## Communications

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## K matrix and unitarity constraints on off-shell T matrix elements

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A discussion of off-shell properties of the T matrix is given based on the damping equation and unitarity. The off-shell function  $\varphi_l(k, q)$  of Baranger *et al.* is shown to be  $\varphi_l(k, q) = \cos \delta_l(k) \langle k | K_l(k^2) | q \rangle$ , where  $\delta_l$  and  $K_l$  are the phase shift and partial-wave K (reaction) operator. The ratio of the imaginary to the real part of the half-off-shell partial-wave T matrix element is shown to be  $\tan \delta_l(k)$ , thus providing a unitarity constraint to be satisfied by any approximate T matrix elements. In addition, the imaginary part of the fully-off-shell T matrix element is shown to be proportional to the product  $\varphi_l(p, k) \varphi_l(k, q)$ . These results hold for both one-body and two-channel identical particle scattering.

A well-known result in the theory of one-body scattering is the Heitler damping equation<sup>1</sup> relating the T and K operators:

$$T = K - i\pi K \delta(E - H_0) T = K - i\pi T \delta(E - H_0) K, \quad (1)$$

where  $H_0$  is the unperturbed part of the Hamiltonian H, and the interaction  $V=H-H_0$ . Equation (1) is a means of guaranteeing unitarity, since any Hermitian K will produce a unitary S matrix.

We have recently shown<sup>2</sup> that an equation similar to (1) holds for the symmetrized T and K operators  $\mathcal{T}$  and  $\mathcal{K}$  that occur in the description of the scattering of identical particles. In particular, if  $\mathcal{T} = T(d) \pm T(e)$  and  $\mathcal{K} = K(d) \pm K(e)$ , where d and erefer to the direct and exchange processes and the + (-) sign indicates bosons (fermions), then<sup>2</sup>

$$\mathbf{\mathcal{T}} = \mathbf{\mathcal{K}} - i\pi\mathbf{\mathcal{K}}\delta(E - H_2)\mathbf{\mathcal{T}} = \mathbf{K} - i\pi\mathbf{\mathcal{T}}\delta(E - H_2)\mathbf{\mathcal{K}} \quad . \tag{2}$$

Here we have assumed a simplified problem wherein there are only two identical particles (1 and 2) interacting with a center of force, so that  $H_i$  describes the plane wave motion of *i* and the bound and continuum states of *j* in the presence of the center of force. Equation (2) has as the direct process particle 2 incident on and emergent from a bound state of 1 while the exchange is that of 1 incident and 2 emergent. Equation (2) expresses unitarity in a two-channel case, and we have used it to derive new coupled equations for direct and exchange *T* and *K* operators.<sup>3</sup> Relatively little use has been made of the damping equation, in part because K is difficult to calculate and in part because Eq. (1) still remains to be solved for T [or Eq. (2) for  $\mathcal{T}$ ] after K (or  $\mathcal{K}$ ) has been determined. Nevertheless, K is an important theoretical quantity and has been used in both formal and computational studies. In this note we use the damping equation and Eq. (3) below to derive some properties of off-shell T matrix elements. We work with T and K, but identical results hold for the identical particle case and can be obtained simply by replacing K, and  $\tilde{K}$  [see Eq. (3) below] and T everywhere by  $\mathcal{K}, \tilde{\mathcal{K}}$ , and  $\mathcal{T}$ .

We have previously studied<sup>4</sup> the quantity  $\tilde{K}$  defined by

$$\tilde{K} = V + V \frac{\vartheta}{E - H} V \equiv \operatorname{Re} T , \qquad (3)$$

where  $\mathcal{P}$  means principal value, and shown that it is related to K. For the case of central interactions, and with  $E = \hbar^2 k^2 / 2M$ , the following halfoff-shell relations hold:

$$\langle k | \tilde{K}_{l}(k^{2}) | q \rangle = \cos^{2} \delta_{l}(k) \langle k | K_{l}(k^{2}) | q \rangle$$
(4a)

and

$$\langle q | \tilde{K}_{l}(k^{2}) | k \rangle = \cos^{2} \delta_{l}(k) \langle q | K_{l}(k^{2}) | k \rangle$$
, (4b)

where the subscript labels the *l*th partial wave and  $\delta_l(k)$  is the usual *l*th order phase shift. Similar equations relate  $\tilde{\mathbf{K}}$  (defined<sup>2</sup> by  $\tilde{\mathbf{K}} = \operatorname{Re} \mathbf{f}$ ) and  $\mathbf{K}$  in

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the identical particle case.

The normalization used to obtain Eqs. (4), and used here also, is  ${}^4$ 

$$-\pi \rho_{k} \langle k | T_{l}(k^{2}) | k \rangle = e^{i\delta_{l}(k)} \sin \delta_{l}(k)$$
(5)

and

$$-\pi\rho_{k}\langle k | K_{l}(k^{2}) | k \rangle = \tan\delta_{l}(k) \quad , \tag{6}$$

where  $\rho_k = Mk/\hbar^2$  is the density of states factor.

We first examine half-off-shell matrix elements of  $T_{l}(k^{2})$  using Eq. (1):

$$\langle q | T_{l}(k^{2}) | k \rangle = \langle q | T_{l}(k^{2}) | k \rangle$$

$$- i \pi \rho_{k} \langle q | T_{l}(k^{2}) | k \rangle \langle k | K_{l}(k^{2}) | k \rangle ,$$

or, solving for  $\langle q | T_{l}(k^{2}) | k \rangle$  and using (6),

$$\langle q | T_{l}(k^{2}) | k \rangle = e^{i\delta_{l}} \cos \delta_{l}(k) \langle q | K_{l}(k^{2}) | k \rangle \quad . \tag{7}$$

Similarly, we find

$$\langle k | T_{l}(k^{2}) | q \rangle = e^{i\delta_{l}} \cos \delta_{l}(k) \langle k | K_{l}(k^{2}) | q \rangle \quad . \tag{8}$$

From this equation we see that the real half-offshell quantity  $\varphi_i(q, k)$  introduced by Baranger *et al.*<sup>5</sup> is just

$$\varphi_{l}(q, k) \equiv e^{-i\delta_{l}(k)} \langle q | T_{l}(k^{2}) | k \rangle = \cos \delta_{l}(k) \langle q | K_{l}(k^{2}) | k \rangle;$$
(9)

 $\varphi_l(k,q)$  is similarly defined. Hence, the symmetric (antisymmetric) part of  $\varphi_l(q,k)$  is given by the symmetric (antisymmetric) part of the half-off-shell K matrix element  $\langle q | K_l(k^2) | k \rangle$ . Equations (7) and (9) provide a simple proof based on unitarity that the phase of the half-off-shell T matrix element is just  $\delta_l(k)$ .<sup>6</sup>

Since K is Hermitian, its matrix elements are real. Furthermore,  $\operatorname{Re}\langle p | T_{l}(k^{2}) | q \rangle = \langle p | \operatorname{Re}T_{l}(k^{2}) | q \rangle$ and similarly for  $\operatorname{Im}T_{l}(k^{2})$ , so that from Eqs. (7) and (8) we easily find

$$\frac{\langle k | \operatorname{Im} T_{i}(k^{2}) | q \rangle}{\langle k | \operatorname{Re} T_{i}(k^{2}) | q \rangle} = \frac{\langle q | \operatorname{Im} T_{i}(k^{2}) | k \rangle}{\langle q | \operatorname{Re} T_{i}(k^{2}) | k \rangle} = \tan \delta_{i}(k) \quad .$$

$$(10)$$

Thus, just as with the on-shell matrix elements, we have that unitarity fixes the ratio of the halfoff-shell elements of  $\operatorname{Re} T_i$  and  $\operatorname{Im} T_i$  to be  $\tan \delta_i(k)$ , an on-shell quantity. While such a condition can be derived from the work of Baranger *et al.*,<sup>5</sup> we see here that it is a direct consequence of unitarity, as expressed in Eq. (1). It is implicitly contained in earlier discussions of off-shell unitarity,<sup>7</sup> but the implications of this result do not seem to have been previously recognized. Equation (10) is a constraint on any approximate method for calculating half-off-shell T matrix elements. Methods based on the construction of a potential will obviously lead to matrix elements of T satisfying (10), as will any method in which  $\varphi_i(k, q)$  is approximated. For other methods (10) may provide a useful check on the validity of the approach, particularly as it clearly demonstrates that the real and imaginary parts of the half-off-shell elements are not independent, just as in the on-shell case. We further see that at a resonance  $[\delta_i(k) = \frac{1}{2}\pi]$ , either one of the following two relations

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$$\langle k | \operatorname{Im} T_{l}(k^{2}) | q \rangle = \infty, \quad \delta_{l}(k) = \frac{1}{2}\pi$$

$$\langle k | \operatorname{Re} T_{l}(k^{2}) | q \rangle = 0, \quad \delta_{l}(k) = \frac{1}{2}\pi$$

must hold, or that both the numerator and denominator of (10) go to zero or to infinity in such a way that their ratio is infinite. Finally, since we expect that  $\delta_i(\infty) = 0$ , Eq. (10) provides a constraint on the analytic behavior of  $\langle k | T_i(k^2) | q \rangle$  as a function of q when  $k^2 \rightarrow \infty$ .

Let us now consider fully-off-shell matrix elements. Separating real and imaginary parts in (1), we have  $[2\text{Re}T = T + T^{\dagger}; 2\text{Im}T = -i(T - T^{\dagger})]$ :

$$\operatorname{Im} T = -\pi K \delta(E - H_0) \operatorname{Re} T$$

$$= -\pi \operatorname{Re} T\delta(E - H_0)K \tag{11}$$

and

or

$$\operatorname{Re} T = K + \pi K \delta (E - H_0) \operatorname{Im} T$$
$$= K + \pi \operatorname{Im} T \delta (E - H_0) K .$$
(12)

By using Eq. (3), Eq. (11) may be reexpressed as

$$\operatorname{Im} T = -\pi K \delta(E - H_0) \tilde{K} , \qquad (13)$$

indicating that the quantity  $\tilde{K}$  plays a basic role in determining the imaginary part of T.

If fully-off-shell partial-wave matrix elements of (13) are taken, we get

$$\langle p | \operatorname{Im} T_{l}(k^{2}) | q \rangle = - \pi \rho_{k} \langle p | K_{l}(k^{2}) | k \rangle \langle k | \tilde{K}_{l}(k^{2}) | q \rangle$$

$$= - \pi \rho_{k} \cos^{2} \delta_{l}(k)$$

$$\times \langle p | K_{l}(k^{2}) | k \rangle \langle k | K_{l}(k^{2}) | q \rangle$$

$$= - \pi \rho_{k} \varphi_{l}(p, k) \varphi_{l}(k, q) .$$

$$(14)$$

The second and third lines of (14) follow on the use of Eqs. (4) and (9), respectively. Knowledge of  $\varphi_i(p, k)$  thus determines the fully-off-shell part of Im $T_i$ ; i.e., as pointed out by Baranger *et al.*, only half-shell quantities are needed to obtain fully off-shell ones. However, we here see that unitarity provides us with a direct relationship: no integrals need be evaluated<sup>5</sup> to find Im $T_i$ . Equation (14) is of course an alternate form of the off-shell unitarity formula.<sup>7</sup>

As implied by Eq. (12), unitarity does not lead to any especially simple expressions for  $\operatorname{Re} T_i$ . Substituting (11) into (12) and taking partial wave matrix elements we easily find

$$\langle p | \operatorname{Re}T_{l}(k^{2}) | q \rangle = \langle p | K_{l}(k^{2}) | q \rangle + \pi \rho_{k} \sin \delta_{l}(k) \cos \delta_{l}(k) \langle p | K_{l}(k^{2}) | k \rangle \langle k | K_{l}(k^{2}) | q \rangle \quad .$$
(15)

The second term on the right-hand side of (15) can be cast into other guises by using Eqs. (9) or (14), but these do not eliminate the presence of the fully-off-shell quantity  $\langle p | K_l(q^2) | q \rangle$ . Unitarity can take us no further and we need some dynamical input to reach the conclusion that  $\langle p | \operatorname{Re} T_l(k^2) | q \rangle$ is also determined by half-on-shell quantities<sup>5</sup> and a knowledge of any bound states.<sup>8</sup> A further discussion of this point and the extension of these results to the multichannel case will be discussed elsewhere.

As noted above, these results all hold for the identical particle case. One need merely replace T, K, and  $\tilde{K}$  by  $\mathcal{T}$ ,  $\mathfrak{K}$ , and  $\tilde{\mathfrak{K}}$ , respectively.

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- <sup>†</sup>Work supported in part by the U.S. Atomic Energy Commission.
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