with β_2 away from the continuum, the contribution of dynamical term evolves from improvement to destruction [Fig. 3(c)]. These have explained the reason why PSS becomes better for energy levels closer to the continuum. Compared with the dynamical effect, the spin-orbit interaction is more sensitive to β_2 on the oblate side. That PSS becomes worse with an increase of $|\beta_2|$ is mainly due to the weaker spin-orbit interaction. On the prolate side, PSS is insensitive to deformation for these doublets with $\Omega = j$ [Figs. 3(b) and 3(d)], and becomes a bit worse with β_2 for the doublets with $\Omega < j$ [Fig. 3(c)], which is attributed to the weaker improvement by the spin-orbit and dynamical terms.

In order to better grasp PSS in deformed nuclei, the single particle energies for all the pseudospin doublets are plotted against the deformation β_2 ranging from -0.3 to 0.5 in Fig. 4. The figure reveals the following points: (i) the energy difference between the pseudospin unaligned and aligned states always remains positive over the range of deformation considered here; (ii) the pseudospin energy splitting is more sensitive to β_2 on the oblate side than that on the prolate side; (iii) the pseudospin energy splitting is smaller for the valence orbits and for the partners just below the Fermi surface. The systematics have been explained well in the preceding analysis.

In summary, we apply the similarity renormalization group theory to transform a general Dirac Hamiltonian into diagonal form. The diagonal elements become Schrödinger-like operators consisting of a nonrelativistic term, a spin-orbit term, a dynamic term, a relativistic modification of kinetic energy, and a Darwin term, which are very useful for exploring the symmetries hidden in the Dirac Hamiltonian for any deformed system. As an example, we have probed 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, we have found that the spin-orbit and dynamical terms play key roles in SS and PSS. The spin energy splitting comes almost entirely from the contribution of the spin-orbit term for prolate nuclei. The extent of this splitting depends on the deformation. Especially for these doublets with $\Omega = j$, the spin energy splitting increases with increasing deformation.

The pseudospin energy splitting is dominated by the nonrelativistic term, the spin-orbit term, and the dynamical term. The energy splitting from the nonrelativistic term is the most serious. The relativistic PSS is significantly improved, which comes mainly from the spin-orbit interaction and the dynamical effect. The spin-orbit interaction always plays a role in favor of PSS, while the dynamical effect depends on the deformation and the particular doublets. When the energy levels develop with the deformation or the quantum numbers of the states toward the continuum, the contribution of the dynamical term evolves from destruction to improvement. This 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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