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The recursion method of a linear operator inversion

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Abstract. A method of inverting a linear operator in a recursively defined basis is developed. The questions of completeness, orthogonality, convergence and numerical stability are discussed. The numerical example of applicability of the method is taken from the Brueckner theory.

1. Introduction

In various fields of the quantum theory, we have to investigate the properties of a resolvent operator $R(E)=(E-H)^{-1}$ corresponding to a linear operator H in a vector space V and depending on a complex parameter E not equal to an eigenvalue of H. In such an investigation, various methods are used. Haydock (1974) derives for any vector $|x_1\rangle \in V$ the expansion of the vector

$$|y_1\rangle = R(E)|x_1\rangle \tag{1}$$

in the form

$$|y_1\rangle = \sum_{k=1}^{\infty} d_k^{(1)}|x_k\rangle \tag{2}$$

where we have slightly changed Haydock's original notation (for details see § 2). The expansion (2) can be considered to be a generalization of the usual power series expansion

$$|y_1\rangle = \sum_{k=1}^{\infty} E^{-k}(H^{k-1}|x_k\rangle) \tag{3}$$

because (3) can be obtained as a special case of (2) (Haydock 1974). The vectors $|x_k\rangle$ are recursively defined by the action of the operator H,

$$b_n|x_{n+1}\rangle = H|x_n\rangle - a_n|x_n\rangle - c_n|x_{n-1}\rangle, \qquad c_1=0 \tag{4}$$

and it is therefore unnecessary to know an inner product in V. The sequences of parameters

$$a_n, b_n, c_{n+1}, \qquad n=1,2,\ldots \tag{5}$$

can be chosen arbitrarily, thus providing a wide flexibility of the definition of the expansion basis $|x_n\rangle$.

The purpose of the present paper is twofold. Firstly, we derive the matrix elements of the resolvent operator $R(E)$ in the Haydock basis (4) (§ 2) and generalize this formalism (§§ 3 and 4). Secondly, we illustrate the practical value of this formalism by a numerical example taken from the Brueckner theory of atomic nuclei (§§ 5 and 6).

2. Action of the resolvent operator and its matrix elements

In the method of Haydock, the coefficients in the expansion (2) are expressed in the product form

$$d_n^{(1)} = \prod_{i=1}^{n} \alpha_i(E), \qquad n = 1, 2, \ldots \tag{6}$$

where $\alpha_n(E) = b_{n-1} f_n(E)$ and the number $b_0 = 1$ is added for convenience. The functions $f_n(E)$ satisfy the condition

$$f_n(E) = (\epsilon_n - b_n c_{n+1} f_{n+1}(E))^{-1}, \qquad n = 1, 2, \ldots \tag{7}$$

where $\epsilon_n = E - a_n$, and, according to Haydock's paper, may be calculated from some initial value given as a rather complicated limit.

In this section, we shall suppose that the values $f_n(E)$ are known and derive the analogue of the expansion (2) for the vector

$$|y_m\rangle = R(E)|x_m\rangle, \qquad m = 1, 2, \ldots. \tag{8}$$

Since the vectors $|x_m\rangle$ are defined by equation (4), they form a complete set in some subspace $\bar{V} \subset V$, invariant with respect to the action of the operator H. Therefore, all the matrix elements of $R(E)$ can be found from $\langle x_n|R(E)|x_m\rangle = \langle x_n|y_m\rangle$.

Let us insert the definition (4) into equation (8) to get

$$b_m|y_{m+1}\rangle = -|x_m\rangle + \epsilon_m|y_m\rangle - c_m|y_{m-1}\rangle, \qquad m = 1, 2, \ldots. \tag{9}$$

The formula

$$|y_m\rangle = \sum_{k=1}^{\infty} d_k^{(m)}|x_k\rangle, \qquad m = 1, 2, \ldots \tag{10}$$

is then valid with the coefficients $d_k^{(m)}$ given by the relation

$$\delta_k^m = \epsilon_m d_k^{(m)} - c_m d_k^{(m-1)} - b_m d_k^{(m+1)}, \qquad k, m = 1, 2, \ldots \tag{11}$$

where δ_k^m is a Kronecker delta. The direct consequence of (11) is the relation

$$d_1^{(m)} = f_1(E) \prod_{i=2}^{m} c_i f_i(E), \qquad m = 2, 3, \ldots \tag{12}$$

which can be proved by means of mathematical induction.

Let us further multiply the vector (8) from the left by the operator $(E-H)$ and use expansion (10). We get

$$|x_m\rangle = \sum_{k=1}^{\infty} d_k^{(m)}(E-H)|x_k\rangle, \qquad m = 1, 2, \ldots. \tag{13}$$

The term by term comparison of both sides of (13) provides the relation

$$\delta^k_m = \epsilon_m d^{(k)}_m - b_{m-1} d^{(k)}_{m-1} - c_{m+1} d^{(k)}_{m+1} \tag{14}$$

where $d^{(k)}_0 = 0$ and $k, m = 1, 2, \ldots$.

There is symmetry between the pair of equations (11) and (14). They differ by the exchange of $b_m \leftrightarrow c_{m+1}$ and lower $\leftrightarrow$ upper indices in the coefficients $d^{(m)}_k$. This symmetry also holds for the initial values (6) and (12) of the recurrence procedure and thus for any coefficient $d^{(m)}_k$. Especially, the relations

$$d^{(m)}_{m+l} = d^{(m)}_m \prod_{i=m+1}^{m+l} b_{i-1} f_i(E), \qquad l, m = 1, 2, \ldots \tag{15}$$

and

$$d^{(m+l)}_m = d^{(m)}_m \prod_{i=m+1}^{m+l} c_i f_i(E), \qquad l, m = 1, 2, \ldots \tag{16}$$

are valid. The following relation, derived from (11) and (14), holds for the remaining unknown values $d^{(m)}_m$:

$$\begin{aligned} d^{(m+1)}_{m+1} &= f_{m+1}(E)(1 + d^{(m)}_m \beta_m), \qquad m = 1, 2, \ldots \\ \beta_m &= b_m c_{m+1} f_{m+1}(E). \end{aligned} \tag{17}$$

This relation implies the final form of the coefficients with identical indices

$$d^{(m+1)}_{m+1} = f_{m+1}(E)\left(1 + \sum_{k=1}^{m} \prod_{i=k}^{m} \beta_i f_i(E)\right), \qquad m = 1, 2, \ldots. \tag{18}$$

Thus, in the expansion

$$\langle x_n | R(E) | x_m \rangle = \sum_{k=1}^{\infty} d^{(m)}_k \langle x_n | x_m \rangle \tag{19}$$

of the resolvent operator, we use the coefficients simply evaluated by means of equations (15), (16) and (18).

3. Generalization of the expansion basis

The orthonormality of the basis vectors $|x_n\rangle$, $n = 1, 2, \ldots$ with respect to some inner product in $\bar{V}$ can be one of the possible restrictions accepted when choosing the coefficients (5). In the case of a general (non-Hermitian) operator H, the orthonormality conditions

$$\langle x_1 | x_{n+1} \rangle = \ldots = \langle x_n | x_{n+1} \rangle = 0, \qquad \langle x_{n+1} | x_{n+1} \rangle = 1 \tag{20}$$

would need $n + 1$ free parameters in the definition of the vector $|x_{n+1}\rangle$, in order to be met.

If we accept the generalization

$$b_n |x_{n+1}\rangle = (H - a_n)|x_n\rangle - \sum_{i=1}^{n-1} c^{(i)}_n |x_{n-i}\rangle, \qquad n = 1, 2, \ldots \tag{21}$$

of the definition (4), where

$$a_n, b_n, c^{(i)}_{n+1}, \qquad n, i = 1, 2, \ldots \tag{22}$$

are arbitrary sequences again, then we are able to make the vectors $|x_n\rangle$, $n=1,2,\ldots$ mutually orthonormal by a special choice of the arbitrary parameters (22). It is easy to show that in the case of a Hermitian operator H, this choice implies $c_n^{(i)}=0$, $i=2, 3,\ldots,n-1$, so that the definition (21) reduces to (4). In the construction of the corresponding sequences (5) given by Haydock (1974), the hermiticity of H is tacitly supposed, because only in this case is the constructed basis actually orthonormal. If some loss of significance occurs in the computation, it is necessary to re-orthogonalize the vector $|x_n\rangle$ to the previously defined ones (Whitehead 1972), so that the generalized definition (21) can be useful even in the case of the Hermitian H. For the generalized recurrence definition (21) of basis vectors we now derive the formalism analogous to that of § 2.

The expansion (10) remains valid in the same form, as well as the relation (6). The recurrence relation (7) for functions $f_n(E)$ becomes more general, namely

$$f_n(E)=\left(\epsilon_n-\sum_{i=1}^{\infty} c_{n+i}^{(i)}\prod_{j=n+1}^{n+i} b_{j-1}f_j(E)\right)^{-1}, \qquad n=1,2,\ldots. \tag{23}$$

Let us first suppose that functions $f_n(E)$ satisfying (23) are known. Then the formulae that are the analogues of the relations (11) and (14) read

$$\delta_k^m=\epsilon_m d_k^{(m)}-b_m d_k^{(m+1)}-\sum_{i=1}^{m-1} c_m^{(m-i)}d_k^{(i)}, \qquad m,k=1,2,\ldots \tag{24}$$

$$\delta_m^k=\epsilon_m d_m^{(k)}-b_{m-1}d_{m-1}^{(k)}-\sum_{i=1}^{\infty} c_{m+i}^{(i)}d_{m+i}^{(k)}, \qquad m,k=1,2,\ldots \tag{25}$$

where $d_0^{(k)}=0$. We obtain, further, the relation (15) in an identical form by means of induction. The lack of symmetry in the present case leads to the more complicated relations

$$b_{k+r}d_k^{(k+r+1)}=\delta_r^0+\epsilon_{k+r}d_k^{(k+r)}-\sum_{l=1}^{r} c_{k+r}^{(r-l+1)}d_k^{(k+l-1)}-\sum_{l=1}^{k-1} c_{k+r}^{(k+r-l)}d_l^{(l)}\prod_{i=l+1}^{k} b_{i-1}f_i(E),$$
$$r=0,1,2,\ldots, \qquad k=2,3,4,\ldots \tag{26}$$

and

$$d_{m+1}^{(m+1)}=f_{m+1}(E)\left(\epsilon_m d_m^{(m)}-\sum_{l=1}^{m-1} c_m^{(m-l)}d_l^{(l)}\prod_{i=l+1}^{m} b_{i-1}f_i(E)\right), \qquad m=1,2,\ldots \tag{27}$$

that correspond to the relations (16) and (17), respectively.

The conclusion reads that the expansion (10), in terms of the generalized basis vectors (21), has the coefficients defined by the formulae (15), (26) and (27), where all the sums and products are finite.

As well as in § 2, the most difficult task here is the calculation of $f_n(E)$. Let us describe our method. It is based on the assumption that the inversion of the matrix $E-H$ in the basis $|x_n\rangle$ is, in principle, possible by inverting the matrix in truncated finite-dimensional space, and then limiting the dimension N to infinity. The truncation of the basis will be simulated by putting $b_N=0$. The recurrence definition (21) then provides N independent vectors $|x_1\rangle,\ldots,|x_N\rangle$, while the vectors $|x_{N+i}\rangle$, $i=1,2,\ldots$, can be put equal to zero as a consequence of a special choice

$c^{(0)}_{N+j}=0$, $i,j=1,2,\ldots$. Any initial values f_{N+1}, $f_{N+2},\ldots$, may be used in the recurrence definition (23) because the functions $f_i(E)$, $i=1,2,\ldots,N$ are uniquely determined by $b_N=0$ (ie $f_N(E)=1/\epsilon_N$ etc).

4. The convergence problems

If we use the formalism of §§ 2 or 3, we must first prove the convergence of the expansion (10) because the vector $|y_m\rangle$ is considered to be a limit of the partial sums

$$|y_m\rangle_N=\sum_{k=1}^{N} d_k^{(m)}|x_k\rangle \tag{28}$$

when $N\to\infty$. In the orthonormal basis, the problem of weak convergence does not arise. For $N>n$, the relations $\langle x_n|x_k\rangle=\delta_k^n$ imply that $\langle x_n|y_m\rangle=d_n^{(m)}$ is exactly valid. When the basis is not orthonormal, the discussion of the convergence, however simple it may be, requires the explicit knowledge of the scalar products of basis vectors and will not be treated here—we suppose the validity of the orthonormality relations (20).

The weak convergence can also be discussed in the basis $|\beta\rangle\neq|x\rangle$, where we can write

$$\langle\beta_i|y_m\rangle_N=\sum_{k=1}^{N}\langle\beta_i|x_k\rangle d_k^{(m)}. \tag{29}$$

For bounded values $\langle\beta_i|x_k\rangle$, it is sufficient to prove the convergence of the series

$$\sum_{k=1}^{\infty}|d_k^{(m)}|. \tag{30}$$

The usual convergence criteria for a series of positive numbers (Korn and Korn 1968) may be used because the ratio $|d_{k+1}^{(m)}|/|d_k^{(m)}|$ is equal to $|\alpha_{k+1}(E)|$ according to (15). Thus, the condition

$$\limsup_{n\to\infty}\,[n(|\alpha_{n+1}(E)|-1)+1]\ln n<-1 \tag{31}$$

is sufficient for the convergence of (30).

Norm of the vectors $|y_m\rangle_N$ is given by the sum

$${}_N\langle y_m|y_m\rangle_N=\sum_{k,l=1}^{N}\langle x_k|x_l\rangle d_k^{(m)}d_l^{(m)}=\sum_{k=1}^{N}(d_k^{(m)})^2$$

and the same criteria can be applied. Since the relation

$$(d_{k+1}^{(m)})^2/(d_k^{(m)})^2=(\alpha_{k+1}(E))^2\leqslant|\alpha_{k+1}(E)|\leqslant 1 \tag{32}$$

must be valid for the corresponding ratio, the convergence in the norm is a consequence of the convergence of the series (30). The condition sufficient for divergence of $|y_m\rangle$ in the norm is

$$\liminf_{n\to\infty}\,[n(|\alpha_{n+1}|^2-1)+1]\ln n\geqslant -1 \tag{33}$$

and implies also the divergence of (30).

The last problem is the convergence of the $f_n(E)$ values when the cutoff parameter N grows to infinity. In fact, we need to prove that the sequence α_{N-k} with k increasing and $N \gg 1$ gives the value α_{n_0} for $n_0 = N - k_0$ independently of the value $N \gg n_0$. The method of proving depends on the parameters (22) used. We give here an outline of the proof for the cases characterized by the existence of the limits

$$\lim_{N\to\infty} \frac{c^{(i)}_{N+i}}{b_{N-1}} = c^{(i)}, \qquad \lim_{N\to\infty} \frac{E - a_N}{b_{N-1}} = \epsilon \neq 0 \tag{34}$$

because the example in the next section belongs to this class.

Firstly, we simplify the situation by putting $c^{(i_0+1)} = c^{(i_0+2)} = \ldots = 0$ for some i_0 and defer the limit $i_0 \to \infty$ as the last step. Secondly, we consider here $i_0 = 1$ only—the discussion of $i_0 > 1$ cases being entirely analogous. Thirdly, we shall consider only the stability of the values α_{n_0} for $n_0 = N - k_0 \gg 1$ since the stability of the remaining values α_{n_1} for $n_1 < n_0$ may be tested numerically.

Without loss of generality ($\alpha \to -\alpha$ transformation if needed), we may choose $\epsilon > 0$ in (34) and using the basic definition (23) (in our $i_0 = 1$ case it is equivalent to (7)) we have

$$\begin{aligned} &\alpha_{n_0} = F(\alpha_{n_0+1})(1 + \mathrm{O}(g(n_0))), \qquad \lim_{n\to\infty} g(n) = 0, \\ &F(\alpha) = (\epsilon - c\alpha)^{-1}. \end{aligned} \tag{35}$$

The stability of α_{n_0} means

$$\alpha_{n_0+1} = \alpha_{n_0}(1 + \mathrm{O}(g(n_0))), \tag{36}$$

so that α_{n_0} is given by solving the equations (35) and (36). The existence of this solution implies that

$$\epsilon^2 \geqslant 4c. \tag{37}$$

We define ψ by the relations $\sinh^2\psi = \epsilon^2 - 4c$, $\operatorname{sgn}\psi = \operatorname{sgn} c$ and get two roots

$$\alpha_{n_0} = \alpha_{0R} = 2(\epsilon - R \sinh\psi)^{-1} \tag{38}$$

where $R = +1$ or $R = -1$. It is a matter of elementary algebra to show that the choice of R which is consistent with the stability condition is given by the relation $R = -\operatorname{sgn} c$. If we avoid the singularity of $F(\alpha)$ by simply putting $F(\epsilon/c) = \infty$, $F(\infty) = 0$, then it is easy to demonstrate that the stability condition (36) is satisfied for any initial value $\alpha_N \neq \alpha_{0S}$ where $S = +\operatorname{sgn} c$. For $0 \leqslant \partial_\alpha F(\alpha_n) = cF^2(\alpha_n) < 1$ with α_n lying in the vicinity of α_0, the sequence α_{N-k}, $k = 1, 2, \ldots$ monotonically decreases (if $F(\alpha_n) < \alpha_n$) or increases (if $F(\alpha_n) > \alpha_n$) to α_0, while for $-1 < \partial_\alpha F(\alpha_n) < 0$ the sequence $(\alpha_{N-k} - \alpha_0)$ changes sign and approaches zero in absolute value.

Since the stable root does not depend on $n > n_0 \gg 1$, we can conclude that for $|\alpha_0| < 1$ the convergence of the series (30) and of the expansion (10) is guaranteed. The result $|\alpha_0| > 1$ implies divergence of (10) and (30) and we have for $\epsilon < 2$, an additional (convergence) restriction on the parameter c,

$$c \leqslant \epsilon - 1. \tag{39}$$

5. An application in nuclear theory

Binding energies of atomic nuclei are calculated in the Brueckner theory by means of the reaction matrix G. The method of the calculation of G in finite nuclei was suggested by Sauer (1970), using the reference reaction matrix G_r as a first step. While the methods of computation of G_r are standard (cf Baranger 1969), the approximate inclusion of the Pauli principle is performed by means of the operator equation

$$(1-G_r\Delta)G=G_r. \tag{40}$$

Sauer solves that equation in a truncated oscillator basis

$$\begin{aligned}\langle k|nl\rangle &= R_{nl}(k)=R_{0l}(k)(-1)^n\left(\frac{n!\Gamma(l+\frac{3}{2})}{\Gamma(n+l+\frac{3}{2})}\right)^{1/2}\mathrm{L}_n^{l+1/2}(\lambda k^2),\\ R_{0l}(k)&=k^l\exp(-\tfrac{1}{2}\lambda k^2)\left(\frac{2\lambda^{l+3/2}}{\Gamma(l+\frac{3}{2})}\right)^{1/2},\end{aligned} \tag{41}$$

where k is a relative impulse of two nucleons, λ is the parameter in a corresponding harmonic potential and $\mathrm{L}_n^{l+1}(x)$ are Laguerre polynomials (eg Gradshteyn and Ryzhik 1971). Sauer uses the operator Δ in the form

$$\begin{aligned}\Delta&=\Delta(Q)-\Delta(I)\\ \Delta(Q)&=\delta_{ll'}\langle nl|Q[\omega-Q(\tfrac{1}{2}e_{\mathcal{NL}}+K_{\mathrm{rel}})Q]^{-1}Q|n'l\rangle\end{aligned} \tag{42}$$

where ω is the available energy (negative). $\frac{1}{2}e_{\mathcal{NL}}$ is a constant approximating to the centre-of-mass energy of the two nucleons, K_{rel} is the relative kinetic energy operator and Q, the approximate Pauli projector, is a diagonal matrix with elements $\langle n,l|Q|n,l\rangle=Q_{\mathcal{NL}}(n,l)$.

Sauer shows numerically that the calculation of $\Delta(Q)$ by means of the truncated matrix inversion converges quite rapidly with increasing cutoff. Nevertheless, the amount of work needed for numerically inverting matrices grows rapidly with their dimension and therefore the present method seems to be more adequate. Let us now demonstrate how it works.

If the matrix Q is non-singular ($Q=I$ is a special case), we put

$$\begin{aligned}&H=-Q(\tfrac{1}{2}e_{\mathcal{NL}}+K_{\mathrm{rel}})Q, \qquad K_{\mathrm{rel}}=k^2, \qquad E=-\omega>0,\\ &|x_1\rangle=R_{n_0l}(k)\end{aligned} \tag{43}$$

and choose

$$\begin{aligned}a_n&=-(1/\lambda)(2n+2n_0-\tfrac{1}{2}+l+\tfrac{1}{2}\lambda e_{\mathcal{NL}})[Q_{\mathcal{NL}}(n+n_0-1,l)]^2,\\ b_n=c_{n+1}&=-(1/\lambda)[(n+n_0)(n+n_0+l+\tfrac{1}{2})]^{1/2}Q_{\mathcal{NL}}(n+n_0,l)Q_{\mathcal{NL}}(n+n_0-1,l),\\ n_0&=0.\end{aligned} \tag{44}$$

Then we get $|x_{n+1}\rangle=R_{n+n_0,l}(k)$ according to definition (6). The formalism of § 2 provides the result

$$\langle m+n_0,l|\Delta(Q)|n+n_0,l\rangle=-Q_{\mathcal{NL}}(m+n_0,l)d_{n+1}^{(m+1)}Q_{\mathcal{NL}}(n+n_0,l). \tag{45}$$

It can happen that $Q_{\mathcal{NL}}(n_0,l)=0$—eg, in ^{4}He we have $Q_{00}(0,0)=0$. Then the space $\tilde{V}$ is one dimensional and the next oscillator function should be taken as the initial vector $|x_1\rangle$. In general, the first non-zero element $Q_{\mathcal{NL}}(n_0,l)$ determines the value of the parameter n_0 which must be used in the case of the singular matrix Q in order to get the non-trivial space $\bar{V}$. For example, in ^{4}He we have $n_0=1$ and the formula

$$Q_{00}(n, l)=1-1/2^{2n+l-1}, \qquad 2n+l>0 \tag{46}$$

which we derive by employing the Trlifaj (1972) expression for Moshinsky coefficients. It is seen that $Q \neq I$ cases may sometimes be calculated on an elementary level.

Formal proof of the convergence of the series (10) or (30) is needed in our case, because the value $\alpha_0=-1$ lies, for any matrix Q, on the boundary of the convergence region. The proof is quite lengthy and will not be given here in detail. We describe only the method of proof.

Firstly, we neglect the exponential contribution of the $Q_{\mathcal{N}\mathcal{L}}(n, l)-1$ values (cf (46)) and get, in the $Q=I$ approximation, the relation (7) in the form

$$\alpha_n=-\frac{[(n-1)(n+l-\frac{1}{2})]^{1/2}}{\lambda(E+\frac{1}{2}e_{\mathcal{N}\mathcal{L}})+2n+l-\frac{1}{2}+[n(n+l+\frac{1}{2})]^{1/2}\alpha_{n+1}}. \tag{47}$$

Secondly, we put $\alpha_n=-1+A_n$ and get

$$A_n/(1-A_n)=B_n+(1+C_n)A_{n+1} \tag{48}$$

where

$$B_n=\frac{\lambda(E+\frac{1}{2}e_{\mathcal{N}\mathcal{L}})+(4n)^{-1}(l+\frac{1}{2})^2+\mathrm{O}(n^{-2})}{n[1+\mathrm{O}(n^{-1})]}, \qquad C_n=n^{-1}+\mathrm{O}(n^{-2}).$$

Thirdly, we show that the correct value A_n is bounded by the values $A_n^{(1)}$ and $A_n^{(2)}$ that are calculated by means of (48) from the initial values $A_N=0$ and $A_N=1$, respectively. The higher the cutoff N is, the closer the values $A_n^{(1)}$ and $A_n^{(2)}$ approach the correct value A_n, so that this phenomenon can be used also in practical calculations for the error determination.

The last step of the proof uses the criterion (31) of the convergence of (30) in the form $nA_n>1$. All the values from the interval $(A_n^{(1)}, A_n^{(2)})$ fulfil this condition after a few iterations of (48), where the number $k=N-n$ of these iterations depends on the magnitude of the value $\lambda(E+\frac{1}{2}e_{\mathcal{N}\mathcal{L}})\geqslant 0$.

Thus, the proof of the convergence of (30) is completed. It implies the convergence of the expansion (10) in the norm. Since we are able to derive the formula

$$R_{nl}(k)=(-1)^n[2\pi^{-1}(\lambda/n)^{1/2}]^{1/2}k^{-1}\sin[2k(n\lambda)^{1/2}-\tfrac{1}{2}l\pi][1+\mathrm{O}(n^{-1/2})], \tag{49}$$

we can conclude that the expansion of $\langle k|y_m\rangle$ also converges.

6. Numerical test

The rate of convergence of $\langle m|\Delta(Q)|n\rangle$ with respect to the cutoff $N\to\infty$ was tested for Q given by (46), $Q=I$, $l=0, 1, \frac{1}{2}e_{\mathcal{N}\mathcal{L}}=0$, $\lambda=1, 2$ and for E varying. A few results are presented in table 1. Using the initial values $\alpha_N=0$ or $\alpha_N=-1$ and increasing N, we get the absolute values of the calculated matrix elements increasing or decreasing, respectively, to the correct value. In such a way, we can get the desired value and also the error estimate. Better results can be obtained using $\alpha_N=\alpha_0(N)$, where the value $\alpha_0(N)$ is a solution of equation (47), where we put $\alpha_n=\alpha_0(N)=\alpha_{n+1}$, $n=N$.

Table 1. The rate of convergence of a few matrix elements $\langle m|(E-T)^{-1}|n\rangle = \langle m|R|n\rangle$. The numbers of the correctly calculated significant digits are given for three different initializations α_N dependent on the cutoff N.

			$\langle 0\|R\|0\rangle$			$\langle 2\|R\|2\rangle$			$\langle 0\|R\|3\rangle$		
E	N	$\alpha_0(N)$ \ α_N	0	−1	$\alpha_0(N)$	0	−1	$\alpha_0(N)$	0	−1	$\alpha_0(N)$
50	8	−0·1122								10	
	7	−0·0995					10		10	8	10
	6	−0·0860				10	9		9	7	9
	5	−0·0718				9	8	10	7	5	7
	4	−0·0566				7	6	7	5	4	5
	3	−0·0404	10	10	10	5	3	5	2	2	2
	2	−0·0229	9	7	9	2	1	2	0	0	0
	1	−0·0000	6	5	6	0	0	0	0	0	0
1	100	−0·9001				10	10		10	10	
	50	−0·8588	10	10	10	9	9	10	8	9	10
	20	−0·7775	6	6	7	4	5	6	4	4	5
	10	−0·6869	4	4	5	3	2	4	2	2	3
	5	−0·5615	2	3	3	2	1	2	1	1	1
0·1	200	−0·9753	8	8	9	6	6	8	5	6	7
	50	−0·9453	4	3	5	3	2	4	3	2	4
	10	−0·8455	2	1	3	0	0	1	0	0	1
0	8000	−0·99986	2			2			2		
	15	−0·9306	1	1	1	0	1	0	0	0	1

An example of an inadequate use, though good test, of the method is a very slowly convergent calculation for $E=0$. The exact result can be obtained by analytic integration—we reach 1% accuracy at $N=8000$. This result can hardly be obtained by matrix inversion, not to speak of the error estimation possibility.

The test was performed on the calculator Compucorp 324 G with 2×80 elementary instructions in the storage.

7. Conclusion

Our work is inspired by Haydock (1974). He gives the expansion of the result of the resolvent operator $R(E)=(E-H)^{-1}$ acting on an arbitrary initial vector $|x_1\rangle$ in terms of the recursively defined basis vectors $|x_n\rangle$, $n=1,2,\ldots$. We derive analogous expansions of the vectors $|y_m\rangle = R(E)|x_m\rangle$, $m=2,3,\ldots$, in the same basis. The expansion coefficients are calculated by means of elementary formulae so that the action of the resolvent operator in the whole space can be easily investigated.

The calculation of the expansion coefficients is based on a recursively evaluated sequence of numbers α_n. The initialization of this sequence represents a serious practical difficulty in Haydock's original paper. We show that this difficulty can be simply overcome by the basis truncation. The initial value $\alpha_N=0$ can then be taken for a large N.

The recursive definition of the vectors $|x_n\rangle$ is very flexible and does not depend on any inner product. It contains three sequences of arbitrary parameters that can be chosen to simplify the structure of the vectors $|x_n\rangle$. If we succeed in relating $|x_n\rangle$ to some simple functions, the problem of evaluating the matrix elements of $R(E)$ becomes trivial.

It can happen that some additional restrictions are necessary for simplifying the vectors $|x_n\rangle$. We introduce further corresponding parameters in the definition of the basis and derive the generalized formulae. The new definition enables us, for example, to orthonormalize the vectors $|x_n\rangle$ for any linear operator H.

The convergence of expansions in the orthonormal basis becomes a very simple problem and is closely connected with the evaluation of α_n. Both the problems are discussed in some detail. Some convergence and numerical stability criteria are explicitly given for a class of operators H which is characterized by the possibility of choosing the arbitrary parameter sequences convergent (cf (34)).

A numerical test confirms the general arguments. The main advantage of using the method lies in the possibility of checking the precision in a simple way. We use two types of the α_n initialization and the two corresponding approximations approach the final result from both sides. In general, the method enables us to influence the precision by increasing the cutoff N of the basis. It is important that only a one-dimensional array α_n is calculated for a given N. At the same time, only a fixed number of matrix elements of $R(E)$ is required in most cases so that much work is saved in comparison to the matrix inversion technique.

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References

Baranger M 1969 *Proc. Int. School of Phys. Enrico Fermi*, Course 40 eds M Jean and R A Ricci (New York: Academic Press)
Gradshteyn I S and Ryzhik I M 1971 *Tablicy Integralov, Summ i Proizv.* (Moscow: Nauka)
Haydock R 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 2120–4
Haydock R and Kelly M J 1975 *J. Phys.* C: *Solid St. Phys.* **8** L290–3
Korn G A and Korn T M 1968 *Mathematical Handbook* (New York: McGraw-Hill)
Sauer P U 1970 *Nucl. Phys.* A **150** 467–77
Trlifaj L 1972 *Phys. Rev.* C **5** 1534–41
Whitehead R R 1972 *Nucl. Phys.* A **182** 290–300