

Separable representations of T matrices valid in the vicinity of off-shell points*

D. J. Ernst, C. M. Shakin, and R. M. Thaler

Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106

(Received 11 July 1973)

The method developed in a previous paper for the construction of separable representations for T matrices is extended. It is shown that the separable representation we propose is valid in the vicinity of specified off-shell points. Since the off-shell points considered include those with arbitrary negative-energy parameters, the method presented here should be of value for the bound-state three-body problem.

I. SEPARABLE REPRESENTATIONS IN A NONORTHONORMAL BASIS

Following our previous study,¹ we consider the rank- N separable potential

$$\mathfrak{U} = VP(PVP)^{-1(P)}PV, \quad (1.1)$$

where P is a projection operator onto a space spanned by a finite set of functions.² Previously we considered the set of N functions $\{|\psi_{k_i^2, k_i}\rangle, |\psi_B\rangle\}$. For the purposes of this work we wish to extend our definitions of the space spanned by P to include the functions³ $\{|\psi_{k_i^2, k_i}\rangle, |\psi_B\rangle, |\psi_{s_j^2, k_j}\rangle\}$. The new feature⁴ in this discussion is the inclusion of the off-shell functions $|\psi_{s_j^2, k_j}\rangle$. These off-shell state vectors are neither mutually orthogonal nor orthogonal to the mutually orthogonal states

$$\{|\psi_{k_i^2, k_i}\rangle, |\psi_B\rangle\}.$$

Thus we must consider how to work with a non-orthogonal set of state vectors.

We have previously discussed the operator given in Eq. (1.1) in the case that P is a projection operator defined such that

$$P = \sum |\Phi_i\rangle\langle\Phi_i|, \quad (1.2)$$

where the state vectors $|\Phi_i\rangle$ are orthonormal. The operator $(PVP)^{-1(P)}$ was defined as an inverse in the subspace, i.e.,

$$(PVP)(PVP)^{-1(P)} = (PVP)^{-1(P)}(PVP) = P. \quad (1.3)$$

We now define an operator Π such that

$$\Pi = \sum |\phi_i\rangle\langle\phi_i|. \quad (1.4)$$

The operator Π is not necessarily a projection operator, since we do not require that the $|\phi_i\rangle$ be either orthogonal or normalized. We do, however, require that the $|\phi_i\rangle$ be linearly independent, and that the N states $|\phi_i\rangle$ span the same subspace

as do the N orthonormal states $|\Phi_i\rangle$.

We now wish to show that \mathfrak{U}' , defined as

$$\mathfrak{U}' = V\Pi(\Pi V\Pi)^{-1(P)}\Pi V, \quad (1.5)$$

is identical to the operator \mathfrak{U} defined in Eq. (1.1). Of course, the operator $(\Pi V\Pi)^{-1(P)}$ which appears in Eq. (1.5) is defined to be an inverse in the subspace, i.e.,

$$(\Pi V\Pi)^{-1(P)}(\Pi V\Pi) = (\Pi V\Pi)(\Pi V\Pi)^{-1(P)} = P. \quad (1.6)$$

The definition of Π implies that

$$\Pi = \Pi P = P\Pi = P\Pi P. \quad (1.7)$$

Thus Eq. (1.5) may be reexpressed as

$$\begin{aligned} \mathfrak{U}' &= (VP)(P\Pi P)\{(P\Pi P)(PVP)(P\Pi P)\}^{-1(P)}(P\Pi P)(PV) \\ &= VP(PVP)^{-1(P)}PV = \mathfrak{U}. \end{aligned} \quad (1.8)$$

In order to construct \mathfrak{U} from the relationship in Eq. (1.5), it is necessary to work in a basis which is not orthonormal. We define the matrix M by

$$(\Pi V\Pi)^{-1(P)} = \sum_{i,j} |\phi_i\rangle M_{ij} \langle\phi_j|, \quad (1.9)$$

and similarly define the matrix \tilde{M} by

$$\begin{aligned} \Pi(\Pi V\Pi)^{-1(P)}\Pi &= \sum_{i,j,k,l} |\phi_i\rangle \tilde{M}_{ij} \langle\phi_j| \\ &= \sum_{i,j,k,l} |\phi_k\rangle \langle\phi_k|\phi_i\rangle M_{ij} \langle\phi_j|\phi_l\rangle \langle\phi_l|. \end{aligned} \quad (1.10)$$

The definition of $(\Pi V\Pi)^{-1(P)}$, Eq. (1.6), may then be written as

$$\sum_{i,j,k,l} |\phi_i\rangle M_{ij} \langle\phi_j|\phi_k\rangle \langle\phi_k|V|\phi_l\rangle \langle\phi_l| = P. \quad (1.11)$$

Multiplication from the left by Π in Eq. (1.11)

gives

$$\begin{aligned} \sum_{i,j,k,l,p} |\phi_p\rangle \langle \phi_p | \phi_i\rangle M_{ij} \langle \phi_j | \phi_k\rangle \langle \phi_k | V | \phi_l\rangle \langle \phi_l | - \sum_p |\phi_p\rangle \langle \phi_p | \\ = \sum_{k,l,p} |\phi_p\rangle \bar{M}_{pk} \langle \phi_k | V | \phi_l\rangle \langle \phi_l | - \sum_p |\phi_p\rangle \langle \phi_p | = 0. \end{aligned} \quad (1.12)$$

Since the states $|\phi_i\rangle$ are linearly independent, it necessarily follows that

$$\sum_k \bar{M}_{pk} \langle \phi_k | V | \phi_l\rangle = \delta_{pl}. \quad (1.13)$$

The potential \mathbf{v} is then given by

$$\mathbf{v} = \sum_{ij} V | \phi_j\rangle \bar{M}_{ij} \langle \phi_j | V, \quad (1.14)$$

with \bar{M}_{ij} given by Eq. (1.13). Thus Eqs. (1.13) and (1.14) provide the explicit formulas necessary to construct \mathbf{v} for the case that the states $|\phi_i\rangle$ are neither normalized nor orthogonal.

It then immediately follows from Eq. (1.1) that

$$\mathbf{v} | \xi_i\rangle = V | \xi_i\rangle \quad (1.15)$$

and likewise

$$\langle \xi_i | \mathbf{v} = \langle \xi_i | V, \quad (1.16)$$

if $|\xi_i\rangle$ is a state vector in the subspace defined by P , i.e., if

$$| \xi_i\rangle = P | \xi_i\rangle. \quad (1.17)$$

Thus we have shown that any vector $|\xi_i\rangle$ in the subspace has the desired property given in Eqs. (1.9) and (1.10). We also note that even if the state vectors $|\phi_i\rangle$ are not normalizable this result holds provided only that the operator V is such that $\langle \phi_i | V | \phi_j\rangle$ exists.

II. SEPARABLE REPRESENTATIONS OF THE POTENTIAL OPERATOR

We now return to the problem posed at the beginning of Sec. I: We consider the set of N state vectors³ $\{|\psi_{k_i^2, k_i}\rangle, |\psi_B\rangle, |\psi_{s_j^2, k_j}\rangle\}$. It is useful to define the various solutions of the off-shell equation for \mathbf{v} ,

$$|\hat{\psi}_{s^2, k}^{(0)}\rangle = |k\rangle + G_0^{(0)}(s^2) \mathbf{v} |\hat{\psi}_{s^2, k}^{(0)}\rangle, \quad (2.1)$$

where the superscript zero identifies the principal value prescription. The corresponding K matrix $\hat{K}(s^2)$,

$$\langle p | \hat{K}(s^2) | q\rangle = \langle p | \mathbf{v} | \hat{\psi}_{s^2, q}^{(0)}\rangle, \quad (2.2)$$

satisfies

$$\hat{K}(s^2) = \mathbf{v} + \mathbf{v} G_0^{(0)}(s^2) \hat{K}(s^2). \quad (2.3)$$

It is now easily shown that

$$|\hat{\psi}_{s_j^2, k_j}^{(0)}\rangle = |\psi_{s_j^2, k_j}^{(0)}\rangle, \quad (2.4)$$

$$|\hat{\psi}_{k_i^2, k_i}^{(0)}\rangle = |\psi_{k_i^2, k_i}^{(0)}\rangle, \quad (2.5)$$

and

$$|\hat{\psi}_B\rangle = |\psi_B\rangle, \quad (2.6)$$

where the functions on the right of Eqs. (2.4)–(2.6) are those solutions which are used to define the P space. Therefore, it follows immediately from Eq. (1.1) that³

$$\langle p | \hat{K}(s_j^2) | k_j\rangle = \langle p | K(s_j^2) | k_j\rangle \quad (2.7)$$

and

$$\langle p | \hat{K}(k_i^2) | k_i\rangle = \langle p | K(k_i^2) | k_i\rangle. \quad (2.8)$$

It is clear, therefore, from the two-potential formula for K that

$$\begin{aligned} \langle p | K(s^2) | q\rangle &= \langle p | \mathbf{v} | \hat{\psi}_{s^2, q}^{(0)}\rangle + \langle \hat{\psi}_{s^2, p}^{(0)} | (V - \mathbf{v}) | \psi_{s^2, q}^{(0)}\rangle \\ &= \langle p | \hat{K}(s^2) | q\rangle + \langle p | R(s^2) | q\rangle. \end{aligned} \quad (2.9)$$

The symmetric function $\langle p | R(s^2) | q\rangle$ satisfies the relation

$$\langle p | R(s_j^2) | k_j\rangle = \langle p | R(k_i^2) | k_i\rangle = 0. \quad (2.10)$$

For simplicity let us consider a rank-one potential \mathbf{v} based on a single off-shell solution³ $|\psi_{s_j^2, k_j}^{(0)}\rangle$:

$$\mathbf{v} = \frac{V |\psi_{s_j^2, k_j}^{(0)}\rangle \langle \psi_{s_j^2, k_j}^{(0)} | V}{\langle \psi_{s_j^2, k_j}^{(0)} | V | \psi_{s_j^2, k_j}^{(0)}\rangle}. \quad (2.11)$$

The K matrix for this choice is found to be

$$\langle p | \hat{K}(s^2) | q\rangle = \frac{\langle p | V | \psi_{s_j^2, k_j}^{(0)}\rangle \langle \psi_{s_j^2, k_j}^{(0)} | V | q\rangle}{\langle \psi_{s_j^2, k_j}^{(0)} | V - V G_0^{(0)}(s^2) V | \psi_{s_j^2, k_j}^{(0)}\rangle} \quad (2.12)$$

For the case $s^2 < 0$, this expression also yields the T matrix

$$\langle p | \hat{t}(s^2) | q\rangle = \langle p | \mathbf{v} | \psi_{s^2, q}^{(+)}\rangle, \quad (2.13)$$

since in this case all the wave functions $|\psi_{s^2, q}^{(\pm)}\rangle$ and $|\psi_{s^2, q}^{(0)}\rangle$ are identical. For $s^2 > 0$ we may find $\hat{t}(s^2)$ from the standard relation between the T matrix and the K matrix.

One may also construct a separable potential \mathfrak{V} from the off-shell wave functions which satisfy outgoing boundary conditions $|\psi_{s_j^2, k_j}^{(+)}\rangle$. In this case, one would have³

$$\langle p | \hat{t}(s_j^2) | k_j \rangle = \langle p | t(s_j^2) | k_j \rangle, \quad (2.14)$$

i.e., the matrix \hat{t} would be equal to t along a single line in the (p, s, q) space. One finds, however, that $\langle k_j | \hat{t}(s_j^2) | q \rangle$ and $\langle k_j | t(s_j^2) | q \rangle$ are not necessarily equal. In the case of the K matrix this equality follows immediately from the Hermiticity of the K matrix. For the T matrix, the addi-

which define the P space, we have

$$\begin{aligned} \langle p | t(s_j^2) | k_j \rangle &= \langle p | K(s_j^2) | k_j \rangle - i \frac{1}{2} \pi \frac{\langle p | K(s_j^2) | s_j \rangle s_j \langle s_j | K(s_j^2) | k_j \rangle}{1 - i \frac{1}{2} \pi s_j \langle s_j | K(s_j^2) | s_j \rangle} \\ &= \langle p | \hat{K}(s_j^2) | k_j \rangle - i \frac{1}{2} \pi \frac{\langle p | \hat{K}(s_j^2) | s_j \rangle s_j \langle s_j | \hat{K}(s_j^2) | k_j \rangle}{1 - i \frac{1}{2} \pi s_j \langle s_j | \hat{K}(s_j^2) | s_j \rangle} \\ &= \langle p | \hat{t}(s_j^2) | k_j \rangle, \end{aligned} \quad (2.15)$$

and similarly

$$\langle k_j | t(s_j^2) | q \rangle = \langle k_j | \hat{t}(s_j^2) | q \rangle. \quad (2.16)$$

Equivalently, we may define the P space through the functions $|\psi_{s_j^2, k_j}^{(+)}\rangle$ and $|\psi_{s_j^2, k_j}^{(-)}\rangle$ to obtain the relations given in Eqs. (2.15) and (2.16).

III. CONCLUSIONS

We have shown how to construct a *separable* potential \mathfrak{V} from the potential V , such that at N points in the (p, q, s) space the K matrix (or the T matrix) for \mathfrak{V} and the K matrix (T matrix) for V are identical. These N points are given by $s = s_j$, $p = q = k_j$. These points may be either off-shell points ($s_j \neq k_j$) or on-shell points ($s_j = k_j$). Furthermore, we have seen that this construction necessarily has the further property that

$$\langle p | \hat{K}(s_j) | k_j \rangle = \langle p | K(s_j) | k_j \rangle \quad (3.1)$$

and

$$\langle k_j | \hat{K}(s_j) | q \rangle = \langle k_j | K(s_j) | q \rangle. \quad (3.2)$$

Thus we see that the K matrix (T matrix) for \mathfrak{V} and the K matrix (T matrix) for V are identical on two intersecting lines, intersecting at the point $s = s_j$, $p = q = k_j$. This implies that at the point $s = s_j$, $p = q = k_j$ any derivative in the plane given by the intersection of the two lines referred to above must be the same for K and \hat{K} . Now it is also clear that the derivatives

$$\left. \frac{\partial}{\partial s} \langle k_j | \hat{K}(s) | k_j \rangle \right|_{s=s_j} = \left. \frac{\partial}{\partial s} \langle k_j | K(s) | k_j \rangle \right|_{s=s_j} \quad (3.3)$$

must be equal as well if Eqs. (3.1) and (3.2) obtain.

tional equality can be achieved if one also includes in the P space the functions $|\psi_{s_j^2, k_j}^{(-)}\rangle$. In our previous work¹ where only on-shell wave functions $|\psi_{k_i^2, k_i}^{(+)}\rangle$ were employed this point did not arise. This is because in that case we may generate the P space with the set of functions $\{|\psi_{k_i^2, k_i}^{(+)}\rangle\}$ or $\{|\psi_{k_i^2, k_i}^{(-)}\rangle\}$ or $\{|\psi_{k_i^2, k_i}^{(0)}\rangle\}$, since these functions are not linearly independent.

It is, perhaps, important to note that the relationship between t and K is such that the identity $\langle q | \hat{K}(s_j^2) | k_j \rangle = \langle q | K(s_j^2) | k_j \rangle$ does not imply $\langle q | \hat{t}(s_j^2) | k_j \rangle = \langle q | t(s_j^2) | k_j \rangle$. If however, we include both $|\psi_{s_j^2, k_j}^{(0)}\rangle$ and $|\psi_{k_j^2, k_j}^{(0)}\rangle$ among the states

This is very easy to prove.

However, we shall not pursue this argument because this is but a special case of the generalized effective range expansion which will be discussed elsewhere. The derivative in any direction at the point $s = s_j$, $p = q = k_j$ is given uniquely if the state vector $|\psi_{s_j^2, k_j}^{(0)}\rangle$ is known. The construction under discussion is one which has the property that $|\psi_{s_j^2, k_j}^{(0)}\rangle = |\hat{\psi}_{s_j^2, k_j}^{(0)}\rangle$. In fact Eqs. (3.1) and (3.2) are another expression of the property. Thus it follows immediately that

$$\langle p | \hat{K}(s^2) | q \rangle \cong \langle p | K(s^2) | q \rangle \quad (3.4)$$

in a volume containing the point $s = s_j$, $p = q = k_j$. This property is now established whether or not $s_j = k_j$, i.e., this property can hold for off-shell as well as on-shell points. Hence it follows that we have the latitude to choose to fit the approximate separable potential off shell as readily as on shell. Similar remarks hold for the T matrix subject to the relations discussed in Sec. II. These are the constructions we sought to establish.

Recently Pieper⁵ has constructed a separable nucleon-nucleon potential based on the method given in Ref. 1. This potential provides a more accurate representation of the data than any other separable potential now available in the literature. This success motivates the present extension. The T matrices in the bound-state three-body problem, for example, are far off shell and evaluated at negative energies. Therefore it may prove advantageous to compromise the on-shell fit in favor of greater accuracy in the off-shell region of greatest importance in the many-body problem.

*Supported in part by the National Science Foundation.

¹D. J. Ernst, C. M. Shakin, and R. M. Thaler, Phys. Rev. C 8, 46 (1973).

²The finite number of orthogonal continuum states $|\psi_i\rangle$ do not define a well behaved projection operator $P = \sum_i |\psi_i\rangle\langle\psi_i|$. This is a consequence of the fact that continuum state vectors are not normalizable. However, the expression in Eq. (1.1) is independent of the norm of the state vectors $|\psi_i\rangle$. This property leads to a proper definition of the operator \mathcal{U} in Eq. (1.1).

³The functions $|\psi_{s_j^2, k_j}\rangle$ are defined in Eqs. (4.9)–(4.11) of Ref. 1. They satisfy $|\psi_{s^2, k}\rangle = |k\rangle + G^{(0)}(s^2)V|\psi_{s^2, k}\rangle$ where $G^{(0)}(s^2)$ is a principal value Green's function. The corresponding K matrix is $\langle p|K(s^2)|q\rangle = \langle p|V|\psi_{s^2, q}\rangle$ and satisfies $K(s^2) = V + VG^{(0)}(s^2)K(s^2)$. Similarly the T -matrix equation is $t(s^2) = V + VG^{(+)}(s^2)t(s^2)$.

⁴Separable approximations to the T matrix for negative energies have been discussed by K. L. Kowalski, Nuovo Cimento 45, 769 (1966).

⁵S. Pieper, Phys. Rev. C 9, 883 (1974).