Chapter 12

Elements of Formal Scattering Theory

12.1 Scattering States

In the previous chapter, we more or less phenomenologically derived the boundary conditions for the scattering states. We now want to introduce a more formal definition. The time-dependent Schrödinger equation

$$\hbar i \ \mid \dot{\psi}(t)\rangle \ = \ H \ \mid \psi(t)\rangle \tag{12.1}$$

with $H = H_0 + V$, and $H_0 = \frac{P^2}{2m}$ has the solution

$$\mid \psi(t)\rangle \ = \ e^{-\frac{i}{\hbar} Ht} \ \mid \psi(0)\rangle \ . \tag{12.2}$$

A reasonable requirement that (12.2) is a scattering state will be to require that long before and after the scattering process $\mid \psi(t)\rangle$ behaves like a free wave packet $\mid \varphi_a(t)\rangle$. Mathematically we can formulate this with the norm as

$$\| \mid \psi_a^{(+)}(t)\rangle - \mid \varphi_a(t)\rangle \| = \| \ e^{-\frac{i}{\hbar} Ht} \mid \psi_a^{(+)}(0)\rangle - e^{-\frac{i}{\hbar} H_0 t} \mid \varphi_a(0)\rangle \ \| \stackrel{t\to-\infty}{\longrightarrow} \ 0 \tag{12.3}$$

where the limit $t \to -\infty$ implies that long before the scattering $\mid \psi_a^{(+)}(0)\rangle$ should behave as a free wave. The index a denotes an arbitrary initial distribution of momenta in the wave packet.

$$\begin{aligned} \| \ e^{\frac{i}{\hbar} Ht} \left(e^{\frac{-i}{\hbar} Ht} \ \mid \varphi_a^{(+)}(0)\rangle \right. \ &- \ \left. e^{-\frac{i}{\hbar} H_0 t} \ \mid \varphi_a(0)\rangle \right) \ \| \\ &= \ \| \mid \psi_a^{(+)}(0)\rangle - e^{\frac{i}{\hbar} Ht} \ e^{-\frac{1}{\hbar} H_0 t} \mid \varphi_a(0)\rangle \ \| \stackrel{t\to-\infty}{\longrightarrow} \ 0 \ . \end{aligned} \tag{12.4}$$

Thus, we can define a scattering state as

$$| \psi_a^{(+)} \rangle \;=\; s - \lim_{t \to -\infty} \; e^{\frac{i}{\hbar} \, Ht} \, e^{-\frac{i}{\hbar} \, H_0 t} \, | \, \varphi_a \rangle \;=\; \Omega^{(+)} \, | \, \varphi_a \rangle \tag{12.5}$$

where we defined the Møller operator

$$\Omega^{(+)} \;:=\; s - \lim_{t \to -\infty} \; W(t) \;=\; s - \lim_{t \to -\infty} \; e^{\frac{i}{\hbar} \, Ht} \, e^{-\frac{i}{\hbar} \, H_0 t} \; . \tag{12.6}$$

In order to show the existence of the Møller operator, we have to show the convergence. Let $t_2 < t_1 < 0$ and consider

$$\begin{aligned} \| \, [W(t_2) - W(t_1)] \, \varphi_a \, \| \;&=\; \| \int_{t_1}^{t_2} \; dt \; \frac{dW(t)}{dt} \; \varphi_a \, \| \\ &\leq\; | \int_{t_1}^{t_2} \; dt \;\; \| \, \frac{dW(t)}{dt} \; \varphi_a \, \| \, | \\ &=\; | \int_{t_1}^{t_2} \; dt \;\; \| \, e^{\frac{i}{\hbar} \, Ht} \; \frac{1}{\hbar} \; (H - H_0) \; e^{-\frac{i}{\hbar} \, H_0 t} \; \varphi_a \, \| \, | \\ &=\; | \int_{t_1}^{t_2} \; dt \; \frac{1}{\hbar} \;\; \| \, V \; e^{-\frac{i}{\hbar} \, H_0 t} \; \varphi_a \, \| \, | \\ &=\; | \int_{t_1}^{t_2} \; dt \; \frac{1}{\hbar} \;\; \| \, V \; \varphi_a(t) \, \| \, | \;\; . \end{aligned} \tag{12.7}$$

The existence of the integral means that the norm $\| \cdot \|$ has to fall off at least as $\frac{1}{|t|^{1+\varepsilon}}$. We already showed that a free wave packet decays as $\frac{1}{|t|^{3/2}}$. If V only exists in a finite range, one only has to integrate over a finite region, and then the fall-off in t is sufficient. To show this, let us consider the norm in (12.7) separately.

$$\| \, V \; \varphi_a(\vec{r}) \, \|^2 \;=\; \int \; d^3x \; V^2(\vec{x}) \;\; | \; \varphi_a(\vec{x}, t) \; |^2 \tag{12.8}$$

We assume that V is square integrable, i.e., a vector in the Hilbert space. If, e.g., V is local and real, e.g., $e^{-\mu r}/r$, this is certainly fulfilled. (V square integrable means $\int \; d^3x \; V^2(\vec{x}) < \infty$.) Then (12.8) becomes

$$\begin{aligned} \int \; d^3x \; V^2(\vec{x}) \;\; | \; \varphi_a(\vec{x}, t) \; |^2 \;&\leq\; \int \; d^3x \;\; | \; V(\vec{x}) \; |^2 \; | \; \varphi_a(\vec{x}, t) \; |^2 \\ &\leq\; \int \; d^3x \; V^2(\vec{x}) \; \frac{c}{t^3} \\ &=\; \frac{c}{t^3} \; \int \; d^3x \; V^2(x) \;\; = \;\; \frac{c}{t^3} \;\; \cdot c' \end{aligned} \tag{12.9}$$

and thus

$$\| \, V \; \varphi_a(\vec{r}) \, \| \leq \; \frac{\bar{c}}{| \; t \; |^{3/2}} \; . \tag{12.10}$$

For the original estimate (12.7) then follows

$$| \int_{t_1}^{t_2} dt \, \frac{1}{\hbar} \, \| V \, \varphi_a(t) \| | \leq | \int_{t_1}^{t_2} dt \, \frac{\bar{c}}{\hbar} \, \frac{1}{| t |^{3/2}} \leq | \frac{1}{| t_2 |^{1/2}} - \frac{1}{| t_1 |^{1/2}} | \stackrel{t \to -\infty}{\longrightarrow} 0 \quad (12.11)$$

Thus, for square-integrable potentials, the Møller operator exists. If $V \doteq V(\vec{r})$, then $V \sim \frac{1}{r^{3/2+\varepsilon}}$ in order to be square integrable. It can actually be shown (Kupsch-Sandhas theorem) that the Møller operators exist if the potential

$$| V(\vec{r}) | \leq \frac{c}{r^{1+\varepsilon}} \quad (12.12)$$

for $r \geq R$, i.e., falls off for large r faster than the Coulomb potential. We can always expand a wave packet $| \varphi_a \rangle \in \mathcal{H}$ with respect to plane waves

$$| \varphi_a \rangle = \int d^3p \; | \vec{p} \rangle \langle \vec{p} \, | \, \varphi_a \rangle = \int d^3p \; | \vec{p} \rangle \; \tilde{\varphi}_a(\vec{p}) \; . \quad (12.13)$$

The scattering state is then given by

$$\begin{aligned} | \psi^{(+)} \rangle &= \Omega^+ \, | \, \varphi_a \rangle \\ &= \int d^3p \; \Omega^+ \, | \, \vec{p} \, \rangle \; \tilde{\varphi}_a(\vec{p}) \\ &= \int d^3p \; | \, \vec{p} \, \rangle^{(+)} \; \tilde{\varphi}_a(\vec{p}) \end{aligned} \quad (12.14)$$

where we define

$$\Omega^{(+)} \; | \, \vec{p} \, \rangle = | \, \vec{p} \, \rangle^{(+)} \; . \quad (12.15)$$

Here that states $| \, \vec{p} \, \rangle^{(+)}$ correspond to the scattering states. The distribution function $\tilde{\varphi}_a(\vec{p})$ is the same for the free wave packet and the scattering state, only the "basis vectors" change when going to scattering states.

12.2 Properties of the Scattering States

In (12.6) we have defined the Møller operator as limit for $t \to -\infty$ of the operator

$$W(t) := e^{\frac{i}{\hbar} Ht} \, e^{-\frac{i}{\hbar} H_0 t} \; . \quad (12.16)$$

To investigate properties of the Møller operator, we consider

$$\lim_{t \to \infty} \| (W(t) - \Omega^+) \varphi \| = \lim_{t \to \infty} (\| W(t) \varphi \| - \| \Omega^+ \varphi \|) = 0 \; , \quad (12.17)$$

from which follows (since $W(t)$ unitary)

$$\lim_{t\to-\infty} \parallel W(t)\varphi \parallel = \parallel \Omega^{(+)}\varphi \parallel = \parallel \varphi \parallel \tag{12.18}$$

from which we can extract that

$$\langle \varphi \mid \varphi \rangle \;=\; \langle \Omega^{(+)}\varphi \mid \Omega^{(+)}\varphi \rangle \;=\; \langle \varphi \mid (\Omega^{(+)})^{\dagger}\; \Omega^{(+)} \mid \varphi \rangle \;, \tag{12.19}$$

or since $\mid \varphi \rangle$ is an arbitrary state

$$(\Omega^{(+)})^{\dagger}\; \Omega^{(}+) \;=\; \mathbf{1} \;. \tag{12.20}$$

The Møller operator is an isometric operator (preserves the norm); however, it is **not** a unitary operator, i.e., a left inverse does not exist. Next we consider

$$\begin{aligned} {}^{(+)}\langle \vec{p}\,' \mid \vec{p}\,\rangle^{(+)} \;=\; \langle \Omega^{(+)}\vec{p}\,' \mid \Omega^{(+)}\vec{p}\,\rangle \;&=\; \langle \vec{p}\,' \mid (\Omega^{(+)})^{\dagger}\; \Omega^{(+)} \mid \vec{p}\,\rangle \\ &=\; \langle \vec{p}\,' \mid \vec{p}\,\rangle \;=\; \delta(\vec{p}\,' - \vec{p}\,) \;. \end{aligned} \tag{12.21}$$

(12.21) shows that the scattering solutions are normalized to a δ-function in the same way the plane waves are. For further studying the properties of the states $\mid p\rangle^{(+)}$, we rewrite $\Omega^{(+)}$ as

$$\begin{aligned} \Omega^{(+)} \;&=\; s - \lim_{t\to-\infty}\; e^{\frac{i}{\hbar}\; Ht}\; e^{-\frac{i}{\hbar}\; H_0 t} \\ &=\; s - \lim_{t\to-\infty}\; e^{\frac{i}{\hbar}\; H(t-\tau)}\; e^{-\frac{i}{\hbar}\; H_0 (t-\tau)} \\ &=\; e^{-\frac{i}{\hbar}\; H\tau}\; \Omega^{(+)}\; e^{\frac{i}{\hbar}\; H_0 \tau} \;. \end{aligned} \tag{12.22}$$

Differentiating with respect to τ and evaluating at $\tau = 0$ leads to

$$0 \;=\; \frac{i}{\hbar}\; H\Omega^{(+)} \;-\; \frac{i}{\hbar}\; \Omega^{(+)}\; H_0$$

from which the so-called "intertwining relation" results:

$$H\Omega^{(+)} \;=\; \Omega^{(+)}\; H_0 \;. \tag{12.23}$$

Applying (12.23) on a plane wave state $\mid \vec{p}\rangle$ gives

$$\begin{aligned} H\Omega^{(+)} \;\mid \vec{p}\,\rangle \;&=\; \Omega^{(+)}\; H_0 \;\mid \vec{p}\,\rangle \\ &=\; \Omega^{(+)}\; \frac{P^2}{2m} \;\mid \vec{p}\,\rangle \\ &=\; \frac{p^2}{2m}\; \Omega^{(+)} \;\mid \vec{p}\,\rangle \;, \end{aligned} \tag{12.24}$$

from which follows

$$H \ \mid \vec{p} \,\rangle^{(+)} \ = \ \frac{p^2}{2m} \ \mid \vec{p} \,\rangle^{(+)} \ , \tag{12.25}$$

which states that the full scattering solution $\mid \vec{p} \,\rangle^{(+)}$ multiplied with H gives the same energy as the free solution $\mid \vec{p} \,\rangle$ multiplied with H_0. This also means that the full solution behaves at large distances similar to the free solution, a boundary condition which we just imposed in the previous chapter. We also showed that $\mid \vec{p} \,\rangle^{(+)}$ are eigenstates to the full Hamiltonian H.

Going to the coordinate space representation should give the results of the previous chapter. For the free Schrödinger equation, we have

$$\begin{aligned} \langle \vec{x} \mid H_0 \mid \vec{p} \,\rangle \ &= \ \int \ d^3x' \ \langle \vec{x} \mid H_0 \mid \vec{x} \,' \rangle \langle \vec{x} \,' \mid \vec{p} \,\rangle \\ &= \ \int \ d^3x' \ \langle \vec{x} \mid -\frac{\hbar^2}{2m} \ \nabla^2 \ \delta(\vec{x} - \vec{x} \,') \mid \vec{x} \,' \rangle \langle \vec{x} \,' \mid \vec{p} \,\rangle \\ &= \ -\ \frac{\hbar^2}{2m} \ \nabla^2 \ \langle \vec{x} \mid \vec{p} \,\rangle \ = \ \frac{p^2}{2m} \ \langle \vec{x} \mid \vec{p} \,\rangle \end{aligned} \tag{12.26}$$

where $\langle \vec{x} \mid \vec{p} \,\rangle = \ \frac{1}{(2\pi\hbar)^{3/2}} \ exp \ \left(\frac{i}{\hbar} \ \vec{p} \cdot \vec{x} \right)$. In a similar fashion, we obtain

$$\langle \vec{x} \mid H \mid \vec{p} \,\rangle^{(+)} \ = \ \left(-\frac{\hbar^2}{2m} \ \nabla^2 + V \right) \ \langle \vec{x} \mid \vec{p} \,\rangle^{(+)} \ = \ \frac{p^2}{2m} \ \langle \vec{x} \mid \vec{p} \,\rangle^{(+)} \tag{12.27}$$

or with $\langle \vec{x} \mid \vec{p} \,\rangle^{(+)} \ = \ \psi^{\dagger}_{\vec{p}}(\vec{x})$

$$\left(-\frac{\hbar^2}{2m} \ \nabla^2 + V \right) \ \psi^{\dagger}_{\vec{p}}(\vec{x}) \ = \ \frac{p^2}{2m} \ \psi^{\dagger}_{\vec{p}}(\vec{x}) \ , \tag{12.28}$$

which is the stationary Schrödinger equation for positive energies. Again, the eigenstates are not normalizable. However, here this is a consequence; in the considerations of the previous chapter it had to be an assumption. We still will have to show that $\mid \vec{p} \,\rangle^{(+)} = \Omega^{(+)} \ \mid \vec{p} \,\rangle$ has the correct asymptotic behavior.

12.3 Integral Equation for $\psi^{(+)}_{\vec{p}}(\vec{x})$

Before being able to set up an integral equation, we have to prove the following statement. Given a function $g(t)$, then for $\varepsilon > 0$

$$\lim_{t \to -\infty} \ g(t) \ = \ -\lim_{\varepsilon \to 0} \int_0^{-\infty} \ dt' \ \varepsilon \ e^{\varepsilon t'} g(t') \ . \tag{12.29}$$

We start from the right-hand side

$$
\begin{aligned}
-\int_0^{-\infty} dt'\ \varepsilon\ e^{\varepsilon t'} g(t') &= -\int_0^{-\infty} \frac{d}{dt'}\ (e^{\varepsilon t'})\ g(t')\ dt' \\
&= g(0)\ +\ \int_0^{-\infty} dt'\ e^{\varepsilon t'}\ \frac{dg(t')}{dt'}\ .
\end{aligned}
\tag{12.30}
$$

As a remark, the limit and the integral operation can be interchanged if both converge separately. Thus we have

$$
\begin{aligned}
\lim_{\varepsilon\to 0}(-\varepsilon)\ \int_0^{-\infty} dt'\ e^{\varepsilon t'} g(t') &= \lim_{\varepsilon\to 0}\ \left[g(0) + \int_0^{-\infty} dt'\ e^{\varepsilon t'}\ \frac{dg(t')}{dt'} \right] \\
&= g(0)\ +\ g(-\infty)\ -\ g(0) \\
&= g(-\infty)\ .
\end{aligned}
\tag{12.31}
$$

With this **"Abel Limit"**, we replace the limit with respect to t by a limit $\varepsilon \to 0$. Now we consider the operators

$$
\begin{aligned}
\Omega^{(+)}\ =\ W(-\infty) &= -\lim_{\varepsilon\to 0} \int_0^{-\infty} \varepsilon\ e^{\varepsilon t} W(t)\ dt \\
&= -\lim_{\epsilon\to 0} \int_0^{-\infty} \varepsilon\ e^{\varepsilon t}\ \varepsilon^{\frac{i}{\hbar}\ Ht}\ e^{-\frac{i}{\hbar} H_0 t}\ dt \\
&= -\lim_{\varepsilon\to 0}\ \varepsilon\ \int_0^{-\infty} e^{\frac{i}{\hbar}\ Ht}\ e^{-\frac{i}{\hbar}(H_0+i\varepsilon)t}\ dt\ .
\end{aligned}
\tag{12.32}
$$

Applying this on a state $|\ \vec{p}\ \rangle$ yields

$$
\begin{aligned}
\Omega^{(+)}\ |\ \vec{p}\ \rangle &= -\lim_{\varepsilon\to 0}\ \varepsilon\ \int_0^{-\infty} dt\ e^{\frac{i}{\hbar}\ (H-E-i\varepsilon)t}\ \ |\ \vec{p}\ \rangle \\
&= \lim_{\varepsilon\to 0}\ \frac{\varepsilon}{\frac{i}{\hbar}\ (H-E-i\varepsilon)}\ \ |\ \vec{p}\ \rangle \\
&= \lim_{\varepsilon\to 0}\ i\varepsilon\ \frac{\hbar}{E+i\varepsilon-H}\ \ |\ \vec{p}\rangle\ \ =\ \lim_{\varepsilon\to 0}\ i\varepsilon\ G(z)\ \ |\ \vec{p}\rangle
\end{aligned}
\tag{12.33}
$$

where in the last step $\hbar \equiv 1$ was set and $z = E + i\varepsilon$. The function

$$
G(z)\ =\ \frac{1}{z-H} \tag{12.34}
$$

is called the **Resolvent of** H. With (12.33) the scattering state can be written as

$$
|\ \vec{p}\ \rangle^{(+)}\ =\ \Omega^{(+)}\ \ |\ \vec{p}\ \rangle\ =\ \lim_{\varepsilon\to 0}\ i\varepsilon\ G(E+i\varepsilon)\ \ |\ \vec{p}\rangle\ . \tag{12.35}
$$

$G(E+i\varepsilon)$ contains the full Hamiltonian in the denominator and cannot be treated in the form (12.35). Therefore, we want to split to equation in such a way that H_0 and V are in separate pieces. We define the **free Resolvent** as

$$G_0(z) \;=\; \frac{1}{z-H_0} \tag{12.36}$$

and consider

$$G_0^{-1}(z) \;-\; G^{-1}(z) \;=\; (z-H_0) \;-\; (z-H) \;=\; -H_0 \;+\; H \;=\; V\;. \tag{12.37}$$

Multiplying (12.37) from the left with $G_0(z)$ and the right with $G(z)$ gives

$$\begin{aligned} G_0(z)\,[G_0^{-1}(z) \;&-\; G^{-1}(z)]\,G(z) \\ &=\; G(z) \;-\; G_0(z) \;=\; G_0(z)\,V\,G(z)\;, \end{aligned}$$

from which follows

$$G(z) \;=\; G_0(z) \;+\; G_0(z)\,V\,G(z)\;. \tag{12.38}$$

The relation (12.38) is called **Hilbert identity** or **Second Resolvent equation**, and has already the typical form of an integral equation. Multiplying (12.37) from the left with $G_0(z)$ gives a different form of the Hilbert identity, namely

$$G(z) \;=\; G_0(z) \;+\; G(z)\,V\,G_0(z)\;. \tag{12.39}$$

By comparison of the last terms in (12.38) and (12.39), we find $G_0(z)\;V\;G(z) \;=\; G(z)\;V\;G_0(z)$. Applying (12.38) on a free state $|\,\vec{p}\,\rangle$ gives

$$\begin{aligned} G(E+i\varepsilon)\;\;|\,\vec{p}\,\rangle \;&=\; G_0(E+i\varepsilon)\;\;|\,\vec{p}\,\rangle \;+\; G_0(E+i\varepsilon)\;V\;G(E+i\varepsilon)\;|\,p\rangle \\ i\varepsilon\;G(E+i\varepsilon)\;\;|\,\vec{p}\,\rangle \;&=\; \frac{i\varepsilon}{E+i\varepsilon-\frac{p^2}{2m}}\;\;|\,\vec{p}\,\rangle \;+\; i\varepsilon\;G_0(E+i\varepsilon)\;V\;G(E+i\varepsilon)\;\;|\,\vec{p}\,\rangle\;, \end{aligned} \tag{12.40}$$

where $H_0\;|\,\vec{p}\,\rangle = \;\frac{p^2}{2m}\;\;|\,\vec{p}\,\rangle$. Carrying out the lim $\varepsilon \to 0$ gives

$$\lim_{\varepsilon\to 0}\;i\varepsilon\;G(E+i\varepsilon)\;\;|\,\vec{p}\,\rangle \;=|\,\vec{p}\,\rangle^{(+)} \;=|\,\vec{p}\,\rangle \;+\; G_0(E+i0)\;V\;\;|\,\vec{p}\,\rangle^{(+)}\;. \tag{12.41}$$

Eq. (12.41) is the **Lippmann-Schwinger equation for states**, and its exists if $V\;|\,\vec{p}\,\rangle^{(+)}$ is a vector out of the Hilbert space, i.e., V is square integrable. The interpretation of (12.41) is that the full scattering state $|\,\vec{p}\,\rangle^{(+)}$ is the sum of an incident plane wave $|\,\vec{p}\,\rangle$ and a "perturbation" $G_0\;V\;|\,\vec{p}\,\rangle^{(+)}$, which is caused by the potential V. From

this we can deduce that (12.41) has the form of the boundary condition as postulated in (11.26). Applying the form (12.39) of the Hilbert identity leads to

$$\begin{aligned} |\,\vec{p}\,\rangle^{(+)} &= i\varepsilon\, G(E+i\varepsilon)\;|\,\vec{p}\,\rangle &&= i\varepsilon\,[1+G(E+i\varepsilon)V]\,G_0(E+i\varepsilon)\;|\,\vec{p}\,\rangle \\ &&&= [1+G(E+i\varepsilon)V]\;|\,\vec{p}\,\rangle \\ &&&= \Omega^{(+)}\;|\,\vec{p}\,\rangle\;, \end{aligned} \tag{12.42}$$

from which we deduce a representation of $\Omega^{(+)}$ as

$$\Omega^{(+)} = 1 + G(E+i\varepsilon)\,V\;. \tag{12.43}$$

However, this representation is not very useful since $G(E+i\varepsilon)$ is not known.

12.4 Coordinate Space Representation of the Lippmann-Schwinger Equation

For obtaining a coordinate space representation, we have to form

$$\begin{aligned} \langle\vec{x}\,|\,\vec{p}\,\rangle^{(+)} &= \langle\vec{x}\,|\,\vec{p}\,\rangle + \int d^3x'\int d^3x''\,\langle\vec{x}\,|\,G_0(E+i0)\;|\,\vec{x}\,'\rangle\langle\vec{x}\,'\,|\,V\,|\,\vec{x}\,''\rangle\langle\vec{x}\,''\,|\,\vec{p}\rangle^{(+)} \\ \psi^{(+)}_{\vec{p}} &= \frac{1}{(2\pi\hbar)^{3/2}}\,e^{\frac{i}{\hbar}\,\vec{p}\cdot\vec{x}} + \int d^3x'\int d^3x''\,G_0^{(+)}(\vec{x},\vec{x}\,')\,V(\vec{x}\,',\vec{x}\,'')\,\psi^{(+)}_{\vec{p}}(\vec{x}\,'')\;. \end{aligned} \tag{12.44}$$

If $V(\vec{x}\,',\vec{x}\,'')$ is assumed to be local, i.e., $V(\vec{x}\,',\vec{x}\,'') = V(\vec{x}\,')\,\delta(\vec{x}\,',\vec{x}\,'')$, this reduces to

$$\psi^{(+)}_{\vec{p}}(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}}\,e^{\frac{i}{\hbar}\,\vec{p}\cdot\vec{x}} + \int d^3x'\,G_0^{(+)}(\vec{x},\vec{x}\,')\,V(\vec{x}\,')\,\psi^{(+)}_{\vec{p}}(\vec{x}\,')\;. \tag{12.45}$$

This is an integral equation, valid for local potentials. The same equation is obtained by solving the stationary Schrödinger equation.

We still have to determine the coordinate space representation of the free Green function $G_0^{(+)}(\vec{x},\vec{x}\,')$:

$$\begin{aligned} G_0^{(+)} &= \langle\vec{x}\,|\,G_0(E+i0)\,|\,\vec{x}\,'\rangle = \langle\vec{x}\,|\;\frac{1}{E+i0-H_0}\;|\,\vec{x}\,'\rangle \\ &= \int d^3p'\,\langle\vec{x}\,|\;\frac{1}{E+i0-H_0}\;|\,\vec{p}\,\rangle\langle|\,\vec{p}\,'\,|\,\vec{x}\,'\rangle \\ &= \int d^3p'\,\langle\vec{x}\,|\,\vec{p}\,'\rangle\langle\vec{p}\,'\,|\,\vec{x}\,'\rangle\;\frac{1}{E+i0-\frac{p'2}{2m}} \end{aligned}$$

$$= \int d^3p' \, \frac{1}{(2\pi\hbar)^3} \, e^{\frac{i}{\hbar} \vec{p}\,'\cdot(\vec{x}-\vec{x}\,')} \, \frac{1}{E + i0 - \frac{p'^2}{2m}} \, . \tag{12.46}$$

Considering that $\vec{p} = \vec{p}\,'$ and using spherical coordinates leads to

$$\begin{aligned} G_0^{(+)}(\vec{x},\vec{x}\,') &= \frac{1}{(2\pi\hbar)^3} \int_0^\infty \int_{-1}^1 \int_0^{2\pi} dp\, p^2 \, d\, cos\, \theta \, d\varphi \, e^{\frac{i}{\hbar} p(x-x')\, cos\, \theta} \, \frac{1}{E + i0 - \frac{p^2}{2m}} \\ &= \frac{m}{2\pi^2\hbar^3} \int_0^\infty dp\, p^2 \, \frac{e^{\frac{i}{\hbar} p(x-x')} - e^{-\frac{i}{\hbar} p(x-x')}}{ip \mid x - x' \mid} \, \frac{1}{2mE + i0 - p^2} \\ &= \frac{m}{2\pi^2\hbar^3} \int_{-\infty}^\infty dp\, p \, \frac{1}{2mE + i0 - p^2} \, \frac{e^{\frac{i}{\hbar} p(x-x')}}{i \mid x - x' \mid} \\ &= \frac{m}{2\pi^2\hbar^3} \int_{-\infty}^\infty dp\, p \, \frac{1}{\frac{2mE}{\hbar^2} + i0 - p^2} \, \frac{e^{ip(x-x')}}{i \mid x - x' \mid} \, , \end{aligned} \tag{12.47}$$

where we used $p = \hbar k$ in the last relation. The integrand has poles for positive energies for $\frac{2mE}{\hbar^2} - k^2 = 0$, and the poles are located at

$$\hbar k_{1/2} = \pm\sqrt{2mE + i\varepsilon} \tag{12.48}$$

from which follows

$$\begin{aligned} \hbar k_1 &= +\sqrt{2mE} + i\varepsilon \\ \hbar k_2 &= -\sqrt{2mE} - i\varepsilon \, . \end{aligned} \tag{12.49}$$

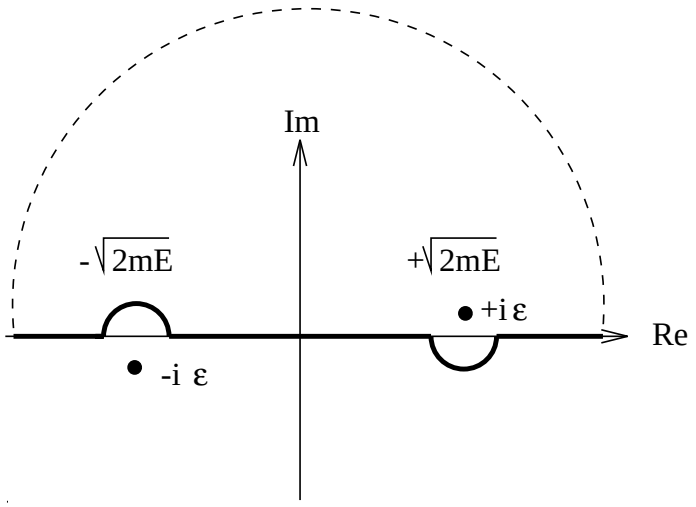

Fig. 12.1 Integration path for evaluating $G_0^{(+)}(\vec{x},\vec{x}\,')$.

To solve (12.47) we continue the function into the complex plane and integrate along the path indicated in Fig. 12.1. Since only $\hbar k_1$ lies inside the contour, we obtain for (12.47) along the path of Fig. 12.1

$$\begin{aligned} \frac{m}{2\pi^2\hbar^3} \qquad & \int_{-\infty}^{\infty} dk \; \frac{k}{\frac{2mE}{\hbar^2} - k^2} \cdot \frac{e^{ik(x-x')}}{i \mid x - x' \mid} \\ = \; & \frac{m}{2\pi^2\hbar^3} \cdot 2\pi i \; Res_{k \to \frac{\sqrt{2mE}}{\hbar}} \; \frac{k}{\frac{2mE}{\hbar^2} - k^2} \; \frac{e^{ik(x-x')}}{i \mid x - x' \mid} \; . \end{aligned} \tag{12.50}$$

We choose to close the contour in the upper half plane, i.e., have $e^{i(k+i\eta)(x-x')} = e^{ik(x-x')} \, e^{-\eta(x-x')}$, which falls off sufficiently fast if we take the upper half circle $\to \infty$. The pole for $+\sqrt{2mE}$ sits in the area enclosed by the contour. Applying the Residue theorem leads to the final expression

$$\langle \vec{x} \mid G_0(E + i0) \mid \vec{x}\,' \rangle \; = \; -\frac{m}{2\pi\hbar^2} \; \frac{e^{i \, \frac{p}{\hbar} \, (x-x')}}{(x - x')} \; . \tag{12.51}$$

With this, (12.45) becomes

$$\psi_{\vec{p}}^{(+)}(\vec{x}) \; = \; \frac{1}{(2\pi\hbar)^{3/2}} \, e^{\frac{i}{\hbar} \, \vec{p} \cdot \vec{x}} \; - \; \frac{m}{2\pi\hbar^2} \int d^3x' \; \frac{e^{\frac{i}{\hbar} \, \vec{p} \cdot (\vec{x} - \vec{x}\,')}}{\mid \vec{x} - \vec{x}\,' \mid} \; V(\vec{x}\,') \; \psi_{\vec{p}}^{(+)}(\vec{x}\,') \tag{12.52}$$

which is the Lippmann-Schwinger equation in coordinate space representation.

12.5 Asymptotic Behavior

In order to make a comparison with the asymptotic boundary conditions imposed in Chapter 11 and better understand their origin, we have to study the asymptotic behavior of (12.52). The first term of the right-hand side corresponds to a plane wave and does already have the desired asymptotic form. We need to study the second term and find out if it behaves asymptotically as an outgoing spherical wave. Expanding $\mid \vec{x} - \vec{x}' \mid^2$ gives

$$\begin{aligned} \mid \vec{x} - \vec{x}\,' \mid^2 = \; \vec{x}^{\,2} \; - \; 2\vec{x} \cdot \vec{x}\,' \; + \; \vec{x}^{\,\prime 2} \; & \approx \; r^2 \; - \; 2\vec{x} \cdot \vec{x}\,' \\ & = \; r^2 \left(1 - \; \frac{2\vec{x} \cdot \vec{x}\,'}{r^2} \right) \end{aligned} \tag{12.53}$$

and thus

$$\begin{aligned} \mid \vec{x} - \vec{x}\,' \mid \; & = \; \sqrt{(\vec{x} - \vec{x}\,')^2} \; \approx \; r \sqrt{\left(1 - \; \frac{2\vec{x} \cdot \vec{x}\,'}{r^2} \right)} \; \approx \; r \left(1 - \; \frac{\vec{x}\vec{x}\,'}{r^2} \right) \\ & = \; r - \; \frac{\vec{x} \cdot \vec{x}\,'}{r} \; , \end{aligned} \tag{12.54}$$

which corresponds to a dipole approximation. Inserting (12.54) into (12.52) and considering that

$$G_0^{(+)}(\vec{x}-\vec{x}\,') \;=\; \frac{m}{2\pi\hbar^2}\,\frac{e^{ikr}}{r}\;e^{-i\left(\frac{k\vec{x}}{r}\right)\,\cdot\vec{x}\,'}\;,$$

we obtain as asymptotic behavior of (12.52)

$$\psi_{\vec{p}}^{(+)} \;\stackrel{r\to\infty}{\longrightarrow}\; \varphi(\vec{x}) \;+\; \left(\frac{-m}{2\pi\hbar^2}\right)\;\int\; d^3x'\;e^{-\frac{ik\vec{x}}{r}\,\cdot\vec{x}\,'}\;V(\vec{x}\,')\;\psi_{\vec{p}}^{(+)}(\vec{x}\,')\;\cdot\;\frac{e^{ikr}}{r} \tag{12.55}$$

which, when compared to the "Sommerfeld radiation condition" (11.30), shows that the Lippmann-Schwinger equation has the correct asymptotic behavior. A comparison with (11.30)

$$\psi_{\vec{p}}^{(sc)}(\vec{x}) \;\stackrel{r\to\infty}{\longrightarrow}\; \varphi_{\vec{p}}(\vec{x}) \;+\; f(\hat{p}\,',\hat{p})\;\frac{e^{ikr}}{r}\;\frac{1}{(2\pi\hbar)^{3/2}}$$

gives

$$\begin{aligned} f(\hat{p}\,',\hat{p}) \;&=\; -m\;4\pi^2\hbar\;\int\;d^3\vec{x}\,'\;\frac{e^{-\frac{i}{\hbar}\;\vec{p}\,'\cdot\vec{x}\,'}}{(2\pi\hbar)^{3/2}}\;V(\vec{x}\,')\;\psi_{\vec{p}}^{(+)}(\vec{x}\,') \\ &=\; -4\pi^2 m\hbar\;\int\;d^3x'\;\langle\vec{p}\,'\mid\vec{x}\,'\rangle\langle\vec{x}\,'\mid V\mid\vec{x}\,'\rangle\langle\vec{x}\,'\mid\vec{p}\,\rangle^{(+)} \\ &=\; -4\pi^2 m\hbar\;\langle\vec{p}\,'\mid V\mid\vec{p}\,\rangle^{(+)}\;. \end{aligned} \tag{12.56}$$

In order to solve for $f(\hat{p}\,',\hat{p})$, one must first solve the Lippmann-Schwinger equation to obtain $\mid\vec{p}\,\rangle^{(+)}$. Similar to the considerations following (11.89), one can consider solving for $f(\hat{p}\,',\hat{p}\,)$ only in an approximate fashion and expand $\mid\vec{p}\,\rangle^{(+)} =\mid p\rangle + \cdots$. If one considers only the first term in the expansion, one obtains the **Born approximation for the scattering amplitude**

$$f(\hat{p}\,',\hat{p}\,)_{Born} \;=\; -4\pi^2 m\hbar\;\langle\vec{p}\,'\mid V\mid\vec{p}\,\rangle\;. \tag{12.57}$$

12.6 The Lippmann-Schwinger Equation as Operator Equation

In its general form (12.52) can be written as

$$\mid\psi_{\vec{p}}^{(+)}\rangle \;=\mid\varphi_p\rangle \;+\; G_0^{(+)}\;V\mid\psi_p^{(+)}\rangle\;. \tag{12.58}$$

Multiplying (12.58) with V and defining $V \mid \psi_p^{(+)}\rangle \;=\; T \mid \varphi_p\rangle$ yields

$$T \mid \varphi_p\rangle \;=\; V \mid \varphi_p\rangle \;+\; V\, G_0^{(+)}\, T \mid \varphi_p\rangle \;. \tag{12.59}$$

Since the plane waves $\mid \varphi_p\rangle$ form a complete set of states, (12.59) is valid as operator equation:

$$T \;=\; V \;+\; V\, G_0^{(+)}\, T \;, \tag{12.60}$$

which is the **Operator Lippmann-Schwinger Equation** or **t-matrix** equation.
In its momentum space representation (12.60) reads

$$\begin{aligned}
\langle \vec{p}\,' \mid T \mid \vec{p}\,\rangle \;&=\; \langle \vec{p}\,' \mid V \mid \vec{p}\rangle \;+\; \int d^3p''\; d^3p'''\; \langle \vec{p}\,' \mid V \mid \vec{p}\,''\rangle\langle \vec{p}\,'' \mid G_0^{(+)} \mid \vec{p}\,'''\rangle\langle \vec{p}\,''' \mid T \mid \vec{p}\,\rangle \\
&=\; \langle \vec{p}\,' \mid V \mid \vec{p}\,\rangle \;+\; \int d^3p''\; \langle \vec{p}\,' \mid V \mid \vec{p}\,''\rangle\; \frac{1}{E + i\varepsilon - \frac{p''^2}{2m}}\; \langle \vec{p}\,'' \mid T \mid \vec{p}\,\rangle \;.
\end{aligned} \tag{12.61}$$

This is an integral equation of Fredholm type, and one has to solve for all values of p'', i.e., off-the-energy-shell. However, one needs for the calculation of physical observables only the values for which $\frac{p''^2}{2m} \;= E = \; \frac{p^2}{2m}$, i.e., one needs only the on-shell values. The reason for this is that for the calculation of cross sections only the asymptotic expansion was used (compared structure of proofs in Chapter 11). The terminology is as follows: Matrix elements for which

$$p'2 \;=\; p^2 \;=\; p_0^2 \quad \text{are called on} - \text{shell} \;,$$

those for which

$$p'^2 \;\neq\; p^2 \;=\; p_0^2 \quad \text{are called half} - \text{shell} \;,$$

and those for which

$$p'^2 \;\neq\; p^2 \;\neq\; p_0^2 \quad \text{are called fully} - \text{off} - \text{shell} \;.$$

Here p_0^2 is defined via the incoming energy $E_{p_0} \;=\; \frac{p_0^2}{2m}$. In terms of the t-matrix, (12.56) can be written as

$$f(\hat{p}\,', \hat{p}\,) \;=\; -4\pi^2 m\hbar\, \langle \vec{p}\,' \mid T \mid \vec{p}\,\rangle \;. \tag{12.62}$$

Let us consider the propagator $G_0^{(+)}$ in (12.61). If we write it as

$$\begin{aligned}
\langle \vec{p}\,' \mid G_0^{(+)} \mid \vec{p}\,\rangle \;&=\; \frac{\delta(\vec{p}\,' - \vec{p}\,)}{E + i\varepsilon - \frac{p'^2}{2m}} \\
&=\; \delta(\vec{p}\,' - \vec{p}\,)\; \left[\frac{\mathcal{P}}{E - \frac{p^2}{2m}} \;-\; i\pi\; \delta\left(E - \frac{p^2}{2m}\right)\right] \;,
\end{aligned} \tag{12.63}$$

where we used the **Cauchy Principal value**

$$\frac{1}{x+i\varepsilon} \;=\; \frac{\mathcal{P}}{x} \;-\; i\pi\;\delta(x) \tag{12.64}$$

then we can consider the approximation

$$\langle \vec{p}\,' \mid G_0^{(+)} \mid \vec{p}\,\rangle \approx\; \delta(\vec{p}\,' - p')(-i\pi)\;\delta\left(E - \;\frac{p^2}{2m}\right)\;, \tag{12.65}$$

which is called k-matrix Born approximation.

The Lippmann-Schwinger equation (12.60) is an integral equation of Fredholm type and can, in principal, be solved by iteration (Neumann series) if the kernel $V\;G_0^{(+)}$ is small, so that the convergence of the series is secured. In terms of (12.60), this iteration can be written out as

$$\begin{aligned} T^{(1)}(z) &= V \\ T^{(2)}(z) &= V \;+\; V\;G_0^{(+)}\;V \\ T^{(3)}(z) &= V \;+\; V\;G_0^{(+)}\;V\;G_0^{(+)}\;V\;. \end{aligned} \tag{12.66}$$

In general this series can be written as

$$T(z) \;=\; \sum_{n=1}^{\infty}\; V(G_0^{(+)}(z)V)^{n-1} \;=\; V\;\sum_{n=0}\;(G_0^{(+)}(z)V)^n \tag{12.67}$$

and is called **Born Series**.

We could have also started from the Lippmann-Schwinger equation for states as given in (12.58). If we define as zeroth order to the full solution $\mid \psi_{\vec{p}}^{(+)}\rangle^0 \;:= \mid \varphi_{\vec{p}}\rangle$, the free solution, then we obtain in first order iteration

$$\mid \psi_{\vec{p}}^{(+)}\rangle^1 \;= \mid \varphi_{\vec{p}}\rangle \;+\; G_0^{(+)}\;V \mid \varphi_{\vec{p}}\rangle \tag{12.68}$$

and in general in n-th order

$$\mid \psi_{\vec{p}}^{(+)}\rangle^n \;=\; \sum_{\nu=0}^{n}\;(G_0^{(+)}V)^{\nu}\;\mid \varphi_{\vec{p}}\rangle\;. \tag{12.69}$$

If this series converges for $n \to \infty$, we obtain in this way a solution for (12.58), which reads

$$\mid \psi_{\vec{p}}^{(+)}\rangle \;=\; \sum_{\nu=0}^{\infty}\;(G_0^{(+)}V)^{\nu}\;\mid \varphi_{\vec{p}}\rangle \tag{12.70}$$

and one can say: If the series (12.70) converges, then the vector defined by the series is a proper scattering state. As we have seen in (12.56), the scattering amplitude can be written as

$$f_E(\hat{p}', \hat{p}) \;=\; -4\pi^2 m\hbar \, \langle \varphi_{\vec{p}\,'} \mid V \mid \psi^{(+)}_{\vec{p}} \rangle \; .$$

Inserting (12.70) yields

$$f_E(\hat{p}', \hat{p}) \;=\; -4\pi^2 m\hbar \, \sum_{\nu=0}^{\infty} \langle \varphi_{\vec{p}\,'} \mid V (G_0^{(+)} V)^{\nu} \mid \varphi_{\vec{p}} \rangle \; . \tag{12.71}$$

Thus, the scattering amplitude can be written as a series

$$\begin{aligned} f_E(\hat{p}', \hat{p}) \;&=\; \sum_{i=1}^{\infty} f_E^{(i)}(\hat{p}', \hat{p}) \\ f_E^{(i)}(\hat{p}', \hat{p}) \;&=\; -4\pi^2 m\hbar \, \langle \varphi_{\vec{p}'} \mid V (G_0^{(+)} V)^{(i-1)} \mid \varphi_{\vec{p}} \rangle \; . \end{aligned} \tag{12.72}$$

Here (i) counts the power of V. The **first** Born approximation for the scattering amplitude, sometimes called **the** Born approximation, is linear in the potential. It is useful to consider a graphical representation of (12.72).

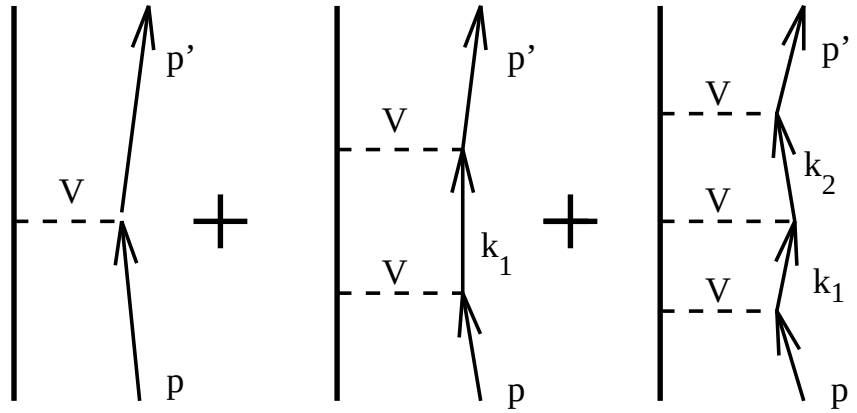

Fig. 12.2 Schematic interpretation of the terms in the perturbation series for $f_E(\hat{p}\,', \hat{p})$.

This graphical series expresses the fact that the scattering can be interpreted as a multiple interaction of the potential. The Born approximation is in this respect also called tree approximation. The line $\vec{k}$ in the second-order approximation characterizes $G_0^{(+)}$, i.e., the free motion of the particle between the multiple scatterings. However, this is not the true free motion since in

$$V \, G_0^{(+)} V \;=\; \int d^3k_1 \; V \, G_0^{(+)} \mid \vec{k}_1 \rangle \langle \vec{k}_1 \mid V \tag{12.73}$$

the momentum $\vec{k}_1$ is an integration variable, and we do not have $\frac{k_1^2}{2m} = \frac{p^2}{2m}$, i.e., $\vec{k}_1$ is not restricted to the on-shell value. We rather have a typical quantum mechanical behavior, during the interaction we have a momentum uncertainty allowed by the uncertainty principle. To stress again, this point of view is only meaningful if the Born series converges.

In the previous considerations, we started from the Lippmann-Schwinger equation (12.58) and derived the Born series (12.70). We also could have started from (12.70) as **definition** of the scattering state, assuming that this definition is only valid within the radius of convergence of the series. Then we can derive the Lippmann-Schwinger equation starting from (12.70).

$$\begin{aligned} \mid \psi_{\vec{p}}^{(+)} \rangle &= \sum_{\nu=0}^{\infty} (G_0^{(+)} V)^{\nu} \mid \varphi_{\vec{p}} \rangle \\ &= \mid \varphi_{\vec{p}} \rangle + G_0^{(+)} V \sum_{\nu=1}^{\infty} (G_0^{(+)} V)^{\nu-1} \mid \varphi_{\vec{p}} \rangle \\ &= \mid \varphi_{\vec{p}} \rangle + G_0^{(+)} V \sum_{\nu=0}^{\infty} (G_0^{(+)} V)^{\nu} \mid \varphi_{\vec{p}} \rangle \\ &= \mid \varphi_{\vec{p}} \rangle + G_0^{(+)} V \mid \psi_p^{(+)} \rangle \ . \end{aligned} \tag{12.74}$$

This shows that we "summed up" the Born series. However, we do not obtain an explicit solution on the right-hand side, but rather the unknown function again. This indicates that in general we do not obtain a closed solution for the scattering state but rather an integral equation.

We can interpret this in a slightly different way. As we shall see, the Born series converges for sufficiently high energies. In that region (12.70) is a reasonable definition and within the radius of convergence the Born series and the Lippmann-Schwinger equation are equivalent. This stays valid for all other energies and thus determines the continuation of the definition (12.70) to energy regions, where the series does not exist.

It is appropriate to describe this approach here since it shows how one obtains an integral equation by summing up multiple interactions of V. This procedure is important with respect to quantum field theory. There the usual practice leads to a Dyson series (an infinite series corresponding to the Born series, represented by Feynman diagrams).

Summing up this series gives an integral equation, which resembles in its form the Lippmann-Schwinger equation, the **Bethe-Salpeter equation**, which, however, has a much more complicated structure.

12.7 The Lippmann-Schwinger Equation for the Bound State

If we assume that V supports a bound state $\mid \psi_b\rangle$ at $E = E_b < 0$, then the Schrödinger equation reads

$$(H_0 + V) \mid \psi_b\rangle = E_b \mid \psi_b\rangle \tag{12.75}$$

or

$$(H_0 - E_b) \mid \psi_b\rangle = -V \mid \psi_b\rangle \; . \tag{12.76}$$

Since $E_b < 0$, there is no regular solution for the case $V = 0$ and we can write

$$\mid \psi_b\rangle = \frac{1}{E_b - H_0} \, V \mid \psi_b\rangle \; , \tag{12.77}$$

which is the homogeneous Lippmann-Schwinger equation for $\mid \psi_b\rangle$. Evaluating the free Green's function for $E = E_b < 0$ (12.51), we see that $\langle \vec{x} \mid \psi_b\rangle \equiv \psi_b(\vec{x}\,)$ has the correct exponential fall-off behavior, namely proportional to $e^{-\sqrt{2m|E_b|}} \, \frac{|x-x'|}{|x-x'|}$.

12.8 The Low Equation

When deriving the Lippmann-Schwinger equation for states or operators, we started from the Hilbert identity given by (12.38). Now we want to start from the alternative form (12.39), namely

$$G(z) = G_0(z) + G(z) \, V \, G_0(z) \; .$$

Similar to Section 12.3, we apply (12.39) on a free state $\mid \vec{p}\,\rangle$, multiplying with $i\varepsilon$ and consider the limit $\varepsilon \to 0$.

$$i\varepsilon \, G(E + i\varepsilon) \mid \vec{p}\,\rangle = \frac{i\varepsilon}{E + i\varepsilon - \frac{p^2}{2m}} \mid \vec{p}\,\rangle + G(E + i\varepsilon) \, V \, \frac{i\varepsilon}{E + i\varepsilon \, \frac{p^2}{2m}} \mid \vec{p}\,\rangle \; . \tag{12.78}$$

Taking the limit $\varepsilon \to 0$ gives

$$\mid \vec{p}\,\rangle^{(+)} = \mid \vec{p}\,\rangle + G(E + i\varepsilon) \, V \mid \vec{p}\,\rangle \; , \tag{12.79}$$

which is the **Low equation for states** (corresponding to (12.41)). Multiplying with V and taking into account the definition $V \mid p\rangle^{(+)} = T \mid p\rangle$ gives

$$V \mid \vec{p}\,\rangle^{(+)} = T \mid p\rangle = (V + V \, G \, V) \mid \vec{p}\,\rangle \tag{12.80}$$

or as operator equation

$$T \;=\; V + V\; G\; V \;. \tag{12.81}$$

For practical calculations, the Low equation is not particularly useful, since it contains the full resolvent $G(z)$. If we assume that the Hamiltonian H has bound states with $H \mid \psi_b\rangle = E_b \mid \psi_b\rangle$ and a continuous spectrum, then we can write the spectral decomposition of $G(z)$ as

$$\begin{aligned} \frac{1}{E \pm i\varepsilon - H} \;&=\; \sum_b \mid \psi_b\rangle \, \frac{1}{E \pm i\varepsilon - E_b} \, \langle \psi_b \mid \\ &+ \int d^3p \;\mid \psi_{\vec{p}}^{(+)}\rangle \, \frac{1}{E \pm i\varepsilon - H} \, \langle \psi_{\vec{p}}^{(+)} \mid \;. \end{aligned} \tag{12.82}$$

$G(z)$ is a holomorphic function for $Im \neq 0$, and $G(z)$ has poles at the binding energies E_b. Inserting (12.82) into (12.81) leads to

$$\begin{aligned} \langle \vec{p}\,' \mid T \mid \vec{p}\,\rangle \;=\; \langle \vec{p}\,' \mid V \mid \vec{p}\,\rangle \;&+\; \sum_b \frac{\langle \vec{p}\,' \mid V \mid \psi_b\rangle\langle \psi_b \mid V \mid \vec{p}\,\rangle}{E - E_b} \\ &+ \int d^3k \, \frac{\langle \vec{p}\,' \mid T^\dagger \mid \vec{k}\,\rangle\langle \vec{k} \mid T^- \mid \vec{p}\,\rangle}{E \pm i\varepsilon - E_k} \;, \end{aligned} \tag{12.83}$$

where the subscript $\pm$ refers to $\pm i\varepsilon$ in $G(E \pm i\varepsilon)$. If $E > 0$, then there are no bound states and the discrete sum over b vanishes. If $E < 0$ is allowed, then $\langle \vec{p}\,' \mid T \mid \vec{p}\,\rangle$ has poles by $E = E_b$, and the residue is separable. [Remark: A function $f(\vec{q}\,', \vec{q}\,)$ is called separable if $f(q', q) = f_1(q')\; f_2(q)$.] The residue can be written as

$$\begin{aligned} \langle \vec{p}\,' \mid V \mid \psi_b\rangle \;=\; \langle \vec{p}\,' \mid (H - H_0) \mid \psi_b\rangle \;&=\; (E - E_{\vec{p}}\,)\langle \vec{p}\,' \mid \psi_b\rangle \\ &=\; (E - E_{\vec{p}}\,)\; \psi_b(\vec{p}\,') \;, \end{aligned} \tag{12.84}$$

where $\psi_b(\vec{p}\,')$ is the bound state wave function for $E = E_b$. Thus, if $E < 0$ is close to E_b, then the t-matrix is dominated by the pole term. The residue is characterized by the corresponding bound state wave functions. As function of $E\langle \vec{p}\,' \mid T(E) \mid \vec{p}\rangle$, has the following behavior:

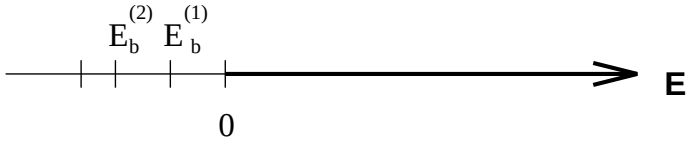

Fig. 12.3 Pole structure of $\langle \vec{p}\,' \mid T(E) \mid \vec{p}\,\rangle$.

There are poles for the bound states and a cut for the continuous spectrum.

12.9 Unitarity Relations

When considering only positive energies, the sum over b vanishes in (12.83). Let us consider the difference of $T^{(+)}$ and $T^{(-)}$ as obtained from (12.83) under the assumption that V is hermitian.

$$\begin{aligned}\langle \vec{p}' \mid T^{(+)}(E) \quad & -T^{(-)}(E) \mid \vec{p}\rangle = \langle \vec{p}' \mid T^{(+)}(E) \mid \vec{p}\rangle - \langle \vec{p}' \mid T^{(-)}(E) \mid \vec{p}\rangle \\ = & \int d^3k \langle \vec{p}' \mid T^{(+)}(E) \mid \vec{k}\rangle \left[\frac{1}{E - E_k + i\varepsilon} - \frac{1}{E - E_k - i\varepsilon}\right] \langle \vec{k} \mid T^{(-)}(E) \mid \vec{p}\rangle.\end{aligned} \tag{12.85}$$

Using the Cauchy principal value $\frac{1}{x \pm i\varepsilon} = \frac{\mathcal{P}}{x} \mp i\pi\delta(x)$, we obtain

$$\langle \vec{p}' \mid T^{(+)}(E) \quad -T^{(-)}(E) \mid \vec{p}\,\rangle \tag{12.86}$$

$$\begin{aligned} = & -2\pi i \int d^3k \langle \vec{p}' \mid T^{(+)}(E_k) \mid \vec{k}\rangle \delta(E - E_k) \langle \vec{k} \mid T^{(-)}(E_k) \mid \vec{p}\rangle \\ = & -2\pi i \int_0^\infty dk\ k^2 \int d\Omega_k \langle \vec{p}' \mid T^{(+)}(E_k) \mid \vec{k}\rangle \delta(k'' - k) \frac{m}{k} \langle \vec{k} \mid T^{()}(E_k) \mid \vec{p}\rangle \end{aligned} \tag{12.87}$$

In the last relation we used $\delta(ax) = \frac{1}{|a|}\delta(x)$, $\delta(\varphi(x))] = \sum_i \frac{1}{|\varphi'(a_i)|}\delta(x - a_i)$, where a_i are the roots of the equation $\varphi(x) = 0$, and $E = \frac{p''^2}{2m}$.
Eq. (12.87) is called the **off-shell unitarity relation**, since in general $\mid \vec{p}\ \mid \neq \mid \vec{p}\,' \mid \neq \mid \vec{k}\ \mid$.

For elastic scattering, i.e., $\mid \vec{p}\ \mid = \mid \vec{p}'\ \mid$, Eq. (12.87) simplifies to

$$\begin{aligned}\langle \vec{p}' \mid T^{(+)}(E_p) \ & - \ T^{(-)}(E_p) \mid \vec{p}\,\rangle \\ & = -2\pi i\ m\ p \int d\Omega_k \langle \vec{p}\,' \mid T^{(+)}(E_p) \mid \vec{k}\,\rangle \langle \vec{k}\ \mid T^{(-)}(E_p) \mid \vec{p}\,\rangle\end{aligned} \tag{12.88}$$

which is usually referred to as **on-shell unitarity relation**.

If we restrict ourselves to the forward direction, i.e., $\vec{p}\,' = \vec{p}$, or equivalently $\theta = 0$, with θ being the angle between $\vec{p}\,'$ or $\vec{p}$, we obtain

$$\begin{aligned}\langle \vec{p}\ \mid T^{(+)}(E) \ - \ T^{(-)}(E) \mid \vec{p}\,\rangle \ & = \ \langle \vec{p}\ \mid T^{(+)} \mid \vec{p}\,\rangle \ - \ \langle \vec{p}\ \mid T^{(+)} \mid \vec{p}\,\rangle^* \\ & = \ 2i\ Im\ \langle \vec{p}\ \mid T^{(+)} \mid \vec{p}\,\rangle\end{aligned} \tag{12.89}$$

and with (12.89)

$$Im\ \langle \vec{p}\ \mid T^{(+)}(E) \mid \vec{p}\,\rangle\ =\ -\pi\ mp \int d\Omega_k\ \mid \langle \vec{p}\ \mid T^{(+)}(E) \mid \hat{k}\rangle \mid^2\ . \tag{12.90}$$

Eq. (12.90) is referred to as **optical theorem** and provides a non-linear relation between the imaginary part of T in forward direction and the absolute value of T integrated over all angles.

12.10 S-Operator

In (12.4) the scattering state was defined via its behavior for large negative times, i.e., long before the scattering event.

$$\mid \psi_a^{(+)}\rangle\ =\ s - \lim_{t\to-\infty}\ e^{iHt}\ e^{-iH_0t} \mid \varphi_a\rangle\ =\ \Omega^{(+)} \mid \varphi_a\rangle\ .$$

In order to completely characterize the scattering event, we need to have the behavior of $\mid \psi_a^{(+)}\rangle$ for large positive t, i.e.,

$$\mid \psi_a^{(+)}(t)\rangle\ =\ e^{-iHt} \mid \psi_a^{(+)}(-\infty)\rangle\ =\ e^{-iHt}\Omega^{(+)} \mid \varphi_a\rangle\ . \tag{12.91}$$

One of the basic boundary condition was that long after the scattering, the state $\mid \psi_a^{(+)}(t)\rangle$ should again behave as a free wave. Thus, in order to characterize the scattering, we should consider the probability coefficients $\mid \langle \varphi_b(t) \mid \psi_a\ ^{(+)}(t)\mid^2$ for large times t. Here $\mid \varphi_b(t)\rangle$ is a free wave.

Define

$$\begin{aligned} S_{ab}\ &=\ \lim_{t\to-\infty}\ \langle \varphi_b(t) \mid \psi_a^{(+)}(t)\rangle \\ &=\ \lim_{t\to\infty}\ \langle e^{-iH_0t}\ \varphi_b \mid e^{-Ht}\ \psi_a^{(+)}\rangle \\ &=\ \lim_{t\to\infty}\ \langle e^{iHt}\ e^{-H_0t}\ \varphi_b \mid \psi_a^{(+)}\rangle \\ &=\ \langle \Omega^{(-)}\ \varphi_b \mid \psi_a^{(+)}\rangle\ =\ \langle \psi_b^{(-)} \mid \psi_a^{(+)}\rangle \end{aligned} \tag{12.92}$$

with

$$\Omega^{(-)}\ :=\ \lim_{t\to\infty}\ e^{iHt}\ e^{-iH_0t} \tag{12.93}$$

and

$$\Omega^{(-)} \mid \varphi_b\rangle\ :=\ \mid \psi_b^{(-)}\rangle \tag{12.94}$$

which characterizes the outgoing scattering state. The existence of $\Omega^{(-)}$ is guaranteed, since the proofs of Section 12.1 never explicitly used the limit $t \to \infty$. Thus, the transition probability from an incoming state to an outgoing state is given by

$$S_{ab}^2 \;=\; |\, \langle \psi_b^{(-)} \mid \psi_a^{(+)} \,\rangle\, |^2 \quad . \tag{12.95}$$

With

$$\begin{aligned} S_{ab} \;=\; \langle \psi_b^{(-)} \mid \psi_a^{(+)} \rangle \;&=\; \langle \Omega^{(-)}\, \varphi_b \mid \Omega^{(+)}\, \varphi_a \rangle \\ &=\; \langle \varphi_b \mid \Omega^{(-)\dagger}\, \Omega^{(+)} \mid \varphi_a \rangle \;:=\; \langle \varphi_b \mid S \mid \varphi_a \rangle \end{aligned} \tag{12.96}$$

we define the **scattering operator** (S-matrix)

$$S \;=\; \Omega^{(-)\dagger}\, \Omega^{(+)} \quad . \tag{12.97}$$

Using the explicit definition of the Møller operators, it can be easily seen that S is unitary. Furthermore, the existence of S depends on the existence of the Møller operators.

12.11 Energy Conservation

In (12.23) the intertwining relation was given as

$$H\Omega^{(\pm)} \;=\; \Omega^{(\pm)}\, H_0 \quad .$$

Its complex conjugate equation reads

$$(\Omega^{(\pm)})^\dagger\, H \;=\; H_0\, \Omega^{\pm\dagger} \quad .$$

From the isometry property of the Møller operators, $\Omega^{(\pm)\dagger}\, \Omega^{(\pm)} \;= \mathbf{1}$, follows

$$(\Omega^{(\pm)})^\dagger\, H\, \Omega^{(\pm)} \;=\; H_0 \quad . \tag{12.98}$$

The last equation leads to the interpretation that $\Omega^{(\pm)}$ can be considered as an operator which transforms H into H_0. From this point of view, we have to conclude that $\Omega^{(\pm)}$ **cannot** be unitary. If it would be, then H and H_0 would have to have the same spectrum.

Since H_0 has only a continuous spectrum, H could not have bound states, which is clearly not the case. We can say that $\Omega^{(\pm)}$ is then and only then unitary, if H does not have bound states.

Let us consider

$$\begin{aligned} SH_0 \;=\; \Omega^{(-)\dagger}\,\Omega^{(+)}\,H_0 \;&=\; \Omega^{(-)\dagger}\,H\,\Omega^{(+)} \\ &=\; H^0\,\Omega^{(-)\dagger}\,\Omega^{(+)} \;=\; H_0 S\ , \end{aligned} \tag{12.99}$$

which shows that $[S, H_0] = 0$. We also have

$$\begin{aligned} H_0 \;\mid \vec{p}\,\rangle \;&=\; E_p \;\mid \vec{p}\,\rangle \\ SH_0 \;\mid \vec{p}\,\rangle \;&=\; E_s\; S \mid \vec{p}\,\rangle \;=\; H_0 S \;\mid \vec{p}\rangle\ , \end{aligned} \tag{12.100}$$

which means that $\mid \vec{p}\,\rangle$ as well as $S \mid \vec{p}\,\rangle$ are eigenstates of H_0 with the same eigenvalue E_p. For the expectation values for H_0 in the initial state (before the scattering) and the final state (after the scattering), we find

$$\begin{aligned} \langle \psi_b^{(-)} \mid H_0 \mid \psi_b^{(-)} \rangle \;&=\; \langle S\psi_a^{(+)} \mid H_0 \mid S\psi_a^{(+)} \rangle \\ &=\; \langle \psi_a^{(+)} \mid S^\dagger H_0 S \mid \psi_a^{(+)} \rangle \\ &=\; \langle \psi_a^{(+)} \mid S^\dagger S\; H_0 \mid \psi_a^{(+)} \rangle \\ &=\; \langle \psi_a^{(+)} \mid H_0 \mid \psi_a^{(+)} \rangle \end{aligned} \tag{12.101}$$

H_0 has a complete spectrum of non-normalizable eigenstates $\{\mid \vec{p}\,\rangle\}$, thus S can be represented in these states. From $[S, t_0] = 0$ follows

$$\begin{aligned} 0 \;=\; \langle \vec{p}\,' \mid [H_0, S] \mid \vec{p}\,\rangle \;&=\; \langle \vec{p}\,' \mid H_0 S \mid \vec{p}\,\rangle \;-\; \langle \vec{p}\,' \mid S H_0 \mid \vec{p}\,\rangle \\ &=\; (E_{p'} - E_p) \langle \vec{p}\,' \mid S \mid \vec{p}\,\rangle\ . \end{aligned} \tag{12.102}$$

From this follows that $\langle \vec{p}\,' \mid S \mid \vec{p}\,\rangle \neq 0$ only if $E_{p'} = E_p$. Therefore, we can write

$$S_{p'p} \;=\; \langle \vec{p}\,' \mid S \mid \vec{p}\,\rangle \;=\; \delta(E_{p'} - E_p) \langle \hat{p}' \mid S \mid \hat{p} \rangle \tag{12.103}$$

where $\hat{p} = \vec{p}/\mid \vec{p}\ \mid$. This means $S_{p'p}$ is defined on-shell.

12.12 Unitarity of the S-Operator

In order to show that S as defined in (12.97) is unitary, we have to show that

$$S^\dagger S \;=\; S S^\dagger \;=\; \mathbf{1}\;. \tag{12.104}$$

The first relation is easy and we use that $\Omega^{(+)\dagger}\,\Omega^{(\pm)} = \mathbf{1}$:

$$\begin{aligned}
\langle \Omega^{(\pm)}\varphi \mid \Omega^{(\pm)}\varphi\rangle &= \lim_{t'\to\mp\infty}\lim_{t\to\mp\infty} \langle e^{iHt'}\, e^{-iH_0t'}\, \varphi \mid e^{iHt}\, e^{-iH_0t}\, \varphi\rangle \\
&\overset{t'=t}{=} \lim_{t\to\mp\infty} \langle e^{iHt}\, e^{-iH_0t}\, \varphi \mid e^{iHt}\, e^{iH_0t}\, \varphi\rangle \\
&= \langle \varphi \mid \mathbf{1} \mid \varphi\rangle \;= \parallel \varphi \parallel^2 \;.
\end{aligned} \tag{12.105}$$

In order to show the other relation, we need to consider the mapping properties of $\Omega^{(\pm)\dagger}$. Applied on a scattering state, it gives

$$\Omega^{(\pm)\dagger} \mid \psi_a^{(\pm)}\rangle \;=\; \Omega^{(\pm)\dagger}\,\Omega^{(\pm)} \mid \varphi_a\rangle \;= \mid \varphi_a\rangle\;. \tag{12.106}$$

This means, applied on a scattering state $\Omega^{(\pm)\dagger}$, gives a full wave packet.

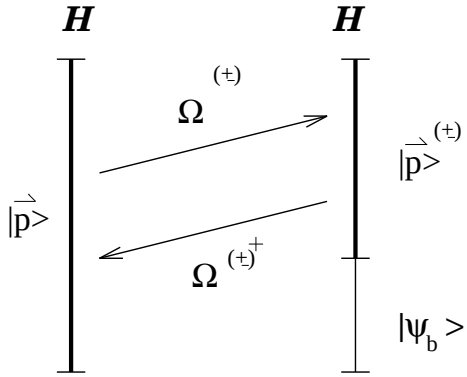

Fig. 12.4 Mapping properties of the Møller operators.

Fig. 12.4 illustrates that

$$\begin{aligned}
\mid p\rangle^{(\pm)} &= \Omega^{(\pm)} \mid \vec{p}\,\rangle \\
\mid \vec{p}\,\rangle &= \Omega^{(\pm)\dagger} \mid \vec{p}\,\rangle^{(\pm)} \quad \text{with} \;\; Ker(\Omega^{(\pm)\dagger}) \;\neq\; 0 \\
0 &= \Omega^{(\pm)\dagger} \mid \psi_n\rangle\;.
\end{aligned} \tag{12.107}$$

Thus $\Omega^{(\pm)}\ \Omega^{(\pm)\dagger} = P_c$, a projection operator on the continuous spectrum. Now consider

$$\begin{aligned} S^\dagger S &= (\Omega^{(-)\dagger}\Omega^{(+)})^\dagger(\Omega^{(-)\dagger}(\Omega^{(-)\dagger}\Omega^{(+)}) &&= \Omega^{(+)\dagger}\Omega^{(-)}\Omega^{(-)\dagger}\ \Omega^{(+)} \\ &&&= \Omega^{(+)\dagger}\ P_c\Omega^{(+)} \ = \ \mathbf{1} \\ SS^\dagger &= (\Omega^{(-)\dagger}\Omega^{(+)})(\Omega^{(-)\dagger}\Omega^{(+)})^\dagger &&= \Omega^{(-)\dagger}\Omega^{(+)}\Omega^{(+)\dagger}\Omega^{(-)} \\ &&&= \Omega^{(-)\dagger}\mathbf{P}_c\ \Omega^{(-)} \ = \ \mathbf{1}\ . \end{aligned} \tag{12.108}$$

As a remark: S is only unitary on the whole Hilbertspace $\mathcal{H}$ if the states $\mid p\rangle^{(+)}$ span the entire space of scattering states.

Let us now consider the probability of scattering into all possible final states

$$\begin{aligned} \int d^3p\ \mid \langle \vec{p}\ \mid S \mid \varphi_a\rangle \mid^2 &= \int d^3p\ \langle \vec{p}\ \mid S \mid \varphi_a\rangle^* \langle \vec{p}\ \mid S \mid \varphi_a\rangle \\ &= \int d^3p\ \langle \varphi_a \mid S^\dagger \mid \vec{p}\ \rangle\langle \vec{p}\ S \mid \varphi_a\rangle \\ &= \langle \varphi_a \mid S^\dagger S \mid \varphi_a\rangle \ = \parallel \varphi_a \parallel^2 \ . \end{aligned} \tag{12.109}$$

Thus, the probability is conserved in the scattering process.

12.13 Transition Operator

In (12.96) the scattering operator was defined as the transition probability

$$\begin{aligned} S_{ba} &= \langle \psi_b^{(-)} \mid \psi_a^{(+)}\rangle \\ &= \langle \varphi_b \mid \psi_a^{(+)}\rangle \ + \ \langle\ \frac{1}{E_b - i\varepsilon - H}\ V\ \varphi_b \mid \psi_a^{(+)}\rangle\ , \end{aligned} \tag{12.110}$$

where we used the Low equation (12.79) for the last step. One also has

$$\begin{aligned} \langle \varphi_b \mid \psi_a^{(+)}\rangle &= \langle \varphi_b \mid \varphi_a\rangle \ + \ \langle \varphi_b \mid G_0(E_a + i\varepsilon)\ V \ \mid \psi_a^{(\pm)}\rangle\ . \\ &= \delta_{ba} \ + \ \frac{1}{E_a - E_b - i\varepsilon}\ \langle \varphi_b \mid V \mid \psi_a^{(+)}\rangle \end{aligned} \tag{12.111}$$

Inserting (12.111) into (12.110) leads to

$$
\begin{aligned}
S_{ba} &= \delta_{ba} + \left[\frac{1}{E_b - E_a + i\varepsilon} - \frac{1}{E_b - E_a - i\varepsilon}\right] \langle \varphi_b \mid V \mid \psi_a^{(+)} \rangle \\
&= \delta_{ba} - 2\pi i\, \delta(E_b - E_a) \langle \varphi_b \mid T^{(+)}(E_a) \mid \varphi_a \rangle \\
&= \delta_{ba} - 2\pi i\, \delta(E_b - E_a)\, T_{ab}^{(+)}(E_a)\ .
\end{aligned}
\tag{12.112}
$$

This suggests that the S operator can be split into two parts according to

$$
S = \mathbf{1} - 2\pi i\, \tau^{(+)} \tag{12.113}
$$

where

$$
\tau_{ba}^{(\pm)} := \delta(E_b - E_a)\, T_{ba}^{(\pm)} \tag{12.114}
$$

describes the scattering. For the interaction $V = 0$ follows $S = \mathbf{1}$.

Thus, $\tau_{ba}^{\pm}$ describes the scattering process and has to appear in the differential cross section. Thus for scattering relevant quantity is $S - \mathbf{1}$, where the scattering in forward direction is subtracted. Due to the δ function $\delta(E_b - E_a)$, $\tau_{ba}^{(\pm)}$ is only defined for $E_b = E_a$, i.e., on-shell. Another way to formulate this is that the S operator only defines the on-shell elements of the T operator. However, this is not enough to define an operator – one has to know the matrix elements for all momenta. From the unitarity of the S operator follows

$$
\begin{aligned}
SS^\dagger &= (\mathbf{1} - 2\pi i \tau^{(+)})(\mathbf{1} + 2\pi i \tau^{(-)}) \\
&= \mathbf{1} - 2\pi i(\tau^{(+)} - \tau^{(-)}) + 4\pi^2\, \tau^{(+)}\tau^{(-)}
\end{aligned}
\tag{12.115}
$$

and from there

$$
\begin{aligned}
\tau^{(+)} - \tau^{(-)} &= -2\pi i\, \tau^{(+)}\tau^{(-)} \\
\delta(E_b - E_a)(T_{ba}^{(+)} - T_{ba}^{(-)}) &= -2\pi i \sum_\alpha \delta(E_b - E_a)\, \delta(E_a - E_\alpha)\, T_{b\alpha}^{(+)} T_{\alpha b}^{(-)}
\end{aligned}
\tag{12.116}
$$

and for $E_0 = E_a$

$$
T_{ba}^{(+)} - T_{ba}^{(-)} = -2\pi i \sum_\alpha \delta(E_b - E_\alpha)\, T_{b\alpha}^{(+)} T_{\alpha a}^{(-)} \tag{12.117}
$$

or explicitly

$$\begin{aligned}\langle \vec{p}\ \mid T^{+}(E_p) - T^{(-)}(E_p) \mid \vec{p}\,' \rangle \;&=\; -2\pi i \int d^3k\ \delta(E_p - E_\alpha) \\ &\quad \langle \vec{p}\ \mid T^{(+)}(E_p) \mid \vec{k}\ \rangle\langle \vec{k}\ \mid T^{(-)}(E_p) \mid \vec{p}\,' \rangle\end{aligned} \tag{12.118}$$

which is the on-shell unitarity relation already derived in (12.89). However, (12.118) contains less information than the unitarity relations derived in Section 12.9, which are given fully-off-shell.

12.14 Cross Section

The cross section should describe the probability that under given initial conditions something is scattered into the direction of $\vec{p}\,'$, where the forward direction should be subtracted. This probability is obviously given by $S - \mathbf{1}$ and can be defined as

$$\begin{aligned} dW &= d^3p' \ \mid -2\pi i\langle \vec{p}\,' \mid T \mid \varphi_{\vec{p}}\ \rangle \mid^2 \\ &= p'^2\ dp'\ d\Omega_{\vec{p}\,'}\ \mid -2\pi i\langle \vec{p}\,' \mid T \mid \varphi_{\vec{p}}\ \rangle \mid^2 \\ &= m\ \sqrt{2mE'}\ dE'\ d\Omega_{\vec{p}}\ 4\pi^2 \mid \langle \vec{p}\,' \mid T \mid \varphi_{\vec{p}}\ \rangle \mid^2 \end{aligned} \tag{12.119}$$

where $p^2 = 2mE$ has been used. Next we need to consider

$$\begin{aligned} \mid \langle \vec{p}\,' \mid T(E_p) \mid \varphi_{\vec{p}}\ \rangle \mid^2 \;&=\; \left| \int d^3p\ \langle \vec{p}\,' \mid T(E_p) \mid \vec{p}\ \rangle\ \tilde{\varphi}_{p_0}(\vec{p}\ ) \right|^2 \\ &=\; \left| \int d^3p\ \delta(E' - E_p) \langle \hat{p}' \mid T(E_p) \mid \hat{p} \rangle\ \tilde{\varphi}_{p_0}(\vec{p}\ ) \right|^2 . \end{aligned} \tag{12.120}$$

For $\tilde{\varphi}_{p_0}(\vec{p}\ )$ being a wave packet which is sharply peaked at $\vec{p} = \vec{p}_0$ and $\langle \hat{p}' \mid T(E_p) \mid \hat{p} \rangle$ being a slowly varying function, we can write

$$|\langle \vec{p}\,' \mid T(E_p) \mid \varphi_{\vec{p}}\ \rangle \mid^2 \approx\ \langle \hat{p}' \mid T(E_{p_0}) \mid \hat{p} \rangle \mid^2 \mid \int d^3p\ \delta(E' - E_p)\ \tilde{\varphi}_{p_0}(\vec{p}\ ) \mid^2$$

and thus

$$\begin{aligned} dW \;&\approx\; 4\pi^2\ mp_0\ d\Omega\ dE\ \mid \langle \hat{p}' \mid T(E_{p_0}) \mid \hat{p} \rangle \mid^2 \int d^3p\ \delta(E' - E_p)\ \tilde{\varphi}_{p_0}(\vec{p}\ ) \mid^2 \\ &=\; 4\pi^2\ mp_0\ d\Omega\ dE \mid \langle \hat{p}' \mid T(E_{p_0}) \mid \hat{p} \rangle \mid^2\ I(E_p)\ . \end{aligned} \tag{12.121}$$

Needed is the scattering into a definite solid angle $d\Omega$, thus one can integrate over the energy

$$dW(\Omega) \;=\; 4\pi^2 \; mp_0 \; d\Omega \;\; | \, \langle \hat{p}' \mid T(E_{p_0}) \mid \hat{p}_0 \rangle^2 \;\; \int \; dE' \; I(E) \; . \tag{12.122}$$

The energy δ-function can be written as
$\delta(E' - E) = \frac{m}{p_0} \delta(\mid \vec{p}' \mid - \mid \vec{p}_0 \mid)$ leading to another factor $\frac{m}{p_0}$ in 12.122.

The differential cross section was defined as the flux scattered into a specific solid angle $d\Omega$ divided by the incoming flux:

$$\begin{aligned} d\sigma \;&=\; \frac{dW(\Omega)}{W_0} \\ &=\; \frac{(2\pi)^4 \; mp_0 \cdot \; \frac{m}{p_0} \; \rho_0 \; \Delta t \;\; | \, \langle \hat{p}' \mid T(E_{p_0}) \mid \hat{p}_a \mid^2 \;\; d\Omega}{\rho_0 \; \Delta t} \end{aligned} \tag{12.123}$$

from which follows

$$\frac{d\sigma}{d\Omega} \;=\; (2\pi)^4 \; m^2 \;\; | \, \langle \hat{p}' \mid T(E_{p_0}) \mid \hat{p}_0 \rangle \mid^2 = \mid f(\hat{p}', \hat{p}) \mid^2 \tag{12.124}$$

which gives the relation between the on-shell t-matrix and the scattering amplitude. For the total cross section this leads to

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega} = (2\pi)^4 m^2 \int \Omega |\langle \hat{p}' | T(E_{p_0} | \hat{p} \rangle|^2 \tag{12.125}$$

12.15 Scattering of Identical Spinless Particles

For identical particles the states have to be symmetric (or antisymmetric) under the exchange of the two particles. Interchanging particle labels corresponds to replacing $\vec{p} \;=\; (p, \theta, \phi)$ by $-\vec{p} \;=\; (p, \pi - \theta, \phi + \pi)$. Similarly, the scattering amplitude has to be symmetric (antisymmetric) under the exchange of 1 and 2, i.e., we have to consider

$$f(\hat{p}', \hat{p}) \;\pm\; f(-\hat{p}', \hat{p}) \;=\; f(\theta, \phi) \;\pm\; f(\pi - \theta, \phi + \pi) \; , \tag{12.126}$$

Since for spinless particles, the interaction is rotationally invariant around the axis along the incoming momentum $\vec{p}$, we drop the dependence on ϕ and have

$$\begin{aligned} \frac{d\sigma}{d\Omega} \;&=\; \mid f_p(\theta) \;+\; f_p(\pi - \theta) \mid^2 \\ &=\; \mid f_p(\theta) \mid^2 \;+\; \mid f_p(\pi - \theta) \mid^2 \;+ 2Re(f^*(\theta) \; f(\pi - \theta)) \; . \end{aligned} \tag{12.127}$$

First, the differential cross section for the scattering of two identical spinless particles is symmetric around 90^o. Second, $\frac{d\sigma}{d\Omega}$ contains three terms, the cross sections for the amplitudes for scattering into the direction (θ, ϕ) for particles interference from $z = -\infty$ and $z = +\infty$ and an influence term, which is a typical quantum mechanical effect, since one must add amplitudes and not intensities.

Next, we consider the scattering of two identical spin $\frac{1}{2}$ particles interacting via a spin-independent potential. Since their spin is a good quantum number, we consider $S = 0$ and $S = 1$ states separately. The total wave function must be antisymmetric. For $S = 0, \chi_{s=0}$ is antisymmetric, thus the spatial part must be symmetric. Thus, we obtain for the cross section in the singlet state

$$\frac{d\sigma_s}{d\Omega} = \mid f(\theta) + f(\pi - \theta) \mid^2 \tag{12.128}$$

For $S = 1, \chi_{s=1}$ is symmetric, thus the spatial part must be antisymmetric, and we obtain

$$\frac{d\sigma_t}{d\Omega} = \mid f(\theta) - f(\pi - \theta) \mid^2 \ . \tag{12.129}$$

Eqs. (12.128) and (12.129) assume that the scattering particles are in a definite spin state, i.e., beam and target are polarized. If this is not the case, i.e., if beam as well as target are unpolarized, i.e., spins are randomly oriented, then we must average over the random spin orientations. This corresponds to the assumption that the four spin states, $S = 0, m_s = 0, S = 1, m_s = \pm 1, 0$ occur with equal frequency. Then the **unpolarized** differential cross section is given by

$$\frac{d\sigma}{d\Omega}\,(unpol) = \frac{1}{4}\,\frac{d\sigma_s}{d\Omega} + \frac{3}{4}\,\frac{d\sigma_t}{d\Omega}\ . \tag{12.130}$$

12.16 The Gellman-Goldberger Relation

The Gellman-Goldberger relation or **two-potential formula** is particularly appropriate when the interaction between the projectile and the target decomposes naturally into two parts: $V = V_0 + V_1$. This division is especially useful if the scattering wave function under the action of one part can be obtained exactly, while the effect of the other can be treated in the same approximation. In this sense, the formula leads to the so-called "distorted-wave Born approximation" and, in other circumstances, to the method of the "final state interaction."

Let us assume that the interaction potential $V = V_0 + V_1$. Then, the corresponding LS equation reads

$$\begin{aligned} T &= (V_0 + V_1) + (V_0 + V_1)\, G_0 T \\ &= (V_0 + V_1) + V_0\, G_0 T + V_1\, G_1 T \end{aligned} \tag{12.131}$$

As a reminder, from (12.58) we had for the scattering state

$$| \vec{p} \rangle^{(+)} = | \vec{p} \rangle + G_0 V \ | \vec{p} \rangle^{(+)}$$

from which follows

$$| \vec{p} \rangle^{(+)} = (1 - G_0 V)^{-1} \ | \vec{p} \rangle = \Omega^{(+)} \ | \vec{p} \rangle \ . \tag{12.132}$$

From the relation (12.39), we obtained the Low equation in the form

$$| \vec{p} \rangle^{(+)} = | \vec{p} \rangle + GV \ | \vec{p} \rangle = (1 + GV) \ | \vec{p} \rangle = \Omega^{(+)} \ | p \rangle \tag{12.133}$$

So we have the different representations of the Møller operator

$$\Omega^{(+)} = (1 - G_0 V)^{-1} = (1 + GV) = 1 + G_0 T \ . \tag{12.134}$$

Multiplying (12.131) from the left with $\Omega_0^{(+)\dagger} := (1 - V_0 G_0)^{-1}$ gives

$$\begin{aligned} (1 - V_0 G_0)^{-1} \ (1 - V_0 G_0) T &= (1 - V_0 G_0)^{-1} \ V_0 + (1 - V_0 G_0)^{-1} \ V_1 \qquad (12.135) \\ &+ (1 - V_0 G_0)^{-1} \ V_1 G_0 T \\ T &= T_0 + (1 - V_0 G_0)^{-1} \ V_1 \ (1 + G_0 T) \qquad (12.136) \end{aligned}$$

where we used that $T_0 = V_0 + V_0 \ G_0 T_0$ as exact solution of the Hamiltonian $H_0 + V_0$. Using the relations (12.134), one obtains

$$T = T_0 + \Omega_0^{(-)\dagger} \ V_1 \ \Omega^{(+)} \tag{12.137}$$

where $\Omega^{(+)}$ is the Møller operator for the full scattering problem. Eq (12.137) is the so-called "two-potential formula." The first term is the scattering amplitude for the potential V_0 alone; in many cases, it is either known or calculable. The second term incorporates the effect of the "residual potential "V_1 and must often be treated approximately. If the interaction V_1 is sufficiently weak, it can be treated in a first order approximation, which means here $\Omega^{(+)} \approx \Omega_0^{(+)}$ so that

$$T \approx T_0 + \Omega_0^{(-)\dagger} \ V_1 \ \Omega_0^{(+)} \tag{12.138}$$

or in terms of matrix elements

$$\langle \vec{p}\,' \mid T \mid \vec{p}\,\rangle \;:=\; T_{fi} \;=\; \langle \vec{p}\,' \mid T_0 \mid \vec{p}\,\rangle \;+\; {}^{(-)}\langle \vec{p}_0\,' \mid V_1 \mid \vec{p}_o\rangle^{(+)} \;. \tag{12.139}$$

The second term is a generalization of the Born approximation in which distorted wave functions $\mid p_0\rangle^{(+)}$ are used to calculate the scattering due to V_1 in the presence of V_0. It is often called the **distorted wave Born approximation**. For instance, in the scattering of protons from nuclei, one might choose V_0 to be the Coulomb potential and V_1 the short-range nuclear force. Then the second term in (12.139) approximates the scattering due to the nuclear force, taking account of the Coulomb repulsion and the consequent reduction in the amplitude of the wave function at small separations. See Ch. Elster, L. C. Liu and R. M. Thaler, "A Practical calculational method for treating Coulomb scattering in momentum space," J. Phys. G **19**, 2123 (1993).

J. Phys. G: Nucl. Part. Phys. 19 (1993) 2123–2134. Printed in the UK

A practical calculational method for treating Coulomb scattering in momentum space

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Received 3 June 1992, in final form 5 July 1993

Abstract. An exact and practical numerical procedure for treating the Coulomb interaction in momentum-space calculations of elastic scattering of charged particles is presented. The method is tested for various interactions over a wide charge, energy and angular momentum range and found to be accurate.

1. Introduction

In a recent paper an exact and practical method for the treatment of the Coulomb interaction in the scattering of protons from nuclei in momentum space has been successfully applied [1] and several new physical results hitherto unascertainable have been presented therein. The interest and necessity to develop an accurate treatment of the Coulomb interaction in momentum space has been further motivated in intermediate-energy proton–nucleus scattering, since it is now well established that the non-locality of the first-order optical potential for proton–nucleus scattering must be treated accurately in order to reproduce experimental data for proton–nucleus elastic scattering at intermediate energies. Recently performed 'full-folding' calculations by several different groups [2–4] have shown clearly that intermediate-energy calculations of proton–nucleus elastic scattering are highly sensitive to the details of the non-locality of the optical potentials, especially near interference minima or at larger scattering angles. Because the non-locality of the proton–nucleus optical potentials has its origin in the non-locality of the elementary proton–nucleon interaction and because the on-shell proton–nucleon amplitude is related to the proton–nucleon scattering cross sections, which are themselves momentum-space observables, it follows that formulating optical potentials directly in the momentum space represents a more natural description of the physics. For this reason, it is of vital interest to be able to treat the Coulomb interaction in momentum space in an exact, numerically reliable way. In view of the importance of this matter, the theoretical basis of the method applied in [1] is examined further in this paper.

The problem of scattering by the long-range Coulomb force is theoretically well understood [5–7], and an established technology is available for the calculation of scattering observables for strongly interacting charged particles. These procedures are defined and carried out in coordinate space [7], whereas, for the reasons stated above, more and more calculations in nuclear physics are being performed in momentum space. It may appear strange that a problem which has a well defined solution in coordinate space should

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occasion difficulty in momentum space. The fact is that the Fourier transform of the so-called coordinate-space Coulomb wavefunction does not exist in a functional sense. The logarithmic singularity due to the long range of the Coulomb force, that can be treated easily in coordinate space, is far more intractable in momentum space.

Vincent and Phatak (VP) have introduced a method for handling the Coulomb-nuclear problem in momentum space [8]. This method has had considerable success and has been widely applied [9]. Its underlying idea is the solution of the problem in momentum space with a cut-off Coulomb force, followed by the matching of the Fourier transform of this solution to the asymptotic Coulomb wave in coordinate space, thus enforcing the correct asymptotic behaviour. Although the method is correct in principle, as we shall show, it is difficult to apply with stable accuracy as a result of the sharp cut-off present in that method. Indeed, some procedures [10, 11] have been recently suggested to dampen the effect of the sharp cut-off.

A different approach has been taken by Alt, Sandhas and collaborators [12, 13], whose work has been performed entirely in momentum space. The long-range Coulomb force is 'suitably' screened by a decreasing radial function, and the screened Coulomb-nuclear problem is then solved as an integral equation. The unscreened limit is taken to be the 'stable' result obtained by increasing the screening radius. This too is a correct-in-principle method which can be made to work. This method has been successfully tested and applied in p–d [$Z_1 Z_2 = 1$] scattering calculations at low energies [13], but is unexplored for high charges Z and high energies, and probably extremely difficult to realize in this regime.

A number of different approximate procedures have also been introduced [14, 15]. Since these procedures are approximate, they must be investigated with care in each instance of application. Clearly, an exact treatment of the scattering of charged particles in momentum space, which is relatively easy to apply and numerically stable, is still of great interest.

All the previous attacks on the inclusion of the long-range Coulomb interaction in momentum-space calculations discussed above [8, 11–14] can be characterized by some sort of Coulomb shielding. If the Coulomb interaction is shielded, it can of course, be treated as an ordinary short-range potential, and for each angular momentum the difference between the full phase shift (shielded point Coulomb plus short-range potential) and the shielded point Coulomb phase shift can be calculated. Such procedures always present the problem that the 'shielding radius' R must be sufficiently large that the non-point Coulomb part of the phase shift has stabilized, that is increasing R gives the same numerical result. On the other hand, if R becomes too large, these procedures are inherently indistinguishable from the non-shielding calculations and suffer from the very disease they were introduced to alleviate. It is thus obviously most desirable to find a practical computational procedure based on a treatment in which the limit $R \to \infty$ is taken analytically, instead of being taken numerically. We suggest such a procedure in this paper.

The algorithm we suggest involves application of the well known two-potential formula to the scattering of a charged particle from a target of like charge (i.e. repulsive Coulomb force). The interaction is separated into the sum of two parts, one of which is the 'point' Coulomb interaction, the other being the short-ranged residuum. Since the Coulomb T-matrix is known analytically, we need only solve for the residual Coulomb-modified transition matrix. It is known that this latter problem can be transformed to the problem of solving a Lippmann–Schwinger equation, for which the input 'potential' is modified through the introduction of the Coulomb distortion [16]. Such a procedure has been attempted by the Hannover Group [17]. However, as those authors pointed out, it is tedious to obtain stable numerical results with that calculational method. It is, therefore, the purpose of this paper to re-examine the derivation of this two-potential formalism to recognize how calculations

may be performed to ensure numerical stability in the most expeditious manner over the widest possible range of conditions. We emphasize that the crucial aspect differentiating our approach from the previous ones is that the limiting procedure for Coulomb shielding is taken *analytically* in our approach. It is this analytic procedure that ensures stable numerical results without introducing any approximation. The details of our considerations appear in condensed form in section 2, so that the calculational method may be easily discerned. Sample calculations are presented in this paper (section 3), so that the reader may see the accuracy obtainable here *vis-a-vis* the coordinate-space results, and those generated by means of the VP algorithm. Finally, we present in section 4 further discussion about our method and the conclusions.

2. The scattering equation and its solution

We wish to calculate elastic scattering of a charged particle in the field of a potential which consists of a long-ranged Coulomb part and a finite-ranged part, i.e. we consider a potential W given by

$$W = V^{\mathrm{C}} + V^{\mathrm{S}} \tag{1}$$

where V^{C} is a repulsive Coulomb potential and V^{S} is an arbitrary short-ranged potential. The familiar two-potential formula for the scattering amplitude is then given as

$$\bar{f}(E,\theta) = \frac{-\eta(E)}{2k_0 \sin^2\frac{\theta}{2}} \mathrm{e}^{-2\mathrm{i}\eta(E)\ln(\sin\theta/2)} - \frac{2\pi^2\mu}{k_0} \sum_l (2l+1)\mathrm{e}^{2\mathrm{i}[\sigma_l(E)-\sigma_0(E)]} \langle k_0|\tau_l(E)|k_0\rangle P_l(\cos\theta) \tag{2}$$

where E is the scattering energy and k_0 is the on-shell momentum defined by $k_0^2 = 2\mu E$. Further

$$\sigma_l(E) = \arg\Gamma(l+1+\mathrm{i}\eta) \tag{3}$$

is the Coulomb phase shift and

$$\eta(E) = Z_1 Z_2 \mu/\hbar k_0. \tag{4}$$

The matrix element $\langle k_0|\tau_l(E)|k_0\rangle$ is related to the Coulomb-modified nuclear phase shift by

$$\langle k_0|\tau_l(E)|k_0\rangle = (-2\pi^2\mu)^{-1} \mathrm{e}^{\mathrm{i}\delta_l(E)} \sin\delta_l(E) \tag{5}$$

which is the on-shell solution of the following Lippmann–Schwinger type equation:

$$\langle k'|\tau_l(E)|k\rangle = \langle k'|U_l|k\rangle + \int \langle k'|U_l|k''\rangle \frac{4\pi k''^2\,\mathrm{d}k''}{E - E'' + \mathrm{i}\varepsilon} \langle k''|\tau_l(E)|k\rangle. \tag{6}$$

Here $\langle k'|U_l|k\rangle$ is the Coulomb-distorted matrix element of the short-range potential V^{S} and is given by

$$\langle k'|U_l|k\rangle = \langle (\phi_l^{\mathrm{C}})^{(+)}(k')|V^{\mathrm{S}}|(\phi_l^{\mathrm{C}})^{(+)}(k)\rangle \tag{7}$$

where $(\phi_l^C)^{(+)}$ is the Coulomb wavefunction. A detailed derivation and justification of the above equations are given in the appendix.

Treating Coulomb scattering in momentum space amounts, therefore, to solving (6). For that purpose, one must find a suitable, reliable way to calculate $\langle k'|U_l|k\rangle$, the short-range potential in a Coulomb basis (7). We will examine this aspect of Coulomb scattering in the remainder of this section.

We first emphasize that the calculation of U_l in terms of momentum-space Coulomb wavefunctions through the relations

$$\langle k'|U_l|k\rangle = \langle(\phi_l^C)^{(+)}(k')|V^S|(\phi_l^C)^{(+)}(k)\rangle$$
$$= (4\pi)^2 \mathcal{N}_l^*(k')\mathcal{N}_l(k) \int \langle\phi_l^C(k')|k'''\rangle k'''^2\,dk'''\langle k'''|V^S|k''\rangle k''^2\,dk''\langle k''|\phi_l^C(k)\rangle \quad (8)$$

cannot be readily carried out. The Hannover group [17] has attempted to use momentum-space Coulomb wavefunctions to obtain the potential U_l (8) by integrating over their rapid oscillations; and, indeed, their approach has not been fruitful in a wider range of applications.

The origin of the above-mentioned difficulty is that the momentum-space Coulomb wavefunctions do not properly exist. To see this more clearly, we first note that the coordinate-space Coulomb wavefunction $\langle r|\phi_l^C(k)\rangle$ may be written as

$$\langle r|(\phi_l^C)(k)\rangle = \hat{M}_l F_l(\eta, kr) \quad (9)$$

where $\hat{M}_l = (2\pi)^{-3/2}e^{i\sigma_l}/kr$, $\eta \equiv \eta(k) = Z_1Z_2\mu/\hbar k$, and the function $(kr)^{-1}F_l(\eta, kr)$ is the regular solution of the radial Schrödinger equation with a potential given by $Z_1Z_2e^2/r$, and is normalized in such a way that

$$F_l(\eta, kr) \overset{r\to\infty}{\to} \sin\left[kr - \frac{l\pi}{2} + \sigma_l(E) - \eta(E)\ln 2kr\right]. \quad (10)$$

The Fourier transform of that function is

$$\langle k''|\phi_l^C(k)\rangle \equiv \mathcal{N}_l \int_0^\infty dr\, r j_l(k''r) F_l(\eta, kr) \quad (11)$$

with $\mathcal{N}_l = (2\pi^2 k)^{-1}e^{i\sigma_l}(-i)^l$. However, equation (11) is not well defined in the sense that the integral is not strongly convergent. In fact, it is easy to see that

$$\int_0^\infty dr\, r j_l(k'r) F_l(\eta, kr) = \frac{2k}{e^{2i\sigma_l} - 1}\int_0^\infty dr\, r^2 j_l(k'r) j_l(kr)$$
$$+ \int_0^\infty dr\, r j_l(k'r)\left[F_l(\eta, kr) - \frac{2ke^{i\sigma_l}}{e^{2i\sigma_l} - 1} r j_l(kr)\right]$$
$$= \frac{\pi}{ke^{2i\sigma_l} - 1}\delta(k - k') + \int_0^\infty dr\, r j_l(k'r)\left[F_l(\eta, kr) - \frac{2ke^{i\sigma_l}}{e^{2i\sigma_l} - 1} r j_l(kr)\right] \quad (12)$$

is of dubious validity. The right-most integral in (12) converges in the case that $F_l(\eta, kr)$ represents scattering from a finite-ranged potential with phase shift σ_l. However, this integral is not well defined in the Coulomb case. This remark is equivalent to the statement that the integral equation in momentum space for the Coulomb wavefunction does not have a well defined solution, or equivalently, that the momentum-space Coulomb wavefunction

considered to be the Fourier transform of the coordinate-space Coulomb function does not exist in the functional sense.

However, despite the difficulty in dealing with (8), the Coulomb-distorted matrix elements of U_l do exist and are well defined, because V^S is a finite-ranged potential. This latter fact underlies our procedure given below.

We choose to express the matrix element $\langle k'|U_l|k\rangle$ as

$$\langle k'|U_l|k\rangle = \int \langle \phi_l^C(k')|r'\rangle r'^2\,\mathrm{d}r'\langle r'|V_l^S|r''\rangle r''^2\,\mathrm{d}r''\langle r''|\phi_l^C(k)\rangle \tag{13}$$

and recommend the use of (13) as the basic procedure to follow in the calculation of the matrix element $\langle k'|U_l|k\rangle$. This integration is numerically stable because the coordinate-space Coulomb wavefunctions are well defined and V^S is short-ranged. Thus, if V^S is known in coordinate space, the prescription for the generation of U_l is simple, i.e. we fold V^S with the r-space Coulomb functions and integrate. If the V^S is known initially in momentum space, the prescription for the generation of U_l involves another step, that is we must first find V^S in coordinate space by Fourier-transforming V^S from momentum space into coordinate space, i.e.

$$\langle r'|V_l^S|r\rangle = \frac{2}{\pi}\int j_l(k''r')k''^2\,\mathrm{d}k''\langle k''|V_l^S|k'''\rangle k'''^2\,\mathrm{d}k'''\,j_l(k'''r). \tag{14}$$

Those Fourier transforms do exist because of the finite range of V^S.

In brief, the calculational feasibility of the matrix element defined by (13), which is the input to the Lippmann–Schwinger equation (6), is an essential point in our treatment of charged-particle scattering in momentum space. In no instance have we had any difficulty in obtaining accurate numerical representations of the matrix element $\langle k'|U_l|k\rangle$. The only practical difficulty that may be encountered with our method is that given a potential in momentum space, it may not always be numerically easy to generate the coordinate-space analogue of that potential. Usually this is just a matter of grid sizes, N, unless the potential has a highly oscillatory behaviour or a non-integrable singularity structure. As a further remark, if the single Fourier transform in one momentum variable exists for all fixed values of the other variable, the double transform poses only the question of construction of an algorithm which is of order N^3 instead of order N^4 which might be implied by the structures of (13) and (14). In addition, those equations are highly vectorizable, so that even linear grids of the order of 10^4 can efficiently be implemented within high-performance vector architectures. No difficulties whatsoever were encountered in any of the cases we explored. Once the matrix elements of U_l are calculated, the momentum-space integral equation for $\langle k|\tau_l(E)|k'\rangle$ (6) can be solved conveniently by matrix inversion with its propagator singularity taken care of by the method of Sloan [18].

3. Calculation of phase shifts

The above procedure has been tested with proton scattering from charged targets. A number of different short-range interaction V^S have been considered. In table 1, we show the results for $l = 0$ phase shifts given by the present theory and by the usual r-space calculations at proton lab kinetic energy T_p between 25 and 800 MeV for a target having a point charge $Z = 20$, which interacts with the proton via a local exponential interaction $V^S(r) = U_0\exp(-\lambda r)$ with $U_0 = -300$ MeV and $\lambda = 770$ MeV c^{-1}. We have also made

comparisons for the proton scattering from a target having $Z = 82$. In order to further test the accuracy of the present theory for high-l partial waves, we have changed the parameters of the exponential interaction by using $\lambda = 280$ MeV c^{-1} while leaving the value of U_0 unchanged. The results are given in table 2, which show very good agreement between the phase shifts given by the present theory and the r-space calculations. We emphasize that the use of a local potential for comparison is only because local potentials can be easily solved exactly in coordinate space. In [1] this method is applied to inherently non-local potential calculations for proton–nucleus scattering.

Table 1. $l = 0$ phase shifts (in degrees) of proton scattering from a target of $Z = 20$ for an exponential short-range interaction with $U_0 = -300$ MeV and $\lambda = 770$ MeV c^{-1}.

	$V^C = 0$		$V^C \neq 0$	
T_p (MeV)	r-space	k-space	r-space	k-space
25	34.31	34.32	6.49	6.50
100	29.49	29.50	23.32	23.31
200	24.28	24.30	22.96	22.97
500	16.89	16.89	17.07	17.07
800	13.35	13.35	13.59	13.59

Table 2. Phase shifts δ_l (in degrees) of proton scattering from a target of $Z = 82$ for an exponential short-range interaction with $U_0 = -300$ MeV and $\lambda = 280$ MeV c^{-1}.

		$V^C = 0$		$V^C \neq 0$	
T_p (MeV)	l	r-space	k-space	r-space	k-space
50	0	126.8	126.8	48.49	48.29
	1	97.84	97.84	22.70	22.62
	2	55.25	55.22	9.93	9.90
	3	23.75	23.73	4.39	4.38
	4	9.87	9.86	1.95	1.94
200	0	77.22	77.10	81.16	81.02
	1	66.25	66.14	62.15	62.06
	2	52.31	52.23	44.88	44.82
	3	38.79	38.73	31.26	31.22
	4	27.56	27.52	21.33	21.31
	5	19.09	19.06	14.41	14.39

In section 1, we mentioned that the VP algorithm [8] in principle gives an exact method but is difficult to use with controllable accuracy. To see this, we compare, in table 3, the phase shifts given by the VP algorithm, the present theory, and the r-space calculations for the case of $Z = 82$ at $T_p = 200$ MeV with the same interaction as given in table 2. For the purpose of discussion, we take the r-space phase shifts to represent the exact solution and calculate the percentage deviation of the momentum-space solutions from the r-space solution. They are given (in %) inside the brackets in table 3. While the present theory always leads to deviations $\leqslant 0.15\%$, which can be improved through the use of more accurate numerical techniques, the deviations given by the VP algorithm depend on the choice of R_m and deteriorate rapidly with a slight increase in R_m. Furthermore, the best choice of R_m depends on the order of the partial wave, as evidenced by table 3. This partial-wave dependence is, however, not known *a priori* since its knowledge would imply that

Table 3. Phase shifts for $V^C \neq 0$ calculated with the coordinate-space method, the present theory, and the Vincent–Phatak theory at various matching radii R_m for the case of $Z = 82$ and $T_p = 200$ MeV. Same short-range interaction as for table 2.

			V–P						
R_m (fm)	r-space	This theory	2.5	3.0	3.5	4.0	4.5	5.0	5.5
δ_0	81.16	81.02 (0.17)	80.71 (0.55)	81.31 (0.18)	81.30 (0.17)	81.64 (0.59)	81.73 (0.70)	82.09 (1.1)	82.19 (1.3)
δ_1	62.15	62.06 (0.14)	61.96 (0.31)	62.06 (0.14)	62.35 (0.32)	62.40 (0.40)	62.78 (1.0)	62.87 (1.2)	63.42 (2.0)
δ_2	44.88	44.82 (0.13)	44.81 (0.61)	44.79 (0.20)	44.92 (0.09)	45.18 (0.67)	45.26 (0.85)	45.69 (1.8)	45.81 (2.1)
δ_3	31.26	31.22 (0.13)	30.61 (2.0)	31.26 (0.0)	31.29 (0.10)	31.43 (0.54)	31.71 (1.4)	31.83 (1.8)	32.31 (3.4)
δ_4	21.33	21.31 (0.09)	21.21 (0.56)	21.06 (1.3)	21.40 (0.33)	21.47 (0.67)	21.65 (1.5)	21.93 (2.8)	22.15 (3.8)
δ_5	14.41	14.39 (0.14)	14.40 (0.07)	14.27 (0.97)	14.32 (0.62)	14.56 (1.0)	14.63 (1.5)	14.92 (3.5)	15.15 (5.1)

one already knows the answer the VP method is trying to provide. Because the interactions encountered in nuclear physics are not of a square-well type but have tails, the 'judicious' choice of R_m can be problematic in VP calculations. In this respect, the technique developed in this work is preferable.

4. Discussion and conclusion

The method presented here has been shown in detail to be theoretically viable. *No approximations* have been made in the theory. Numerical calculations based on this *exact* method can be as accurate as required.

The suggested method is computationally very straightforward. The momentum space calculation of the angular-momentum decomposed T-matrix element, $\langle k_0|\tau_l(E)|k_0\rangle$, consists of the solution of the standard Lippmann–Schwinger equation, equation (6), with the matrix element $\langle k'|U_l|k\rangle$

$$\begin{aligned}\langle k'|U_l|k\rangle &= \langle(\phi_l^C)^{(+)}(k')|V^S|(\phi_l^C)^{(+)}(k)\rangle \\ &= \int \langle(\phi_l^C)^{(+)}(k')|r\rangle\, dr\, r^2\langle r|V_l^S|r'\rangle\, dr'\, r'^2\langle r'|(\phi_l^C)^{(+)}(k)\rangle \\ &= (k'k(2\pi)^2)^{-1}\int F_l(\eta(k'),k'r)\, dr\, r\langle r|V_l^S|r'\rangle\, dr'\, r' F_l(\eta(k),kr'). \qquad (15)\end{aligned}$$

If V^S is given in momentum space, an additional step is required, namely, we must generate the coordinate-space matrix element $\langle r|V_l^S|r'\rangle$ from $\langle k'|V_l^S|k\rangle$ through the relation given in (14).

This procedure is obviously very easy to carry out if one is already in the position to solve a Lippmann–Schwinger-type equation in momentum space, since it only requires a modification of the input potential matrix.

One might ask why we cannot first Fourier-transform the non-local nucleon–nucleon amplitude to coordinate space, then formulate a coordinate-space optical potential and solve the Coulomb-nuclear problem in the coordinate space? The answer resides in the fact that a non-local potential cannot be solved easily in coordinate space; and that some approximate procedures have to be used. These approximations inevitably obscure the genuine aspects of the strong-interaction physics. For this very reason, recent microscopic theories of hadron–nucleus optical potentials are all formulated and calculated in the momentum space. It is precisely in this context that our momentum-space method, though requiring twice the Fourier transform, represents an important achievement in finding an exact solution to the problem.

Acknowledgments

The authors are grateful for helpful, critical discussions with R Brandenburg, A Picklesimer, and P C Tandy. All three made important contributions to this work, primarily, by demonstrating that many of our previous attempts to find a practical solution of this problem were impractical or incorrect. One of us (RMT) gratefully acknowledges the gracious hospitality of the department of physics of The Ohio State University, where he visited while this work was in progress, and where most of the work was carried out. This work was supported in part by the National Science Foundation under grants PHY-8719526 and PHY-8858250, and by the Office of Nuclear Physics of the Department of Energy. The computational support of the Ohio Supercomputer Center under grant PDS150 is gratefully acknowledged.

Appendix

In this appendix we present a formal derivation of the two-potential formula (2) for the case where the potential can be separated into the sum of two potentials; one of which is the Coulomb potential. Because of the long-range nature (or the $\sim r^{-1}$ dependence) of the Coulomb interaction, it is well known that one must establish rigorous results by considering at first a shielded Coulomb potential and then taking the limiting process in which the shielding radius R goes into infinity. Although these considerations are by no means new [6, 16], we will carry out this line of analysis in the framework of the two-potential theory. Our analysis should serve to remind us of the delicacy with which the limiting procedure has to be treated. More importantly, we show how the Coulomb shielding limit $R \to \infty$ can be taken *analytically* so that the use of (7) or (13) is fully justified.

We consider a potential W given by

$$W = V^{C} + V^{S} \tag{16}$$

where V^{C} is the repulsive Coulomb potential and V^{S} is an arbitrary short-ranged potential. The short-ranged potential V^{S} may, of course, contain electromagnetic contributions. In the case where we study the scattering of a charged particle from a nuclear target, for example, we may write $V^{S} = V^{N} + (V^{CD} - V^{C})$, where V^{N} is the nuclear part of the interaction, V^{CD} the Coulomb potential due to the actual charge distribution, and V^{C} is the point Coulomb potential. Obviously, $(V^{CD} - V^{C})$ is short-ranged. The full Hamiltonian is then given as $H = H_0 + W$, where H_0 is the free Hamiltonian. For the reason stated above, we shall first consider $\hat{W} = \hat{V}^{C} + V^{S}$, with the cut-off Coulomb potential $\hat{V}^{C}$ defined as

$$\hat{V}^{C}(r) = \begin{cases} V^{C} & \text{if } r < R \\ 0 & \text{if } r > R. \end{cases} \tag{17}$$

We shall, of course, eventually take the limit $R \to \infty$. Because the treatment of Coulomb scattering involves a non-uniform or weak limiting process, it should occasion no surprise that the point in the development at which R goes to infinity is crucial.

Applying the two-potential formula to $\hat{W}$, we obtain

$$T = \hat{T}^{C} + (\hat{\Omega}^{C})^{(-)\dagger} V^{S} \Omega^{(+)} \tag{18}$$

for the transition amplitude. Without loss of generality, we can assume that the short-range interaction V^{S} is spin independent and spherically symmetric. In the angular momentum decomposed form, equation (18) then gives

$$\langle k_0 | T_l(E) | k_0 \rangle = \langle k_0 | \hat{T}_l^{C}(E) | k_0 \rangle + \langle (\hat{\phi}_l^{C})^{(-)}(k_0) | V^{S} | \psi_l^{(+)}(k_0) \rangle \tag{19}$$

for the on-shell matrix element of T_l, where $k_0^2 = 2\mu E$. E is the energy and μ is the reduced mass of the system. Both $\hat{T}^{C}(E)$ and $|\hat{\phi}^{C}(k_0)\rangle$ are properly defined, since $\hat{V}^{C}$ is of finite range. The phase shift $\hat{\sigma}_l(E)$ corresponding to the cut-off Coulomb potential is given by

$$\hat{\sigma}_l(E) = \sigma_l(E) - \eta \ln 2k_0 R \tag{20}$$

where

$$\sigma_l(E) = \arg\Gamma(l + 1 + i\eta) \tag{21}$$

is the Coulomb phase shift and the Sommerfeld parameter η is given by

$$\eta(E) = Z_1 Z_2 e^2 \mu/\hbar k_0. \tag{22}$$

In (20), we have neglected a contribution to the phase shift, which is less than $\eta/2k_0R$ in magnitude and is easily seen to disappear for large values of R as discussed in [6].

The usual relation between the in and out states then allows us to write

$$\langle(\hat{\phi}_l^C)^{(-)}(k_0)| = e^{2i\hat{\sigma}_l(E)}\langle(\hat{\phi}_l^C)^{(+)}(k_0)| \tag{23}$$

so that (19) may be expressed as

$$\langle k_0|T_l(E)|k_0\rangle = \langle k_0|\hat{T}_l^C(E)|k_0\rangle + e^{2i\hat{\sigma}_l(E)}\langle(\hat{\phi}_l^C)^{(+)}(k_0)|V^S|\psi_l^{(+)}(k_0)\rangle. \tag{24}$$

The full solution $|\psi_l^{(+)}(k_0)\rangle$ satisfies the integral equation

$$|\psi_l^{(+)}(k_0)\rangle = |(\hat{\phi}_l^C)^{(+)}(k_0)\rangle + \hat{G}_C^{(+)}(E)V^S|\psi_l^{(+)}(k_0)\rangle \tag{25}$$

where $\hat{G}_C^{(+)}(E)$ is the resolvent of the pure cut-off Coulomb Hamiltonian, $\hat{H}_C = H_0 + \hat{V}_C$, i.e. $\hat{G}_C^{(+)}(E) = (E - \hat{H}^C + i\varepsilon)^{-1}$. From (25) we instantly obtain a central result for the present treatment, namely

$$\langle(\hat{\phi}_l^C)^{(+)}(k)|V^S|\psi_l^{(+)}(k_0)\rangle = \langle(\hat{\phi}_l^C)^{(+)}(k)|V^S|(\hat{\phi}_l^C)^{(+)}(k_0)\rangle + \langle(\hat{\phi}_l^C)^{(+)}(k)|V^S\hat{G}_C^{(+)}(E)V^S|\psi_l^{(+)}(k_0)\rangle. \tag{26}$$

We now define operators $U_l(E)$ and $\tau_l(E)$ whose relevant matrix elements are given by

$$\langle k|U_l|k'\rangle \equiv \langle(\hat{\phi}_l^C)^{(+)}(k)|V^S|(\hat{\phi}_l^C)^{(+)}(k')\rangle \tag{27}$$

and

$$\langle k|\tau_l|k'\rangle \equiv \langle(\hat{\phi}_l^C)^{(+)}(k)|V^S|\psi_l^{(+)}(k')\rangle. \tag{28}$$

It is clearly our intent eventually to substitute ϕ_l^C for $\hat{\phi}_l^C$ in (27) and (28). The following considerations represent part of the justification for so doing. First we note that the true Coulomb potential V^C is a local potential, so that in coordinate space we have (for $r < R$)

$$\begin{aligned}\langle r|(\hat{\phi}_l^C)^{(+)}(k)\rangle = {} & j_l(kr)\hat{N}_l(k, R) \\ & - kj_l(kr)\int_r^R dr' r'^2 h_l^+(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle \\ & - kh_l^+(kr)\int_0^r dr' r'^2 j_l(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle\end{aligned} \tag{29}$$

where $j_l(kr)$ is the regular spherical Bessel function and $h_l^+(kr) = n_l(kr) + ij_l(kr)$ is the irregular outgoing-wave spherical Bessel function. We can rewrite (29) as

$$\begin{aligned}\langle r|(\hat{\phi}_l^C)^{(+)}(k)\rangle = {} & j_l(kr)[\hat{N}_l(k, R) - k\int_0^R dr' r'^2 h_l^+(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle] \\ & + kj_l(kr)\int_0^r dr' r'^2 h_l^+(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle \\ & - kh_l^+(kr)\int_0^r dr' r'^2 j_l(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle \\ = {} & j_l(kr)C_l(k, R) + kj_l(kr)\int_0^r dr' r'^2 h_l^+(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle \\ & - kh_l^+(kr)\int_0^r dr' r'^2 j_l(kr')V^C(r')\langle r'|(\hat{\phi}_l^C)^{(+)}(k)\rangle\end{aligned} \tag{30}$$

where the choice of $\hat{N}_l(k, R)$ fixes $C_l(k, R)$. If we choose $C_l(k, R)$ to be

$$C_l(k, R) = C_l(k) = C_0(k) \prod_{s=1}^{l} \left(1 + \frac{(\eta^2(k))}{s^2}\right)^{1/2} \tag{31}$$

where $C_0(k)$ is given by

$$C_0(k) = \left(\frac{2\pi\eta(k)}{e^{2\pi\eta(k)} - 1}\right)^{1/2} \tag{32}$$

then we find that the solution to (30) becomes

$$\langle r|(\hat{\phi}_l^C)^{(+)}(k)\rangle = \begin{cases} \langle r|\phi_l^C(k)\rangle & \text{if } r < R \\ \dfrac{1}{kr}\sin(kr - l\pi/2 + \sigma_l - \eta\log 2kR) & \text{if } r > R. \end{cases} \tag{33}$$

The Coulomb wavefunction shown in (33) is the usual Coulomb wavefunction, normalized such that

$$\langle r|\phi_l^C(k)\rangle \overset{r\to\infty}{\to} \frac{1}{kr}\sin(kr - l\pi/2 + \sigma_l - \eta\log 2kr). \tag{34}$$

The requirement that the states $\langle r|(\hat{\phi}_l^C)^{(+)}\rangle$ be a complete orthonormal set of states is clearly met by the states shown in (33).

What we have shown is that for R sufficiently large, and for $\langle r|(\hat{\phi}_l^C)^{(+)}(k)\rangle$ appropriately normalized we do *not* need to take the limit $R \to \infty$ numerically, since our procedure gives the same matrix elements (with a V^S of finite range) independent of the value of R. Consequently, the $\hat{}$-symbol may be removed in the definitions of the matrix elements in (27) and (28). In other words, equation (27) becomes

$$\langle k|U_l|k'\rangle = \langle(\phi_l^C)^{(+)}(k)|V^S|(\phi_l^C)^{(+)}(k')\rangle \tag{35}$$

and (28) becomes

$$\langle k|\tau_l(E)|k_0\rangle = \langle(\phi_l^C)^{(+)}(k)|V^S|\psi_l^{(+)}(k_0)\rangle. \tag{36}$$

With this in mind, we may rewrite (26) as

$$\langle k|\tau_l(E)|k_0\rangle = \langle k|U_l|k_0\rangle + \int \langle k|U_l|k'\rangle \frac{4\pi k'^2\,dk'}{E - E' + i\varepsilon}\langle k'|\tau_l(E)|k_0\rangle \tag{37}$$

where we have inserted a complete set of Coulomb wavefunctions. (Clearly, this procedure only holds for a repulsive Coulomb potential, which does not have a discrete spectrum.) This leaves $\hat{G}_C^{(+)}(E)$ in the familiar form of a free resolvent. Note that all the phases disappear in (37). Since (37) is the standard integral equation of scattering, it follows that we can readily generate $\langle k_0|\tau_l(E)|k_0\rangle$, which is the required matrix element on the right in (24), provided that we can generate $\langle k|U_l|k'\rangle$ and provided also that $\langle k|U_l|k'\rangle$ behaves like a finite-ranged potential. Such is indeed the case, as should be clear from the discussions above.

It remains to be shown that, upon taking the $R \to \infty$ limit, the $\langle k_0|\hat{T}_l^C(E)|k_0\rangle$ in (19) may be identified with the usual Coulomb T-matrix element. This demonstration is given in standard text [7] in scattering theory and will not be repeated here. We have, therefore, proved (2), (7), and (13).

The procedure we have developed above suggests that we may directly calculate $\langle k_0|\tau_l(E)|k_0\rangle = (-2\pi^2\mu)^{-1}\exp[i\delta_l(E)]\sin\delta_l(E)$ by solving (37). To this end, we must, of course, be able to produce the matrix elements $\langle k'|U_l|k\rangle$ to use as inputs into (37). This has been discussed in the main text.

In summary, we have presented a method which states that the Coulomb-distorted matrix elements of the short-ranged potential can be calculated with the use of unscreeened Coulomb wavefunctions. This derivation forms the theoretical basis for our procedure of computing Coulomb distortions in momentum space as indicated by (13). We emphasize, that this does not require taking the often unstable numerical limit of a cutoff R going to infinity.

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