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Kinetic few-body propagator by exact inversion

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Abstract. We present an exact formula for matrix elements of the free many-body propagator in the oscillator basis. It has the structure $(a+bz)/(c+dz)$ where a, b, c and d are polynomials in the energy variable ω and the auxiliary function $z(\omega)$ is defined by the continued fraction.

1. Introduction

The motivation of the present paper stems from the Schrödinger equation

$$H\psi = -\omega\psi \qquad H = T + V \qquad \omega > 0 \tag{1}$$

for the A-body system with $T = k_1^2 + k_2^2 + \ldots + k_A^2$ and with any realistic two-particle interaction $V = \Sigma\, V_{ij}$. Let us consider an equivalent Lippmann–Schwinger form of (1):

$$\psi + \frac{1}{\omega + T} V\psi = 0. \tag{2}$$

This is not only a starting point for the derivation of the three-body Faddeev equations and their $A > 3$ generalisations (cf, e.g., Vanzani 1978) but also a formulation of a bound-state problem which has definite numerical advantages (Gareev *et al* 1977). The point is that in the standard harmonic-oscillator basis, the large matrix elements of the kinetic-energy operator T appear in the denominator.

In practical applications (cf, e.g., Truhlík 1978) the numerical integration of the matrix elements of the full resolvent $(\omega + T)^{-1}$ is used. An alternative approach based on exact matrix inversion is also possible due to the sparse structure of the matrix representation of T. This approach was suggested by Bassichis and Strayer (1978) for $A = 1$ and was extended by Znojil (1979) to cases where $A > 1$.

In the present paper we remove certain difficulties connected with the $A > 1$ generalisation and derive an exact algebraic formula for an arbitrary matrix element of $(\omega + T)^{-1}$ in the oscillator basis (§ 2). Its properties are discussed in the appendix and in §§ 3 and 4.

2. Algebraic formula

We apply the Haydock (1974) expansion to the function (free propagator)

$$\frac{1}{\omega + k_1^2 + \ldots + k_A^2} = \lambda \sum_{n=0}^{\infty} d_{n+1}(\lambda\omega) L_n^{\beta-1}(\lambda k_1^2 + \ldots + \lambda k_A^2)$$
$$\beta = l_1 + l_2 + \ldots + l_A + \tfrac{3}{2}A \tag{3}$$

using a complete set of Laguerre polynomials $L_n^{\beta-1}$ defined, for example, by Gradshteyn and Ryzhik (1971). In terms of the auxiliary sequence $\alpha_1, \alpha_2, \ldots$ satisfying the recurrence relations

$$\begin{aligned} &\alpha_1 = (\beta + \lambda\omega - \beta\alpha_2)^{-1} \\ &\alpha_{m+1} = [2 + (\beta + \lambda\omega)/m - (1 + \beta/m)\alpha_{m+2}]^{-1} \qquad m = 1, 2, \ldots \end{aligned} \tag{4}$$

the expansion coefficients d_{n+1} in (3) are defined explicitly as products:

$$d_{n+1}(\lambda\omega) = \alpha_{n+1} d_n(\lambda\omega) = \alpha_1 \alpha_2 \ldots \alpha_{n+1} \qquad n = 0, 1, \ldots . \tag{5}$$

It is proved in the appendix that α's are continued fractions defined uniquely by (4) and that expansion (3) is convergent for any oscillator parameter $\lambda > 0$, binding energy $\omega > 0$ and angular momenta $l_j \geqslant 0$, $j = 1, 2, \ldots, A$.

Next we investigate the matrix elements of the propagator $(\omega + T)^{-1}$

$$K_A = \langle n_1 l_1 \ldots n_A l_A \ldots | (\omega + T)^{-1} | n_1' l_1 \ldots n_A' l_A \ldots \rangle \tag{6}$$

in the oscillator basis

$$\begin{aligned} &|n_1 l_1 \ldots n_2 l_2 \ldots n_A l_A \ldots\rangle = |n_1 l_1\rangle |n_2 l_2\rangle \ldots |n_A l_A\rangle \times \text{angular part} \\ &\langle k|nl\rangle = R_{nl}(k) = (2\lambda^{l+\frac{3}{2}})^{1/2} p_l(n) k^l \exp(-\tfrac{1}{2}\lambda k^2) L_n^{l+\frac{1}{2}}(\lambda k^2) \\ &p_l(n) = (-1)^n [n!/\Gamma(n + l + \tfrac{3}{2})]^{1/2}. \end{aligned} \tag{7}$$

The K_A are diagonal in the angular quantum numbers and are defined as A-tuple integrals.

Using expansion (3), the separation of variables is achieved by the well known identity

$$\begin{aligned} &L_n^{l_1+\ldots+l_A+3A/2-1}(\lambda k_1^2 + \lambda k_2^2 + \ldots + \lambda k_A^2) \\ &\quad = \sum_{i_1+i_2+\ldots+i_A=n} L_{i_1}^{l_1+\frac{1}{2}}(\lambda k_1^2) L_{i_2}^{l_2+\frac{1}{2}}(\lambda k_2^2) \ldots L_{i_A}^{l_A+\frac{1}{2}}(\lambda k_A^2). \end{aligned} \tag{8}$$

The corresponding matrix elements (Talmi integrals) of the single separated factors $\langle n_1 l | L_m^{l+\frac{1}{2}}(\lambda k) | n_2 l\rangle = [n_1|m|n_2]_l$ are given by the closed expression

$$[n|m|n']_l = (-1)^{n+m+n'} \sum_{p=m}^{n+n'} \binom{p}{m} B(nln'l, l+p) \tag{9}$$

where $B(nln'l, p')$ are the Brody–Moshinsky (1960) coefficients. Hence, the A-tuple integration of the investigated matrix element K_A may be performed in an explicit way by inserting expansions (3) and (8) in (6). The final algebraic formula reads

$$\begin{aligned} K_A = \lambda \sum_{m_1=|n_1-n_1'|}^{n_1+n_1'} [n_1|m_1|n_1']_{l_1} \sum_{m_2=|n_2-n_2'|}^{n_2+n_2'} [n_2|m_2|n_2']_{l_2} \ldots \\ \sum_{m_A=|n_A-n_A'|}^{n_A+n_A'} [n_A|m_A|n_A']_{l_A} d_{1+m_1+m_2+\ldots+m_A}(\lambda\omega). \end{aligned} \tag{10}$$

Note that the sum is finite and the coefficients d are defined by (5) and (4) as the finite products of the convergent continued fractions α_m, $m = 1, 2, \ldots 1 + \Sigma_{i=1}^{A}(n_i + n_i')$.

For some purposes the necessary number of different continued fractions may be lowered by algebraic cancellations of the type

$$d_2(\lambda\omega)=\alpha_1\alpha_2=\frac{\alpha_2}{\beta+\lambda\omega-\beta\alpha_2}, \tag{11}$$

etc. In accordance with the general prescription (cf Znojil 1978, appendix 2), the systematic cancellations lead to the polynomial formula

$$\begin{aligned} d_{n+1}(\lambda\omega)&=\frac{P(J-n-1)}{(n+1)P(J)} \qquad J\geqslant n+1 \\ P(i)&=A_i(\omega)+B_i(\omega)z(\omega) \qquad i=0,1,\ldots J \end{aligned} \tag{12}$$

which is to be used instead of (5). Here, $z(\omega)$ is the continued fraction defined by (4) for $m=J$,

$$z(\omega)=\alpha_{J+1}=\cfrac{1}{2+\dfrac{\beta+\lambda\omega}{J}-\cfrac{(J+\beta)/J}{2+\dfrac{\beta+\lambda\omega}{J+1}-\cfrac{(J+\beta+1)/(J+1)}{2+\ldots}}}, \tag{13}$$

and A_i, B_i, $i=0,1,\ldots J$ are polynomials of degree i and $i-1$, respectively, in the energy variable ω. They may be written in terms of the linear combination of the confluent hypergeometric functions, but the simplest definition is given by the three-term recurrence

$$\begin{aligned} P(J+1-m)&=(\lambda\omega+2m+\beta-2)P(J-m)/m \\ &\quad-(m+\beta-1)P(J-m-1)/(m+1) \qquad m=J-1,J-2,\ldots 1 \end{aligned} \tag{14}$$

initialised by

$$P(0)=J \qquad P(1)=(\lambda\omega+2J+\beta-2)-(\beta+J-1)z(\omega). \tag{15}$$

For any given set of quantum numbers (truncated oscillator basis), we may choose $J\geqslant 1+\max\sum_{i=1}^{A}(n_i+n_i')$ so that just one continued fraction is necessary for all matrix elements. Hence each sum (10) is really equal to the ratio of two polynomials in ω and z as stated in the abstract. Let us illustrate this for the lowest s-wave states ($l_i=0$). The closed form of the matrix elements is

$$\begin{aligned} \left\langle 00,\ldots 00\left|\frac{1}{\omega+T}\right|00,\ldots 00\right\rangle&=\lambda\frac{P(J-1)}{P(J)}=\frac{\lambda}{\beta+\lambda\omega-\beta\alpha_2}=\lambda\alpha_1 \\ \left\langle 10,00,\ldots\left|\frac{1}{\omega+T}\right|10,00,\ldots\right\rangle&=\lambda\frac{P(J-1)-P(J-2)+\frac{5}{6}P(J-3)}{P(J)} \\ &=\lambda\frac{\beta+\lambda\omega+(\frac{3}{2}-\beta)\alpha_3}{(\beta+\lambda\omega)^2+2\lambda\omega+\beta-(\beta+\lambda\omega)(1+\beta)\alpha_3} \\ \left\langle 10,00,\ldots\left|\frac{1}{\omega+T}\right|00,\ldots,10,00\ldots\right\rangle&=\lambda\frac{P(J-1)-(\frac{3}{2})^{1/2}P(J-2)}{P(J)} \\ &=\lambda\frac{1-\sqrt{6}\alpha_2}{\beta+\lambda\omega-\beta\alpha_2}, \end{aligned} \tag{16}$$

etc.

3. Numerical properties

A computational application of an exact algebraic formula is not necessarily better than the standard numerical techniques because of the possible loss of precision ϵ. We shall show that in our case a rigorous estimate of numerical errors is available.

First, we note that there are three sources of the possible loss of precision $\epsilon = \epsilon_1 + \epsilon_2 + \epsilon_3$, namely the calculation of $d(\lambda\omega)$, $[n|m|n']$ and the final summation (10) respectively. The evaluation of $d_{n+1}(\lambda\omega) = \alpha_1\alpha_2 \ldots \alpha_{n+1}$ is discussed in the appendix, with the conclusion that the value of ϵ_1 (error in $d(\lambda\omega)$ or $z(\omega)$) may be made practically negligible by the proper choice of the initialisation α_N in (4). The sufficient value of the cut-off N is usually very small, except for the case of an extremely small value of the binding energy parameter $\lambda\omega$, which would require either $N > 100$ or an improved initialisation (cf table 1 and the appendix for details).

Table 1. Differences α_4(evaluated) $-$ α_4(exact) illustrating the convergence and stability of the auxiliary continued fractions ($J = \beta = 3$). Example: -55 in the row 10^{-5} means α_4(evaluated) $-$ α_4(exact) $= -55 \times 10^{-5}$.

$\lambda\omega$	0·1			0·5			5	
α_4(exact)	0·560604155			0·479698107			0·244986186	
Units of δ	10^{-5}	10^{-6}	10^{-8}	10^{-4}	10^{-6}	10^{-7}	10^{-4}	10^{-7}
N / α_N	30	60	120	10	20	30	5	10
20				−50	−118	−71		
0	−55	−25	−37	−30	−84	−51	−9	−7
$1-\bar{A}_N^{(1)}$	−8	−2	−2	−4	−7	−3		
$1-\bar{A}_N^1-\bar{A}_N^2$	+4	+1	+1					
$1-(\lambda\omega/N)^{1/2}$				+8	+15	+7		
1	+221	+61	+78	+102	+219	+179		

The second component ϵ_2 is, unfortunately, significantly enhanced by errors in the tabulated Brody–Moshinsky coefficients. It is necessary to recalculate the tables of the overlap coefficients $[n|m|n']$. At the same time we minimise ϵ_2 by employing the symmetry of the Talmi integrals

$$\frac{[m_1|m_3|m_2]_l}{p_l(m_1)p_l(m_2)} = \int_0^\infty \mathrm{d}t\, t^{l+\frac{1}{2}} L_{m_1}^{l+\frac{1}{2}}(t) L_{m_2}^{l+\frac{1}{2}}(t) L_{m_3}^{l+\frac{1}{2}}(t)$$

$$= \frac{(-1)^{m_3} 2^l}{\Gamma(\frac{3}{2}) p_l^2(m_1) p_l^2(m_2)} \sum_{p=m_3}^{m_1+m_2} (-1)^p \binom{p}{m_3} (2p+2l+1)!!\, Z_{m_1 m_2}^{(p)} \tag{17}$$

$$Z_{m_1 m_2}^{(p)} = \sum_{r=\max(0,\, p-m_2)}^{\min(p,\, m_1)} \frac{\binom{m_1}{r}\binom{m_2}{p-r}}{(2l+2r+1)!!\,(2l+2p-2r+1)!!} \tag{18}$$

where we choose $m_3 = \max(n, n', m)$ and $m_1 = \min(n, n', m)$ to eliminate some of the sign changes.

Thus, provided that $\epsilon_2 \sim 0$, the final precision of K_A will be determined practically by ϵ_3. Since the typical values of $d(\lambda\omega)$ are of the order of unity, the loss of precision ϵ in the sum (10) will be determined roughly by the order of the maximal term (pivot). The

empirical fit $[n|n|n]\sim 7\cdot 5^n$ leads to the estimated number $\epsilon \simeq \epsilon_3 \simeq n \lg 7\cdot 5 \simeq \frac{7}{8}n$ of incorrect decimal digits where $n = \max(n_i, n_i')$ corresponds to the truncation of the oscillator basis. The linear growth of ϵ with n is quite acceptable in practice and enables us to specify *a priori* the possible higher-precision requirements in the computer code.

For practical purposes the code is to be complemented also by the remultiplication of the identity

$$(\omega + T)(\omega + T)^{-1} = (\omega + T)K_A = 1. \tag{19}$$

This is a very simple test (sum of $3A$ terms only) and it determines practically the actual value of ϵ. The numerical example of such a test is shown in table 2.

Table 2. Loss of precision ϵ (in decimal digits) in K_A for $A = 2$, $l = 0$ and $\omega = \lambda = 1$.

		n_2	0		1		3
		n_1	0	5	2	5	3
n_2'	n_1'						
0	1		0	0	0	0	0
0	3		0	2	0	2	1
1	4		0	3	1	3	1
4	4		0	3	0	3	2

4. Concluding remarks

The applicability of our formula for K_A is not restricted to the Lippmann–Schwinger equation (2) or its connected-kernel descendants. That is, K_A also defines the kernel of the reference spectrum form of the Bethe–Goldstone equation in Brueckner theory,

$$Q\frac{1}{\omega + QTQ}Q - \frac{1}{\omega + T} = -\frac{1}{\omega + T}P\frac{1}{K_A}P\frac{1}{\omega + T} \tag{20}$$

where $A = 2$ and $P = 1 - Q$ denotes the so called Pauli projector and defines here the truncated oscillator subspace (cf also equation (4) of Znojil (1976)).

It is important that in the formula for K_A the transition to the many-body ($A > 1$) case is quite straightforward. Even the bad asymptotic behaviour of ψ in the oscillator basis may partially be improved, in analogy with the $A = 1$ case (Gareev *et al* 1977). Using the identity (2), i.e. the transformation

$$\psi \to -(\omega + T)^{-1}V\psi,$$

we replace the oscillator function $\tilde{R}_{nl}(r) = \langle r|nl\rangle = \mathrm{i}^{2n+l}\lambda^{-3/2}R_{nl}(r/\lambda)$ by its asymptotically correct modification

$$\begin{aligned}-\langle r|(\omega + T)^{-1}V_l(r)|nl\rangle &= K_{l+\frac{1}{2}}(\gamma r)\int_0^r \mathrm{d}\xi\,\xi^2 I_{l+\frac{1}{2}}(\gamma\xi)V_l(\xi)\tilde{R}_{nl}(\xi) \\ &\quad + I_{l+\frac{1}{2}}(\gamma r)\int_r^\infty \mathrm{d}\xi\,\xi^2 K_{l+\frac{1}{2}}(\gamma\xi)V_l(\xi)\tilde{R}_{nl}(\xi).\end{aligned} \tag{21}$$

With the asymptotically well behaved MacDonald functions K and I and for $\gamma^2 = k_2^2 + k_3^2 + \ldots + k_A^2 + \omega$, this leads to the correct exponential asymptotic behaviour in the coordinate $r = r_1$.

Appendix. Properties of the continued fractions

(i) Let us assume that the recurrence relations (4) are initialised by the arbitrary value α_N for sufficiently large N. Then, after a few applications of (4), the value of α_{N-k}, $k \gg 1$, $N \gg k$ becomes independent of α_N. This may be shown most easily by putting $\alpha_{m+1} = 1 - A_{m+1}$. Then the recurrence (4) has the form of the rational mapping

$$y = \frac{a + bx}{c + dx} \qquad b > 0,\ c > 0,\ d > 0 \tag{A.1}$$

with

$$a = a_m = \omega/m \qquad b = b_m = 1 + \beta/m$$
$$c = c_m = 1 + \omega/m \qquad d = d_m = 1 + \beta/m \tag{A.2}$$

and $x = A_{m+2}$, $y = A_{m+1}$, and it becomes roughly independent of the index m for a sufficiently large value $m \gg 1$. A repeated application of (A.1) gives A_{N-k} approaching zero from below. The practical consequence of this is the numerical stability of the algorithm represented by the recurrence (4) with arbitrary initialisation.

(ii) A more detailed investigation of the values of α_m for large m must take into account the changes of m. Again, we may consider (4) as mapping (A.1). For $4a > -(c-b)^2/d$, it may be proved that the fixed point $\bar{x}$ of this mapping is given by the plus-sign root

$$\bar{x} = \frac{2a}{c - b + [(c-b)^2 + 4ad]^{1/2}} \tag{A.3}$$

of the corresponding quadratic equation. With the exact values of the parameters (A.2) we thus get

$$\bar{x} = \bar{A}_m^{(1)} = \frac{2\omega}{\omega - \beta + [(\omega + \beta)^2 + 4\omega m]^{1/2}}. \tag{A.4}$$

Of course, due to the changes of m in the repeated use of (4) the approximation $A_{m+1} \simeq \bar{A}_m^{(1)}$ may be used for $m \gg 1$ only. Nevertheless, the leading-order term gives $\alpha_{m+1} \simeq 1 - (\omega/m)^{1/2}$ and implies the convergence of the infinite sum (3).

(iii) The preceding procedure (subtracting the fixed-point approximation) may be repeated by putting $A_{m+1} = A_{m+1}^{(1)} = \bar{A}_m^{(1)} + A_{m+1}^{(2)}$ and in general

$$A_{m+1}^{(k)} = \bar{A}_m^{(k)} + A_{m+1}^{(k+1)} \qquad k = 1, 2, \ldots. \tag{A.5}$$

In the $(k+1)$th step, the mapping $x = A_{m+2}^{(k+1)} \to y = A_{m+1}^{(k+1)}$ has the form (A.1) again and the fixed point $\bar{A}_m^{(k+1)}$ exists and is given by (A.3). The corresponding parameters

$$\begin{aligned} a &= a_m^{(k+1)} = -(\bar{A}_m^{(k)} - \bar{A}_{m+1}^{(k)})(b_m^{(k)} - d_m^{(1)} A_m^{(k)}) \\ b &= b_m^{(k+1)} = b_m^{(k)} - d_m^{(1)} \bar{A}_{m+1}^{(k)} \\ c &= c_m^{(k+1)} = c_m^{(k)} + d_m^{(1)} \bar{A}_{m+1}^{(k)} \\ d &= d_m^{(k+1)} = d_m^{(k)} = d_m^{(1)} \end{aligned} \tag{A.6}$$

where $k = 1, 2, \ldots$ are defined in the recurrent way from the initialisation (A.2) ($k = 1$). For $m \gg 1$, the leading term of $\bar{A}_m^{(k)}$ behaves like $m^{-k/2}$ for $k \geqslant 1$. This may be proved from explicit formulae for $k = 1$ and 2, and then using the smallness of $\bar{A}_m^{(k)} - \bar{A}_{m+1}^{(k)} = O(m^{-(k+1)/2})$ for all $k \geqslant 3$. In this way we obtain an alternative representation

$$\alpha_{m+1} = 1 - \bar{A}_m^{(1)} - \bar{A}_m^{(2)} - \bar{A}_m^{(3)} - \ldots \tag{A.7}$$

of our continued fraction as an infinite series.

(iv) In table 1 a few examples are shown. We observe an acceleration of convergence and a monotonous decrease of $z(\omega) = \alpha_{J+1}$ ($J = 3$) with increasing of $\lambda\omega$. The numerical stability is illustrated by the 'mad' initialisation $\alpha_N = 20$. The tabulated deviation $\delta = \alpha_4$ (evaluated) $- \alpha_4$ (exact) considered as a function of the initialisation α_N is monotonous and has a zero in the interval (0, 1). Because of this, and because of the changing sign of $\bar{A}^{(k)} \sim (-1)^k$, the sequence of partial sums of (A.7) (including the trivial pair 0 and 1) generates the lower and upper bounds of α_{J+1} and represents an extremely useful initialisation for (4). For example, for $\lambda\omega = 0{\cdot}1$ and $\alpha_{30} = 0$ (simple truncation) table 1 shows that the value α_4 (evaluated) $= \alpha_4$(exact) $+ \delta = 0{\cdot}56060 - 55 \times 10^{-5} = 0{\cdot}56005$ is lower than the exact value by 0·1% while for $\alpha_{60} = 0$ (double cut-off) or $\alpha_{30} = 1 - \bar{A}_{30}^{(1)}$ (improved initialisation) this error is reduced by an order of magnitude.

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