CHAPTER - 3

INTEGRAL FORM OF THE SCHRÖDINGER EQUATION AND OFF-SHELL SCATTERING

3.1 Lippmann-Schwinger equation

In the previous chapter we have introduced the concept of Jost solution and Jost function and constructed expressions for the regular, physical and principal value wave functions in terms of them. We have noted that the Jost function corresponding to a particular partial wave has two important properties.

(i) Its phase is the negative of the phase shift for the partial wave, and

(ii) its zeroes in the upper half of the complex k plane correspond to the energies of the bound states which occur in that partial wave. Thus the Jost function for a two-particle system is directly related to the observable of the system. The phase shifts for a two-particle system can be used to describe two-particle or on-shell scattering amplitudes for the system. However, if we consider a many-particle system, the various pairs of particles do not scatter elastically from each other such that we require the knowledge of two-particle off-shell amplitudes to deal with the

situation. We devote this chapter to bring out the basic philosophy underlying off-energy-shell potential scattering and describe certain aspects of the two-body T and K matrix calculation.

Following our notations of chapter 2 we begin with the three dimensional Schrödinger equation

$$(\nabla^2 + k^2)\, \psi(\underline{r}) = v(r)\, \psi(\underline{r}) = \rho(\underline{r}). \qquad (3.1)$$

The Green's function $G_o(\underline{r}, \underline{r}')$ satisfies the Schrödinger equation with a delta function source

$$(\nabla^2 + k^2)\, G_o(\underline{r}, \underline{r}') = \delta(\underline{r}-\underline{r}'). \qquad (3.2)$$

In terms of $G_o(\underline{r}, \underline{r}')$ we can write a formal integral equation for $\psi(\underline{r})$ as follows

$$(\nabla^2 + k^2)\, \psi(\underline{r}) = \int d^3r'\ \rho(\underline{r}')\ \delta(\underline{r}-\underline{r}'). \qquad (3.3)$$

Using (3.2) and (3.3) we have

$$(\nabla^2 + k^2)\, \psi(\underline{r}) = \int d^3r' \rho(\underline{r}')\ (\nabla^2 + k^2)\ G_o(\underline{r}, \underline{r}'). \qquad (3.4)$$

Thus a particular solution of (3.4) is

$$\psi_1(\underline{r}) = \int d^3r' \, \rho(\underline{r}') \, G_o(\underline{r},\underline{r}'). \tag{3.5}$$

The general solution of (3.1) is the sum of the particular solution and a solution of the homogeneous equation

$$(\nabla^2 + k^2) \, \varphi(\underline{r}) = 0. \tag{3.6}$$

Thus

$$\psi(\underline{r}) = \varphi(\underline{r}) + \int d^3r' \, G_o(\underline{r},\underline{r}') \, v(\underline{r}') \, \psi(\underline{r}'). \tag{3.7}$$

Equation (3.7) represents the integral equation for the wave function. From (3.6) we have

$$\varphi(\underline{r}) = Ae^{-i\underline{k}.\underline{r}} + Be^{-i\underline{k}.\underline{r}}. \tag{3.8}$$

The particular integral $\psi_1(\underline{r})$ can be expanded in terms of the complete orthogonal set $\varphi(\underline{r})$ giving

$$\psi_1(\underline{r}) = \int d^3k' \, A(\underline{k}') \exp(i\underline{k}'.\underline{r}). \tag{3.9}$$

Operating $(\nabla^2 + k^2)$ on (3.9) we get back the differential form of Schrodinger equation provided

$$\rho(\underline{r}) = \int d^3k' \, (k^2 - k'^2) \, A(\underline{k}') \, e^{i\underline{k}'.\underline{r}}. \tag{3.10}$$

Multiplying (3.10) by $\exp(-i\underline{k}''.\underline{r})$ and integrating over r we get

$$A(\underline{k}') = \frac{1}{(2\pi)^3 (\underline{k}^2 - \underline{k}'^2)} \int d^3r \ \rho(r) \exp(-i\underline{k}'.\underline{r}). \quad (3.11)$$

Combining (3.9) and (3.11)

$$\psi_1(r) = (2\pi)^{-3} \int \frac{d^3k'}{(k^2-k'^2)} \int d^3r' v(r') \psi(\underline{r}') \exp[i\underline{k}'. (\underline{r}-\underline{r}')]. \quad (3.12)$$

Comparison of (3.5) and (3.12) yields

$$G_o(\underline{r},\underline{r}') = (2\pi)^{-3} \int \frac{d^3k'}{k^2-k'^2} \exp[i\underline{k}'. (\underline{r}-\underline{r}')] . \quad (3.13)$$

Equation (3.13) represents the integral form of Green's function. An integral equation embodies the boundary condition within it through an appropriate Green's function. The Green's function which represents an outgoing spherical wave in addition to the incident plane wave has the form

$$G_o^+(\underline{r},\underline{r}') = (2\pi)^{-3} \lim_{\epsilon \to 0} \int \frac{\exp[i\underline{k}'. (\underline{r}-\underline{r}')]}{k^2 - k'^2 + i\epsilon} d^3k'. \quad (3.14)$$

Clearly the term + $i\epsilon$ in the denominator defines the singularity of the Green's function and goes to zero after the integral has been performed. The superscript $+$ on G_o relates to the outgoing wave boundary condition. Carrying out the integrations in (3.14) over the directions of k and using Cauchy's theorem one gets

$$G_o^+ (\underline{r},\underline{r}') = - \frac{\exp (ik|\underline{r}-\underline{r}'|)}{4\pi |\underline{r}-\underline{r}'|}. \qquad (3.15)$$

Substituting (3.15) in (3.7) we obtain

$$\psi^+ (\underline{r}) = e^{i\underline{k}\underline{r}} - \frac{1}{4\pi} \int d^3r' \frac{\exp(ik |\underline{r}-\underline{r}'|)}{|\underline{r} - \underline{r}'|} v(\underline{r}') \psi^+(\underline{r}'). \qquad (3.16)$$

In (3.16) if we allow r to tend to ∞ we find

$$\psi^+ (\underline{r}) \underset{r\to\infty}{\to} e^{i\underline{k}.\underline{r}} + \frac{e^{ikr}}{r} \left(-\frac{1}{4\pi}\right) \int d^3r' e^{-i\underline{k}'.\underline{r}'} v(\underline{r}') \psi^+ (\underline{r}'), \qquad (3.17)$$

where we have used the asymptotic behavior of the free particle Green's function

$$G^+ (\underline{r},\underline{r}') \underset{r\to\infty}{\longrightarrow} -\left(\frac{1}{4\pi}\right) \frac{e^{ikr}}{r} e^{-i\underline{k}'.\underline{r}'} \qquad (3.18)$$

with $\underline{k}'$ directed along r and defined by $\underline{k}' = k\hat{r}$. From (3.17) we obtain the integral expression for the scattering amplitude $f(\theta)$ as

$$f(\theta) = -\frac{1}{4\pi}\int d^3r' \, e^{-i\underline{k}'\cdot\underline{r}'} \, v(\underline{r}') \, \psi^+(\underline{r}'). \tag{3.19}$$

It is convenient to define a quantity proportional to the scattering amplitude

$$T(\underline{k}',\underline{k}) = -4\pi f(\theta) = \int d^3r \, e^{-i\underline{k}'\cdot\underline{r}} \, v(\underline{r}) \, \psi^+_{\underline{k}}(\underline{r}). \tag{3.20}$$

We shall call $T(\underline{k}',\underline{k})$ the T matrix, or transition amplitude, which describes the physical situation in which there is an incident plane wave in the entrance channel and scattered outgoing wave in all other channels. Similarly, we define $v(\underline{k}',\underline{k})$ to be

$$v(\underline{k}',\underline{k}) = \int d^3r \; e^{-i\underline{k}'\cdot\underline{r}} \, v(\underline{r}) \, e^{i\underline{k}\cdot\underline{r}} \tag{3.21}$$

The quantity $v(\underline{k}',\underline{k})$ may be called the V matrix or potential matrix. If the plane wave $e^{i\underline{k}\underline{r}}$ is substituted for the wave function $\psi^+_{\underline{k}}(\underline{r})$ in the definition of the T matrix, the V matrix is obtained. The V matrix is then the Born approximation to the T matrix.

Multiplying (3.16) by $e^{-i\underset{\sim}{k}'.\underset{\sim}{r}}$ $v(r)$ and integrating over all space we get

$$T(\underset{\sim}{k}',\underset{\sim}{k}) = v(\underset{\sim}{k}',\underset{\sim}{k}) + \int d^3r' \int d^3r \exp(-i\underset{\sim}{k}'.\underset{\sim}{r})\, v(\underset{\sim}{r})\, G^+(\underset{\sim}{r},\underset{\sim}{r}')\, v(\underset{\sim}{r}')\, \psi^+(\underset{\sim}{r}'). \qquad (3.22)$$

Combining (3.14) and (3.22) we obtain

$$T(\underset{\sim}{k}',\underset{\sim}{k}) = v(\underset{\sim}{k}',\underset{\sim}{k}) + \int \frac{d^3k''}{(2\pi)^3} \frac{v(\underset{\sim}{k}',\underset{\sim}{k}'')\, T(\underset{\sim}{k}'',\underset{\sim}{k})}{k^2 - k'^2 + i\epsilon}\,. \qquad (3.23)$$

This is referred to as the Limppmann-Schwinger equation [37].

3.2 Off-energy-shell potential scattering

The Lippmann Schwinger equation gives a direct relation between T matrix and V matrix eliminating in the intermediate step the problem of finding the wave function. It thus appears that we have considerably simplified the algebra involved in the calculation of T matrices. But unfortunately the situation is not that simple. To solve (3.23) we must find $T(\underset{\sim}{k}',\underset{\sim}{k})$ not only when energy is conserved, that is, when $k' = k$, but also for all other values of k'. In all scattering processes energy is conserved. From this point of view T matrices for $k \neq k'$ may be regarded as unphysical amplitudes. The necessity for including these physically unmeasurable

contributions in the integral equation for $T(\underline{k}',\underline{k})$ may be delineated as follows. Using (3.7), (3.14) and (3.20) we can write

$$\psi^+(\underline{r}) = e^{i\underline{k}.\underline{r}} + \int \frac{d^3k'}{(2\pi)^3} \frac{\exp(i\underline{k}'.\underline{r})\ T(\underline{k}',\underline{k})}{k^2-k'^2 + i\epsilon} \quad . \qquad (3.24)$$

We see that a knowledge of the T matrix $T(\underline{k}',\underline{k})$ for all values of k' is equivalent to a knowledge of the wave function itself. Let us examine the relation of T matrix on-energy-shell to the wave function in (3.24). To do so we rewrite (3.24) in the form

$$\psi^+(\underline{r}) = e^{i\underline{k}.\underline{r}} + \int \frac{d^3k'}{(2\pi)^3} \frac{\exp(i\underline{k}'.\underline{r})\ T(\hat{k}\underline{k}',\underline{k})}{k^2-k'^2 + i\epsilon}$$

$$+\int \frac{d^3k'}{(2\pi)^3} \frac{\exp(i\underline{k}'.\underline{r})\left\{T(\underline{k}',\underline{k}) - T(\hat{k}\underline{k}',\underline{k})\right\}}{k^2 - k'^2 + i\epsilon} . \qquad (3.25)$$

Here $\hat{\underline{k}}'$ is a unit vector in the direction of $\underline{k}'$. In (3.25) the second term represents the contribution to the wave function from the on-energy shell T matrix while the third term gives the contribution from the off-shell region. To perform the integral in the second term we take the expression for the T matrix given in (3.20) and insert it in the second term of (3.25). Using the Legendre expansions for the plane

waves that occur in the integral and carrying out integrations over k' we can show that

$$\int \frac{d^3 k'}{(2\pi)^3} \frac{\exp(i\underline{k}'.\underline{r}) \exp(-ik\hat{\underline{k}}'.\underline{r}')}{k^2 - k'^2 + i\epsilon} = -\frac{1}{4\pi k} \sum_{\ell=0}^{\infty} (2\ell+1)$$

$$\times\, w_\ell^+(kr)\, u_\ell(kr')\, P_\ell(\cos\theta_{rr'}) \qquad (3.26)$$

where $\theta_{rr'}$ is the angle between the directions of $\underline{r}$ and $\underline{r}'$. Introducing Legendre expansion for the plane wave that occurs in the eexpression for $G_o(\underline{r},\underline{r}')$ [Eq. (3.15)] we get

$$G_o^+(\underline{r},\underline{r}') = -\frac{1}{4\pi k} \sum_{\ell=0}^{\infty} (2\ell+1)\, P_\ell(\cos\theta_{rr'})$$

$$\times \begin{cases} u_\ell(kr)\, w_\ell^+(kr') & , \ r < r' \\ w_\ell^+(kr)\, u_\ell(kr') & , \ r > r' \end{cases}$$

in agreement with (2.44).

Comparing (3.26) and (3.27) we see that the right hand side of (3.26) is just the Legendre expansion of the outgoing wave Green's function when $r > r'$. Outside the range of the potential where r must be greater than r', the second term in (3.25) is then simply

$$\int \frac{d^3 k'}{(2\pi)^3} \frac{\exp(i\underline{k}'.\underline{r})\, T(\underline{k}',\underline{k})}{k^2 - k'^2 + i\epsilon} = \int d^3 r'\, G^+(\underline{r},\underline{r}')\, v(\underline{r}')\, \psi_{\underline{k}}^+(\underline{r}') \qquad (3.28)$$

which is the full scattered wave.

Thus we see that T matrix "on-the-energy-shell" implies knowledge of the wave function beyond the range of interaction. Contrary to this the T matrix "off-the-energy-shell" suggests the knowledge of the wave function within the range of interaction. Interestingly, we are not in the know of what is happening within the interaction region. We are collecting scattering data with the help of detector placed well beyond the range of interaction. So off-shell contributions are really unmeasurable quantities. The need to include these quantities in the integral equation for $T(\underline{k}',\underline{k})$ is equivalent to the need to evaluate the wave function inside the potential.

As already noted in nuclear scattering involving more than two bodies, energy and momentum are not necessarily conserved because momentum can be absorbed by the other particles. This is called a virtual process which can be described in terms of the off-shell T matrix elements. This is what makes knowledge of the off-energy behavior of the two nucleon T matrix basic to the understanding of nuclear scattering involving a many-nucleon system. Furthermore, in the domain of nucleon-nucleon interactions, there is no well established law of interaction and the question as to whether or not only two-body forces are important is not yet properly understood. Certain qualitative features are of course well known, such as existence of a long range (one pion exchange type interaction) and presumably

a short range spin orbit force. These and other features of the two-body forces have significant effects not only on the behavior of the two-body system but also on more general systems consisting of more than two-nucleons. More specifically, the off-shell elements of a two-body potential have more readily observable effects on the behavior of a few-body system $N > 2$ than a mere study of two-body system would reveal. The three-body system, being the simplest one with $N > 2$, affords a unique opportunity of learning more about the qualitative features of a two body potential and of deciding on questions like the adequecy of two-body forces for the description of more complex nuclear phenomena. Again, to resolve the ambiguity in the effective nucleon-nucleon interaction one must study problems such as nuclear matter, p-p bremsstrahlung three-body bound states and scattering phenomena etc., which involve off-energy-shell T matrix elements.

3.3 K (reactance) matrix

The Lippmann-Schwinger equation for the T matrix given by (3.23) cannot be solved by simple analytical methods. One usually takes recourse to approximation techniques, which can be demonstrated by writing (3.23) in the operator form namely

$$T = V + V \frac{1}{E-H_o + i\epsilon} V + V \frac{1}{E - H_o + i\epsilon} V \frac{}{E - H_o + i\epsilon} V + \ldots \tag{3.28a}$$

where E is the kinetic energy operator and H_o the free-particle Hamiltonian.

For the whole series in (3.28a) the unitarity condition is satisfied but for a finite order in the series the condition is violated. If the power series is rapidly convergent, this violation may not seriously affect the numerical results. For instance, a weak inelastic process may not seriously deplete the incident state, and a first order Born approximation could give reliable results. When the incident state is seriously damped by such a process, the restrictions of unitarity must be taken into account to obtain accurate results. So for practical applications one often wants a formulation that permits approximate calculation incorporating the conditions of unitarity. This can be accomplished by introducing operator $\mathcal{K}$ through Caley transformation

$$S = \frac{1 - \frac{i\mathcal{K}}{2}}{1 + \frac{i\mathcal{K}}{2}} \tag{3.29}$$

Here $\mathcal{K}$ is connected to the reactance operator K by

$$\mathcal{K} = 2\pi\delta\,(E-H_o)K\,. \tag{3.30}$$

The K matrix (reaction Matrix) refer to a physical situation in which there is a plane wave in the incident channel and standing scattered waves in all other channels.

Relations similar to (3.30) hold between an operator τ and the usual T matrix. In analogy to (3.29) and (3.30) we have

$$S = 1 - i\tau \tag{3.31}$$

and

$$\tau = 2\pi\delta(E-H_o)T. \tag{3.32}$$

Comparing (3.29) and (3.31) we have

$$\tau = \kappa - \frac{i\kappa\tau}{2}. \tag{3.33}$$

Now using (3.30) and (3.32) in (3.33) we can write

$$T = K - i\pi K\ \delta(E - H_o)T \tag{3.34}$$

and equivalently

$$K = T + i\pi T\ \delta(E - H_o)\ K. \tag{3.35}$$

Equations (3.34) and (3.35) and usually termed as Heitler damping equation. To use the damping equation, one usually assumes that K is known from some previous approximate

calculation ; then T is determined from this equation. We shall see that so long K is hermitian, the T matrix obtained from this equation will satisfy the unitary condition.

Equations (3.34) or (3.35) was derived as a relation between on-the-energy shell matrix elements. Such matrix elements are not sufficient by themselves to determine the operator K. We shall fix the off-the-energy-shell matrix elements by assuming that (3.34) holds both for on and off-energy shell or in other words it is a generally valid operator relation.

As usual we consider the Lippmann-Schwinger equation

$$T = V + V \frac{1}{E - H_o + i\epsilon} T \qquad (3.36)$$

and substitute it in (3.35) to get

$$K = V + V \frac{P}{E - H_o} K \qquad (3.37)$$

where

$$\frac{P}{E - H_o} = \frac{1}{E - H_o + i\epsilon} + i\pi\delta (E - H_o). \qquad (3.38)$$

The operator $\frac{P}{E - H_o}$ is called the principal value Green's function written as

$$\frac{P}{E - H_o} = \lim_{\epsilon \to 0} \frac{1}{2} \left[\frac{1}{E - H_o + i\epsilon} + \frac{1}{E - H_o - i\epsilon} \right] \quad (3.39)$$

The principal value Green's function is thus a superposition of outgoing and ingoing wave Green's function. Equation (3.37) has the same structure as the integral equation for T ; only the definition of the Green's function is changed. As an outgoing state was involved in the T matrix, we can associate a new type of state with K . Obviously this new state will contain standing waves, in addition to the usual incident plane wave. We can show that K need not be obtained exactly to maintain unitarity since any Hermitian operator $\tilde{K}$, when inserted into the damping equation, will yield a T matrix satisfying the unitarity condition.

To see this let us introduce

$$T = \tilde{K} + i\pi T^{\dagger} \delta(E - H_o) \tilde{K} \quad . \quad (3.40)$$

This together with (3.34) yields

$$T = \tilde{K} - i\pi T^{\dagger} \delta(E-H_o)\, T - \pi^2 T^{\dagger} \delta(E-H_o)\, \tilde{K}\, \delta(E-H_o)\, T$$

$$T^{\dagger} = \tilde{K} + i\pi T^{\dagger} \delta(E-H_o)\, T - \pi^2 T^{\dagger} \delta(E-H_o)\, \tilde{K}\, \delta(E-H_o)\, T$$

and

$$T - T^{\dagger} = - 2\pi i T^{\dagger} \delta(E - H_o) T. \qquad (3.41)$$

Thus any Hermitian K matrix leads to a T matrix satisfying proper unitarity condition. This fact is quite encouraging to initiate development of description of physical process in terms of the K matrix. But unfortunately, the solution of the integral equation for the K matrix is more difficult than that for the T matrix. This can be seen as follows.

From (3.36) we can write

$$T = V + V G_o^{+} T \qquad (3.42)$$

Again the full wave Green's function G^{+} is written as

$$\begin{aligned} G^{+} &= G_o^{+} + G_o^{+} V G^{+} \\ &= G_o^{+} + G_o^{+} V G_o^{+} + G_o^{+} V G_o^{+} V G_o^{+} + \ldots\ldots \end{aligned} \qquad (3.43)$$

From (3.42) we have

$$\begin{aligned} T &= V + V G_o^{+} T \\ &= V + V G_o^{+} T + V G_o^{+} V G_o^{+} V + \ldots\ldots \\ &= V + V \left[G_o^{+} + G_o^{+} V G_o^{+} + G_o^{+} V G_o^{+} V G_o^{+} + \ldots\ldots \right] V \\ &= V + V G^{+} V, \end{aligned} \qquad (3.44)$$

where we have used the iterated version of G from (3.43).

So the Lippmann-Schwinger equation has a formal solution. In contrast to this the K matrix equation

$$K = V + V \frac{P}{E - H_o} K$$

cannot be written in the form

$$K \neq V + V \frac{P}{E - H} V \qquad (3.45)$$

because of the fact that the principal value Green's function does not have Lippmann-Schwinger iteration like the ordinary Green's function [30] .

Formal solutions are crucial for developing iteration techniques to solve Lippmann-Schwinger equation. For the K matrix iterative techniques are not applicable because of the restriction put in (3.45) and so determination of K is not possible. Keeping this in mind kouri and Levin have developed a formalism to obtain the K operator without solving the integral equation (3.37). In the next chapter we describe their method with particular emphasis on the off-shell scattering.