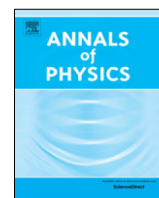




Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Derivation of K -matrix reaction theory in a discrete basis formalism

Y. Alhassid^a, G.F. Bertsch^{b,*}, P. Fanto^a^a Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, USA^b Department of Physics and Institute for Nuclear Theory, University of Washington, Box 351560, Seattle, WA 98195, USA

ARTICLE INFO

Article history:

Received 16 April 2020

Accepted 14 June 2020

Available online 18 June 2020

Keywords:

Reaction theory

 K -matrix S -matrix

Nuclear theory

ABSTRACT

The usual derivations of the S and K matrices for two-particle reactions proceed through the Lippmann–Schwinger equation with formal definitions of the incoming and outgoing scattering states. Here we present a simpler alternative derivation that is carried out completely in the Hamiltonian representation, using a discrete basis of configurations for the scattering channels as well as the quasi-bound configurations of the combined fragments. We use matrix algebra to derive an explicit expression for the K matrix in terms of the Hamiltonian of the internal states of the compound system and the coupling between the channels and the internal states. The formula for the K matrix includes explicitly a real dispersive shift matrix to the internal Hamiltonian that is easily computed in the formalism. That expression is applied to derive the usual form of the S matrix as a sum over poles in the complex energy plane. Some extensions and limitations of the discrete-basis Hamiltonian formalism are discussed in the concluding remarks and in the Appendix.

© 2020 Elsevier Inc. All rights reserved.

1. Introduction

The K -matrix formalism for reactions between particles with an internal structure is widely used in many domains of physics, including molecular collisions [1], mesoscopic physics [2,3], hadronic spectra [4], nuclear reactions [5], and statistical reaction theory in general [6]. Its advantage over the competing R -matrix theory [7–9] is a simplified connection between internal states of the

* Corresponding author.

E-mail address: bertsch@uw.edu (G.F. Bertsch).

compound system and the channel wave functions of the incoming or outgoing particles.¹ In particular, in the K -matrix approach, the Hamiltonian dynamics within the internal states can be treated by well-known configuration-interaction (CI) methods [10]. However, the derivation of equations relating the K matrix to the Hamiltonian can be rather obscure in the literature. The derivations often start from the Lippmann–Schwinger equation and its associated T matrix, which is already several steps removed from the Hamiltonian equation expressed in a computationally transparent basis [6,11–14]. Here we carry out the derivations starting from a representation of the Hamiltonian H in a discrete basis. As a benefit, we find an expression for the dispersive couplings of the internal states to the continuum that is computationally quite simple. In contrast, many derivations in the literature suppress these terms in the final formulas.

A simple version of our formalism has been applied in nuclear reaction theory [15,16]. In the Mazama code introduced in Ref. [15], the diagonal S -matrix element is computed for one specific channel, providing the elastic cross section in that channel and the total reaction cross section. Here we consider a general scattering problem of any number of two-particle channels.

2. Discrete-basis formulation of the scattering problem

2.1. Discretized two-particle Hilbert space

The Hilbert space of the two-particle scattering system consists of two subspaces. The first contains configurations, labeled by λ , that are used to construct internal wave functions of the compound system; the scattering wave function amplitude for each internal configuration λ will be denoted ψ_λ . The second subspace contains all the scattering channels. Each channel c is defined by the set of configurations having the same internal structures for the two particles and differing only in the relative coordinate between the particles' centers of mass. We introduce a discretized mesh of separation distances $r_n = R_0 + n\Delta r$ ($n = 0, 1, \dots$) with finite spacing Δr . The channel wave function in channel c then consists of the set of amplitudes $\varphi_c(n)$ of the configurations on the mesh points,

$$\vec{\varphi}_c = \{\varphi_c(0), \varphi_c(1), \dots\}. \quad (1)$$

R_0 is assumed to be sufficiently large such that potential interactions between the reactants at larger distances $r > R_0$ can be ignored. The first configuration $\varphi_c(1)$ is connecting to the internal states, either directly or through some extension of the chain into the interacting region. A less restrictive definition of the channel wave function that allows for a potential interaction $V_c(r)$ in each channel c is given in the [Appendix](#).

2.2. Hamiltonian matrix elements

2.2.1. Channel hamiltonian

The Hamiltonian in the channel space is taken to be the kinetic energy operator of the relative motion of the two particles. It is approximated by the second-order difference formula on neighboring mesh points. Following nomenclature from condensed-matter physics, we denote the Hamiltonian matrix element between adjacent states in the channel by t_c (here $t_c = \hbar^2/2M_c(\Delta r)^2$ where M_c is the reduced mass of the two fragments). Then the Hamiltonian matrix H^c describing the relative motion of the fragments in channel c has the matrix elements

$$H_{n,n'}^c = -t_c\delta_{n,n'+1} + (2t_c + E_c)\delta_{n,n'} - t_c\delta_{n,n'-1}, \quad (2)$$

where E_c is the summed energy of the two reactants at rest. In the region $r_n > R_0$ the Hamiltonian is invariant under translations, so its eigenfunctions at energy E can be expressed as a superposition

¹ We use the term 'particles' both for the elementary constituents and the (possibly composite) reactants in the initial or final states of the reaction.

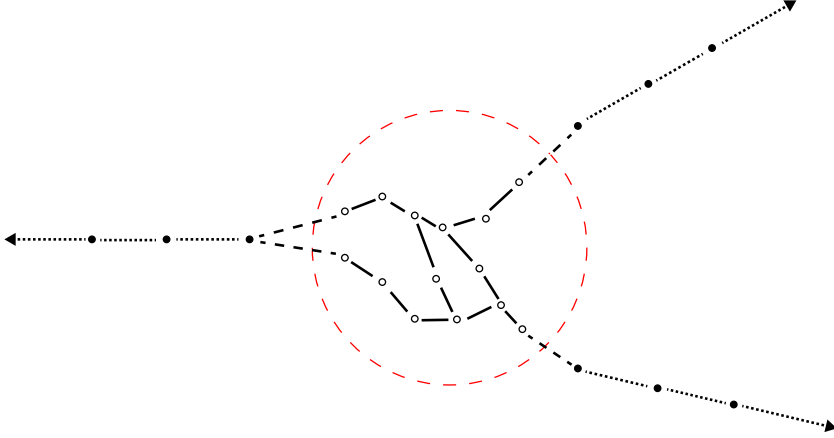


Fig. 1. Connectivity of the discretized Hamiltonian. The internal states are enclosed in the large dashed circle. Small open circles represent states of the internal Hamiltonian and the solid lines indicate off-diagonal matrix elements of the internal Hamiltonian. Solid circles represent the discretized channel configurations. They are coupled to each other through the dotted lines to generate the channel Hamiltonian. The dashed lines denote matrix elements $v_{\lambda,c}$ connecting the channels to the internal states.

of an incoming wave and an outgoing wave with wave number k_c and amplitudes $a_c^{(-)}$ and $a_c^{(+)}$, respectively

$$\varphi_c(n) = a_c^{(-)} e^{-ik_c r_n} - a_c^{(+)} e^{ik_c r_n} . \quad (3)$$

Using $[H^c \vec{\varphi}_c](n) = E \varphi_c(n)$ for $n > 0$ together with (3), the energy-momentum dispersion is given by

$$E - E_c = 2t_c(1 - \cos \kappa_c) . \quad (4)$$

where $\kappa_c = k_c \Delta r$. In the continuum limit, Eq. (4) reduces to the usual quadratic dispersion $E - E_c = (\hbar^2/2M_c)k_c^2$.

2.2.2. Interaction with internal states

The Hamiltonian matrix elements involving states in the interaction region $r \leq R_0$ are of two kinds: those strictly between internal states and those that connect with the channel wave functions at the $n = 1$ site. We denote the latter matrix elements connecting the internal state λ with channel c by $v_{\lambda,c}$. Fig. 1 demonstrates the states and the Hamiltonian matrix elements that connect them.

We consider N_i internal states and N_c channels, and assume that the internal state Hamiltonian is diagonal with energies E_λ . For each channel c , the wave function is regular at $n = 0$, i.e., $\varphi_c(0) = 0$. At radial site $n = 1$ the scattering wave function satisfies the Hamiltonian equation

$$-t_c \varphi_c(2) + (2t_c + E_c) \varphi_c(1) + \sum_{\lambda=1}^{N_i} v_{\lambda,c} \psi_\lambda = E \varphi_c(1) , \quad c = 1, \dots, N_c , \quad (5)$$

while the corresponding equations for the internal-state amplitudes are

$$\sum_{c=1}^{N_c} v_{\lambda,c} \varphi_c(1) + E_\lambda \psi_\lambda = E \psi_\lambda , \quad \lambda = 1, \dots, N_i . \quad (6)$$

Eliminating the internal state amplitudes ψ_λ from Eqs. (6) and substituting in Eqs. (5), we find

$$-t_c \varphi_c(2) + (2t_c \cos \kappa_c) \varphi_c(1) + \sum_{\lambda, c'} \frac{v_{\lambda,c} v_{\lambda,c'}}{E - E_\lambda} \varphi_{c'}(1) = 0 . \quad (7)$$

3. D matrix

Substituting the channel wave function form (3) in Eqs. (7) yields a set of coupled linear equations relating the vector of outgoing amplitudes $\vec{a}^{(+)} = (a_1^{(+)}, a_2^{(+)}, \dots, a_{N_c}^{(+)})$ to the vector of incoming amplitudes $\vec{a}^{(-)} = (a_1^{(-)}, a_2^{(-)}, \dots, a_{N_c}^{(-)})$

$$t_c a_c^{(-)} + \sum_{\lambda c'} \frac{v_{\lambda c} v_{\lambda c'}}{E - E_{\lambda}} e^{-ik_{c'}} a_{c'}^{(-)} = t_c a_c^{(+)} + \sum_{\lambda c'} \frac{v_{\lambda c} v_{\lambda c'}}{E - E_{\lambda}} e^{ik_{c'}} a_{c'}^{(+)}, \quad (8)$$

where we have absorbed a factor of $e^{-ik_c R_0}$ in $a_c^{(-)}$ and a factor of $e^{ik_c R_0}$ in $a_c^{(+)}$.

In principle, we could define an $N_c \times N_c$ matrix that transforms $\vec{a}^{(-)}$ to $\vec{a}^{(+)}$ but this is not the S -matrix. The S -matrix preserves the total probability flux and requires the amplitudes $a_c^{(\pm)}$ to be normalized to the unit flux. To change to flux-normalized variables, we note that, for a tridiagonal channel Hamiltonian, the probability current $J_c(n \rightarrow n+1)$ from a site n to the neighboring site $n+1$ is given by

$$J_c(n \rightarrow n+1) = iH_{n,n+1}^c [\varphi_c(n) \varphi_c^*(n+1) - \varphi_c^*(n) \varphi_c(n+1)] \quad (9)$$

up to a channel-independent constant. Applying (9) to the wave functions $a_c^{(\pm)} e^{\pm ik_c r_n}$ for the Hamiltonian (2), we find for the current J_c in channel c

$$J_c = \pm 2t_c \sin \kappa_c |a_c^{(\pm)}|^2, \quad (10)$$

which is independent of n . The flux-normalized amplitudes are thus

$$b_c^{(\pm)} = a_c^{(\pm)} / d_c, \quad (11)$$

where

$$d_c = (2t_c \sin \kappa_c)^{-1/2}. \quad (12)$$

Eqs. (8) can be rewritten for the flux-normalized amplitudes $b_c^{(\pm)}$

$$d_c t_c b_c^{(-)} + \sum_{\lambda c'} \frac{v_{\lambda c} v_{\lambda c'}}{E - E_{\lambda}} d_{c'} e^{-ik_{c'}} b_{c'}^{(-)} = d_c t_c b_c^{(+)} + \sum_{\lambda c'} \frac{v_{\lambda c} v_{\lambda c'}}{E - E_{\lambda}} d_{c'} e^{ik_{c'}} b_{c'}^{(+)}. \quad (13)$$

Dividing both sides of the equation by $d_c t_c$, we obtain

$$D \vec{b}^{(-)} = D^* \vec{b}^{(+)}, \quad (14)$$

where the matrix D is defined by.²

$$D_{c,c'} = \delta_{c,c'} + 2\pi \sum_{\lambda=1}^{N_i} \frac{W_{\lambda c} W_{\lambda,c'}}{E - E_{\lambda}} d_{c'}^2 t_{c'} e^{-ik_{c'}} \quad (15)$$

with

$$W_{\lambda c} = \frac{1}{\sqrt{2\pi}} \frac{v_{\lambda c}}{d_c t_c}. \quad (16)$$

D^* is obtained from D by simply replacing $e^{-ik_{c'}} \rightarrow e^{ik_{c'}}$. The S matrix is defined by $\vec{b}^{(+)} = S \vec{b}^{(-)}$ and, using Eq. (14), is given by

$$S = D^{*-1} D. \quad (17)$$

² The definitions include factors of 2π and $(2\pi)^{-1/2}$ following the convention in the literature [6].

4. K matrix

The K matrix is defined from the S matrix by the implicit relation

$$S = \frac{1 + iK}{1 - iK} . \quad (18)$$

Substituting Eq. (17) in Eq. (18), and solving for K , we express K in terms of D and D^*

$$K = -i(D + D^*)^{-1}(D - D^*) . \quad (19)$$

In the following we derive an explicit expression for the matrix elements of K . Using Eq. (15), we have

$$\frac{D + D^*}{2} = 1 + W^T(E - H)^{-1}V , \quad \frac{D - D^*}{2} = -i\pi W^T(E - H)^{-1}W , \quad (20)$$

where

$$H = \sum_{\lambda} |\lambda\rangle E_{\lambda} \langle \lambda| \quad (21)$$

is the internal state Hamiltonian of the compound system. The matrix V is defined by

$$V_{\lambda c} = \pi W_{\lambda c} \cot \kappa_c , \quad (22)$$

where we have used $d_c^2 t_c = (2 \sin \kappa_c)^{-1}$.

Substituting Eq. (20) in (19), we find

$$K = -(1 + X)^{-1}X \tan \kappa = -[1 - (1 + X)^{-1}] \tan \kappa , \quad (23)$$

where the matrix X is defined by

$$X = W^T(E - H)^{-1}V , \quad (24)$$

and $\tan \kappa$ is a diagonal matrix with elements $\tan \kappa_c$ along its diagonal.

To invert $1 + X$ we use the operator identity $B^{-1}(B - A)A^{-1} = A^{-1} - B^{-1}$ with $A = E - H$ and $B = E - H + VW^T$ to find

$$(E - H + VW^T)^{-1}VW^T(E - H)^{-1} = (E - H)^{-1} - (E - H + VW^T)^{-1} . \quad (25)$$

Multiplying by W^T on the left and by V on the right, we obtain

$$YX = X - Y , \quad (26)$$

where

$$Y = W^T(E - H + VW^T)^{-1}V . \quad (27)$$

Solving (26), we find $(1 + X)^{-1} = 1 - Y$. Substituting in (23), we find

$$K = -Y \tan \kappa = -W^T(E - H + VW^T)^{-1}V \tan \kappa = -\pi W^T(E - H + VW^T)^{-1}W , \quad (28)$$

where we have used Eq. (22).

The final expression for K is thus

$$K = \pi W^T(H + \Delta - E)^{-1}W , \quad (29)$$

where W is given in Eq. (16) and describes the coupling matrix of the channels to the internal states, while $\Delta = -VW^T$ is the real shift matrix

$$\Delta_{\lambda\lambda'} = -\pi \sum_c W_{\lambda c} W_{\lambda' c} \cot \kappa_c . \quad (30)$$

The above expression for K has the same form as the usual K matrix, c.f. Eq. (18) of Ref. [3]. However, our term includes the real shift matrix Δ that is usually ignored in expressions for the K

matrix. In other derivations of the S matrix, this shift arises from off-shell couplings to the channels; see, e.g., Eqs. (28–30) of Ref. [6]. In our approach, this shift arises naturally from the matrix algebra.

The K matrix in (29) is real symmetric, which guarantees that the S matrix in (18) is symmetric and unitary.

5. S matrix

To find an explicit expression for the S matrix, we use again the operator identity $B^{-1}(B-A)A^{-1} = A^{-1} - B^{-1}$ but now for $A = E - (H + \Delta)$ and $B = E - (H + \Delta - i\pi WW^T)$. We obtain

$$\begin{aligned} i\pi[E - (H + \Delta - i\pi WW^T)]^{-1}WW^T[E - (H + \Delta)]^{-1} \\ = [E - (H + \Delta)]^{-1} - [E - (H + \Delta - i\pi WW^T)]^{-1}. \end{aligned} \quad (31)$$

Multiplying by πW^T on the left and by W on the right, we find

$$i\pi ZK = K + \pi Z, \quad (32)$$

where

$$Z = W^T[E - (H + \Delta - i\pi WW^T)]^{-1}W, \quad (33)$$

and we have used the expression (29) for the K matrix. Relation (32) can be rewritten in the form

$$\frac{K}{1 - iK} = -\pi Z. \quad (34)$$

Using the relation (18) between the S matrix and the K matrix, we find

$$S = 1 + 2i\frac{K}{1 - iK} = 1 - 2\pi iZ \quad (35)$$

where we have used (34) to obtain second equality. We thus find an explicit expression for S

$$S = 1 - 2\pi iW^T[E - (H + \Delta - i\pi WW^T)]^{-1}W, \quad (36)$$

which includes both a real shift Δ and an imaginary shift $-i\pi WW^T$ to the Hamiltonian H . This expression coincides formally with Eqs. (28–30) in Ref. [6] for the S matrix in the absence of background scattering.

6. Concluding remarks

We have described an alternative derivation of the K matrix of scattering theory, as shown for the Hamiltonian specified by Eqs. (2), (5) and (6). Using this derivation, we are able to avoid imposing formal structures such as the continuum Green's functions of Lippmann–Schwinger reaction theory. In practice, it is well-suited to many-body Hamiltonians of equal-mass particles, in which case it may be difficult to identify a relative coordinate. This includes nuclei and atomic condensates where common practice follows the Hartree–Fock or Hartree–Fock–Bogoliubov approximations and their extensions in the CI framework. For large systems, this approach needs much less computational effort than other reaction formalisms, which rely on explicit antisymmetrization and/or the use of a Jacobi coordinate representation to separate out a channel wave function $\varphi_c^r(r)$ in the relative coordinate r of the two particles.

In the above derivation, we left unspecified the exact relationship of the usual channel wave function φ_c^r to the discrete-basis wave function $\tilde{\varphi}_c$. These quantities have different dimensions: the components of $\tilde{\varphi}_c$ are dimensionless amplitudes in the CI formalism while φ_c^r has dimension $[\text{length}]^{-1/2}$, the same as ordinary coordinate-space wave functions. The formal connection between the two is not obvious, since it is difficult to separate out a relative coordinate wave function unless it is already defined in the CI basis. Our approach only involves the role of the relative coordinate at large separations, where the absence of interactions leads to the simplified Hamiltonian approximation in Eq. (2).

The present formalism might be applicable to problems in nuclear reaction theory such as fission [17]. It should also simplify the treatment of the interaction between droplets of atomic condensates, such as the fusion reaction described in Ref. [18].

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

We thank J.J. Rehr for discussion on possible applications to molecular reactions. The work of Y.A. and P.F. was supported in part by the U.S. DOE grant No. DE-SC0019521, and by the U.S. DOE NNSA Stewardship Science Graduate Fellowship under cooperative agreement No. DE-NA0003864.

Appendix. Potential interactions in the channels

Our definition of the channel Hamiltonian requires that the starting point at R_0 be beyond the range of the interaction in the given channel. This is obviously inefficient if there are long-range potential interactions between the reactants. As in other formulations of reaction theory, the present framework can include elastic scattering potentials $V_c(r)$ in the channels to reduce the size of the interaction zone.

We define a mesh for which $n = 1$ is the point where the channel configurations interact with the internal ones. First we solve the one-dimensional Schrödinger equation for the channel wave function $U_c(n)$ in the absence of all coupling terms $v_{\lambda,c}$

$$-t_c U_c(n-1) + [V_c(n) + 2t_c + E_c - E]U_c(n) - t_c U_c(n+1) = 0 \quad (1 \leq n \leq N), \quad (\text{A.1})$$

where $V_c(n)$ is the channel potential at site n . The wave function $U_c(n)$ is assumed to be real and can be written in terms of incoming and outgoing wave functions, $I_c(n)$ and $I_c^*(n)$, respectively,

$$U_c(n) = i[I_c(n) - I_c^*(n)]. \quad (\text{A.2})$$

At the upper mesh points where the potential $V_c(n)$ can be ignored, the incoming wave $I_c(n)$ has the following asymptotic form

$$I_c(n) = e^{-i\delta_c} e^{-i\kappa_c n}, \quad (\text{A.3})$$

where δ_c is the phase shift for scattering in a potential V_c .

At $n = 1$, the real wave function U_c satisfies the Hamiltonian equation

$$[2t_c \cos \kappa_c + V_c(1)]U_c(1) - t_c U_c(2) = 0, \quad (\text{A.4})$$

where we have used $U_c(0) = 0$ and the dispersion relation (4).

After including the interaction $v_{\lambda,c}$ with the internal wave function amplitudes, the channel wave function acquires a different mixture of incoming and outgoing waves

$$\varphi_c(n) = a_c^{(-)} I_c(n) - a_c^{(+)} I_c^*(n). \quad (\text{A.5})$$

Eliminating the internal state amplitudes, the Hamiltonian equation acting at site $n = 1$ has the form (7) but with the additional contribution of the channel potential

$$[2t_c \cos \kappa_c + V_c(1)]\varphi_c(1) - t_c \varphi_c(2) + \sum_{c'=1}^{N_c} \sum_{\lambda=1}^{N_i} \frac{v_{\lambda,c} v_{\lambda,c'}}{E - E_\lambda} \varphi_{c'}(1) = 0. \quad (\text{A.6})$$

Multiplying Eq. (A.4) by $\varphi_c(1)$, and subtracting it from Eq. (A.6) multiplied by $U_c(1)$, we obtain

$$-t_c [\varphi_c(2)U_c(1) - U_c(2)\varphi_c(1)] + \sum_{c',\lambda} U_c(1) \frac{v_{\lambda,c} v_{\lambda,c'}}{E - E_\lambda} \varphi_{c'}(1) = 0. \quad (\text{A.7})$$

Inserting Eqs. (A.2) and (A.5) in Eq. (A.7) and simplifying, yields

$$-it_c \mathcal{W}_c(a_c^{(-)} - a_c^{(+)}) + \sum_{c',\lambda} U_c(1) \frac{v_{\lambda,c} v_{\lambda,c'}}{E - E_\lambda} (a_{c'}^{(-)} I_{c'}(1) - a_{c'}^{(+)} I_{c'}^*(1)) = 0, \quad (\text{A.8})$$

where

$$\mathcal{W}_c = I_c(1)I_c^*(2) - I_c^*(1)I_c(2). \quad (\text{A.9})$$

In analogy with the Wronskian of a second-order differential operator, $\mathcal{W}_c(n) = I_c(n)I_c^*(n+1) - I_c^*(n)I_c(n+1)$ is independent of the mesh position n and thus can be evaluated in the asymptotic regime to give

$$\mathcal{W}_c = 2i \sin \kappa_c. \quad (\text{A.10})$$

The current $J_{n,n+1}^{c(\mp)}$ is given an expression similar to Eq. (9) but with the wave functions $a_c^{(-)}I_c$ and $a_c^{(+)}I_c^*$. It is proportional to \mathcal{W}_c and is thus independent of the mesh position, leading to the same result (10) as in the case without potential interactions. As in the main text, we introduce the flux-normalized variables

$$b_c^{(\pm)} = a_c^{(\pm)}/d_c. \quad (\text{A.11})$$

Inserting Eq. (A.11) into Eq. (A.8), multiplying both sides by d_c , and separating the terms in that are proportional to $b_c^{(-)}$ and $b_c^{(+)}$ yields

$$\sum_{c'} \left(\delta_{cc'} + \sum_{\lambda} U_c(1) \frac{d_c v_{\lambda c} v_{\lambda c'} d_{c'}}{E - E_{\lambda}} I_{c'}(1) \right) b_{c'}^{(-)} = \sum_{c'} \left(\delta_{cc'} + \sum_{\lambda} U_c(1) \frac{d_c v_{\lambda c} v_{\lambda c'} d_{c'}}{E - E_{\lambda}} I_{c'}^*(1) \right) b_{c'}^{(+)}. \quad (\text{A.12})$$

Thus, the S matrix is given by $S = (D^*)^{-1}D$, where the D matrix is now defined by

$$D_{cc'} = \delta_{cc'} + \sum_{\lambda} U_c(1) \frac{d_c v_{\lambda c} v_{\lambda c'} d_{c'}}{E - E_{\lambda}} I_{c'}(1). \quad (\text{A.13})$$

The corresponding S matrix can be shown to be unitary and symmetric.

Finally, in the absence of a channel potential, $I_c(1) = e^{-ik_c}$, $U_c(1) = 2 \sin \kappa_c$, and the D matrix in Eq. (A.13) reduces to Eq. (15).

References

- [1] X.H. Lin, Y.G. Peng, Y. Wu, et al., *Chem. Phys.* 522 (2019) 10.
- [2] Y.V. Fyodorov, H.-J. Sommers, *Phys. Rev. Lett.* 76 (1996).
- [3] Y. Alhassid, *Rev. Modern Phys.* 72 (2000) 895.
- [4] R.S. Longacre, A. Etkin, K.J. Foley, et al., *Phys. Lett. B* 177 (1986) 223.
- [5] T. Kawano, P. Talou, H.A. Weidenmüller, *Phys. Rev. C* 92 (2015) 044617.
- [6] G.E. Mitchell, A. Richter, H.A. Weidenmüller, *Rev. Modern Phys.* 82 (2010) 2845.
- [7] E.P. Wigner, L. Eisenbud, *Phys. Rev.* 72 (1947) 29.
- [8] A.M. Lane, R.G. Thomas, *Rev. Modern Phys.* 30 (1958) 257.
- [9] P. Descouvemont, D. Baye, *Rep. Progr. Phys.* 73 (2010) 036301.
- [10] P.O. Löwdin, *Phys. Rev.* 97 (1955) 1474.
- [11] R.H. Dalitz, *Rev. Modern Phys.* 33 (1961) 471.
- [12] C. Mahaux, H.A. Weidenmüller, *Shell-Model Approach to Nuclear Reactions*, North-Holland, Amsterdam, 1969.
- [13] S.U. Chung, J. Brose, R. Hackmann, et al., *Ann. Phys.* 4 (1995) 404.
- [14] John R. Taylor, *Scattering Theory of Non-Relativistic Collisions*, Dover Publications, Mineola, 2006.
- [15] P. Fanto, G.F. Bertsch, Y. Alhassid, *Phys. Rev. C* 98 (2018) 014604, see its Supplemental Material for the Mazama code.
- [16] G.F. Bertsch, D.A. Brown, E.D. Davis, *Phys. Rev. C* 98 (2018) 014611.
- [17] G.F. Bertsch, W. Younes, *Ann. Phys.* 403 (2019) 68.
- [18] Y. Shin, M. Saba, T.A. Pasquii, et al., *Phys. Rev. Lett.* 92 (2004) 050405.