New symmetry in many-body effective Hamiltonians: An example of rotating nuclei

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A general class of many-body Hamiltonians containing one- and two-body interactions that obey at least one dichotomic symmetry are considered. A rich subset in that class with several important physical applications (such as, e.g., in nuclear superfluidity and/or particle number nonconserving Hamiltonians) are studied from a unitary-group structure point of view. Those Hamiltonians are shown to obey a symmetry called further on $\mathcal{P}$ symmetry. A corresponding Casimir operator is constructed together with its eigenvalues and the implied classification of the spectra is illustrated on a nuclear-physics example with a single-j shell Hamiltonian. The most general form of a $\mathcal{P}$-symmetric Hamiltonian is discussed.

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There exist numerous problems in physics that involve many-body Hamiltonians with one-, two-, three-... body effective interactions leading to nonscalar energy operators as, e.g., in theory of deformed atomic nuclei and in applications of atomic, solid-state, and particle physics. One of the main difficulties encountered is that the solution methods, usually approximate, drastically change from one form of the interaction to another. Here we would like to follow an algebraic approach based on the unitary-group properties of the Hamiltonians in question. A known advantage of such an approach is the relative simplicity of the underlying algorithms which may be viewed as practically independent of the actual form of the (many-body) interactions. A disadvantage is often related to the dimensionality of the Hamiltonian matrices which too often and too quickly become prohibitively large. Needless to say, any symmetry that may arise, offers at the same time a better physics insight and facilitates the solution. In this paper we would like to introduce a symmetry called further on $\mathcal{P}$ symmetry. This symmetry is obeyed by many effective Hamiltonians used in various branches of physics—yet seemingly not used in literature.

For particle-number conserving interactions $\mathcal{P}$ symmetry leads to a block-diagonal structure of the Hamiltonian, each block characterized by the particle number $\mathcal{N}$ and $\mathcal{P}$-quantum number associated with $\mathcal{P}$ symmetry. For an important class of the particle-number *not* conserving Hamiltonians $\mathcal{P}$ symmetry leads to another type of conservation law whose knowledge may be equally useful. To render our presentation more specific we will focus on a nuclear-physics context.

In majority of the nuclear-structure calculations addressing, e.g., the phenomenon of collective rotation and pairing, the effective Hamiltonians used have the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}(1) + \hat{\mathcal{H}}(2) + \hat{\mathcal{H}}(\mathrm{rot}) \ , \tag{1}$$

in which the one-body and two-body interaction terms $\hat{\mathcal{H}}(1)$ and $\hat{\mathcal{H}}(2)$, respectively, are expressed as

$$\hat{\mathcal{H}}(1) + \hat{\mathcal{H}}(2) = \sum_{\alpha\beta} h_{\alpha\beta} c^+_\alpha c_\beta + \frac{1}{2} \sum_{\alpha\beta} \sum_{\gamma\delta} v_{\alpha\beta;\gamma\delta} c^+_\alpha c^+_\beta c_\delta c_\gamma \ . \tag{2}$$

Usually $h_{\alpha\beta}$ represents an average field Hamiltonian and $v_{\alpha\beta;\gamma\delta}$ a residual interaction, for instance, pairing. In this work we consider an important two-dimensional rotation problem within either cranking or particles-rotor approximations which are quite standard in nuclear physics. Therefore

$$\hat{\mathcal{H}}(\mathrm{rot}) = \hat{\mathcal{H}}_{\mathrm{cranking}} \equiv -\omega \hat{j}_x = -\omega \sum_{\alpha\beta} (\hat{j}_x)_{\alpha\beta} c^+_\alpha c_\beta \tag{3}$$

or

$$\hat{\mathcal{H}}(\mathrm{rot}) = \hat{\mathcal{H}}_{p\text{-rotor}} \equiv \frac{(I - \hat{j}_x)^2}{2\mathcal{J}} \ . \tag{4}$$

Here and in the following we denote the collective-rotation axis $\mathcal{O}_x$ and the corresponding one-body angular momentum operator $\hat{j}_x$.

We would like to emphasize that the rotation term, although of great importance in, e.g., high-spin nuclear physics, does not need to be included; all conclusions of this study apply equally well for $\hat{\mathcal{H}}(\mathrm{rot}) = 0$. We are going to demonstrate that most of the standard forms of $\hat{\mathcal{H}}(1)$ with dichotomic symmetry operators such as "signature," $\hat{R}_x \equiv \exp(i\pi\hat{j}_x)$ or "simplex" $\hat{S}_x \equiv \hat{\pi}\hat{R}_x$($\hat{\pi}$ parity) and many-forms of $\hat{\mathcal{H}}(2)$ as, e.g., monopole pairing, obey $\mathcal{P}$ symmetry which so far has not been exploited in analyses of spectra. We will also present the most general form of an effective Hamiltonian satisfying such a symmetry. Parity, an obvious dichotomic symmetry important in many applications may easily be incorporated. In fact in an extension of the present algorithm to "realistic" nuclear Hamiltonians, parity and $\mathcal{P}$ symmetry lead to a further simplification; each block of a given $\mathcal{P}$ quantum number splits into two subblocks of opposite parities. Corresponding results will be published elsewhere.

Let us begin by formulating an algebraic context of our physical problem in Eqs. (1)–(4). Knowing that Hamiltonian (1) commutes with a dichotomic symmetry operator $\hat{S}$ (e.g., $\hat{R}_x$ or $\hat{S}_x$) we will choose the single-nucleonic basis $\{|\alpha\rangle \equiv c_\alpha^+|0\rangle\}$ in such a way that $\hat{s}|\alpha\rangle = s_\alpha|\alpha\rangle$, where $s_\alpha = \pm i$. Let the total number of individual-nucleonic states in this basis be n. To simplify presentation, suppose that n is even and that the numbers of the basis states with $s_\alpha = +i$ and $s_\alpha = -i$, n_+ and n_-, respectively, satisfy $n_+ = n_- = n/2$. Let us introduce an auxiliary set of operators

$$\hat{g}_{\alpha\beta} \equiv \hat{N}_{\alpha\beta} \equiv c_\alpha^+ c_\beta;\ (s_\alpha = +i,\ s_\beta = +i)\ , \tag{5a}$$

$$\hat{g}_{\alpha'\beta'} \equiv \hat{N}_{\alpha'\beta'} \equiv c_{\alpha'} c_{\beta'}^+;\ (s_{\alpha'} = -i,\ s_{\beta'} = -i)\ , \tag{5b}$$

$$\hat{g}_{\alpha\beta'} \equiv \hat{B}_{\alpha\beta'}^+ \equiv c_\alpha^+ c_{\beta'}^+;\ (s_\alpha = +i,\ s_{\beta'} = -i)\ , \tag{5c}$$

$$\hat{g}_{\alpha'\beta} \equiv \hat{B}_{\alpha'\beta} \equiv c_{\alpha'} c_\beta;\ (s_{\alpha'} = -i,\ s_\beta = +i)\ . \tag{5d}$$

With the above restrictions on the s-quantum numbers each set of operators contains $n^2/4$ elements and the whole ensemble in Eqs. (5a)–(5d) contains n^2 operators.

It is now straightforward to prove that the operators $\{\hat{g}_{kl}\}$ in (5) satisfy the commutation relations

$$[\hat{g}_{kl}, \hat{g}_{pq}] = \delta_{lp}\hat{g}_{kq} - \delta_{kq}\hat{g}_{pl};\quad k,l,p,q = 1,2\ldots,n\ , \tag{6}$$

which are known to define an algebra of a unitary group in n dimensions, $\mathcal{U}(n)$.

Let us observe a difference between our representation of this $\mathcal{U}(n)$ algebra, that mixes c^+c^+ and c^+c operators, Eq. (5), and the one based exclusively on the $\hat{N}_{\alpha\beta} = c_\alpha^+ c_\beta$ operators [1] which naturally obey the commutation relations $[\hat{N}_{\alpha\beta}, \hat{N}_{\gamma\delta}] = \delta_{\beta\gamma}\hat{N}_{\alpha\delta} - \delta_{\alpha\delta}\hat{N}_{\gamma\beta}$; $\alpha,\beta,\gamma,\delta = 1,2\ldots,n$, that are identical to those in (6). Observe also that the operators $\hat{N}_{\alpha\beta}$, $\hat{B}_{\alpha\beta}^+$, and $\hat{B}_{\alpha\beta}$ unrestricted by the dichotomic symmetry conditions in Eqs. (5a)–(5d) obey the commutation relations characteristic for the generators of an SO($2n$) group rather than those for $\mathcal{U}(n)$, cf. Ref. [2]. An important physical consequence of the above property is that the Hamiltonians constructed out of generators (6) may, but do not need to conserve the particle number, a feature that is very useful in some applications.

It will be convenient to define a Casimir operator

$$\hat{P} \equiv \sum_{k=1}^{n} \hat{g}_{kk} \to [\hat{P}, \hat{g}_{rs}] = 0;\quad r,s = 1,2,\ldots,n\ . \tag{7}$$

We will also define a generalized pairing two-body interaction

$$\hat{\mathcal{H}}(2) \to \hat{\mathcal{H}}(\text{pairing}) = \sum_{\alpha\alpha'}\sum_{\beta\beta'} v_{\alpha\alpha',\beta\beta'} c_\alpha^+ c_{\alpha'}^+ c_{\beta'} c_\beta \tag{8a}$$

$$= \frac{1}{2}\sum_{\alpha\beta}\left(\sum_{\alpha'} v_{\alpha\alpha',\beta\alpha'}\right)\hat{g}_{\alpha\beta} + \frac{1}{2}\sum_{\alpha'\beta'}\left(\sum_{\alpha} v_{\alpha'\alpha,\beta'\alpha}\right)\hat{g}_{\alpha'\beta'} - \sum_{\alpha\alpha'}\sum_{\beta'\beta} v_{\alpha\alpha',\beta\beta'}\hat{g}_{\alpha\beta'}\hat{g}_{\alpha'\beta}\ , \tag{8b}$$

where the summation indices obey the restrictions of Eq. (5). Expression (8a) gives the standard monopole pairing Hamiltonian as a particular case. Restricted to the above (still quite rich) pairing interactions the original cranking Hamiltonian in Eq. (1) takes the form

$$\hat{\mathcal{H}} = \sum_{\alpha\beta}[h_{\alpha\beta} - \omega(\hat{j}_x)_{\alpha\beta}]\hat{g}_{\alpha\beta} + \sum_{\alpha'\beta'}[h_{\alpha'\beta'} - \omega(\hat{j}_x)_{\alpha'\beta'}]\hat{g}_{\alpha'\beta'} - \sum_{\alpha\alpha'}\sum_{\beta\beta'} v_{\alpha\alpha',\beta\beta'}\hat{g}_{\alpha\beta'}\hat{g}_{\alpha'\beta} \tag{9}$$

in which the first two terms of Eq. (8b) having a one-body character have been included in the one-body Hamiltonian, thus leading to its simple modification. The particles-rotor form of the Hamiltonian can also be expressed in terms of $\hat{g}_{kl}$ generators. Because of the commutation relations in (7) we may look for the solutions which are at the same time the eigenstates of $\hat{\mathcal{H}}$ and $\hat{\mathcal{P}}$

$$\hat{\mathcal{H}}|\psi_\rho\rangle = E_\rho|\psi_\rho\rangle \quad\text{and}\quad \hat{\mathcal{P}}|\psi_\rho\rangle = p_\rho|\psi_\rho\rangle\ . \tag{10}$$

The fact that the Hamiltonian of interest, Eq. (9), has been expressed in terms of a unitary-group generators implies the possibility of constructing its eigenstates in terms of the corresponding irreducible representations of the $\mathcal{U}(n)$. An elegant scheme for such a construction has been proposed by Gelfand and Zetlin [3]. We have solved Eq. (10) by constructing first the matrix representations of the $\hat{g}_{pq}$ generators in the Gelfand-Zetlin basis $\{|GZ;\mu\rangle\}$ and then diagonalizing $\hat{\mathcal{H}}$. We will not repeat the description here (for details see, e.g. Refs. [1,4]. Nevertheless it will be useful to recall that for the antisymmetric irreps, adequate for the multifermion systems,

$$\hat{g}_{kk}|GZ;\mu\rangle = \mu_k|GZ;\mu\rangle; \tag{11}$$

μ_k may take only the values 0 or 1 and consequently the eigenvalues possible of the $\hat{\mathcal{P}}$ operator in Eq. (7) are $p = 0,1,2,\ldots,n$. The related p values label $(n+1)$ antisymmetric irreducible representations of the $\mathcal{U}(n)$ group and it can be shown that the corresponding irrep. dimensions are $\mathcal{N}(p,n) = \binom{n}{p}$ (see also Ref. [5]). Once the $\hat{g}_{kl}$ generators are calculated, the whole numerical difficulty reduces to calculating the matrix elements h_{kl}

and $v_{kk',l'l}$ in Eq. (9).

It will be of advantage to discuss the physical interpretation of Casimir operator $\mathcal{P}$ first. Following our notation we have

$$\hat{\mathcal{P}} = \sum_{k=1}^{n} \hat{g}_{kk} = \sum_{\alpha=1}^{n_+} \hat{g}_{\alpha\alpha} + \sum_{\alpha'=1}^{n_-} \hat{g}_{\alpha'\alpha'} = \sum_{\alpha=1}^{n_+} c_\alpha^+ c_\alpha + \sum_{\alpha'=1}^{n_-} c_{\alpha'} c_{\alpha'}^+ = \hat{\mathcal{N}}^+ - \hat{\mathcal{N}}^- + n_- , \quad (12)$$

where the $\hat{\mathcal{N}}^+$ and $\hat{\mathcal{N}}^-$ operators satisfy

$$\hat{\mathcal{N}}^+ \equiv \sum_{\alpha=1}^{n_+} c_\alpha^+ c_\alpha, \quad \hat{\mathcal{N}}^- \equiv \sum_{\alpha'=1}^{n_-} c_{\alpha'}^+ c_{\alpha'} . \quad (13)$$

Their eigenvalues, $\mathcal{N}^+$ and $\mathcal{N}^-$, give the numbers of particles with $s = +i$ and $s = -i$, respectively. It is straightforward to prove that $\hat{\mathcal{P}}, \hat{\mathcal{N}}^+, \hat{\mathcal{N}}^-, \hat{\mathcal{N}} \equiv \hat{\mathcal{N}}^+ + \hat{\mathcal{N}}^-$ and $\hat{\mathcal{H}}$ in (1) all commute. One can thus infer from the proportionality $\hat{\mathcal{P}} \sim (\hat{\mathcal{N}}^+ - \hat{\mathcal{N}}^-)$ that the Casimir operator introduced earlier characterizes the difference between the numbers of particles occupying the states of the opposite S symmetries. In other words, the irreducible representations, with the dimensions $\mathcal{N}(p,n)$ introduced above contain those and only those basis vectors $|GZ,\mu\rangle$ for which $\Delta\mathcal{N}_\mu \equiv (\mathcal{N}_\mu^+ - \mathcal{N}_\mu^-)$ are equal (to a common constant). It then follows that for the systems with even particle numbers $\mathcal{N} \equiv (\mathcal{N}^+ + \mathcal{N}^-)$, the p eigenvalues satisfy $p = 0, 2, 4 \ldots$ while the systems with the odd particle numbers have $p = 1, 3, \ldots$.

Let us observe that a Hamiltonian expressible in terms of the generators (5) may in general contain the interactions which do not conserve the number of particles (for instance, terms $\sim \hat{B}^+\hat{B}^+, \sim \hat{B}^+\hat{B}^+\hat{B}^+, \sim \hat{\mathcal{N}}\hat{B}^+$, etc.). In such a case a (p,n)-irreducible representation will generate matrix elements connecting states with different particle numbers of the same parity and, necessarily, with the same $(\mathcal{N}^+ - \mathcal{N}^-)$. [Hamiltonians of this more general form are not of interest in the context of Hamiltonian (1) that preserves the number of particles.] Knowing in addition that $\hat{\mathcal{N}}^+$ and $\hat{\mathcal{N}}^-$ commute with $\hat{\mathcal{H}}$ and that $\hat{\mathcal{P}}|GZ,\mu\rangle = p_\mu|GZ,\mu\rangle$ while $\hat{\mathcal{N}}^+|GZ,\mu\rangle = \mathcal{N}_\mu^+|GZ,\mu\rangle$, we may always order the GZ states within a (p,n) irrep. by grouping them according to a common particle number, $\mathcal{N} \equiv \mathcal{N}^+ + \mathcal{N}^-$, thus bringing the corresponding total matrix into a block-diagonal form, each block characterized by the particle number $\mathcal{N}$.

Let us mention that the most general form of a two-body interaction which obey the $\mathcal{P}$ symmetry and preserves the particle number is

$$\hat{\mathcal{H}}(\mathcal{P}\text{ symmetric}) = \sum_{\alpha\alpha'} \sum_{\beta\beta'} v_{\alpha\alpha',\beta\beta'}, c_\alpha^+ c_{\alpha'}^+ c_{\beta'} c_\beta + \sum_{\alpha\beta} \sum_{\gamma\delta} v_{\alpha\beta,\gamma\delta} c_\alpha^+ c_\beta^+ c_\delta c_\gamma + \sum_{\alpha'\beta'} \sum_{\gamma'\delta'} v_{\alpha'\beta',\gamma'\delta'} c_{\alpha'}^+ c_{\beta'}^+ c_{\delta'} c_{\gamma'} , \quad (14)$$

where, as before, the indices without a "prime" refer to the $s = +i$ and the indices with a "prime" to the $s = -i$ nucleon basis states. By exchanging the order of $c_\beta^+ c_\delta$ and $c_{\beta'}^+ c_{\delta'}$ operators in the above Hamiltonian we may express the two last terms in Eq. (14) in terms of the generators 5(a)–5(b) with once again a trivial modification of the original one-body Hamiltonian. Any other (two-body, three-body, etc.) interactions will obviously lead to the same symmetry properties of the corresponding many-body Hamiltonians *if they can be expressed using generators* (6).

The results of this procedure corresponding to a model space of a $j = \frac{11}{2}$ shell, i.e., $n = 2j + 1 = 12$ with $N = 6$ particles are illustrated below. We have diagonalized the Hamiltonian of the particles-rotor form, i.e., replacing the cranking term in Eq. (9) by $(I - \hat{j}_x^{\text{total}})^2/(2\mathcal{J})$. It is convenient to slightly modify our notation by introducing

$$P \equiv p - n_- = (\mathcal{N}^+ - \mathcal{N}^- + n_-) - n_- = \mathcal{N}^+ - \mathcal{N}^- . \quad (15)$$

Following the arguments presented above, it can be relatively easy to show, using combinatorial arguments, that various P blocks of the Hamiltonian contain for the fixed-particle number $N(=6)$ submatrices of dimensions $d_{P=0} = 400$, $d_{P=\pm 2} = 225$ (two blocks), $d_{P=\pm 4} = 36$ (two blocks), and $d_{P=\pm 6} = 1$ (two blocks). The energy spectra in function of spin for the lowest solutions of each block (yrast line for each P symmetry) are presented in Fig. 1 for illustration. The related $P = \pm 2$, ± 4, and ± 6 solutions are degenerated at $I = 0$ (cf. Fig. 1). It is worth emphasizing that the difference between the energies of the solutions of the opposite P values that are degenerate at $I = 0$ (P splitting) should not be confused with the signature splitting, whose illustrations are abundant in

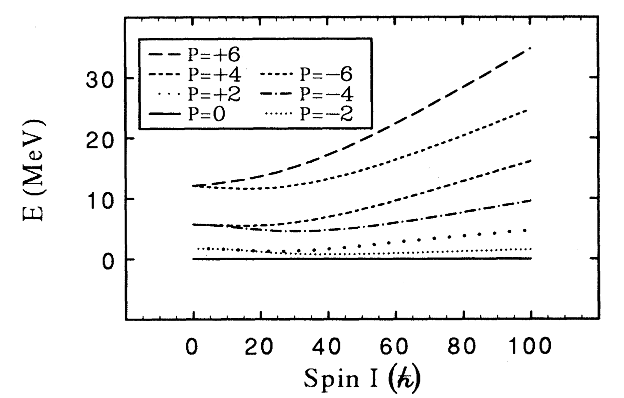

FIG. 1. Many-body solutions of the particle-rotor Hamiltonian for $N = 6$ particles within the single $j = \frac{11}{2}$ shell. The Hamiltonian parameters are $J = 60\hbar^2$ MeV^{-1} for the rotor, $G = 0.33$ MeV for the pairing, and the deformation $\chi = 2.4$ for the deformed j shell. The corresponding single-particle energies are $\chi[3m_\alpha^2 - j(j+1)]/j(j+1)$, according to standard notation. Only the lowest solutions for each P value are given. The $P = 0$ yrast line has been normalized to zero, to express more clearly the relative positions of the excited bands. Note the increasing excitation with increasing $|P|$, a result easily understandable in terms of the physical interpretation of the $\hat{\mathcal{P}}$ operator.

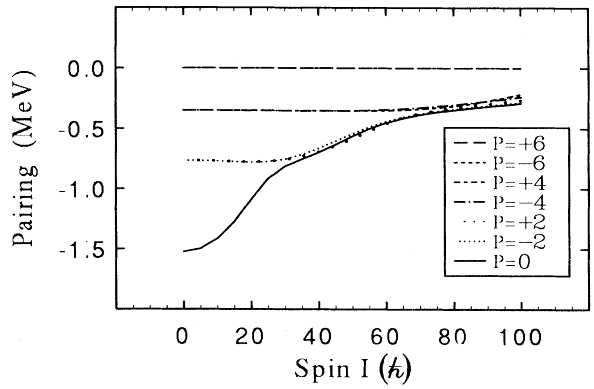

FIG. 2. The expectation values of the monopole pairing Hamiltonian for the solutions of Fig. 1. Note the decreasing effect of pairing within the many-body solutions of increasing $|P|$. The physical interpretation of this effect becomes obvious from the physical interpretation of the $\hat{\mathcal{P}}$ operator (see text).

the literature. In fact the P splitting for an even system corresponds to two states of the same signature.

It will also be instructive to present an illustration of the expectation values of the pairing Hamiltonian within the many-body solutions of Fig. 1. The corresponding results are given in Fig. 2. The two bands with $P = \pm 6$ are unique in a sense that they correspond to maximally aligned configurations (all 6 nucleons on 6 states with either all of them with $s = +i$ or all of them having $s = -i$). Within $j = \frac{11}{2}$ shell there is only one many-body state for each configuration of this type and since no nucleonic pair can be "pairing coupled" there, we have $\langle \hat{\mathcal{H}}(\text{pairing}) \rangle = 0$ independently of spin. The yrast line corresponds to $P = 0$, i.e., to the configuration in which maximum of the nucleonic states can interact *via* pairing.

An important prediction related to high-spin properties of nuclei at this point is the possibility of new types of crossings between the rotational bands corresponding to *the same parity and the same signature but differing by p-quantum numbers.* Such bands should manifest crossings with negligible band interactions. The above prediction has an important qualitative character: P-quantum number can be defined, e.g., in terms of the standard cranking model in nuclear-structure physics.

To summarize: We have discussed the symmetry properties of a typical effective nuclear Hamiltonian commonly used to describe rotating nuclei, from the point of view of the theory of representations of the unitary groups. We have demonstrated the existence of a new symmetry, called by us $\mathcal{P}$ symmetry, applicable to a still very rich subensemble of general, usually non-R(3)-scalar effective Hamiltonians. Although the formalism has been developed with the nuclear-physics context in mind, it may have much more applications in other branches of physics, e.g., those problems in which variable numbers of particles are studied. The rotation term considered important in the nuclear-physics context may be neglected for the applications other than nuclear, thus simplifying the solutions. Extensions to a realistic (nuclear-physics) context will be published elsewhere.

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