An efficient projection algorithm and its application to the spurious center-of-mass motion problem

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Abstract

Based on the correspondence of projection to an eigenvalue problem via the underlying group structure, we generalize the projection algorithm proposed by Morrison \textit{et al}. This algorithm is eligible for large-scale computations, because we can avoid the accumulation of errors. As an example, we apply it to the spurious c.m. motion in a multi-$\hbar\omega$ shell-model calculation. In comparison with Lawson’s method, the present method is exact and nevertheless does not need longer CPU time. It is pointed out that the exact treatment of the spurious c.m. motion is crucial to some physical quantities.

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In the numerical treatment of a Hamiltonian in a large space, we often need an efficient algorithm for projection, in connection to conservation laws or spurious motions. For instance, the $J$ (angular-momentum) projection accelerates shell-model calculations in many cases. A more serious problem is the spurious center-of-mass (c.m.) motion: since we sometimes use a Hamiltonian which may excite the spurious motion, it is important to project it out of basis vectors. In this report we extensively develop a projection algorithm, which was first proposed in Ref. [1] for the $J$ projection, and apply it to the c.m. motion problem within the regime of multi-$\hbar\omega$ shell-model calculations.

Suppose that, in an $N$-dimensional ($N$ is finite) Hilbert space $V$, we have relevant and irrelevant components. The projection operator $P$ picks up only the relevant components, eliminating the irrelevant ones. We now introduce a certain hermitian operator $H_P$, which satisfies $H_P V \subseteq V$ and has degenerate eigenvalues within $V$. We denote the eigenvalues by $\mu_0, \mu_1, \cdots, \mu_{n-1}$ ($n < N$). Eigenvectors associated with each eigenvalue $\mu_k$ span a subspace $W_k$ ($k = 0, 1, \cdots, n - 1$). The full space $V$ is equal to the direct sum of $W$’s:

$$V = \bigoplus_{k=0}^{n-1} W_k.$$  

Any vector $|v\rangle \in V$ is expanded as

$$|v\rangle = \sum_{k=0}^{n-1} c_k |v^{(k)}\rangle,$$  

where $|v^{(k)}\rangle \in W_k$ (i.e. $H_P |v^{(k)}\rangle = \mu_k |v^{(k)}\rangle$). It is postulated that the relevant components belong exclusively to $W_0$, which is attached to the eigenvalue $\mu_0$; $PV = W_0$ and $P|v\rangle \propto |v^{(0)}\rangle$.

(We can straightforwardly extend our discussion to the case that the relevant subspace is a sum of a few $W$’s.) The projection can then be redefined as an eigenvalue problem with respect to $H_P$, as will be illustrated below.

It is crucial to find such an operator $H_P$ with a simple form. The projection is normally linked to a certain group structure. As is well-known, conservation corresponds to a symmetry, and therefore to a group. A spurious motion occurs when we ignore a symmetry to be satisfied. This symmetry leaves its trace in a group structure in the enlarged space. In both cases, the relevant components are characterized by a specific representation of the corresponding group. Then a Casimir operator of the group can be adopted as $H_P$; for instance, $H_P = \mathbf{J}^2$ in the $J$ projection. The condition $H_P V \subseteq V$ is required in order that the group structure holds within $V$.

For a given vector $|v\rangle \in V$, $|v^{(0)}\rangle$ is obtained in the following manner, by applying the Lanczos diagonalization algorithm [2] with respect to $H_P$. Having a set of basis vectors $\Gamma_{n'} \equiv \{|v\rangle, H_P |v\rangle, \cdots, (H_P)^{n'-1} |v\rangle\}$ with the Gram-Schmidt orthogonalization, $H_P$ is represented by a tridiagonal matrix. We denote the $(i,j)$ component of this matrix by $(H_P)_{ij}$. At a certain $n' (\leq n)$, $(H_P)^{n'} |v\rangle$ is no longer linearly independent of $\Gamma_{n'}$ because of the degenerate eigenvalues. Then $|v^{(k)}\rangle$ is obtained by solving a system of coupled linear equations

$$\sum_j (H_P)_{ij} x_j^{(k)} = \mu_k x_i^{(k)} \quad (i = 1, \cdots, n'),$$  

where $x_i^{(k)}$ yields the expansion coefficient of $|v^{(k)}\rangle$ for the Lanczos bases and $x_1^{(k)} = c_k$ of Eq. (3). Since $H_P$ is tridiagonal now, the sum over $j$ on the left-handed side of Eq. (3) runs
from $i-1$ to $i+1$ at most. What we need is the eigenvector $|v^{(0)}\rangle$. The probability $\langle v|P|v\rangle$ is given by $|x^{(0)}_i|^2$. It has been known that solving Eq. (3) from $i = n'$ to 1 with a small initial value of $x^{(0)}_{n'}$ is advantageous, in order to keep rounding errors small [2].

Because of the group structure, $\mathcal{H}_P$ has highly degenerate eigenvalues; $n \ll N$. For the $J$ projection in shell-model calculations, $n$ is the number of possible $J$ values in the space $V$, being several tens even for the M-scheme shell-model space with $N \sim 10^6$ [3]. In the above algorithm, we can keep the number of bases small ($n' \leq n$). As far as we know $\mu_0$ in advance, the inverse iteration method is immediately applicable to obtain $|v^{(0)}\rangle$. However, solving Eq. (3) from $i = n'$ to 1 is more efficient, because we reach $|v^{(0)}\rangle$ with a small number of operations. The Lanczos method has an advantage for these reasons, although $n$ is not quite large.

It is noted that, by using $\mathcal{H}_P$, we can explicitly construct the projection operator $P$ as

$$P = \prod_{k=1}^{n-1} \left( \frac{\mathcal{H}_P - \mu_k}{\mu_0 - \mu_k} \right). \tag{4}$$

Each factor $(\mathcal{H}_P - \mu_k)/(\mu_0 - \mu_k)$ eliminates the irrelevant component $|v^{(k)}\rangle \in W_k$ with $k \neq 0$, leaving $|v^{(0)}\rangle$ at last. Despite its mathematical exactitude, this procedure is not numerically efficient. First of all, we always need an $n$-fold operation of $\mathcal{H}_P$, in contrast to $n' (\leq n)$ in the present algorithm. Moreover, in the process eliminating $|v^{(k)}\rangle$, other irrelevant components may be enhanced, causing serious numerical errors. We take the $J = 0$ projection as an example, with $\mathcal{H}_P = J^2$ and $\mu_k = k(k+1)$. We operate $(\mathcal{H}_P - \mu_k)/(\mu_0 - \mu_k)$ on $|v\rangle$ from $k = 1$ to $n - 1$. The irrelevant component $|v^{(1)}\rangle$ is removed at the first step. However, if a small amount of the $W_{n-1}$ component is contained in $|v\rangle$, this component is enhanced by the factor $[n(n-1)-2]/2 \sim O(n^2)$. After several steps, the $W_{n-1}$ component is repeatedly enhanced and eventually dominates over the relevant component, giving rise to a loss of precision for the relevant component in practical floating-point computations. It is numerically advantageous to enhance the relevant component, which corresponds to a single eigenvalue $\mu_0$, rather than to remove many irrelevant components. In the present algorithm, the relevant component is enhanced because of the order of solving Eq. (3).

Morrison et al. have pointed out the equivalence between projection and an eigenvalue problem for some cases, particularly for the $J$ projection [1]. They proposed the Lanczos algorithm with $\mathcal{H}_P = J^2$. However, it has not been discussed how to obtain $\mathcal{H}_P$ in general cases, since one has not fully realized the underlying group structure in the correspondence of the projection to an eigenvalue problem. Furthermore, only the case of $[H, \mathcal{H}_P] = 0$ was discussed in Ref. [4]. Generalizing their argument, we have now developed the projection algorithm systematically.

Since we apply the Lanczos method, $\mathcal{H}_P$ as well as $H$ do not have to be represented in a matrix form [4]. The present algorithm may be extended even to the case that $n$ (and therefore $N$) is infinite or the eigenvalues of $\mathcal{H}_P$ are continuous. In such cases, however, the degree of convergence with finite $n'$ strongly depends on the vector $|v\rangle$. We have restricted ourselves to the finite $N$ cases in this article, by which the convergence for $n'$ is assured.

We next demonstrate the present projection method for the spurious c.m. motion in a multi-$\hbar \omega$ shell-model calculation. Shell-model calculations in multi-$\hbar \omega$ spaces are under current interest, in relation to a microscopic description of nuclei [5] and to a research on light unstable nuclei [6]. Because the origin of the coordinate space is fixed in the shell
model, the c.m. motion, which is irrelevant to the nuclear structure itself, is included in the model space. With the harmonic-oscillator (h.o.) single-particle wavefunctions, the c.m. motion is also expanded in terms of the h.o. representation, which forms a $U(3)$ group. It is desired to constrain the c.m. mode to the 0s orbit. For this purpose, we take

$$\mathcal{H}_P = \frac{1}{2AM} P^2 + \frac{AM\omega^2}{2} R^2 - \frac{3}{2} \hbar \omega,$$

where $R$ and $P$ denotes c.m. coordinate and momentum. This is indeed proportional to a Casimir operator (linear Casimir operator) of the $U(3)$ group, and is expressed up to two-body operators within the shell-model space,

$$\mathcal{H}_P = \frac{1}{A} \left[ \sum_i \left( \frac{1}{2M} P_i^2 + \frac{M\omega^2}{2} r_i^2 - \frac{3}{2} \hbar \omega \right) + \sum_{i<j} \left( \frac{1}{M} p_i \cdot p_j + M\omega^2 r_i \cdot r_j \right) \right].$$

The 0s mode corresponds to the eigenvalue $\mu_0 = 0$.

In order for the c.m. motion to be well-defined inside the model space $V$, $\mathcal{H}_P V \subseteq V$ should be satisfied. Otherwise the model space should be extended. We consider a model space with the $\hbar \omega$-type truncation; $V$ is a direct sum of subspaces characterized by the number of oscillator quanta $m$, $V = \bigoplus_m V^{(m)}$. Each subspace $V^{(m)}$ is expanded by direct products of the relative motion and the c.m. motion, both of which have specific numbers of oscillator quanta, $V^{(m)} = \bigoplus_k [V^{rel}_m \otimes W^{m}].$ A resummation as $W_k = \bigoplus_r [V^{rel}_r \otimes W^{m}_r]$ leads to the expression of Eq.(5). The space $W_k$ is characterized by the symmetric representation $[k]$ of the c.m. $U(3)$ group and has $\mu_k = k\hbar \omega$. Obviously $\mathcal{H}_P V \subseteq V$ is satisfied. All the components outside $W_0$ are regarded as spurious components. The corresponding projection operator $P$ of Eq.(5) has been discussed in Ref. [8]. Unlike the $J$ projection, we do not necessarily demand that the shell-model Hamiltonian $H$ should commute with $\mathcal{H}_P$, under the presence of a core or inactive particles.

The present projection is incorporated into the shell-model diagonalization. The Lanczos method is usually employed in diagonalizing a shell-model Hamiltonian. When the single-particle energies consist only of kinetic energy and the effective interaction depends only on relative coordinates with the h.o. bases, the shell-model Hamiltonian can be made commutable with $\mathcal{H}_P$. Even in such cases with $[H, \mathcal{H}_P] = 0$ (i.e. $[H, P] = 0$), the present projection is useful to cut off numerical errors. It may be applied in the Lanczos iterations of $H$ at a certain interval, as well as to the initial vector.

For the spurious c.m. motion problem, the so-called Lawson’s method has conventionally been used. The original Hamiltonian is amended as
\[ H' = H + \lambda H_P \quad (\lambda > 0) \]  

The \( H_P \) term shifts up the spurious components and reduces their admixture in low-lying states. The quality of this prescription for large \( \lambda \) can be assessed by perturbation theory. By regarding \( \lambda H_P \) as an unperturbed Hamiltonian and \( H \) as a perturbation, an eigenvector of \( H' \) is approximated by

\[ |v_\lambda \rangle \cong |v(0)\rangle - \sum_{k=1}^{n-1} \eta_k |v^{(k)}\rangle; \quad \eta_k = \frac{1}{\lambda k \hbar \omega} \langle v^{(0)} | H | v^{(k)} \rangle \sim O(\lambda^{-1}) . \]  

As far as \([H, H_P] \neq 0\), \( \eta_k \) does not vanish. Notice that \( \eta_1 \) is the largest in general, because of the energy denominator. The corresponding energy is

\[ E_\lambda \equiv \langle v_\lambda | H' | v_\lambda \rangle \cong E^{(0)} - \sum_{k=1}^{n-1} \eta_k \langle v^{(0)} | H | v^{(k)} \rangle + O(\lambda^{-2}) , \]

where \( E^{(0)} \equiv \langle v^{(0)} | H | v^{(0)} \rangle \). Thus the influence of the spurious modes on the wavefunctions and energies is proportional to \( \lambda^{-1} \), not diminishing rapidly as \( \lambda \) increases. On the other hand, as we set larger \( \lambda \), the convergence with respect to \( H' \) becomes slower, because the \( H_P \) term dominates and fine splitting due to \( H \) is not easily attained. Moreover, even if the influence of the spurious motion is small for energies, it is not necessarily negligible for transition properties, particularly when there is some cancellation.

We have carried out a numerical test for the \(^{10}\)Be nucleus. In the lowest configuration we have six nucleons in the \( p \)-shell, on top of the \(^4\)He core. We take the model space \( V \) spanned by up to the \( 3\hbar \omega \) excitations \((n = 4)\). For \( H \), the single-particle energies are determined from the Woods-Saxon potential with the parameters of Ref. \([11]\). The Millener-Kurath \([12]\) and USD \([13]\) two-body interactions are taken for the \((s-p-sd)\)-shell, while the M3Y \(NN\) effective interaction \([14]\) is used for the rest. This Hamiltonian is adopted just for a numerical test, putting aside its physical appropriateness. As a matter of fact, the negative-parity levels have too high excitation energies.

As in Fig. 1, the subroutine for the c.m. projection is incorporated into the shell model code VECSSE \([3,15]\). The present projection technique is compared with Lawson’s method. For the \( \lambda \) parameter in Lawson’s method, we take 0 (i.e. no care of c.m. motion), 1, 5 and 20, with \( \hbar \omega = 45A^{-1/3} - 25A^{-2/3} = 15.5 \) MeV. The CPU time on HITAC S3800/480 is presented in Table 1. Both the positive- and negative-parity states are computed up to \( J = 4 \), and 5–7 lowest eigenstates are computed for each \( J^P \), with the convergence criterion of 0.1 keV. While the present method gives an exact projection, it does not make the CPU time so long. In Lawson’s prescription, it takes a longer CPU time as \( \lambda \) increases, because more iterations (i.e. more Lanczos bases) are necessary to fulfill the convergence criterion. While for \( \lambda = 1 \) the iteration number is almost the same as that in the present projection, it costs almost twice as many iterations for \( \lambda = 20 \), resulting in longer CPU time than the exact projection. The calculated energies are presented in Table 1. The energy eigenvalues of Lawson’s method do not rapidly converge for increasing \( \lambda \); the 100 keV discrepancy remains even with \( \lambda = 20 \). The excitation energies, on the other hand, are rather stable. For \( \lambda = 0 \), the spurious component dominates the lowest \( 1^- \) state with \( E_x = 13.998 \) MeV, while the third lowest \( 1^- \) state consists mainly of the \( W_0 \) component, whose energy is presented in
Table II. As a measure of admixture of the spurious components, the expectation value of $\mathcal{H}_P$ is also shown for $4^+_1$.

We turn to the transition properties. Some of the calculated results are presented in Table III. The $E1$ transition strengths are rather susceptible to the contamination of the spurious c.m. motion, since the bare $E1$ operator $T(E1) = e\sqrt{3/4\pi}\sum_{i\in p} r_i$ has the isoscalar part proportional to $R$. Here $r_i$ denotes the coordinate of the $i$-th nucleon and the sum runs over all the protons. A simple modification of $T'(E1) = e\sqrt{3/4\pi}\sum_{i\in p}(r_i - R)$ reduces the influence of the spurious motion [16]. However, we do not find apparent improvement for Lawson’s method in Table III. On the other hand, the present method yields equal values between $T$ and $T'$, since the c.m. excitation is entirely removed.

A similar treatment for the $E2$ transition to $T'(E1)$ requires two-body operators, and hence is not popular. We here assume the usual one-body $E2$ operator with the bare charges. Compared with the exact values, Lawson’s method works well in most cases. However, the $1^-_2 \rightarrow 2^-_1$ transition, whose strength is not large, shows a significant discrepancy. Even when excitation energies seem good for a physical discussion, the influence of the spurious motion may be serious for transition strengths, particularly for relatively small ones.

In summary, we have developed a projection algorithm, extending the method of Ref. [1]. The projection is redefined as an eigenvalue problem of a Casimir operator of the underlying group. On this ground, the Lanczos diagonalization technique can be utilized also for projection. This algorithm is efficient particularly in large-scale computations, because numerical errors do not accumulate severely. We have applied it to eliminate the spurious c.m. motion in a multi-$\hbar\omega$ shell-model calculation. Whereas the present method is exact, it does not need longer CPU time than Lawson’s method. The present algorithm is useful, or even crucial, to evaluate physical quantities sensitive to admixture of the c.m. excitation.

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TABLES

TABLE I. CPU time (sec) for diagonalization of \( H \), with the c.m. motion handled by the present algorithm or Lawson’s method.

| Projection     | \( \lambda = 0 \) | \( \lambda = 1 \) | \( \lambda = 5 \) | \( \lambda = 20 \) |
|----------------|-------------------|-------------------|-------------------|-------------------|
|                | 586               | 523               | 535               | 560               | 629               |

TABLE II. Eigenenergy of the ground state and excitation energies (MeV). \( \langle \mathcal{H}_P \rangle \) value is also shown for \( 4^+_1 \) in the parenthesis.

|              | Exact            | \( \lambda = 0 \) | \( \lambda = 1 \) | \( \lambda = 5 \) | \( \lambda = 20 \) |
|--------------|-----------------|-------------------|-------------------|-------------------|-------------------|
| \( E(0^+_1) \) | -375.845        | -376.691          | -376.453          | -376.142          | -375.950          |
| \( E_x(2^+_1) \) | 4.246           | 4.200             | 4.212             | 4.229             | 4.240             |
| \( E_x(4^+_1) \) | 17.922          | 17.617            | 17.707            | 17.821            | 17.888            |
| \( \langle \mathcal{H}_P \rangle / \hbar \omega \) | (0.0)            | (1.3 \times 10^{-1}) | (1.5 \times 10^{-2}) | (3.3 \times 10^{-3}) | (3.9 \times 10^{-4}) |
| \( E_x(1^-_1) \) | 19.266          | 19.125            | 19.166            | 19.263            | 19.269            |
| \( E_x(3^-_1) \) | 19.409          | 18.234            | 19.476            | 19.445            | 19.422            |

TABLE III. \( B(E1) (e^2\text{fm}^2) \) and \( B(E2) (e^2\text{fm}^4) \).

|              | Exact            | \( \lambda = 0 \) | \( \lambda = 1 \) | \( \lambda = 5 \) | \( \lambda = 20 \) |
|--------------|-----------------|-------------------|-------------------|-------------------|-------------------|
| \( B(E1; 0^+_1 \rightarrow 1^-_2) \) by \( T \) | 0.901            | 0.292             | 0.953             | 0.888             | 0.898             |
| \( B(E1; 0^+_1 \rightarrow 1^-_2) \) by \( T' \) | 0.901            | 0.498             | 0.690             | 0.878             | 0.896             |
| \( B(E2; 0^+_1 \rightarrow 2^+_1) \) | 13.167           | 12.905            | 12.949            | 13.045            | 13.121            |
| \( B(E2; 1^-_1 \rightarrow 3^-_1) \) | 2.059            | 1.807             | 2.047             | 2.059             | 2.059             |
| \( B(E2; 1^-_1 \rightarrow 2^-_1) \) | 0.011            | 0.413             | 0.265             | 0.002             | 0.004             |
FIG. 1. Illustration of the present projection algorithm incorporated into the Lanczos diagonalization of $H$. The basis vectors ($|v_i^{(0)}\rangle$) are generated so as to stay inside $W_0$. 