A New Method for Determining K-Matrix Elements

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Abstract

Formal solutions to the integral equation for the K operator are difficult to obtain because the principal value Green's function does not have a Lippmann-Schwinger iteration. We introduce a new Hermitian operator $\tilde{K} = V + V[\not{P}/(E - H)]V$ in this paper and show that its on-shell and half-off-shell partial wave matrix elements are equal to $\cos^2 \delta_l$ times those of the usual K operator. From these the fully off-shell values of K can be determined.

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In recent work on the validity of a separable approximation to a local (central) potential, Ernst et. al. [1] have employed an explicit solution to the integral equation for the K operator:

$$K(E) = V + V \frac{\mathcal{P}}{E - H_0} K(E) \quad (1)$$

Here H_0 is the kinetic energy operator, V is the potential, $\mathcal{P}$ means the principal value and the full Hamiltonian H is

$$H = H_0 + V$$

The explicit solution to eq.(1) whose off-shell matrix elements are used in [1] is of the form

$$K(E) = V + V G^{(0)}(E) V \quad (2)$$

where the full Green's function $G^{(0)}(E)$ appearing in (2) is not $\mathcal{P}/(E - H)$ but is a quantity to be found by construction [1].

Replacement of $G^{(0)}(E)$ in (2) by $\mathcal{P}/(E - H)$ does not give a solution to (1), as pointed out by a number of authors, eg. [2,3,4]. In fact formal solutions to (1), while they can be written out [3], are not given in any simple form containing $\mathcal{P}/(E - H)$ because this operator does not have a Lippmann-Schwinger iteration similar to that of the outgoing wave Green's function $(E + i\epsilon - H)^{-1}$. However replacement of $G^{(0)}$ by $\mathcal{P}/(E - H)$ does define an Hermitian operator $\tilde{K}(E)$:

$$\tilde{K}(E) = V + V \frac{\mathcal{P}}{E - H} V \quad (3)$$

We have recently studied [4] the on-shell properties of $\tilde{K}(E)$ and have proved the following results. First, on-shell, partial-wave matrix elements of $\tilde{K}$ are proportional to those of K :

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

where $E = \hbar^2 k^2 / 2M$ and $\delta_\ell(k)$ is the usual phase shift. Second, the standing wave state $|x_k^0\rangle$ defined by

$$|x_k^0\rangle = |k\rangle + \frac{\mathcal{P}}{E - H} V |k\rangle \quad (5)$$

which may be transformed to

$$|\chi_k^0\rangle = P|k\rangle + \frac{P}{E - H_0} \tilde{K}(E) |k\rangle, \quad (6)$$

yields the same on-shell, K-matrix elements as does the usual standing wave solution $|\psi_k^0\rangle$ defined by

$$|\psi_k^0\rangle = |k\rangle + \frac{P}{E - H_0} K(E) |k\rangle \quad (7)$$

in the sense that the ratio of the irregular to the regular solution in (5) is $\tan \delta_\ell(k)$. The quantity P in (6) is an operator such that $\tilde{K} = KP$; we display forms for P below.

These results show that one can use $\tilde{K}(E)$ to determine on-shell matrix elements of $K(E)$. In this note, we extend our results to the case of off-shell matrix elements of $\tilde{K}_\ell(E)$. In particular we prove that eq. (4) also relates the half-off-shell matrix elements of $\tilde{K}_\ell(E)$ and $K_\ell(E)$.

As a means of introducing some notation, we first give a simpler proof of (4) than stated in [4]. Our normalization is such that

$$-\pi \rho_k \langle k | T_\ell(k^2) | k \rangle = e^{i\delta_\ell(k)} \sin \delta_\ell(k) \quad (8)$$

and

$$-\pi \rho_k \langle k | K_\ell(k^2) | k \rangle = \tan \delta_\ell(k), \quad (9)$$

where $\rho_k = Mk/\hbar^2$ and $T(E)$ is the usual transition operator:

$$T(E) = V + V (E + i\epsilon - H)^{-1} V, \quad \epsilon \rightarrow 0^+. \quad (10)$$

Comparing eqs (3) and (10) we find

$$\tilde{K}(E) = \text{Re } T(E), \quad (11)$$

and taking diagonal, on-shell matrix elements for the ℓ th partial wave we get

$$\langle k | \tilde{K}_\ell(k^2) | k \rangle = \text{Re } \langle k | T_\ell(k^2) | k \rangle.$$

By using eqs. (8) and (9) in this result we easily obtain

$$\begin{aligned} \langle k | \tilde{K}_L(k^2) | k \rangle &= \cos \delta_L(k) \sin \delta_L(k) / (-\pi \rho_k) \\ &= \cos^2 \delta_L(k) \langle k | K_L(k^2) | k \rangle, \text{ QED.} \end{aligned} \quad (4)$$

Let us now consider the off-shell behaviour. The damping equation relating T and K is

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

whose solutions are

$$T(E) = [1 + i\pi K(E) \delta(E - H_0)]^{-1} K(E) \quad (12a)$$

and

$$T(E) = K(E) [1 + i\pi \delta(E - H_0) K(E)]^{-1} \quad (12b)$$

From (11) and (12) we find

$$\tilde{K}(E) = [1 + \pi^2 [K(E) \delta(E - H_0)]^2]^{-1} K(E) \equiv PK(E) \quad (13a)$$

and

$$\tilde{K}(E) = K(E) [1 + \pi^2 [\delta(E - H_0) K(E)]^2]^{-1} = K(E) P' \quad (13b)$$

An equivalent set of relationships are [4]

$$\tilde{K}(E) = K(E) [1 - \pi^2 \delta(E - H_0) V \delta(E - H) V] \quad (14a)$$

and

$$\tilde{K}(E) = [1 - \pi^2 V \delta(E - H) V \delta(E - H) V \delta(E - H_0)] K(E) \quad (14b)$$

these latter results can be derived from eqs (3), (10) and (12).

The results we obtain can be derived from either eqs (13) or (14); we choose to work with (14a). Using $E = \hbar^2 k^2 / 2M$ and taking matrix elements of the l th partial wave between states $\langle p |$ and $| q \rangle$, eq(14a) becomes

$$\begin{aligned} \langle p | \tilde{K}_L(k^2) | q \rangle &= \langle p | K_L(k^2) | q \rangle \\ &- \pi^2 \rho_k^2 \langle p | K_L(k^2) | k \rangle \langle k | T_L(k^2) | k \rangle \langle k | T_L^\dagger(k^2) | q \rangle, \end{aligned} \quad (15)$$

where we have used

$$\langle k | T(k^2) | k \rangle = \langle k | V | \phi_k^+ \rangle$$

with $|\psi_k^+\rangle$ being the usual outgoing wave solution.

Now, $\langle k|T_\ell(k^2)|k\rangle$ is proportional to $\exp(i\delta_\ell)\sin\delta_\ell$, and from the damping equation we have

$$\begin{aligned}\langle K|T_\ell^+(k^2)|q\rangle &= \langle k|K_\ell(k^2)|q\rangle \left[1 + \frac{1\pi\rho_k \langle k|K_\ell(k^2)|k\rangle}{1 - 1\pi\rho_k \langle k|K_\ell(k^2)|k\rangle} \right] \\ &= \frac{\langle k|K_\ell(k^2)|q\rangle}{1 + i \tan \delta_\ell(k)}.\end{aligned}$$

Using this result and eq.(8) in (15) leads to

$$\begin{aligned}\langle p|\tilde{K}_\ell(k^2) - K_\ell(k^2)|q\rangle &= \pi\rho_k \sin \delta_\ell(k) \cos \delta_\ell(k) \\ &\times \langle p|K_\ell(k^2)|k\rangle \langle k|K_\ell(k^2)|q\rangle,\end{aligned}\quad (16)$$

which is the basic result of this paper.

If we now take $q = k$ we find

$$\langle p|\tilde{K}_\ell(k^2) - K_\ell(k^2)|k\rangle = -\sin^2\delta_\ell(k) \langle p|K_\ell(k^2)|k\rangle$$

or

$$\langle p|\tilde{K}_\ell(k^2)|k\rangle = \cos^2\delta_\ell(k) \langle p|K_\ell(k^2)|k\rangle. \quad (17)$$

Similarly, for $p = k$, we also get

$$\langle k|\tilde{K}_\ell(k^2)|q\rangle = \cos^2\delta_\ell(k) \langle k|K_\ell(k^2)|q\rangle, \quad (18)$$

a result that follows from the Hermiticity of $\tilde{K}$ and K . Equations (17) and (18) are the half-off shell extensions of eq. (4), thus proving that for either on-shell or half-off-shell matrix elements one can calculate $\tilde{K}_\ell$ and then relate it in the same (simple) manner to the corresponding matrix elements of K_ℓ for both cases.

From these equations, we see that the fully off-shell values of $K_\ell(E)$ can also be obtained from $\tilde{K}_\ell(E)$. That is, if we use (17) and (18) to replace the product of half-off-shell matrix elements of K_ℓ in (16) with those of $\tilde{K}_\ell$, then we get

$$\begin{aligned} \langle p | \tilde{K}_\ell(k^2) | q \rangle &= \langle p | K_\ell(k^2) | q \rangle + \frac{\pi p k \tan \delta_\ell}{\cos^2 \delta_\ell} \\ &\times \langle p | \tilde{K}_\ell(k^2) | k \rangle \langle k | \tilde{K}_\ell(k^2) | q \rangle . \end{aligned} \quad (19)$$

This equation therefore gives the fully off-shell values of $K_\ell(E)$ in terms of the off-shell values of $\tilde{K}_\ell(E)$ and the on-shell values (i.e., $\delta_\ell(k)$).

Hence, while $\tilde{K}(E)$ is not the solution of (1), it is closely related to the solution: a determination of off-shell elements of $\tilde{K}$ leads to an evaluation of those of K itself. We therefore have shown formally that K can be found without either solving the integral equation (1) or constructing the operator $G^{(0)}$. This may prove to be of aid in determining off-shell values of the T matrix.

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