Recurrence relations for reaction matrices

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The general structure of an exact Pauli projector is employed in the derivation of relations between Brueckner reaction matrices that are defined for a different number of occupied states (corresponding either to different nuclei or different truncations of the Pauli projector). A numerical example is given showing the truncation influence in ^{4}He.

[NUCLEAR STRUCTURE Accurate methods of calculating nuclear reaction matrices.]

Having an identity projector

$$I=\sum_{i\in C_0}|i\rangle\langle i| \tag{1}$$

in a Hilbert space $\mathcal{H}=\mathcal{H}_0$, we may divide all states $i\in C_0$ into separate groups $D_1, D_2, \ldots$ and define the subspaces $\mathcal{H}_\alpha\subset\mathcal{H}$ by the projectors

$$Q_\alpha=\sum_{i\in C_\alpha}|i\rangle\langle i|\,,$$
$$C_\alpha=C_{\alpha-1}-D_\alpha,\quad \alpha=1,2,\ldots. \tag{2}$$

In this case, simple algebraic manipulations[1] enable us to replace the inversion of a large matrix (linear operator in $\mathcal{H}$) by a succession of inversions of smaller matrices. This may have important numerical advantages in some special cases.[2] In application, this algebraic replacement is a basic step in solving the Schrödinger equation by the successive partitioning method[3] and proved to be very useful in practical calculations,[4] i.e., as a guide for making approximations.

In the present paper, we shall consider an application of this algebraic scheme to solving the Bethe-Goldstone equation[5]

$$G_\alpha=V-VB_\alpha G_\alpha,$$
$$B_\alpha=\frac{Q_\alpha}{Q_\alpha K Q_\alpha},\quad K=T+\omega \tag{3}$$

defining the two-body Brueckner reaction matrix $G=G_\alpha$. Here, V is a two-nucleon potential, $\omega=-E>0$ is a parameter (E is the so-called starting energy), and T denotes the kinetic energy operator. The Pauli projector is given by Eq. (2) in terms of uncorrelated two-particle wave functions $|i\rangle$.[5,6] Since the matrix K in the energy denominator is nondiagonal and nonsingular and the solution of Eq. (3) should be as exact as possible, the present problem of improving the solution method for Eq. (3) differs substantially from the repeated introduction of an effective interaction as presented, e.g., in Ref. 4.

As an initial step of finding $G=G_\alpha$, the reference matrix G_0 defined with the trivial propagator $Q_0=I$ should be found numerically by solving Eq. (3) for $\alpha=0$ on a mesh of grid points in the k-space.[6] The second step is also standard—an explicit solution of Eq. (3) for $\alpha=1$ may be identified with the formula of Tsai and Kuo[7]

$$G_1=G_0+G_0\Delta_1 G_0\,,$$
$$\Delta_1=B_0P_1\frac{1}{P_1(B_0-B_0G_0B_0)P_1}P_1B_0\,,\quad P_1=I-Q_1\,. \tag{4}$$

A simple reinterpretation of Eq. (4) considered in a restricted two-nucleon space $\mathcal{H}_R=\mathcal{H}_{\alpha-1}$, $\alpha=2,3,\ldots$ provides finally a relation

$$G_\alpha=G_{\alpha-1}+G_{\alpha-1}\Delta_\alpha G_{\alpha-1},$$
$$Q_{\alpha-1}-Q_\alpha=R_\alpha=\sum_{i\in D_\alpha=C_{\alpha-1}-C_\alpha}|i\rangle\langle i|\,, \tag{5}$$
$$\Delta_\alpha=B_{\alpha-1}R_\alpha\frac{1}{R_\alpha(B_{\alpha-1}-B_{\alpha-1}G_{\alpha-1}B_{\alpha-1}R_\alpha}R_\alpha B_{\alpha-1}$$

for G_α that solves Eq. (3) not only in $\mathcal{H}_R$ but also in the usual space $\mathcal{H}=\mathcal{H}_0$ and is defined in terms of $G_{\alpha-1}$. Here, only the inversion in the subspace defined by the projector R_α is needed.

The most exciting possibility of application of Eq. (5) stems from the shell model structure of nuclei. In a broad interval of the mass number A, the same $|i\rangle$ may be used[5] so that both $Q_{\alpha-1}$ and Q_α may be interpreted as correct Pauli projectors. In this sense, Eq. (5) uses the given reaction matrix $G_{\alpha-1}$ in the simple evaluation of G_α corresponding to a heavier nucleus.

As the complement to Eq. (5), the backward recurrence $G_{\alpha+1}\to G_\alpha$ may be derived as well: We put $\alpha=1$ for simplicity. Supposing knowledge of G_2, we may write the reference spectrum equation for G_1

$$G_1 = G_2 - G_2(B_1 - B_2)G_1 . \tag{6}$$

Denoting by

$$A = R_2 K R_2, \quad B = R_2 K Q_2 = C^+, \quad D = Q_2 K Q_2 \tag{7}$$

the matrices defined in corresponding subspaces, we get matrix identities

$$\begin{aligned} &Q_2 B_2 Q_2 = D^{-1}, \\ &R_2 B_1 R_2 = (A - BD^{-1}C)^{-1} = F^{-1}, \\ &Q_2 B_1 R_2 = -D^{-1} C F^{-1}, \\ &Q_2 B_1 Q_2 = D^{-1} + D^{-1} C F^{-1} B D^{-1} . \end{aligned} \tag{8}$$

In the matrix notation

$$Q_1 K Q_1 = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{9}$$

we have

$$\begin{aligned} B_1 - B_2 &= Q_1(B_1 - B_2)Q_1 \\ &= \begin{pmatrix} F^{-1} & -F^{-1}BD^{-1} \\ -D^{-1}CF^{-1} & D^{-1}CF^{-1}BD^{-1} \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ -D^{-1}C \end{pmatrix} \begin{pmatrix} F^{-1} & 0 \\ 0 & F^{-1} \end{pmatrix} (1, -BD^{-1}) \end{aligned} \tag{10}$$

so that

$$\begin{aligned} &G_1 = G_2 - G_2 \frac{1}{K} S_2 R_2 \frac{1}{R_2 S_2 R_2} R_2 S_2 \frac{1}{K} G_1 , \\ &S_2 = K - K B_2 K = P_2 \frac{1}{P_2 (1/K) P_2} P_2, \quad P_2 = I - Q_2 . \end{aligned} \tag{11}$$

Hence we obtain the resulting relation

$$\begin{aligned} &G_1 = G_2 + G_2 \bar{\Delta}_2 G_2 , \\ &\bar{\Delta}_2 = -\frac{1}{K} S_2 R_2 \frac{1}{R_2 [S_2 + S_2 (1/K) G_2 (1/K) S_2] R_2} R_2 S_2 \frac{1}{K} \end{aligned} \tag{12}$$

expressing G_1 in terms of G_2 without using "intermediate" projectors Q_1 or $I - Q_1$.

Together with Eq. (5), Eq. (12) represents our main result, namely the explicit solution of the reference spectrum equations of the type (6) convenient for the simultaneous calculation of neighboring nuclei. Really, this is not the only possible application. Although the initialization of the backward recurrence by the trivial ($Q_n = 0$) value $G_n = V$ does not lead to a new formula,[8] some other initializations (nuclear matter or local density[8] approximated G_n) seem to be a very promising prospect of solving Eq. (3) in a region of heavy nuclei. Unfortunately, we were not successful in overcoming the technical difficulties yet.

The situation in the forward recurrence (5) is more favorable. Since even the reference matrix G_0 is a good approximation to G[5], the second term in Eq. (5) respresents a small correction. Therefore, the direct use of the continued fraction formulas obtained from Eq. (5) by iteration, e.g.,

$$\begin{aligned} G_2 = G_0 &+ G_0 \Delta_1 G_0 + (G_0 + G_0 \Delta_1 G_0) B_1 R_2 \\ &\times \frac{1}{R_2 (B_1 - B_1 G_0 B_1 - B_1 G_0 \Delta_1 G_0 B_1) R_2} \\ &\times R_2 B_1 (G_0 + G_0 \Delta_1 G_0) , \end{aligned} \tag{13}$$

etc., represents a reasonable approximation strategy. The step-by-step increase of cutoff N [growing of the finite set $(C_0 - C_\alpha) \subset (C_0 - C_{\alpha+1}) \subset \cdots \subset (C_0 - C_n)$] allows one to preserve the fixed maximal (computer limited) dimension of matrices to be inverted. The direct precision test for stopping the calculation (error determination) is at our disposal in each step (cf., Table I).

We must stress that an important component of applicability of Eq. (5) is represented by various technical simplifications.

(1) *The B_α evaluation.* We easily derive the relation

$$B_\alpha = B_{\alpha-1} - B_{\alpha-1} R_\alpha \frac{1}{R_\alpha B_{\alpha-1} R_\alpha} R_\alpha B_{\alpha-1} . \tag{14}$$

Although Eq. (14) is similar to Eq. (5), the matrix dimensions are much smaller here due to the diagonality of $K = T + \omega$ with respect to the angular quantum numbers. Furthermore, the simple harmonic oscillator (HO) form of functions $|i\rangle = |n_1 l_1, n_2 l_2, \ldots\rangle$ is mostly used[5] in light nuclei. The band structure of K in the HO basis reduces Eq. (14) to the use of the inversion method of Ref. 2. The ordering of the basis $|i\rangle$ into groups according to the growing total energy

$$\begin{aligned} &|0 l_1, 0 l_2, \ldots\rangle ; \\ &|0 l_1, 1 l_2, \ldots\rangle , |1 l_1, 0 l_2, \ldots\rangle ; \\ &|0 l_1, 2 l_2, \ldots\rangle , |1 l_1, 1 l_2, \ldots\rangle , |2 l_1, 0 l_2, \ldots\rangle ; \end{aligned} \tag{15}$$

plus the exclusion of all the vectors with $Q_\alpha |i\rangle = 0$ enables us to perform the matrix inversion of the quasitridiagonal matrix[2] $Q_\alpha K Q_\alpha = Q_\alpha (T + \omega) Q_\alpha$ in the single-particle HO representation with practically arbitrary precision. For nuclei up to ^{40}Ca, this was tested using the computer code GIER. The convergence proved to be quick: For obtaining 4 (or 6) significant digits in the lowest matrix elements of B_α the number of iterations (= maximal dimension of the matrices) was equal to 10 (or 20, respectively).

(2) *Transformation of variables.* The two-nu-

TABLE I. Exact reaction matrix element $\langle 0000 | G | 0000 \rangle$ (MeV) for ^{4}He and its convergence with respect to the cutoff N (first column). The same with neglect of the c.m. off-diagonal influence (second column). In further columns, the independence of results with respect to change of the partial wave cutoff l_{max} and the number of c.m. grid points N_B is shown.

	l_{max}	0	0	0	2	4
	N_B	16	16	32	32	32
N	c.m.	All	Diag.	All	All	All
0		−17.4166	−17.1900			
1		−14.5863		−14.586 7		
2		−14.4464	−14.2654	−14.446 8		
3		−14.4289	−14.2405	−14.429 3		
4		−14.4267	−14.2357	−14.427 11	−14.427 18	
5		−14.4264	−14.2357	−14.426 80		
6		−14.4263	−14.2351	−14.426 70	−14.426 80	−14.426 80
9		−14.4263	−14.2350	−14.426 70	−14.426 79	−14.426 79

cleon potential V is diagonal in one of the relative variables [e.g., momenta $\vec{k}_r = (\vec{k}_1 - \vec{k}_2)/\sqrt{2}$, $\vec{K}_c = (\vec{k}_1 + \vec{k}_2)/\sqrt{2}$] and Q_α is defined in terms of single-particle functions[5] $\langle \vec{k}_1, \vec{k}_2 | i \rangle$. For HO functions $|i\rangle$, the transformation of Q_α to the relative representation is usually performed[5] using the Moshinsky brackets.[9] In our case, an adequate calculational method consists in the use of the recurrent evaluation of $\langle \vec{k}_r, \vec{K}_c | i \rangle$ as described in Ref. 10.

In conclusion, we return to our numerical example with the ^{4}He nucleus and a simple separable potential V. The results given in Table I display the advantages of the presented formulas most convincingly:

(a). The monotonic character of the convergence confirms that we are allowed to use an extrapolated error estimate and to pick up an optimal cutoff, N, thus avoiding unnecessary calculations.

(b). We see in Table I that the reliability of all numerical methods may carefully be tested; using low N saves time (e.g., N_B characterizes the integration precision).

(c). Physically motivated approximations may be tested precisely by using optimal N. In the example considered, the influence of higher partial waves of V (the Mongan potential[11] in $^1D_2$ and $^1G_4$ channels was used) due to coupling by exact Q_α proved to be extremely small ($\sim 10^{-3}$% for $^1D_2$). On the other side, the precision of the standard c.m. system-diagonal approximation[5] seems to be insufficient.

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