Projector Operators for the No-Core Shell Model*

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Abstract—Projection operators for the use within the ab initio no-core shell model are suggested.

1. INTRODUCTION

The shell model is a recognized tool for microscopic studies of nuclear structure. The no-core shell model (NCSM) [1−3], the version of the shell model where all A nucleons are spectroscopically active, is widely used now (see, e.g., [3−6]) for ab initio calculations of light nuclei (up through $A = 16$) with modern realistic nucleon−nucleon and three-nucleon forces.

The NCSM utilizes the basis of Slater determinants of single-particle oscillator states. These basis functions are known to have spurious contributions of center-of-mass (CM) excitations. The wave functions of physically acceptable eigenstates of the intrinsic NCSM Hamiltonian

$$H_A = \frac{1}{A} \sum_{i<j}^{A} \frac{(\mathbf{p}_i - \mathbf{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} \qquad (1)$$
$$+ \sum_{i<j<k}^{A} V_{NNN,ijk},$$

where m is the nucleon mass, $V_{NN,ij}$ is the two-nucleon interaction (including both strong and electromagnetic components), and $V_{NNN,ijk}$ is the three-nucleon interaction, should be arranged as spurious-free linear combinations of basis states.

To achieve this, the auxiliary Hamiltonian

$$H_{\mathrm{NCSM}} = H_A + \beta \widetilde{Q}_0 \qquad (2)$$

is conventionally diagonalized within the NCSM instead of the Hamiltonian (1). Here,

$$\widetilde{Q}_0 \equiv H_{\mathrm{CM}} - \frac{3}{2}\hbar\Omega, \qquad (3)$$
$$H_{\mathrm{CM}} = T_{\mathrm{CM}} + U_{\mathrm{CM}} \qquad (4)$$

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is the harmonic oscillator CM Hamiltonian, T_{CM} is the CM kinetic energy operator, and

$$U_{\mathrm{CM}} = \frac{1}{2} Am\Omega^2 \mathbf{R}^2, \qquad (5)$$

where

$$\mathbf{R} = \frac{1}{A} \sum_{i=1}^{A} \mathbf{r}_i. \qquad (6)$$

The term $\beta\widetilde{Q}_0$ with large enough parameter β has no effect on the intrinsic states of the A-body system owing to the translational invariance of the Hamiltonian (1); it shifts up in energy spurious CM-excited states and projects out the spurious contributions in the low-lying eigenstates. As a result, the physical low-lying eigenstates of (2) correspond to the $0\hbar\Omega$ CM excitation and are independent of the choice of β.

I suggest below a projection operator P_{CM} that can be used to project out spurious CM-excited components and to obtain spurious-free linear combinations of basis Slater determinants that can be used as a new spurious-free basis for direct diagonalization of the intrinsic Hamiltonian (1). The complete spurious-free basis corresponding to the $0\hbar\Omega$ CM excitations is much smaller than the basis of all Slater determinants including all $\varkappa\hbar\Omega$ CM excitations with $\varkappa \leq N$, where N is the maximal oscillator quanta of the $N\hbar\Omega$ NCSM model space used in the calculations. Therefore, it is expected that the use of the projection operator P_{CM} will significantly simplify the NCSM studies of nuclear structure, will make it possible to arrange the calculations in larger $N\hbar\Omega$ model spaces with the same computer facilities and hence to improve the accuracy of the NCSM predictions, etc.

I note also that the so-called m scheme is conventionally utilized in the NCSM applications; i.e., the basis Slater determinants are used that do not have definite values of the orbital angular momentum L, of the total angular momentum J, and of the total

spin S. The m scheme makes it possible to use well-developed computational methods and available respective computer codes. However, the basis of the m-scheme Slater determinants is very large since it includes all states with all possible values of $J \leq J_{\max}$, $L \leq L_{\max}$, and $S \leq S_{\max}$, where the maximal values $J_{\max}$, $L_{\max}$, and $S_{\max}$ are large enough in modern NCSM applications and depend on the particular nucleus under consideration and on the $N\hbar\Omega$ model space used in the calculations.

I suggest below the projection operators P_J, P_L, and P_S on the states with definite J, L, and S values. These projection operators as well as P_{CM} can be easily utilized within the existing NCSM codes to reduce the number of the basis states significantly.

2. CM-PROJECTOR P_{CM}

Let

$$\Psi = \sum_{\varkappa=0}^{N} \alpha_\varkappa \Psi_\varkappa \tag{7}$$

be a vector (wave function) defined in the $N\hbar\Omega$ model space; N is the maximal possible CM-excitation quanta in this model space. Equation (7) represents an expansion of Ψ in a series of functions $\Psi_\varkappa$ with definite CM-excitation quanta $\varkappa = 0, 1, \ldots, N$. The functions $\Psi_\varkappa$ are the eigenfunctions of the harmonic oscillator CM Hamiltonian:

$$H_{\mathrm{CM}} \Psi_\varkappa = \left(\varkappa + \frac{3}{2} \hbar\Omega \right) \Psi_\varkappa. \tag{8}$$

Owing to Eq. (8), the operator $\widetilde{Q}_0$ defined by Eq. (3) acts as an antiprojector: it projects out the spurious-free component $\Psi_{\mathrm{sf}} \equiv \Psi_0$ of the wave function:

$$\widetilde{Q}_0 \Psi_{\mathrm{sf}} = 0. \tag{9}$$

We can also define antiprojectors

$$\widetilde{Q}_\varkappa \equiv H_{\mathrm{CM}} - \left(\varkappa + \frac{3}{2} \right) \hbar\Omega \tag{10}$$

which project out components with given values of the CM excitation quanta $\varkappa$:

$$\widetilde{Q}_\varkappa \Psi_\varkappa = 0. \tag{11}$$

We can extract the spurious-free content $\widetilde{\Psi}_{\mathrm{sf}}$ of Ψ by the subsequent use of the operators (10):

$$\Psi_1 = \widetilde{Q}_1 \Psi, \tag{12a}$$

$$\Psi_2 = \widetilde{Q}_2 \Psi_1, \tag{12b}$$

$$\cdots$$

$$\widetilde{\Psi}_{\mathrm{sf}} \equiv \Psi_N = \widetilde{Q}_N \Psi_{N-1}. \tag{12c}$$

Equations (12) are equivalent to the following equation:

$$\widetilde{\Psi}_{\mathrm{sf}} = \widetilde{P}\Psi, \tag{13}$$

where the operator

$$\widetilde{P} = \prod_{\varkappa=1}^{N} \widetilde{Q}_\varkappa. \tag{14}$$

Let us call $\widetilde{P}$ a quasi-projector. Mathematically, $\widetilde{P}$ is not a projection operator since it does not fit the standard property of the projection operators

$$P^2 = P. \tag{15}$$

The function Ψ is a superposition (7) of the spurious-free $\Psi_{\mathrm{sf}} \equiv \Psi_0$ and spurious components $\Psi_\varkappa$ with $\varkappa \neq 0$. The standard projection operator property (15) guarantees that

$$P\Psi = \alpha\Psi_{\mathrm{sf}}. \tag{16}$$

Instead of (16), the quasi-projector $\widetilde{P}$, when applied to Ψ, results in

$$\widetilde{P}\Psi = \widetilde{\Psi}_{\mathrm{sf}} = D\alpha\Psi_{\mathrm{sf}}. \tag{17}$$

The constant D can be easily calculated using Eqs. (8) and (10):

$$D = (-1)^N N! (\hbar\Omega)^N. \tag{18}$$

To become a projector, the quasi-projector $\widetilde{P}$ should be normalized:

$$P = \frac{1}{D}\widetilde{P}. \tag{19}$$

In applications, one can use either $\widetilde{P}$ or P. Really, it is usually needed to extract from Ψ its normalized spurious-free component Ψ_{sf}. The multiplier α is usually unknown. Hence, after using either the quasi-projector (14) or the projector (19), one needs to normalize either the function $D\alpha\Psi_{\mathrm{sf}}$ or the function $\alpha\Psi_{\mathrm{sf}}$. Clearly, the same computational efforts are required to normalize the functions $D\alpha\Psi_{\mathrm{sf}}$ and $\alpha\Psi_{\mathrm{sf}}$.

3. OTHER USEFUL PROJECTORS

The same idea can be utilized for the construction of other useful projectors. As an example, let us construct the projector on the states with a definite value of the angular momentum.

Let $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ be the standard orbital momentum operator. Its eigenvalues are known to be $L(L + 1)$. We now define the operators

$$\widetilde{Q}_L \equiv \hat{L}^2 - L(L + 1) \tag{20}$$

and

$$\widetilde{P}_L^{L_{\max}} = \prod_{\kappa=0}^{L-1} \widetilde{Q}_\kappa \prod_{\kappa=L+1}^{L_{\max}} \widetilde{Q}_\kappa, \qquad (21)$$

where $L_{\max}$ is the maximal accessible orbital momentum in the given $N\hbar\Omega$ shell model space. The nonnormalized quasi-projector (21) can be used like the CM nonnormalized quasi-projector (14) to extract the (nonnormalized) component with a definite value of the orbital momentum L by the algorithm described briefly by Eq. (13) or in more detail by Eqs. (12).

The projector $P_L^{L_{\max}}$ can be expressed as

$$P_L^{L_{\max}} = \frac{1}{D_L^{L_{\max}}} \widetilde{P}_L^{L_{\max}}, \qquad (22)$$

where

$$D_L^{L_{\max}} = \prod_{\kappa=0}^{L-1} [\kappa(\kappa+1) - L(L+1)] \qquad (23)$$

$$\times \prod_{\kappa=L+1}^{L_{\max}} [\kappa(\kappa+1) - L(L+1)].$$

The structure of the projectors $P_J^{J_{\max}}$, $P_S^{S_{\max}}$, and $P_T^{T_{\max}}$ on the states with given values of the total angular momentum J, total spin S, or isospin T is exactly the same. The only difference is that, in the case of an odd-A system, one should use half-integer J, T, or S values and modify, respectively, the products in Eqs. (21) and (23).

The standard projection operator property (15) is valid for all projectors (but not quasi-projectors) discussed above.

4. CONCLUSIONS

Expressions of the projection operators on the states with a definite value of the angular momentum, in the form of an expansion in powers of the $SU(2)$ generators, are known in the literature (see, e.g., [7]). However, in the general case, this polynomial includes an infinite number of terms and is inconvenient for use in nuclear shell model applications. As was shown above, in the case of the shell model, the projector can be taken in the form of a finite polynomial in generators that is much more useful for applications. The suggested projectors $P_L^{L_{\max}}$, $P_J^{J_{\max}}$, $P_S^{S_{\max}}$, and $P_T^{T_{\max}}$ are of this form.

The CM projector P_{CM} is also suggested as a finite expansion in powers of a simple CM harmonic oscillator operator H_{CM}. To the best of my knowledge, similar expressions for the CM projector were never discussed in the literature.

The Lanczos iteration approach is utilized in the modern shell model codes; i.e., the basis vectors are obtained successively by acting using the Hamiltonian on the vector obtained at the previous step. The intrinsic Hamiltonian (1) and the NCSM Hamiltonian (2) cannot produce CM excited states or change the value of the total angular momentum of the state. Hence, it is possible to project only the pivot vector (the initial vector in the Lanczos iteration approach) on the spurious-free subspace with the given definite value of the total angular momentum J; all the rest of the basis vectors will be produced spurious-free and with the same value of J by the Lanczos iterations.

Formally, one can use the projected pivot vector and the intrinsic Hamiltonian (1) instead of the auxiliary Hamiltonian (2) in NCSM applications. However, it is well known that spurious states will be produced in the Lanczos iteration approach owing to computer noise (round-off errors). The term $\beta\widetilde{Q}_0$ in Eq. (2) stabilizes the NCSM calculations, reducing the computer noise if β is sufficiently large. Therefore, it looks reasonable to utilize the auxiliary Hamiltonian (1) in the applications; probably, it is reasonable to add the term $\gamma J(J+1)$ with sufficiently large γ to the Hamiltonian (2) to reduce the computer noise in calculations of the states with a definite value J of the total angular momentum.

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