Comment on an alternative to the resonating group method

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This comment refers to a recent work by Raphael, Tandy, and Tobocman. The danger of incorporating cluster approximation in many-body Lippmann-Schwinger equations is emphasized. A certain type of antisymmetrization of Lippmann-Schwinger equations may lead to continuum spurious spectra. In particular it is pointed out that the cluster model equations introduced by these authors have highly suppressed (unphysical) incoming and outgoing waves. Contrary to claims made by these authors, it is stressed that Lippmann's identity is true.

[NUCLEAR REACTIONS Many-body Lippmann-Schwinger equations; cluster model of Raphael, Tandy, and Tobocman; spurious continuum spectra.]

The success of the resonating group method[1] (RGM) confirms the existence of cluster structure in nuclei. One may try to incorporate the physical ideas of the cluster model in an exact many-body formulation. It is shown that certain types of many-body Lippmann-Schwinger equations are not suitable for this purpose. Such approximations may suppress mathematical mechanisms for the rearrangement processes. This then leads to highly reduced wave functions and weak effective intercluster potentials. Secondly we would like to exhibit a new type of continuous spurious spectrum in addition to the more familiar discrete one[2] which may arise in a certain unconnected version of antisymmetrized many-body Lippmann-Schwinger equations. We demonstrate these in connection with a recent work by Raphael, Tandy, and Tobocman (RTT).[3] RTT proposed an alternative to the RGM, which looks attractive since the intercluster interactions of RTT are energy independent in contrast to energy dependent effective interactions in the RGM. Working with the scattering wave function, we arrive at the final equation for the scattering amplitude of RTT. This alternative approach shows in a transparent way the problems one encounters incorporating cluster approximations in the formulation of RTT.

We adopt the notation of RTT without further explanation. We denote two-body fragmentation channels by a and indistinguishable partitions in a channel by $\alpha(j)$, $j=1,2,\ldots,N_a$. Let us consider energetically the lowest two-body fragmentation channel such as $n-\alpha, \alpha-\alpha$ in five or eight nucleon systems, below the threshold for another channel. The scattering states to an initial partition $\alpha(j)$, defined by $\psi_{a(j)}=\lim_{\epsilon\to 0} i\epsilon G\Phi_{a(j)}$, obey the basic set of the Lippmann-Schwinger equations[4].

$$|\psi_{a(j)}\rangle = |\Phi_{a(j)}\rangle\delta_{jk} + G_{\alpha(k)}V_{\alpha(k)}|\psi_{a(j)}\rangle, \quad k=1,2,\ldots,N_a, \tag{1}$$

where $\Phi_{a(j)}$ satisfies $(E-H_{\alpha(j)})\Phi_{a(j)}=0$.

The fully antisymmetric state $\psi^{(a)}$ defined by[3]

$$|\psi^{(a)}\rangle = \sum_{j=1}^{N_a}(-1)^{\sigma_{\alpha(j)}}P_\alpha(j)\,|\psi_{a(1)}\rangle \equiv \mathcal{A}_{\alpha(1)}|\psi_{a(1)}\rangle \tag{2}$$

satisfies the set of N_a Lippmann-Schwinger equations

$$|\psi^{(a)}\rangle = \Phi_{a(j)} + G_{\alpha(j)}V_{\alpha(j)}|\psi^{(a)}\rangle, \quad j=1,2,\ldots,N_a. \tag{3}$$

Because of Eq. (1), one obviously needs all Lippmann-Schwinger equations (3) in order to exclude the states $\psi_{a(j)}$ which are not fully antisymmetrized. The set (3) can be the starting point for various formulations. Firstly, one may decompose $\psi^{(a)}$ into Yakubovski components and set up Yakubovski equations.[5] Secondly, one may keep the full $\psi^{(a)}$, introducing dummy variables, and arrive at a coupled set of equations, as demonstrated by Sandhas[5] for distinguishable particles. In both cases the other sets, corresponding to different two-body fragmentations (even if energetically closed), have to be included. Thereby, the kernel gets highly complicated, containing resolvent operators corresponding to various subclusters. The coupling scheme will show up

in specific distributions of particle variables, as has been demonstrated explicitly for three particles.[4] Clearly the number of coupled unknown functions involved can be extremely large. Instead one may, similar to the procedure applied by Tobocman[6] to the transition operators, average the set (3) for the state $\psi^{(a)}$ over all partitions and arrive at one equation,

$$|\psi^{(a)}\rangle = \frac{1}{N_a}\mathcal{G}_{\alpha(1)}\Phi_{a(1)} + \frac{1}{N_a}\mathcal{G}_{\alpha(1)}G_{\alpha(1)}V_{\alpha(1)}|\psi^{(a)}\rangle . \tag{4}$$

Obviously Eq. (4), by its very construction, excludes the nonantisymmetric states. However, Eq. (4) now may have spurious solutions of a new type, which we exhibit explicitly. The homogeneous problem corresponding to Eq. (4) can be factorized in the following manner [we set $(-1)^{\sigma_{\alpha(j)}}=1$ by a suitable choice of $P_\alpha(j)$]:

$$\left(1-\frac{1}{N_a}\sum_{j=1}^{N_a}G_{\alpha(j)}V_{\alpha(j)}\right)=\frac{1}{N_a}\left(\sum_j G_{\alpha(j)}\right)(E-H) . \tag{5}$$

Thus spurious solutions will be defined by[2]

$$\sum_j G_{\alpha(j)}\Theta = 0 \tag{6}$$

or

$$\left(1+\frac{1}{N_a}\sum_j G_{\alpha(j)}V^{\alpha(j)}\right)\tilde{\theta}=0 , \tag{7}$$

where $\tilde{\theta}=G_0\Theta$. We decompose as $\tilde{\theta}=\sum_j\tilde{\theta}_{\alpha(j)}$, where the $\tilde{\theta}_j$'s are defined by

$$\tilde{\theta}_{\alpha(j)} = -\frac{1}{N_a}G_{\alpha(j)}V^{\alpha(j)}\tilde{\theta} . \tag{8}$$

Equation (8) can be rewritten as

$$\left(1+\frac{1}{N_a}G_{\alpha(j)}V^{\alpha(j)}\right)\tilde{\theta}_{\alpha(j)} = -\frac{1}{N_a}G_{\alpha(j)}V^{\alpha(j)}\sum_{i\neq j}\tilde{\theta}_{\alpha(i)} . \tag{9}$$

For the sake of simplicity we now consider a three-body system; then Eq. (9) becomes

$$(1+\tfrac{1}{3}G_{\alpha(j)}V^{\alpha(j)})\,\tilde{\theta}_{\alpha(j)} = -\tfrac{1}{3}G_{\alpha(j)}V^{\alpha(j)}\sum_{i\neq j}\tilde{\theta}_{\alpha(i)} . \tag{10}$$

As with the derivation of the Faddeev equation, we solve Eq. (10) for $\tilde{\theta}_{\alpha(j)}$ and get

$$\tilde{\theta}_{\alpha(j)} = \tilde{\theta}^{\,0}_{\alpha(j)} - (G^{-1}_{\alpha(j)}+\tfrac{1}{3}V^{\alpha(j)})^{-1}\tfrac{1}{3}V^{\alpha(j)} \times\sum_{i\neq j}\tilde{\theta}_{\alpha(i)} , \tag{11}$$

where $\tilde{\theta}^{\,0}_{\alpha(j)}$ satisfies

$$(G_0^{-1}-\tfrac{2}{3}V^{\alpha(j)})\tilde{\theta}^{\,0}_{\alpha(j)}=0 . \tag{12}$$

Introducing the two-body t matrix $t^{\alpha(j)}_{(2/3)}$, defined by

$$(G_0^{-1}-\tfrac{2}{3}V^{\alpha(j)})^{-1}\tfrac{2}{3}V^{\alpha(j)} = G_0 t^{\alpha(j)}_{(2/3)} , \tag{13}$$

Eq. (11) can be rewritten as

$$\tilde{\theta}_{\alpha(j)} = \tilde{\theta}^{\,0}_{\alpha(j)} - \tfrac{1}{2}G_0 t^{\alpha(j)}_{(2/3)}\sum_{i\neq j}\tilde{\theta}_{\alpha(i)} . \tag{14}$$

Equation (14) is the Faddeev type equation and defines spurious continuum states whenever $\tilde{\theta}^{\,0}_{\alpha(j)}$ exists. The function $\tilde{\theta}^{\,0}_{\alpha(j)}$ is a plane wave of relative motion of the two clusters which, however, have a smaller binding energy due to the reduced intracluster interaction $\frac{2}{3}V^{\alpha(j)}$. Thus, one gets continuous spurious solutions starting at the spurious threshold above the physical one defined by the reduced binding energies. In addition one has, of course, a discrete spectrum of spurious solutions corresponding to the homogeneous problem.

Thus Eq. (4) has highly undesirable features which are not unexpected since the full physical information enforces "blowing up"[5] and not shrinking. However, one may now introduce the cluster approximation for $G_{\alpha(j)}$,

$$G_{\alpha(j)} = |\phi_{\alpha(j)})\mathcal{G}_{\alpha(j)}\,(\phi_{\alpha(j)}| \tag{15}$$

[which is the same as Eq. (19) of RTT], and one gets

$$|\psi^{(a)}\rangle = \frac{1}{N_a}\mathcal{G}_{\alpha(1)}\Phi_{a(1)} + \frac{1}{N_a}\mathcal{G}_{\alpha(1)}|\phi_{\alpha(1)})\,\mathcal{G}_{\alpha(1)}(\phi_{\alpha(1)}|\,V_{\alpha(1)}|\psi^{(a)}\rangle . \tag{16}$$

Here $\mathcal{G}_{\alpha(j)}$ is the free propagator for the relative motion of two clusters. $\phi_{\alpha(j)}$ in round brackets describes the internal motion of two fragments. Equation (16) shows that the kernel is now connected and $\psi^{(a)}$ has the structure

$$|\psi^{(a)}\rangle = \mathcal{G}_{\alpha(1)}|\phi_{\alpha(1)}\chi(1)\rangle . \tag{17}$$

Here $\chi(1)$ describes the relative motion of the two clusters in the partition $\alpha(1)$ and depends on the intercluster distance. Equations (16) and (17) yield the following equation for χ:

$$\chi(1) = \frac{1}{N_a}\chi^0(1) + \frac{1}{N_a}\mathcal{G}_{\alpha(1)}(\phi_{\alpha(1)}|\,V_{\alpha(1)}\mathcal{G}_{\alpha(1)}|\phi_{\alpha(1)}\chi(1)\rangle , \tag{18}$$

where χ^0 is a plane wave of relative motion of the two fragments. First of all we note that in Eq.

(18) the spurious threshold has disappeared and it is free from continuous spuriosities. This is welcome. However, the cluster approximation also suppressed parts of the physical wave function. Equation (4) appears to contain an incoming wave Φ in the partition channel $\alpha(j)$ only with strength $1/N_a$. This, however, is not true. It is well known[7] that the second term on the right-hand side of Eq. (4) will contribute the remaining strength $(N_a-1)/N_a$ of the incoming wave $\Phi_{\alpha(j)}$. This is possible because of the continuous parts in the spectral representation of the resolvent operators $G_{\alpha(j)}$. After cluster approximation, the continuous parts are excluded and the passage of rearrangement parts $\alpha(k)$ of the wave function through the resolvent $G_{\alpha(j)}$, $j\neq k$ is forbidden. The kernel of Eq. (18) allows only outgoing waves and the asymptotic behavior of $\psi^{(a)}$ is reduced from amplitudes of strength 1 to amplitudes of strength $1/N_a$. By continuity, this reduces $\psi^{(a)}$ or χ also in the interior region and thus leads to a much too small T matrix and intercluster effective interactions.

In order to demonstrate this explicitly we use Eq. (18) to write the equation for the antisymmetrized transition amplitude [Eq. (24) of RTT]. We define the T matrix by

$$T(\vec{k},\vec{k}_0)\equiv\langle\phi_{\alpha(1)}\vec{k}|\,V_{\alpha(1)}\mathcal{A}_{\alpha(1)}|\,\phi_{\alpha(1)}\chi(1)\rangle\,, \quad (19)$$

where $\vec{k}_0$ is the initial momentum. Using Eq. (19) in Eq. (18), we get

$$T(\vec{k},\vec{k}_0)=\frac{1}{N_a}U(\vec{k},\vec{k}_0)+\frac{1}{N_a}\int d\vec{k}'U(\vec{k},\vec{k}')\frac{1}{k_0^2-k'^2+i\epsilon}T(\vec{k}',\vec{k}_0)\,, \quad (20)$$

where we take $\hbar=2m_\alpha=1$, where m_α is the reduced mass between the fragments. The effective interaction U is defined by

$$U(\vec{k},\vec{k}')=\langle\phi_{\alpha(1)}\vec{k}\,|\,V_{\alpha(1)}\mathcal{A}_{\alpha(1)}|\,\phi_{\alpha(1)}\vec{k}'\rangle\,. \quad (21)$$

Equation (20) is the same as Eq. (62) of RTT. Equation (20) has a nice and attractive appearance as the antisymmetrization is fully incorporated and the potential energy is energy independent. However, the potential is much too weak due to the factor $1/N_a$. This has been noted by RTT in a numerical study of dineutron-dineutron scattering where it gave much too small a cross section. They, therefore, *discarded that equation.* Instead, they proposed an equation where the driving term was modified. We would like to show now that in doing so RTT were in fact inconsistent within their own formulation and Eq. (20) should have resulted. For the sake of clarity and simplicity, we confine ourselves to three particles and adopt the notation $\alpha(j)\equiv j$, thus $\phi_{\alpha(j)}\equiv\phi_j$, $V_{\alpha(j)}\equiv V_j$, etc. Equation (22) of RTT for the antisymmetrized transition amplitude is

$$T_\alpha=\tfrac{1}{3}V_1\mathcal{A}_1G_1\mathcal{A}_1G_1^{-1}+\tfrac{1}{3}V_1\mathcal{A}_1G_1T_\alpha\,. \quad (22)$$

Again Eq. (22) is not connected and it may have spuriosities too, as we have seen in the context of Eq. (4), since it results also from an averaging process. After cluster approximation one gets from Eq. (22)

$$T(\vec{k},\vec{k}_0)=Z(\vec{k},\vec{k}_0)+\int d\vec{k}'\frac{U(\vec{k},\vec{k}')}{3}\left(\frac{1}{k_0^2-k'^2+i\epsilon}\right)\times T(\vec{k}',\vec{k}_0), \quad (23)$$

with

$$Z(\vec{k},\vec{k}_0)=\langle\phi_1\vec{k}|\,\tfrac{1}{3}V_1\mathcal{A}_1G_1\mathcal{A}_1G_1^{-1}|\,\phi_1\vec{k}_0\rangle\,. \quad (24)$$

Using the well established Lippmann identity

$$G_kG_1^{-1}|\,\phi_1\vec{k}_0\rangle=\delta_{k1}|\,\phi_1\vec{k}_0\rangle\,, \quad (25)$$

the driving term is given by

$$Z(\vec{k},\vec{k}_0)=\tfrac{1}{3}\langle\phi_1\vec{k}|\,V_1\mathcal{A}_1|\,\phi_1\vec{k}_0\rangle=\tfrac{1}{3}U(\vec{k},\vec{k}_0)\,. \quad (26)$$

Thus from Eq. (23) one arrives at

$$T=\frac{1}{N_a}U+\frac{1}{N_a}U\mathcal{G}T\,,\quad N_a=3 \quad (27)$$

which has also been given in RTT [Eq. (62)].

Equation (27), which is the correct consequence of Eq. (22) and the cluster approximation, has been discarded, however, by RTT due to the smallness of the interaction. Instead they claim that Eq. (25) is not valid. RTT calculate Z in the following different manner. Obviously one may rewrite Z as [Eq. (27) of RTT]

$$Z(\vec{k},\vec{k}_0)=\langle\phi_1\vec{k}|\,V_1\mathcal{A}_1|\,\phi_1\vec{k}_0\rangle+\tfrac{1}{3}\langle\phi_1\vec{k}|\,V_1\mathcal{A}_1G_1[\mathcal{A}_1,V_1]|\,\phi_1\vec{k}_0\rangle\,. \quad (28)$$

First we note that $\langle\theta|\equiv\langle\phi_1\vec{k}|\,V_1\mathcal{A}_1$ is a square integrable function where all the variables are confined to a finite region of space. Then by obvious cancellations and making use of

$$\mathcal{A}_1|\,\phi_1\vec{k}_0\rangle=|\,\phi_1\vec{k}_0\rangle+|\,\phi_2\vec{k}_0\rangle+|\,\phi_3\vec{k}_0\rangle\,,$$

we get

$$\langle\theta|G_1[\mathcal{A}_1,V_1]|\,\phi_1\vec{k}_0\rangle=\langle\theta|G_1V^1|\,\phi_2\vec{k}_0\rangle-\langle\theta|G_1V^2|\,\phi_2\vec{k}_0\rangle+\langle\theta|G_1V^1|\,\phi_3\vec{k}_0\rangle-\langle\theta|G_1V^3|\,\phi_3\vec{k}_0\rangle\,. \quad (29)$$

Using the resolvent identity, we have

$$\langle\theta|G_1V^2|\,\phi_2\vec{k}_0\rangle=\langle\theta|G_0V^2|\,\phi_2\vec{k}_0\rangle+\langle\theta|\{G_1V^1G_0\}V^2|\,\phi_2\vec{k}_0\rangle\,. \quad (30)$$

Two comments are now in order. With the cluster approximation, the first term

$$\langle\theta|G_0V^2|\phi_2\vec{k}_0\rangle=\langle\theta|\phi_2\vec{k}_0\rangle$$

is absent, which allows the passage of $|\phi_2\vec{k}_0\rangle$ through G_0 contained in G_1. This is a necessary requirement for the mathematical formulation which should not be destroyed by any approximation whatsoever. Secondly, the curly brackets indicate the order of integration in the manifold integral, which should not be changed in general. As is shown in Ref. 7 one can calculate the second term on the right-hand side of Eq. (30) as

$$\begin{aligned}\langle\theta|\{G_1V^1G_0\}V^2|\phi_2\vec{k}_0\rangle&=\langle\theta|G_1V^1\{G_0V^2|\phi_2\vec{k}_0\rangle\}\\&+\langle\theta|(G_1-G_0)V^2|\phi_2\vec{k}_0\rangle-\langle\theta|G_1V^1|\phi_2\vec{k}_0\rangle\\&=\langle\theta|G_1V^1|\phi_2\vec{k}_0\rangle-\langle\theta|G_1\vec{H}_0|\phi_2\vec{k}_0\rangle.\end{aligned}\quad(31)$$

Here $\vec{H}_0=\vec{H}_0-\overleftarrow{H}_0$, where the arrows on the operator of kinetic energy H_0 denote differentiation to the right of left, respectively. Since θ is square integrable and does not allow the variables $\vec{x}$ in $G_1(\vec{x},\vec{x}')$ to go to infinity, the surface integral at infinity which results after using the Gauss theorem to evaluate H_0 (Ref. 7) will vanish. This is because $G_1(\vec{x},\vec{x}')$ for x' at infinity will have the asymptotic form of a breakup behavior, whereas $|\phi_2\vec{k}_0\rangle$ has the form of a two-body fragmentation.[7] Thus from Eqs. (28) to (31) we get

$$\langle\theta|G_1[\mathcal{A}_1,V_1]|\phi_1\vec{k}_0\rangle=-\langle\theta|\phi_2\vec{k}_0\rangle-\langle\theta|\phi_3\vec{k}_0\rangle\quad(32)$$

and

$$\begin{aligned}Z(\vec{k},\vec{k}_0)&=\langle\phi_1\vec{k}|V_1\mathcal{A}_1|\phi_1\vec{k}_0\rangle\\&-\tfrac{1}{3}\langle\phi_1\vec{k}|V_1\mathcal{A}_1|\phi_2\vec{k}_0\rangle-\tfrac{1}{3}\langle\phi_1\vec{k}|V_1\mathcal{A}_1|\phi_3\vec{k}_0\rangle\\&=\tfrac{1}{3}\langle\phi_1\vec{k}|V_1\mathcal{A}_1|\phi_1\vec{k}_0\rangle=\tfrac{1}{3}U(\vec{k},\vec{k}_0),\end{aligned}\quad(33)$$

which is in agreement with Eq. (26).

RTT, however, evaluated the second term on the right-hand side of Eq. (28) using again the cluster approximation [see Eq. (A9) of Appendix of RTT] and could not therefore find the correct result. Ironically, the resulting Z got larger, and thus the cross section, which led them to "conclude" that Eq. (25), is not valid.

According to the arguments presented and the numerical results of RTT, we conclude that the cluster approximation applied to Eq. (4) for the wave function or to Eq. (22) for the antisymmetrized transition operator is not adequate. Though it eliminates continuous spuriosities, it also suppresses the main part (N_a can be large) of the wave function or the effective intercluster potential and thus leads to a "not acceptable" poor approximation of the cross section.

Another defect of all these equations in the single cluster approximation—Eq. (20) or (27) [Eq. (62) or Eq. (24) of RTT] and Eq. (20) of RTT—is that the kernels of all these equations are too weak because of the presence of the factors $(N_a)^{-1}$ in them. This is also related to the wrong asymptotic behavior of Eq. (18). The kernel of RGM [Eq. (16) of RTT] does not have this undesirable feature. So in any practical calculation, when N_a is large, the full solution of the equations proposed in RTT will be nearly equal to their Born approximations. RTT did not notice this defect in their numerical calculation because the full solution of their problem was nearly equal to their Born approximation and hence their result agreed approximately with that of RGM. This is clear from a comparison of Figs. 1 and 3 of RTT.

This undesirable feature also shows up if one distributes particle variables in the Lippmann-Schwinger equation. We exemplify that for the simplest case of three particles, where the information of the set (3) of $N_a=3$ equations can be summarized as[4]

$$\psi^{(a)}_{(123)}=\Phi(123)+G_1V^2\psi^{(a)}_{(231)}+G_1V^3\psi^{(a)}_{(312)}.\quad(34)$$

This equation defines the fully antisymmetric state uniquely and is free from spuriosity. This can be proved immediately by operating with $(1-G_0V^1)$ from the left, which yields

$$\psi^{(a)}_{(123)}=G_0V^1\psi^{(a)}_{(123)}+G_0V^2\psi^{(a)}_{(231)}+G_0V^3\psi^{(a)}_{(312)}.\quad(35)$$

By cyclic permutation we conclude that

$$\psi^{(a)}_{(123)}=\psi^{(a)}_{(231)}=\psi^{(a)}_{(312)},\quad(36)$$

which shows that Eq. (34) in fact defines the antisymmetric solution of the Schrödinger equation. Clearly, this coupling scheme corresponds to the Faddeev-Lovelace choice and the proof of uniqueness is just the one given by Sandhas.[5] Equation (34) therefore appears to be a better starting point than the averaged Eq. (4), which is not connected and, in addition, is spurious. However, with respect to cluster approximation, it is as bad as Eq. (4). After that approximation, the kernel no longer allows the occurrence of channel states $\Phi(231)$ and $\Phi(312)$ and only ingoing and outgoing waves of the channel state $\Phi(123)$ are present. Thus two asymptotic partitions are eliminated completely and one survives with the strength 1 for one partition, whereas the cluster approximation in Eq. (4) reduces all three asymptotic partitions to strengths $\frac{1}{3}$.

Moreover, the cluster approximation to Eq.

(34) has been studied in a bound state problem in comparison with the solution to the full problem.[8] It turned out that again the continuum part of the resolvent operator G_1 was very important and the restriction to the bound state part gave only a poor approximation.

Finally we note that the cluster approximation does not cause these undesirable features if applied for the Faddeev components for 3 particles, where each component carries only one type of asymptotic partition. Thereby at least the strength of the asymptotic amplitude is not reduced.

We conclude that the many-body Lippmann-Schwinger equations studies are not suitable for cluster approximations and the Lippmann identity, which has been questioned by RTT, is correct.

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