CHAPTER - 6
OFF-SHELL T AND K MATRICES - GENERAL FORMALISM

In possession of the off-shell wave functions with different boundary conditions one would like to construct expressions for the T and K matrices in terms of them. The half-off-shell T and K matrices are given by simple relations involving generalized Jost functions. In contrast to this the situation is little complicated for the off-shell case. For a potential which is regular at the origin the desired results can be obtained by using the operator equations (5.4) and (5.30). However, if the potential has a \( \frac{1}{r} \) singularity at the origin the wave function approach needs certain modification to deal with the situation. The plan of the present chapter is as follows:

We first describe how the wave function \( \psi^+_l(k,q,r) \) and \( \psi^D_l(k,q,r) \) could be used to calculate the fully off-shell T and K matrices in the case of regular potentials. Subsequently we modify this approach for potentials which have \( \frac{1}{r} \) singularity. This modification amounts to deriving expressions for T and K matrices which do not involve the potential explicitly. We conclude by noting that the results of Kouri and Levin follow from our treatment.
Combining (5.4), (5.7) and (5.11) we obtain the fully off-shell T matrix in the form

\[ \langle p | T_\ell(k^2) | q \rangle = \frac{2}{\pi pq} \int_0^\infty u_\ell(pr) v(r) \psi^+(k,q,r) \, dr. \quad (6.1) \]

Similarly (5.7), (5.30) and (5.36) can be combined to get

\[ \langle p | K_\ell(k^2) | q \rangle = \frac{2}{\pi pq} \int_0^\infty u_\ell(pr) v(r) \psi^P(k,q,r) \, dr. \quad (6.2) \]

Inserting the expression for \( \psi^+ \) and \( \psi^P \) from (5.16) and (5.38) the results in (6.1) and (6.2) can be conveniently expressed as

\[
\langle p | T_\ell(k^2) | q \rangle = \frac{2}{\pi pq} \left[ \int_0^\infty dr \, u_\ell(pr) v(r) \left\{ \beta_\ell(r) - \left( \frac{k}{q} \frac{\text{Im } f_\ell(k,q)}{\text{Re } f_\ell(k,q)} \right) \times \left[ \cos \delta(k) \alpha_\ell(r) - \sin \delta(k) \gamma_\ell(r) + i(\sin \delta(k) \alpha_\ell(r) + \cos \delta(k) \gamma_\ell(r)) \right] \right\} \right]
\]

\[ \tag{6.3} \]

and

\[
\langle p | K_\ell(k^2) | q \rangle = \frac{2}{\pi pq} \left[ \int_0^\infty dr \, u_\ell(pr) v(r) \left\{ \beta_\ell(r) - \left( \frac{k}{q} \frac{\text{Im } f_\ell(k,q)}{\text{Re } f_\ell(k,q)} \right) \times \left[ \cos \delta(k) \alpha_\ell(r) - \sin \delta(k) \gamma_\ell(r) \right] \right\} \right],
\]

\[ \tag{6.4} \]

where

\[
\alpha_\ell(r) = \cos \frac{l\pi}{2} \text{Re } f_\ell(k,r) + \sin \frac{l\pi}{2} \text{Im } f_\ell(k,r) \quad (6.5a)
\]

\[
\beta_\ell(r) = \cos \frac{l\pi}{2} \text{Im } f_\ell(k,q,r) - \sin \frac{l\pi}{2} \text{Re } f_\ell(k,q,r) \quad (6.5b)
\]
Equations (6.3) and (6.4) form the basis for computing off-shell $T$ and $K$ matrices by the wave function approach for regular potentials.

Looking at (6.3) and (6.4) we see that the matrix elements of the $T$ operator / $K$ operator have been expressed as a single quadrature over the potential sandwiched between a plane wave and an appropriate wave function. If the potential has $1/r$ singularity at the origin the matrix elements will involve certain integrals which are difficult to perform. This calls for deriving expressions for $T$ and $K$ matrices which do not involve potential \cite{44} explicitly. To accomplish this we closely follow the work of Picker, Reddish and Stephenson \cite{45} which was devised to calculate the half-off-shell $T$ matrix. In this work we are, however, interested in the off-shell $K$ matrix.

Following the notations used in chapter 5 we introduce the wave operator

$$\Omega(E) = 1 + G^S_0(E) K(E). \quad (6.6)$$

Therefore

$$G^S_0(E) K(E) = \Omega(E) - 1. \quad (6.7)$$
Taking (6.6) in the mixed representation
\[
\langle r | \Omega(E) | q lm \rangle = \left( \frac{2}{\pi} \right)^\frac{3}{2} j^*_\lambda(qr) y_{\lambda m}(r) + \left\langle r | g_0 S E | r' \right\rangle x \int dr \langle r | K(E) | q lm \rangle
\]
and
\[
(k^2 - \rho^2)^{-1} \langle plm | K(E) | q lm \rangle = \frac{2}{\pi} \int_0^\infty r^2 dr j^*_\lambda(qr)
\]
\[
x \left[ \eta_\lambda(k,q,r) - j^*_\lambda(qr) \right],
\]
\[
(6.8)
\]
In writing (6.8) and (6.9) we have assumed the potential to be central. The function \( \Omega(k,q,r) \) satisfies the differential equation
\[
\left[ \frac{k^2}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} - v(r) \right] \eta_\lambda(k,q,r)
\]
\[
= (k^2 - q^2) j^*_\lambda(qr).
\]
Outside the range of interaction the solution of (6.10) is given by
\[
\eta_\lambda(k,q,r) = j^*_\lambda(qr) + A_\lambda(k,q) \eta_\lambda(kr).
\]
(6.11)
The spherical Neumann function \( \eta_\lambda \) is included in (6.11) in order to incorporate the standing wave boundary condition involved in the \( K \) matrix determination. To facilitate the calculation we now rewrite (6.9) in the form
\[ \langle p\ell m | K(E) | q\ell m \rangle = \left( \frac{2}{\pi} \right) (k^2 - p^2) \int_0^\infty r^2 dr \, j_\ell (pr) \, A_\ell (k, q) \, \eta_\ell (kr) + \left( \frac{2}{\pi} \right) (k^2 - p^2) \int_0^\infty r^2 dr \, j_\ell (pr) \left[ -J_\ell (k, q, r) - j_\ell (qr) \right] - A_\ell (k, q) \, \eta_\ell (kr) \]. \quad (6.12)

Using the integral
\[ \int_0^\infty r^2 dr \, j_\ell (pr) \, \eta_\ell (kr) = - \left( \frac{k}{k - p} \right)^{-1} \left( \frac{p}{k} \right)^l \] \quad (6.13)
in the first term on the right hand side of (6.12), we get
\[ \langle p\ell m | K(E) | q\ell m \rangle = - \left( \frac{2}{\pi} \right) k^{-1} \left( \frac{p}{k} \right)^l A_\ell (q, k) + \left( \frac{2}{\pi} \right) (k^2 - p^2) \int_0^\infty r^2 dr \, j_\ell (pr) \left[ -J_\ell (k, q, r) - j_\ell (qr) \right] - A_\ell (q, k) \, \eta_\ell (kr) \]. \quad (6.14)

The half-off-shell version of (6.14) is obtained by substituting \( p = k \). We thus have
\[ A_\ell (q, k) = - \frac{1}{2} \sqrt{k} \, k \, \langle k\ell m | K(E) | q\ell m \rangle. \quad (6.15) \]

Inserting (6.15) in (6.14) we get
\[ \langle p\ell m | K(E) | q\ell m \rangle = \langle p\ell m | K(k^2) | q\ell m \rangle = \left( \frac{p}{q} \right)^l \langle k\ell m | K(k^2) | q\ell m \rangle + \left( \frac{2}{\pi} \right) \frac{k^2 - p^2}{pq} \int_0^\infty dr \, pr \, j_\ell (pr) \left[ -J_\ell (k, q, r) - qr \, j_\ell (qr) \right] + \frac{1}{2} \sqrt{k} \, q \, \langle k\ell m | K(k^2) | q\ell m \rangle \, kr \, \eta_\ell (kr) \]. \quad (6.16)
To deduce (6.16) we have also employed the relation (5.36). Equation (6.16) represents the basic formula for computing the off-shell $K$ matrix for potentials singular at the origin. This equation does not involve the potential explicitly. The term inside the squared bracket is singular at the origin. In fact, as $r \to 0$ this term goes as

$$\frac{1}{2} \pi q \left< k \ell m | K(k^2) | q \ell m \right> (2\ell - 1) !! (kr)^{-\ell}.$$ 

Since

$$pr j_{\ell}^*(pr) \sim (pr)^{l+1} r \to 0$$

the integrand on the right hand side of (6.16) is regular despite this singularity. Thus we see that with the above modification the wave function approach is also useful to deal with potentials which are not regular at the origin.

We now proceed to show that (6.3) and (6.4) can be combined to write the basic relation between the off-shell matrix elements of the operator $K$ and $\hat{K}$ as deduced by Kouri and Levin. From (6.3) the real part of the $T$ matrix is given by

$$\text{Re} \left< p | T_{\ell}(k^2) | q \right> = \frac{2}{\pi pq} \left[ \int_0^\infty dr u_{\ell}(pr) v(r) \right]_{\ell} \beta_{\ell}(r)$$

$$\left. - \frac{\ell}{q} \frac{\text{Im} f_{\ell}(k,q)}{|f_{\ell}(k)|} \left[ \cos \delta_{\ell}(k) \alpha_{\ell}(r) - \sin \delta_{\ell}(k) \gamma_{\ell}(r) \right] \right\}.$$  (6.17)

We have seen that the real part of $T$ matrix is related to the matrix element of the altered $K$ by
Equations (6.4), (6.17) and (6.18) can be combined to get

\[
\langle p \mid \tilde{K}_k(k^2) \mid q \rangle = \langle p \mid K_k(k^2) \mid q \rangle.
\]  

(6.18)

Equations (6.4), (6.17) and (6.18) can be combined to get

\[
\begin{align*}
\langle p \mid \tilde{K}_k(k^2) \mid q \rangle & - \langle p \mid K_k(k^2) \mid q \rangle \\
& = \frac{2}{\pi \rho q} \int_0^{\infty} dr \ u_\ell \ (pr) \ v(r) \left[ \frac{\alpha_\ell(x)}{\cos \delta_\ell} - (\cos \delta_\ell' \ - \sin \delta_\ell') \right] x \left( \frac{k}{q} \right) \frac{\text{Im} f_\ell(k, q)}{|f_\ell(k)|}.
\end{align*}
\]  

(6.19)

Equation (6.19) can now be simplified by using \( \text{Re} \langle k \mid T_k(k^2) \mid q \rangle \) in terms of Jost functions and \( \text{Re} \langle p \mid T_k(k^2) \mid k \rangle \) obtained by substituting \( q = k \) in (6.17). In particular, we use the following relations for the real part of the half-off-shell \( T \) matrices.

\[
\text{Re} \langle k \mid T_k(k^2) \mid q \rangle = \langle k \mid \tilde{K}_k(k^2) \mid q \rangle = \left( \frac{k}{q} \right) \frac{2 \text{Im} f_\ell(k, q) \cos \delta_\ell(k)}{\pi q |f_\ell(k)|}.
\]  

(6.20)

and

\[
\begin{align*}
\text{Re} \langle p \mid T_k(k^2) \mid k \rangle = \langle p \mid \tilde{K}_k(k^2) \mid k \rangle & = \frac{2}{\pi \rho k} \int_0^{\infty} dr \ u_\ell \ (pr) \ v(r) x \left\{ \gamma_\ell(r) - \frac{\text{Im} f_\ell(k)}{|f_\ell(k)|} \right\} (\cos \delta_\ell' \ - \sin \delta_\ell') \} \right].
\end{align*}
\]  

(6.21)

In view of (6.20), (6.21) and the fact that \( \sin \delta_\ell(k) = \frac{\text{Im} f_\ell(k)}{|f_\ell(k)|} \), (6.19) can be simplified to
Equation (6.22) shows that the off-shell K matrix obtained by the wave function approach satisfies the relation between the off-shell elements of $\widetilde{K}$ and $\tilde{K}$ of Kouri and Levin c.f. (4.23). The half-off-shell ($p = k$) and on-shell ($p = q = k$) versions of (6.22) yield the corresponding expressions given in (4.22) and (4.6).

The constraint derived by Kouri and Levin in (4.24) follows from our approach in a rather straightforward way since the phase of the half-off-shell $T$ matrix is the phase shift.

Thus there is no physical uncertainty in using the wave function approach developed here. The calculational advantages of our method will be made clear in the next two chapters.