Separable Representations of Two-Body Interactions*

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Consideration is given to the approximation in which an arbitrary potential is replaced by a separable potential. A method is presented which permits the construction of a rank-N separable potential which has the property that the resulting T matrix is exact on the energy shell and half off the energy shell at N selected bound state and/or continuum energies. This construction yields a T matrix that is correct off the energy shell in the vicinity of the N on-shell points.

I. INTRODUCTION

We begin by defining the T matrix in the angular momentum decomposition, $t(\omega)$, for an arbitrary two-body potential V, through the operator equation,

$$t = V + VG_0(\omega)t\,, \tag{1.1}$$

with

$$G_0(\omega) = (\omega - h_0)^{-1}\,. \tag{1.2}$$

Here h_0 is the kinetic energy operator. We may put $\omega = E + i\epsilon$ if we desire the solution appropriate to the outgoing wave boundary condition for the Lippmann-Schwinger equation (we use units with $\hbar^2 = 2m = 1$ and thus $E = k^2$), viz.,

$$|\psi^{(+)}_{E,k}\rangle = |k\rangle + G_0^{(+)}(E)V|\psi^{(+)}_{E,k}\rangle\,. \tag{1.3}$$

Equation (1.1) also has the formal solution,

$$t(\omega) = V + V\mathcal{G}(\omega)V\,, \tag{1.4}$$

with

$$\mathcal{G}(\omega) = (\omega - H)^{-1}\,, \tag{1.5}$$

and

$$H = h_0 + V\,. \tag{1.6}$$

It is well known that in the vicinity of a bound state pole at $\omega = -\epsilon_B$, with bound state wave function $|\psi_B\rangle$, we may write,

$$t(\omega) \simeq \frac{V|\psi_B\rangle\langle\psi_B|V}{\omega + \epsilon_B}\,. \tag{1.7}$$

Further it is easy to see that the separable potential,

$$V_{\rm sep} = V|\psi_B\rangle\lambda\langle\psi_B|V\,, \tag{1.8}$$

will give rise to a T matrix with a pole at $\omega = -\epsilon_B$, (and the appropriate residue) if λ is chosen as

$$\begin{aligned}(1/\lambda) &= \langle\psi_B|VG_0(-\epsilon_B)V|\psi_B\rangle \\ &= \langle\psi_B|V|\psi_B\rangle\,.\end{aligned} \tag{1.9}$$

It is obvious that we have used the equation,

$$|\psi_B\rangle = G_0(-\epsilon_B)V|\psi_B\rangle\,, \tag{1.10}$$

to obtain Eq. (1.9).

Indeed with λ^{-1} given by Eq. (1.9), the T matrix for $V_{\rm sep}$, $\hat{t}(\omega)$, is

$$\hat{t}(\omega) = \frac{V|\psi_B\rangle\langle\psi_B|V}{\lambda^{-1} - \langle\psi_B|VG_0(\omega)V|\psi_B\rangle} \tag{1.11}$$

$$= \frac{V|\psi_B\rangle\langle\psi_B|V}{\langle\psi_B|V[G_0(-\epsilon_B) - G_0(\omega)]V|\psi_B\rangle} \tag{1.12}$$

$$= \frac{V|\psi_B\rangle\langle\psi_B|V}{\langle\psi_B|[V - VG_0(\omega)V]|\psi_B\rangle}\,. \tag{1.13}$$

The quantity,

$$D(\omega) = \langle\psi_B|[V - VG_0(\omega)V]|\psi_B\rangle\,, \tag{1.14}$$

has the property

$$\lim D(\omega) = (\omega + \epsilon_B)\,, \quad \omega \to -\epsilon_B\,. \tag{1.15}$$

We may also define the *form factors*

$$\begin{aligned}|g_B\rangle &= V|\psi_B\rangle \\ &= G_0^{-1}(-\epsilon_B)|\psi_B\rangle \\ &= -(\epsilon_B + h_0)|\psi_B\rangle\,,\end{aligned} \tag{1.16}$$

and rewrite Eq. (1.12) as

$$\hat{t}(\omega) = \frac{|g_B\rangle\langle g_B|}{\langle g_B|[G_0(-\epsilon_B) - G_0(\omega)]|g_B\rangle}\,. \tag{1.17}$$

The separable representation given above has been designated in the literature as the unitary pole approximation (UPA).[1] This approximation has been studied for singlet and triplet nucleon-nucleon interactions.[2] Further, the UPA provides the first term of a more general expansion, the unitary pole expansion,[3] whose accuracy has also been checked numerically.

Because the separable representation of two-body interactions is so useful particularly in the solution of the three-body problem, it is important to understand how one may achieve an optimal

representation of a *realistic* interaction in terms of separable interactions of low rank. The method we develop here is capable of dealing with two-body potentials which are of a general nature and which may have any number of bound states or resonances.

II. SEPARABLE REPRESENTATION

We pose the problem as to whether we can find a rank-one separable potential for which the eigenfunction of the corresponding Hamiltonian is identical to the eigenfunction of the original Hamiltonian, Eq. (1.6). This can be accomplished at one value of the energy parameter. Let us define a separable potential $\mathcal{U}$ as

$$\mathcal{U}=|v\rangle\lambda\langle v|\,. \tag{2.1}$$

The outgoing-wave eigenfunction, $|\phi^{(+)}_{E,k_E}\rangle$, of $H=h_0+\mathcal{U}$ satisfies the Lippmann-Schwinger equation

$$|\phi^{(+)}_{E,k_E}\rangle=|k_E\rangle+\lambda G_0^{(+)}(E)|v\rangle\langle v|\phi^{(+)}_{E,k_E}\rangle\,, \tag{2.2}$$

where $k_E^2=E$. For such a separable potential Eq. (2.2) has the solution

$$|\phi^{(+)}_{E,k_E}\rangle=|k_E\rangle+\frac{\lambda G_0^{(+)}(E)|v\rangle\langle v|k_E\rangle}{1-\lambda\langle v|G_0^{(+)}(E)|v\rangle}\,. \tag{2.3}$$

The outgoing-wave eigenfunction, $|\psi^{(+)}_{E,k_E}\rangle$, of the Hamiltonian $H=h_0+V$ is given by

$$|\psi^{(+)}_{E,k_E}\rangle=|k_E\rangle+G_0^{(+)}(E)V|\psi^{(+)}_{E,k_E}\rangle\,. \tag{2.4}$$

If $|\phi^{(+)}_{E,k_E}\rangle$ and $|\psi^{(+)}_{E,k_E}\rangle$ are to be identical, then comparing Eqs. (2.3) and (2.4), we see that we must have

$$G_0^{(+)}(E)V|\psi^{(+)}_{E,k_E}\rangle=G_0^{(+)}(E)|v\rangle\,. \tag{2.5}$$

This equality need only hold to within a multiplicative constant, which we can set equal to unity without loss of generality. We can achieve the equality given in Eq. (2.5) if we choose $|v\rangle$ to be

$$|v\rangle=V|\psi^{(+)}_{E,k_E}\rangle\,. \tag{2.6}$$

With this choice of $|v\rangle$ it becomes possible to equate Eqs. (2.3) and (2.4), so as to determine λ. We find immediately that

$$1=\frac{\lambda\langle\psi^{(+)}_{E,k_E}|V|k_E\rangle}{1-\lambda\langle\psi^{(+)}_{E,k_E}|VG_0^{(+)}(E)V|\psi^{(+)}_{E,k_E}\rangle}\,, \tag{2.7}$$

or

$$\begin{aligned}(1/\lambda)&=\langle\psi^{(+)}_{E,k_E}|V|k_E\rangle+\langle\psi^{(+)}_{E,k_E}|VG_0^{(+)}(E)V|\psi^{(+)}_{E,k_E}\rangle\\&=\langle\psi^{(+)}_{E,k_E}|V|\psi^{(+)}_{E,k_E}\rangle\,.\end{aligned} \tag{2.8}$$

Thus we have obtained a solution to the problem posed, viz.,

$$\mathcal{U}=V|\psi^{(+)}_{E,k_E}\rangle(\langle\psi^{(+)}_{E,k_E}|V|\psi^{(+)}_{E,k_E}\rangle)^{-1}\langle\psi^{(+)}_{E,k_E}|V\,. \tag{2.9}$$

Although we have derived this result for a single positive energy, it is evident that this result holds equally well for a bound state, and in that case yields the unitary pole approximation discussed in Sec. I.

If we wish to reproduce the wave function at a number of different energies, E_n, we may easily generalize the above procedure. The result is

$$\mathcal{U}=\sum_{i,j}V|\psi_i\rangle\langle\psi_i|M|\psi_j\rangle\langle\psi_j|V\,, \tag{2.10}$$

where $|\psi_i\rangle$ stands for $|\psi^{(+)}_{E_i,k_{Ei}}\rangle$ or $|\psi_{B_i}\rangle$ and the matrix M is defined by the relation

$$\delta_{ik}=\sum_j\langle\psi_i|M|\psi_j\rangle\langle\psi_j|V|\psi_k\rangle=\sum_j\langle\psi_i|V|\psi_j\rangle\langle\psi_j|M|\psi_k\rangle\,. \tag{2.11}$$

At the energy E_n, $|\psi_n\rangle$ is an eigenstate of both $\mathcal{H}=h_0+\mathcal{U}$ and $H=h_0+V$, since obviously

$$\mathcal{U}|\psi_n\rangle=V|\psi_n\rangle\,, \tag{2.12}$$

and

$$\langle\psi_n|\mathcal{U}=\langle\psi_n|V\,. \tag{2.13}$$

Thus the two half-shell T matrices, $\langle p|t(E_n)|k_{E_n}\rangle$ and $\langle p|\hat{t}(E_n)|k_{E_n}\rangle$ are clearly equal. If we diagonalize the Hermitian matrix M by means of a unitary transformation U, we then find that

$$\mathcal{U}=\sum_i V|\hat{\psi}_i\rangle\langle\hat{\psi}_i|M|\hat{\psi}_i\rangle\langle\hat{\psi}_i|V\,, \tag{2.14}$$

where

$$|\hat{\psi}_i\rangle=\sum_j U_{ij}|\psi_j\rangle\,. \tag{2.15}$$

Thus if we define λ_i to be

$$\lambda_i\equiv\langle\hat{\psi}_i|M|\hat{\psi}_i\rangle \tag{2.16}$$

and

$$|v_i\rangle\equiv V|\hat{\psi}_i\rangle\,, \tag{2.17}$$

we may rewrite Eq. (2.14) as

$$\mathcal{U}=\sum_i|v_i\rangle\lambda_i\langle v_i|\,. \tag{2.18}$$

For the interaction given by Eq. (2.14), or equivalently, Eq. (2.18), the wave function $|\phi^{(+)}_{E,k_E}\rangle$ is given by

$$|\phi^{(+)}_{E,k_E}\rangle=|k_E\rangle+G_0^{(+)}(E)\sum_{i,j}|v_i\rangle\Gamma_{ij}(E)\langle v_j|k_E\rangle \tag{2.19}$$

and the corresponding T matrix is given by

$$\langle p|\hat{t}(E)|k\rangle=\sum_{i,j}\langle p|v_i\rangle\Gamma_{ij}(E)\langle v_j|k\rangle\,, \tag{2.20}$$

where $\Gamma_{ij}(E)$ is defined by the relation

$$\sum_j\Gamma_{ij}(E)\langle\psi_j|[V-VG_0^{(+)}(E)V]|\psi_k\rangle=\delta_{ik}\,. \tag{2.21}$$

In the case where $\mathcal{U}$ is taken to be of rank one,

Eqs. (2.19)–(2.21) reduce to

$$|\phi^{(+)}_{E,k_E}\rangle = |k_E\rangle + \frac{G_0^{(+)}(E)V|\psi^{(+)}_{E_1,k_{E1}}\rangle\langle\psi^{(+)}_{E_1,k_{E1}}|V|k_E\rangle}{\langle\psi^{(+)}_{E_1,k_{E1}}|[V-VG_0^{(+)}(E)V]|\psi^{(+)}_{E_1,k_{E1}}\rangle} \tag{2.22}$$

and

$$\langle p|\hat{t}(E)|k\rangle = \frac{\langle p|V|\psi^{(+)}_{E_1,k_{E1}}\rangle\langle\psi^{(+)}_{E_1,k_{E1}}|V|k\rangle}{\langle\psi^{(+)}_{E_1,k_{E1}}|[V-VG_0^{(+)}(E)V]|\psi^{(+)}_{E_1,k_{E1}}\rangle} . \tag{2.23}$$

The procedure outlined above thus allows one to find a separable potential of rank N, which reproduces the exact wave functions at N predetermined energies.

III. EXPANSION OF AN OPERATOR IN TERMS OF A COMPLETE ORTHONORMAL SET OF STATES

The considerations of the previous sections suggest that it may prove profitable to discuss the expansion of a general operator in terms of a complete orthonormal set of state vectors. We postulate a discrete set of orthonormal states $\{|N\rangle\}$ which are complete in the Hilbert space under discussion. An operator $\mathcal{A}$ may be expressed in terms of these states as

$$\mathcal{A} = \sum_{N,M} |N\rangle\langle N|\mathcal{A}|M\rangle\langle M| . \tag{3.1}$$

We now consider a subspace of the full Hilbert space, spanned by a finite subset of the states $\{|N\rangle\}$. We indicate this set of states as $\{|\nu\rangle\}$, and the subspace they define as $\mathcal{H}_p$. From these states we may construct a projection operator p, which projects onto $\mathcal{H}_p$. We write p explicitly as

$$p = \sum_{\nu} |\nu\rangle\langle\nu| . \tag{3.2}$$

We also define the complementary projection operator q, by the relation

$$p+q = 1 . \tag{3.3}$$

In the usual way, we may approximate $\mathcal{A}$ by truncating the series in Eq. (3.1). If $\mathcal{A}$ is Hermitian and we wish the approximate operator to be Hermitian, then we must truncate the left and right series in the same way. Thus we write

$$\mathcal{A}_{T(p)} = \sum_{\nu,\mu} |\nu\rangle\langle\nu|\mathcal{A}|\mu\rangle\langle\mu| , \tag{3.4}$$

or

$$\mathcal{A}_{T(p)} = p\mathcal{A}p . \tag{3.5}$$

Clearly, matrix elements of $\mathcal{A}$ and $\mathcal{A}_{T(p)}$ between states in $\mathcal{H}_p$ will be identical, i.e.,

$$\langle\mu|\mathcal{A}_{T(p)}|\nu\rangle = \langle\mu|\mathcal{A}|\nu\rangle . \tag{3.6}$$

However, all other matrix elements of $\mathcal{A}_{T(p)}$ vanish.

At this point it is instructuve to rewrite the identity, Eq. (3.5) as

$$\mathcal{A}_{T(p)} = p\mathcal{A}p = (p\mathcal{A}p)(p\mathcal{A}p)^{-1}(p\mathcal{A}p) , \tag{3.7}$$

where $(p\mathcal{A}p)^{-1}$ is defined so that

$$(p\mathcal{A}p)^{-1}(p\mathcal{A}p) = (p\mathcal{A}p)(p\mathcal{A}p)^{-1} = p . \tag{3.8}$$

We must now, of course, further restrict ourselves to operators $\mathcal{A}$ and states $|\nu\rangle$ such that $(p\mathcal{A}p)^{-1}$ exists. From Eq. (3.7), it is easy to see that we can construct another approximation to $\mathcal{A}$,

$$\mathcal{A}_{X(p)} = \mathcal{A}p(p\mathcal{A}p)^{-1}p\mathcal{A} . \tag{3.9}$$

Clearly $\mathcal{A}_{X(p)}$, and $\mathcal{A}_{T(p)}$ share the property that

$$p\mathcal{A}_{X(p)}p = p\mathcal{A}_{T(p)}p = p\mathcal{A}p . \tag{3.10}$$

However, the operator $\mathcal{A}_{X(p)}$ has the further property that

$$p\mathcal{A}_{X(p)}q = p\mathcal{A}q \tag{3.11}$$

and

$$q\mathcal{A}_{X(p)}p = q\mathcal{A}p , \tag{3.12}$$

whereas

$$p\mathcal{A}_{T(p)}q = q\mathcal{A}_{T(p)}p = 0 . \tag{3.13}$$

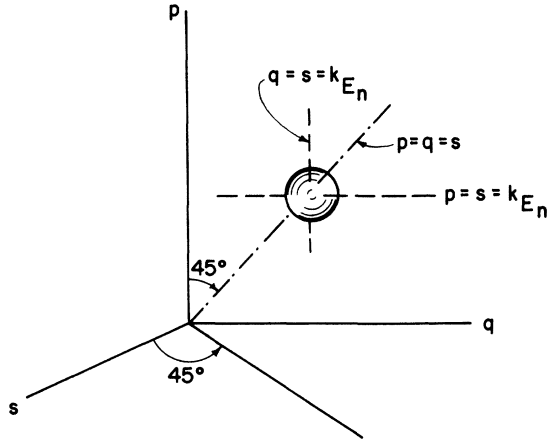

FIG. 1. The s, q, p space represented as a three-dimensional Euclidian space in which the s, q, p axes are taken to be orthogonal. The lines $p=s=k_{E_n}$ and $q=s=k_{E_n}$ are the lines along which the T matrix, $\langle p|t(s^2)|q\rangle$, is given exactly by the separable approximation under discussion. These are, of course, the "half-shell" lines. The line $p=q=s$ is the "on-shell" line. The shaded volume around the point $s=p=q=k_{E_n}$ is the region around the completely on-shell point for which the difference between the separable approximation and the exact result is negligible.

Thus $\mathcal{A}_{X(p)}$ has the property that

$$p\mathcal{A}_{X(p)} = p\mathcal{A} \tag{3.14}$$

and

$$\mathcal{A}_{X(p)}\, p = \mathcal{A} p\,. \tag{3.15}$$

Of course, both $\mathcal{A}_{X(p)}$ and $\mathcal{A}_{T(p)}$ share the property that in the limit $p = 1$,

$$\mathcal{A}_{X(1)} = \mathcal{A}_{T(1)} = \mathcal{A}\,. \tag{3.16}$$

An interesting insight into this construction may be obtained by taking the operator $\mathcal{A}$ to be separable, i.e., we assume

$$\mathcal{A} = |a\rangle\langle a|\,. \tag{3.17}$$

The choice

$$p = |\eta\rangle\langle\eta| \tag{3.18}$$

then yields

$$\mathcal{A}_{X(p)} = |a\rangle\langle a| = \mathcal{A}\,, \tag{3.19}$$

for any choice of $|\eta\rangle$ such that $\langle a|\eta\rangle \neq 0$. On the other hand $\mathcal{A}_{T(p)}$ would be

$$\mathcal{A}_{T(p)} = |\eta\rangle\langle\eta|\mathcal{A}|\eta\rangle\langle\eta|\,, \tag{3.20}$$

which would reproduce $\mathcal{A}$ only if $|\eta\rangle = |a\rangle$.

The connection of these remarks with the result of the previous sections must by now be self evident. If we take $\mathcal{H}_p$ to be the space spanned by the N-state vectors $[|\psi_i\rangle]$ of the previous section[4] and further choose $\mathcal{A}$ to be the potential operator V, then we see that

$$\mathcal{U} = V_{X(p)} = Vp(pVp)^{-1}pV\,. \tag{3.21}$$

Now since

$$\mathcal{U}p = Vp\,, \tag{3.22}$$

it follows immediately that

$$\langle k|\mathcal{U}|\psi_i\rangle = \langle k|V|\psi_i\rangle = \langle k|t(E_i)|k_{E_i}\rangle \tag{3.23}$$

and hence both V and $\mathcal{U}$ have identical half-shell matrix elements at the energies E_i. It follows trivially from the Lippmann-Schwinger equation that the wave functions $\langle r|\psi_i\rangle \equiv \langle r|\psi^{(+)}_{E_i,k_{Ei}}\rangle$ must also then be identical since

$$|\psi^{(+)}_{E,k_E}\rangle = |k_E\rangle + \int G_0^{(+)}(E)|k\rangle\, dk \langle k|t(E)|k_E\rangle\,. \tag{3.24}$$

IV. OFF-SHELL CONSIDERATIONS

We have seen that at the energies E_n, corresponding to the states $|\psi^{(+)}_{E_n k_{En}}\rangle$ used to construct $\mathcal{U}$, the half-off-shell T matrix, $\langle p|t(E_n)|k_{E_n}\rangle$, is reproduced exactly by $\mathcal{U}$. One may use the effective-range formula to generate the first term in an expansion of the fully on-shell T matrix about the energy E_n. The effective range formula[5] for the lth partial wave may be expressed as

$$\frac{d}{dk^2}\left[k^{2l+1}\cot\delta(k)\right]\Big|_{k=k_{En}} \equiv \tfrac{1}{2}\rho(k_{E_n}) = \int_0^R \left[\bar{\psi}_{E_n,k_{En}}{}^2(r) - \psi_{E_n,k_{En}}{}^2(r) - u^2(k_{E_n},r)\right] dr + \tfrac{1}{2}\hat{\rho}(k_{E_n},R)\,. \tag{4.1}$$

Here $\bar{\psi}_{E_n,k_{En}}(r)$ is the asymptotic form of $\psi_{E_n,k_{En}}(r) \equiv \langle r|\psi_{E_n,k_{En}}\rangle$ continued in to the origin, viz.,

$$\bar{\psi}_{E_n,k_{En}}(r) = k^l_{E_n}(k_{E_n}r)\left[\cot\delta(k_{E_n})\, j_l(k_{E_n}r) - n_l(k_{E_n}r)\right], \tag{4.2}$$

with $j_l(kr)$ and $n_l(kr)$ the usual spherical Bessel functions and $u(kr) \equiv k^l(kr)n_l(kr)$. Also, $\hat{\rho}(k,R)$ is given by

$$\tfrac{1}{2}\hat{\rho}(k,R) = \lim_{\bar{k}\to k}\left\{[k^2-\bar{k}^2]^{-1}\left[u(\bar{k},R)\frac{d}{dR}u(k,R) - u(k,R)\frac{d}{dR}u(\bar{k},R)\right]\right\}.$$

Since $\psi_{E_n,k_{En}}(r)$ is a solution for both potentials V and $\mathcal{U}$, $\rho(k_{E_n})$ is identical for both potentials. Thus the derivative of the fully on-shell T matrix $\hat{t}(E_n)$ is correct.

The three-dimensional space associated with the three variables of the fully off-shell T matrix, $\langle p|t(s^2)|q\rangle$, is depicted in Fig. 1. At the center of the shaded volume is the point $p = s = q = k_{E_n}$, where E_n is the energy of one of the states $|\psi^{(+)}_{E_n,k_{En}}\rangle$ used in Eq. (3.18) to construct the separable potential $\mathcal{U}$. Since $\mathcal{U}$ produces the exact half-off-shell T matrices, $\langle p|t(E_n)|k_{E_n}\rangle$ and $\langle k_{E_n}|t(E_n)|q\rangle$, the use of $\mathcal{U}$ in place of V is exact along the dashed lines $p = s = k_{E_n}$ and $q = s = k_{E_n}$. Further, Eq. (4.1) demonstrates that the rate of change of t along the on-shell line $p = q = s$ is also given correctly by $\mathcal{U}$. Thus, we know that $\mathcal{U}$ correctly produces the first terms in an expansion of $\langle p|t(s^2)|q\rangle$ about the fully on-shell point in three linearly independent, but not "orthogonal," directions (i.e., along the three lines, $p = s = k_{E_n}$, $q = s = k_{E_n}$, and $p = q = s$). We may write an expansion in the three "orthogonal" variables, p, q, and s, of the function $\tau(p,q;s^2)$ defined by

$$\tau(p,q{:}s^2) = s^{2l+1}\cot\delta(s)\left(\frac{s}{p}\right)^l\left(\frac{s}{q}\right)^l\frac{\langle p|t(s^2)|q\rangle}{\langle s|t(s^2)|s\rangle}\,. \tag{4.3}$$

One can, of course, equally well expand $\langle p|t(s^2)|q\rangle$ instead of $\tau(p,q;s^2)$, but the result for τ is consider-

ably simpler. The leading terms in an expansion of τ are

$$\tau(p,q;s^2)=k_{E_n}^{2l+1}\cot\delta(k_{E_n})+(p^2-k_{E_n}{}^2)\frac{\partial}{\partial p^2}\tau(p,k_{E_n};k_{E_n}{}^2)|_{p=k_{En}}+(q^2-k_{E_n}{}^2)\frac{\partial}{\partial q^2}\tau(k_{E_n},q;k_{E_n}{}^2)|_{q=k_{En}}$$
$$+(s^2-k_{E_n}{}^2)\frac{\partial}{\partial s^2}\tau(k_{E_n},k_{E_n};s^2)|_{s=k_{En}}, \tag{4.4}$$

where we have made use of the fact that $\tau(p,q;s^2)$ is a function[6] of p^2 and q^2. The derivatives with respect to p^2 and q^2 are derivatives of the half-shell T matrices which are given correctly by $\mathfrak{V}$. These derivatives may be written in terms of the wave functions $\psi_{E_n,k_{En}}(r)$ by[7]

$$\frac{\partial}{\partial p^2}\tau(p,k_{E_n};k_{E_n}{}^2)=\frac{\partial}{\partial q^2}\tau(k_{E_n},q;k_{E_n}{}^2)\equiv\bar\rho(k_{E_n})/2=k_{E_n}^{l}\cot\delta(k_{E_n})\int_0^\infty dr(k_{E_n}r)j_l(k_{E_n}r)[\psi_{E_n,k_{En}}(r)-\bar\psi_{E_n,k_{En}}(r)]. \tag{4.5}$$

The term involving the derivative with respect to s^2 can be written in terms of Eqs. (4.1) and (4.5) by using

$$\frac{d}{ds^2}\tau(s,s;s^2)|_{s=kEn}=\frac{\partial}{\partial p^2}\tau(p,k_{E_n};k_{E_n}{}^2)|_{p=k_{En}}+\frac{\partial}{\partial q^2}\tau(k_{E_n},q;k_{E_n}{}^2)|_{q=k_{En}}+\frac{\partial}{\partial s^2}\tau(k_{E_n},k_{E_n};s^2)|_{s=k_{En}}. \tag{4.6}$$

This gives for the leading terms in the expansion of $\tau(p,q;s^2)$

$$\tau(p,q;s^2)\cong k_{E_n}^{2l+1}\cot\delta(k_{E_n})+\tfrac{1}{2}(p^2+q^2-2k_{E_n}{}^2)\bar\rho(k_{E_n})+\tfrac{1}{2}(s^2-k_{E_n}{}^2)[\rho(k_{E_n})-2\bar\rho(k_{E_n})], \tag{4.7}$$

where $\rho(k_{E_n})$ and $\bar\rho(k_{E_n})$ are given in terms of $\psi_{E_n,k_{En}}(r)$ in Eqs. (4.1) and (4.5).

This is the complete generalization of the effective range theory, as it gives the expansion of the fully off-shell T matrix in terms of the wave function at one energy. Since $\mathfrak{V}$ correctly reproduces the wave function at the energy E_n, it correctly reproduces the fully off-shell T matrix in the region near k_{E_n} [the shaded volume in Fig. (1)] where Eq. (4.7) is valid.

As the half-off-shell T matrix can be written $\langle k|V|\psi^{(+)}_{E_n,k_{En}}\rangle$, it is clear that the knowledge of the wave function $|\psi^{(+)}_{E_n,k_{En}}\rangle$ is equivalent to the knowledge of the half-off-shell T matrix. We may write the fully off-shell T matrix in terms of the wave function defined by

$$\langle p|t(s^2)|k\rangle=\langle p|V|\psi^{(+)}_{s^2,k}\rangle. \tag{4.8}$$

From the equation for $|\psi^{(+)}_{s^2,k}\rangle$ in momentum space,

$$\langle p|\psi^{(+)}_{s^2,k}\rangle=|k\rangle+(s^2-p^2+i\eta)^{-1}\langle p|t(s^2)|k\rangle, \tag{4.9}$$

we see that the expansion of $\langle p|t(s^2)|k\rangle$ in Eq. (4.7) also gives an expansion of the "Bethe-Goldstone" wave function $\langle p|\psi^{(+)}_{s^2,k}\rangle$ in a region of momentum space centered about $p=s=k=k_{E_n}$.

The Kowalski-Noyes[8] representation of the fully off-shell T matrix follows immediately from the formula for the scattering from the sum of two potentials and the use of the potential $\mathfrak{V}$. If we define the wave operator Ω as

$$\Omega^{(+)}(s^2)=1+\mathcal{G}^{(+)}(s^2)V, \tag{4.10}$$

we have

$$|\psi^{(+)}_{s^2,k}\rangle=|k\rangle+\mathcal{G}^{(+)}(s^2)V|k\rangle=\Omega^{(+)}(s^2)|k\rangle \tag{4.11}$$

for the off-shell wave function. In terms of the wave operator, $\Omega^{(+)}_{\rm sep}(s^2)$, for the separable potential, defined by

$$\Omega^{(+)}_{\rm sep}(s^2)=1+(s^2-h_0-\mathfrak{V}+i\eta)^{-1}\mathfrak{V}, \tag{4.12}$$

$\Omega^{(+)}(s^2)$ is given by

$$\Omega^{(+)}(s^2)=\Omega^{(+)}_{\rm sep}(s^2)+(s^2-h_0-\mathfrak{V}+i\eta)^{-1}(V-\mathfrak{V})\Omega^{(+)}(s^2), \tag{4.13}$$

which yields for the fully off-shell T matrix with s^2 equal to E_n,

$$\langle p|t(E_n)|q\rangle=\langle p|\hat t(E_n)|q\rangle+\langle p|\Omega^{(-)\dagger}_{\rm sep}(E_n)[V-\mathfrak{V}]\Omega^{(+)}(E_n)|q\rangle. \tag{4.14}$$

For $\mathfrak{V}$ taken to be of the form of a separable potential of rank one, $\langle p|\hat t(E_n)|q\rangle$ is given by Eq. (2.23) to be

$$\langle p|\hat t(E_n)|q\rangle=\frac{\langle p|V|\psi^{(+)}_{E_n,k_{En}}\rangle\langle\psi^{(+)}_{E_n,k_{En}}|V|q\rangle}{\langle\psi^{(+)}_{E_n,k_{En}}|V-V[1/(E_n-h_0+i\eta)]V|\psi^{(+)}_{E_n,k_{En}}\rangle}. \tag{4.15}$$

Now we note that

$$\langle\psi^{(+)}_{E_n,k_{En}}\Big|V-V\frac{1}{k_{E_n}{}^2-h_0+i\eta}V\Big|\psi^{(+)}_{E_n,k_{En}}\rangle=\langle\psi^{(+)}_{E_n,k_{En}}|V\Big[1-\frac{1}{k_{E_n}{}^2-h_0+i\eta}V\Big]|\psi^{(+)}_{E_n,k_{En}}\rangle$$

$$=\langle\psi^{(+)}_{E_n,k_{En}}|V|k_{E_n}\rangle=\langle k_{E_n}|t(E_n)|k_{E_n}\rangle^*\,, \tag{4.16}$$

so that

$$\langle p|\hat{t}\,(E_n)|\,q\rangle=\frac{\langle p|t(E_n)|k_{E_n}\rangle\langle k_{E_n}|t(E_n)|\,q\rangle^*}{\langle k_{E_n}|t(E_n)|k_{E_n}\rangle^*}. \tag{4.17}$$

Thus in terms of the real off-shell factor defined by

$$F(k_{E_n},q)=\langle k_{E_n}|t(E_n)|\,q\rangle/\langle k_{E_n}|t(E_n)|k_{E_n}\rangle\,, \tag{4.18}$$

the fully off-shell T matrix, Eq. (4.14), becomes

$$\langle p|t(E_n)|\,q\rangle=F(k_{E_n},p)\langle k_{E_n}|t(E_n)|k_{E_n}\rangle F(k_{E_n},q)+R(p,k_{E_n},q)\,. \tag{4.19}$$

This is just the Kowalski-Noyes[8] decomposition of the fully off-shell T matrix, which here follows simply from the scattering from the sum of two potentials, $\mathcal{U}$ and $V-\mathcal{U}$. The remainder term is given by

$$R(p,k_{E_n},q)=\langle p|\Omega^{(-)\dagger}_{\rm sep}(E_n)[V-\mathcal{U}]\Omega^{(+)}(E_n)|\,q\rangle\,, \tag{4.20}$$

from which it is clear that $R(p,k_{E_n},q)=0$ if either $p=k_{E_n}$ or $q=k_{E_n}$.

The use of more than one wave function in the construction of $\mathcal{U}$ will, of course, yield correctly the factorable term in Eq. (4.14) plus an approximation to the remainder term, $R(p,k_{E_n},q)$. Because one expects the factorable term in Eq. (4.14) to dominate the remainder term near a resonance, an appealing choice of the functions would be to choose them at the real energies where resonances occur. There does not exist, however, any simple quantitative criterion[9] to estimate the region where the factorable term does dominate. One might choose the states to construct $\mathcal{U}$ as those which are solutions to the Lippmann-Schwinger equation at the complex energies where the on-shell T matrix is singular.[10] The use of eigenstates at real energies, as suggested here, has the advantage that one does not have to solve the auxiliary problem of locating poles in the complex plane and solving the Lippmann-Schwinger equation at these energies. Also, if the poles of the T matrix are quite far from the real axis, the use of a single function on the real axis might be able to include the effects of several of these singularities over an extended energy region.

An alternate choice for the states used to construct $\mathcal{U}$ could be the eigenstates of the kernel operator $\mathcal{K}(E)=G_0^{(+)}(E)V$, i.e.,

$$G_0^{(+)}(E)V|\,\mathfrak{N}_i(E)\rangle=\mathfrak{N}_i(E)|\,\mathfrak{N}_i(E)\rangle\,, \tag{4.21}$$

where $|\,\mathfrak{N}_i(E)\rangle$ is regular at the origin and a purely outgoing wave at infinity. Weinberg[11] has noted that the Born series is divergent at any energy E where there exists an eigenstate with eigenvalue $|\,\mathfrak{N}_i(E)|\geq 1$. He has therefore suggested that one construct the separable potential $Vp(pVp)^{-1}pV$ by choosing p to be that space spanned by those states $|\,\mathfrak{N}_i(E)\rangle$ whose eigenvalues have magnitude greater than 1. The wave function $|\psi^{(+)}_{E,k_E}\rangle$ is the solution of the integral equation

$$|\psi^{(+)}_{E,k_E}\rangle=|\phi^{(+)}_{E,k_E}\rangle+\bar{\mathcal{G}}^{(+)}(E)[V-\mathcal{U}]|\psi^{(+)}_{E,k_E}\rangle\,, \tag{4.22}$$

with

$$[h_0+\mathcal{U}]|\phi^{(+)}_{E,k_E}\rangle=E|\phi^{(+)}_{E,k_E}\rangle \tag{4.23}$$

and

$$\bar{\mathcal{G}}^{(+)}(E)=(E-h_0-\mathcal{U}+i\eta)^{-1}\,. \tag{4.24}$$

The Born series which arises from iterating equation (4.22) will now be convergent, since the states $|\,\mathfrak{N}_i(E)\rangle$ are now eigenstates of the new kernel with eigenvalue zero, i.e.,

$$\bar{\mathcal{G}}^{(+)}(E)[V-\mathcal{U}]|\,\mathfrak{N}_i(E)\rangle=0\,. \tag{4.25}$$

The states $|\,\mathfrak{N}_i(E)\rangle$ are inconvenient because they depend on E, the energy at which one is solving the problem. It has been noted,[12] however, that the use of an energy-independent state which is similar in appearance to $|\,\mathfrak{N}_i(E)\rangle$ can be used to construct $\mathcal{U}$ and that this will lead to considerable improvement in the convergence of the Born series. The point is only that insofar as $\mathcal{U}=Vp(pVp)^{-1}pV$ is a good representation of $\mathcal{U}$, then $(V-\mathcal{U})$ may be expected to be a weak interaction for which the Born series may converge.

APPENDIX

Here we provide an alternate derivation of the separable T matrix given in Eq. (2.20). We begin

with the Lippmann-Schwinger equation,

$$|\psi^{(+)}_{E,k_E}\rangle = |k_E\rangle + G_0^{(+)}(E)V|\psi^{(+)}_{E,k_E}\rangle\,, \tag{A1}$$

and multiply this equation by V, to obtain

$$V|\psi^{(+)}_{E,k_E}\rangle = V|k_E\rangle + VG_0^{(+)}(E)V|\psi^{(+)}_{E,k_E}\rangle\,. \tag{A2}$$

We now replace $(V|\psi^{(+)}_{E,k_E}\rangle)$ by the truncated expansion

$$(V|\psi^{(+)}_{E,k_E}\rangle) = \sum_{i=1}^{N} a_i(E)V|\psi_i\rangle\,, \tag{A3}$$

where the $|\psi_i\rangle$ are such that

$$H|\psi_i\rangle = E_i|\psi_i\rangle\,. \tag{A4}$$

We may then obtain the coefficients $a_i(E)$ from the relation

$$\sum_{i=1}^{N} \langle\psi_j|V - VG_0^{(+)}(E)V|\psi_i\rangle a_i(E) = \langle\psi_j|V|k_E\rangle\,. \tag{A5}$$

Thus, we may solve for the coefficients $a_i(E)$. The result is

$$a_i(E) = \sum_j \langle\psi_i|\,F(E)|\psi_j\rangle\langle\psi_j|V|k_E\rangle\,, \tag{A6}$$

where $F(E)$ is given by

$$\sum_j \langle\psi_i|\,F(E)|\psi_j\rangle\langle\psi_j|[V - VG_0^{(+)}(E)V]|\psi_k\rangle = \delta_{ik}\,. \tag{A7}$$

The half-shell T matrix is, in this approximation,

$$\begin{aligned}\langle k'|t(E)|k_E\rangle &= \langle k'|V|\psi^{(+)}_{E,k_E}\rangle \\ &\simeq \sum_{i=1}\langle k'|V|\psi_i\rangle a_i(E) \\ &= \sum_{j,k}\langle k'|V|\psi_j\rangle\langle\psi_j|\,F(E)|\psi_k\rangle\langle\psi_k|V|k_E\rangle \\ &\equiv \langle k'|\hat{t}(E)|k_E\rangle\,. \end{aligned} \tag{A8}$$

We have thus shown that the expansion, Eq. (A3), is equivalent to the use of the separable potential $\mathcal{U}$.

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