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On the spectrum of the many-body Pauli projector

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Abstract. Spectrum of the Pauli projector of a quantum many-body system is studied using the methods of operator algebra. It is proven that the kernel of the complete many-body projector is identical to the kernel of the sum of two-body projectors. Since the kernel of the many-body Pauli projector defines an allowed subspace of the complete Hilbert space, it is argued that a truncation of the many-body model space following the two-body Pauli projectors is a natural way of solving the Schrödinger equation for the many-body system. These relations clarify the role of many-body Pauli forces in a multicluster system.

Keywords. Pauli projector; many-body quantum system; forbidden states; allowed subspace.

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1. Introduction

Recent prediction of a quantum phase transition (QPT) in the ^{12}C ground state nucleus within the frame of *ab initio* techniques [1] based on the chiral effective field theory potentials has inspired new research interest on the structure of this important quantum object. The question of whether it is possible to observe the effect of the QPT within the framework of a 3α cluster model, is of great importance. Another interesting property of this nucleus is its special structure, associated with the Bose–Einstein condensation [2]. Although the 3α cluster model for the structure of the lowest ^{12}C states seems very natural due to strong binding of nucleons inside the α clusters, there are serious problems, associated with the removal of Pauli forbidden states in macroscopic cluster models.

When one deals with a two-body quantum system, the spectrum of Pauli projector consists of just two numbers, 0 and 1. However, the spectrum of Pauli projector for the 3-body quantum system belongs to the interval [0; 3], i.e. it can be any real number from that interval [3]. Our numerical calculations for the 3-alpha system confirmed this statement [4].

The problem of removal of Pauli forbidden states (FS) in a quantum many-body system has been discussed extensively for a long time [3–8]. The most popular system for the study of projection techniques is ^{12}C as 3α. When using a deep $\alpha\alpha$-potential of the BFW form [9], there are three Pauli forbidden states in partial waves $|0S\rangle$, $|2S\rangle$ and $|2D\rangle$ for each of the two-body $\alpha\alpha$-subsystems. For a realistic description of the system one has to eliminate all FS from the solution of the three-body Schrödinger equation by using the supersymmetric transformation (SUSY) [10], the orthogonal condition model (OCM) [11] or the method of orthogonalising pseudopotentials (OPP) [12]. The resulting solution of the Schrödinger equation strongly depends on the orthogonalisation method. The first evidence of a strong influence of the orthogonalisation techniques on the quality of the three-body wave function was found in the beta decay study of the ^{6}He halo nucleus into the $\alpha+d$ continuum [13,14], where the ^{6}He nucleus was described as an $\alpha+n+n$ two-neutron halo state. Very recently it was found that the same effect can be observed in the astrophysical capture reaction $\alpha+d \rightarrow {}^6\mathrm{Li}+\gamma$ within the three-body model [15–17]. In both processes, the three-body wave function obtained using the SUSY orthogonalisation techniques failed to describe the experimental data, while the OPP method gives a very good description. The success of the OPP method is connected with its property to yield a nodal behaviour of the three-body scattering and bound-state wave functions at short distances due to Pauli blocking,

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while the SUSY transformation of the initial potential does not keep this realistic property.

Coming back to the 3α problem, we note that within the OPP method, it was found [4] that the energy spectrum of the ground 0^+ and first excited 2_1^+ states is highly sensitive to the description of the $\alpha\alpha$-Pauli forbidden states. The alternative direct orthogonalisation method [7] is based on the separation of the complete Hilbert functional space into two parts, allowed and forbidden, by the Pauli principle 3α states. The allowed subspace is defined by the kernel of the complete three-body projector. However, it was found that in the 3α system there are so called 'almost forbidden states' [7], which correspond to the almost zero eigenvalues of the sum of two-body projectors, $\hat{P} = \sum_i \hat{P}_i$, where each $\hat{P}_i$ is the projector on Pauli-forbidden states in the i-th two-body subsystem. Whether to eliminate these states or to keep them in the three-body model space is a serious question. In the first case one has a strong underbinding, while the second way results in a large overbinding. A solution was suggested in ref. [7] to use the microscopic description of the forbidden states and not to use the FS of the BFW potential. Such a solution gives 'normal' three-body FS contrary to the three-body FS derived from the potential. However, from the physical viewpoint, this is not realistic, as the forbidden states should be associated with two-body potentials which describe the experimental data, binding energies and phase shifts.

On the other hand, the complete projector is more than the sum of two-body projectors (see ref. [3]):

$$\hat{\Gamma} = \sum_{i=1}^{3} \hat{P}_i - \sum_{i\neq j=1}^{3} \hat{P}_i \hat{P}_j + \sum_{i\neq j\neq k=1}^{3} \hat{P}_i \hat{P}_j \hat{P}_k - \cdots, \tag{1}$$

where

$$\hat{P}_i = \sum_f \hat{\Gamma}_i^{(f)}, \tag{2}$$

and $\hat{\Gamma}_i^{(f)}$ is the projecting operator to the f-wave forbidden state in the two-body subsystem $(j+k)$, $(i,j,k) = (1,2,3)$, and their cyclic permutations. Here two-body projectors do not commute with each other: $\hat{P}_i\hat{P}_j \neq \hat{P}_j\hat{P}_i$ and $\hat{P}_i^2 = \hat{P}_i$. However, they commute with the complete projector: $\hat{P}_i\hat{\Gamma} = \hat{\Gamma}\hat{P}_i = \hat{P}_i$. The sums on the right-hand side of eq. (1) contain terms like $\hat{P}_1\hat{P}_2\hat{P}_1$, $\hat{P}_1\hat{P}_2\hat{P}_3$, $\hat{P}_2\hat{P}_1\hat{P}_3$, $\hat{P}_1\hat{P}_2\hat{P}_1\hat{P}_2$, $\hat{P}_1\hat{P}_2\hat{P}_3\hat{P}_1$ etc. due to the above non-commutativity.

One has to note that the method of OPP, as well as the direct diagonalisation techniques [7] use only the first term of the expansion for the operator $\hat{\Gamma}$. The question is, whether neglecting the next terms of the complete projector in these methods is a good approximation? In other words, are the three-body Pauli forces negligible? Our estimation for the overlap of the $|0S\rangle$ forbidden states from different subsystems was around 1.367 which means that terms like $\hat{P}_i\hat{P}_j$ can give additional non negligible contribution to the projector if they do not mutually cancel each other. On the other hand, for the 3α system the microscopic calculations show negligible contribution from three-body Pauli forces [7]. Thus, a possible contribution of the three-body Pauli forces to the full projector must be examined in a strong mathematical way.

2. Main theorems

A way to relate the spectrum of the complete projector $\hat{\Gamma}$ with the sum of the two-body projectors $\hat{P}$ is based on the algebra of the operators $\hat{P}_i$. The final result can be formulated as a

Theorem 1. *The complete many-body projector $\hat{\Gamma}$ is related to the sum of the two-body projectors $\hat{P} = \sum_i \hat{P}_i$ as*

$$\hat{\Gamma} = 1 - \lim_{m\to\infty} (1-\hat{P})^m. \tag{3}$$

Proof. We define the operator $\hat{\Gamma}_n$ as a sum of the first n terms in the expansion of eq. (1):

$$\hat{\Gamma}_n = \sum_{i=1}^{3} \hat{P}_i - \sum_{i\neq j=1}^{3} \hat{P}_i\hat{P}_j + \sum_{i\neq j\neq k=1}^{3} \hat{P}_i\hat{P}_j\hat{P}_k - \cdots + (-1)^{(n-1)} \sum_{i1\neq i2\cdots} \hat{P}_{i1}\hat{P}_{i2}\cdots\hat{P}_{in}.$$

With this definition, we shall prove the relation

$$\hat{\Gamma}_m = 1 - (1-\hat{P})^m \tag{4}$$

for any value of m. The proof will be done by using the technique of mathematical induction. According to this method, first we check and confirm that eq. (4) is correct for $m = 1$. Then, at the next step assuming that it is correct for $m = n$, we prove the above equation for the case $m = n+1$. By multiplying the operator $\hat{\Gamma}_n$ from the left side by the two-body operator $\hat{P}$ and using the commutation relations of the projectors $\hat{P}_i$ we can write the relation

$$\hat{P}\hat{\Gamma}_n = \sum_{i=1}^{3} \hat{P}_i + \sum_{i\neq j=1}^{3} \hat{P}_i\hat{P}_j$$

$$- \sum_{i\neq j=1}^{3} \hat{P}_i \hat{P}_j - \sum_{i\neq j\neq k=1}^{3} \hat{P}_i \hat{P}_j \hat{P}_k$$
$$+ \sum_{i\neq j\neq k=1}^{3} \hat{P}_i \hat{P}_j \hat{P}_k + \cdots + (-1)^{(n-1)}$$
$$\times \sum_{i1\neq i2\cdots} \hat{P}_{i1} \hat{P}_{i2} \cdots \hat{P}_{in} \hat{P}_{in+1}$$
$$= \hat{P} + (-1)^{(n+1)} \sum_{i1\neq i2\cdots} \hat{P}_{i1} \hat{P}_{i2} \cdots \hat{P}_{in} \hat{P}_{in+1}. \quad (5)$$

In the last equation, all the terms are cancelled except the first and the last ones. It gives us the relation

$$\sum_{i1\neq i2\cdots} \hat{P}_{i1} \hat{P}_{i2} \cdots \hat{P}_{in} \hat{P}_{in+1}$$
$$= (-1)^{(n+1)} \hat{P}(\hat{\Gamma}_n - 1). \quad (6)$$

On the other hand, from the definition of the operator $\hat{\Gamma}_n$ one can write

$$\hat{\Gamma}_{n+1} = \hat{\Gamma}_n + (-1)^n \sum_{i1\neq i2\cdots} \hat{P}_{i1} \hat{P}_{i2} \cdots \hat{P}_{in} \hat{P}_{in+1}. \quad (7)$$

Now on the basis of relation (6), one can write the reccurent formula:

$$\hat{\Gamma}_{n+1} - 1 = (1-\hat{P})(\hat{\Gamma}_n - 1)$$
$$= (1-\hat{P})^2(\hat{\Gamma}_{n-1} - 1)$$
$$= \cdots = (1-\hat{P})^n(\hat{\Gamma}_1 - 1). \quad (8)$$

By using the definition of the operator $\hat{\Gamma}_1 = \hat{P}$, finallly we come to the relation

$$\hat{\Gamma}_{n+1} = 1 - (1-\hat{P})^{(n+1)}. \quad (9)$$

The proven relation (3) enables us to define the allowed many-body model space, which corresponds to the kernel of the operator $\hat{\Gamma}$. Thus we come to the following theorem.

Theorem 2. *The kernel of the operator* $\hat{P} = \sum_i \hat{P}_i$ *is identical to the kernel of the complete many-body Pauli projector* $\hat{\Gamma}$.

Proof. Let Ψ belong to the kernel of the operator $\hat{P}$, i.e. it is an eigenfunction of the operator $\hat{P}$ corresponding to the eigenvalue $\lambda = 0$: $\hat{P}\Psi = 0$. Then, from relation (3) one can find $\hat{\Gamma}\Psi = 0$.

Now, let Ψ belong to the kernel of the operator $\hat{\Gamma}$. It means that for any small positive number ϵ there is a large number N and for any $n > N + 1$:

$$||(1-\hat{P})^n\Psi - \Psi|| \leq \epsilon. \quad (10)$$

Now

$$||(1-\hat{P})\Psi - \Psi|| = ||\hat{P}\Psi||$$
$$\leq ||(1-\hat{P})\Psi - (1-\hat{P})^n\Psi|| + ||(1-\hat{P})^n\Psi - \Psi||$$
$$\leq ||1-\hat{P}||||\Psi - (1-\hat{P})^{n-1}\Psi|| + \epsilon$$
$$= (||1-\hat{P}|| + 1)\epsilon = \epsilon_1.$$

Consequently, the function Ψ belongs to the kernel of the operator $\hat{P}$.

3. Summary and conclusion

These theorems clarify the role of many-body Pauli forces in a multicluster system. We have developed a method for the three-body quantum system. An extension to the case of quantum systems containing more than three particles is straightforward.

The results of the present work can be used when solving the Schrödinger equation for many-body quantum system. Since the kernel of the projecting operator defines an allowed subspace, it is good enough to expand a probe wave function of the many-body Hamiltonian over the eigenstates of the operator $\hat{P} = \sum_i \hat{P}_i$ corresponding to its zero eigenvalue. The obtained results indicate that a truncation of the allowed model space following the operator $\hat{P}$ is a natural procedure. This is valid even for the case when the operators $\hat{P}_i$ and $\hat{P}_j$ $(i \neq j)$ overlap strongly.

The obtained results can be applied for the study of nuclear structure in cluster models where a nucleus is described as a system of a few interacting clusters: $^{12}C = 3\alpha$, $^{9}Be = \alpha + \alpha + n$, $^{16}O = 4\alpha$ etc. A nuclear interaction between these clusters includes both two-body $V(\alpha-\alpha)$, $V(\alpha-n)$ and many-body $V(\alpha-\alpha-\alpha)$, $V(\alpha-\alpha-n)$ forces. As was proved in Theorem 2, all the Pauli forces as part of nuclear interaction in these multicluster systems, can be described by the sum of two-body projection operators such as $\hat{P}(\alpha-\alpha)$ and $\hat{P}(\alpha-n)$. This result allows one to simplify calculations for the solution of the Schrödinger equation for multicluster systems.

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