On-shell $T$-matrices in multiple scattering

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Abstract

The transition operator $T$ for the scattering of a particle from $N$ potentials $V_j(x)$ can be expanded into a series featuring the transition operators $t_j$ associated with the individual potentials. For $V_j(x)$ both absolutely and square integrable in $x$, we show, using an analytic continuation argument, that if $T$ is on-shell, i.e. in $< k | T(\sigma^2 \pm i0) | k' >$, $|k| = |k'| = \sigma$, then each $t_j$ is also on-shell.

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I. INTRODUCTION

In his booklet “Surprises in Theoretical Physics” Peierls [1] devotes a section to off-shell effects in multiple scattering. He observes that in the single scatterer case the on-shell T-matrix does not fix the potential uniquely and one can try to get off-shell information by looking at multiple scattering. Indeed, the full T-matrix can be expanded in one-scatterer ones, where in the latter also off-shell contributions are present. However, as observed by Baqi Bég [2] for a two-scatterer situation this is not the case for non-overlapping potentials. Also in periodic systems, treated by means of the KKR-method, only the on-shell single scatterer T-matrices occur [3]. The above approaches make use of partial wave expansions and this raises the question whether these can be avoided. Below we show that this is indeed the case and that an analyticity argument can be used instead.

In order to appreciate the situation, it is useful to consider the classical scattering of a particle by two fixed non-overlapping finite range potentials. Originally the particle is moving freely and after leaving the range of the first potential it moves freely again, its energy being unchanged, until it enters the range of the second potential. Quantum-mechanically the situation is different. The wave function extends throughout space at all times. Nevertheless only the on-shell single scatterer T-operators are involved and one might think that this property is the quantum analogue of the classical situation. However, this is not the case. Below we show that for a large class of overlapping potentials the on-shell T-matrix property still holds.

II. GENERAL BACKGROUND

We consider the situation of a three-dimensional Schrödinger particle in the field of $N$ potentials

\[ H = p^2 + \sum_{j=1}^{N} V_j(x) = H_0 + V. \]  \hspace{1cm} (2.1)

A typical example is $V_j(x) = \Phi(x - x_j)$, where the $x_j$’s are points in space. $N$ can be infinite as in the lattice case. Then $\Phi(x)$ must have sufficient decay at infinity. The associated T-matrix is

\[ T(z) = V + V[z - H]^{-1}V, \quad z = E + i\varepsilon = k_0^2 + i\varepsilon. \]  \hspace{1cm} (2.2)

Expanding $T(z)$ in terms of the individual scatterer T-operators

\[ t_j(z) = V_j + V_j R_j(z) V_j, \quad H_j = H_0 + V_j, \quad R_j(z) = [z - H_j]^{-1}, \]  \hspace{1cm} (2.3)

we obtain the series

\[ T(z) = \sum_j t_j(z) + \sum_{j \neq h} t_j(z)R_0(z)t_h(z) + \sum_{j \neq h \neq k} t_j(z)R_0(z)t_h(z)R_0(z)t_k(z) + \ldots \]  \hspace{1cm} (2.4)

Here the free resolvent $R_0(z) = [z - H_0]^{-1}$ contains both $\delta$-function and Cauchy principal value contributions with the result that the $t_j$’s need not be on-shell even if $T(z)$ itself is on-shell. With on-shell we mean that $|k_1| = |k_2| = k_0$ in $<k_1|T(k_0^2 + i\varepsilon)|k_2>$. 

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Below we show that for potentials that are both absolutely and square integrable only the on-shell parts of the individual T-matrices contribute to the on-shell part of $T(z)$. In the next section we do so for non-overlapping potentials, whereafter we treat the general case.

III. NON-OVERLAPPING POTENTIALS

We start off with the objects

$$X_{\alpha}(z) = < k_{1}| t_{j}(z) \exp[i\alpha \sqrt{H_{0}}] R_{0}(z) t_{h}(z)| k_{2} > |k_{1}|=|k_{2}|=k_{0}$$

$$\quad = < k_{1}| M_{j}(z) \varphi_{j} \exp[i\alpha \sqrt{H_{0}}] R_{0}(z) \varphi_{h} N_{h}(z)| k_{2} > |k_{1}|=|k_{2}|=k_{0},$$

$$Y_{\alpha}(z) = < k_{1}| \exp[-i\alpha \sqrt{H_{0}}] t_{j}(z) \exp[i\alpha \sqrt{H_{0}}] R_{0}(z) t_{h}(z)| k_{2} > |k_{1}|=|k_{2}|=k_{0}$$

$$\quad = \exp[-i\alpha k_{0}] X_{\alpha}(z) \quad (3.1)$$

where $j \neq h$, $z = k_{0}^{2} + i\varepsilon$, $k_{0} > 0$, $\varepsilon > 0$, $\alpha > 0$, $V_{j}(x) = \varphi_{j}(x)^{2}$ (so $\varphi_{j}(x)$ is purely imaginary for those $x$ for which $V_{j}(x)$ is negative, but this does not matter in the following) and

$$M_{j}(z) = \varphi_{j}\{1 + \varphi_{j} R_{j}(z) \varphi_{j}\}, \quad N_{h}(z) = \{1 + \varphi_{h} R_{h}(z) \varphi_{h}\} \varphi_{h}. \quad (3.2)$$

First, consider the limit as $\varepsilon \downarrow 0$ of

$$X_{0}(z) = Y_{0}(z) = < k_{1}| t_{j}(z) R_{0}(z) t_{h}(z)| k_{2} > . \quad (3.3)$$

We assume that each $V_{j}(x)$ is both absolutely and square integrable. Thus $< k_{1}| \varphi_{j}$ and $\varphi_{h}| k_{2} >$ are square integrable and moreover each $\varphi_{j} R_{j}(z) \varphi_{j}$ has a limit as $\varepsilon \downarrow 0 \quad [4, 7]$. Now

$$X_{\alpha}(z) = \int d\mathbf{k} \exp[i\alpha \sqrt{k^{2}}][z - k^{2}]^{-1} < k_{1}| M_{j}(z) \varphi_{j}| \mathbf{k} > < \mathbf{k}| \varphi_{h} N_{h}(z)| \mathbf{k}_{2} >$$

$$\quad = \int d\mathbf{k} \exp[i\alpha \sqrt{k^{2}}][z - k^{2}]^{-1}$$

$$\quad \int d\mathbf{x} d\mathbf{y} < k_{1}| M_{j}| \mathbf{x} > \varphi_{j}(\mathbf{x}) < \mathbf{x}| \mathbf{k} > < \mathbf{k}| \mathbf{y} > \varphi_{h}(\mathbf{y}) < \mathbf{y}| N_{h}| \mathbf{k}_{2} >$$

$$\quad = (2\pi)^{-3} \int d\mathbf{k} \exp[i\alpha \sqrt{k^{2}}][z - k^{2}]^{-1}$$

$$\quad \int d\mathbf{x} d\mathbf{y} < k_{1}| M_{j}| \mathbf{x} > \varphi_{j}(\mathbf{x}) \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})] \varphi_{h}(\mathbf{y}) < \mathbf{y}| N_{h}| \mathbf{k}_{2} >$$

$$\quad = -\pi^{-1} \int_{-\infty}^{+\infty} dkk \exp[i\alpha \sqrt{k^{2}}][k^{2} - z]^{-1} < k_{1}| M_{j}\bar{K}(k^{2} + i0) N_{h}| \mathbf{k}_{2} > , \quad (3.4)$$

where $\bar{K}(z)$ is defined by the kernel

$$< \mathbf{x}| \bar{K}(z)| \mathbf{y} > = \varphi_{j}(\mathbf{x}) \frac{\exp[i\sqrt{2}|\mathbf{x} - \mathbf{y}|]}{4\pi i|\mathbf{x} - \mathbf{y}|} \varphi_{h}(\mathbf{y}),$$

$$< \mathbf{x}| \bar{K}(k^{2} + i0)| \mathbf{y} > = \varphi_{j}(\mathbf{x}) \frac{\exp[ik|\mathbf{x} - \mathbf{y}|]}{4\pi i|\mathbf{x} - \mathbf{y}|} \varphi_{h}(\mathbf{y}). \quad (3.5)$$
We now suppose that $V_j(x)$ is non-vanishing only on the bounded set $A_j$ in coordinate space and that the sets $A_j$ and $A_h$, $j \neq h$, do not overlap, i.e. they have a minimal distance $d > 0$. Then the denominator in $< x | \tilde{K}(k^2 + i0) | y >$ is $\geq d^{-1}$, so $\tilde{K}(k^2 + i0)$ and $< k_1 | M_j \tilde{K}(k^2 + i0) N_h | k_2 >$ can be continued analytically as entire functions of $\varsigma$, $k \to \varsigma \in \mathbb{C}$, with exponential decay in the upper halfplane. Defining $\sqrt{\varsigma^2}$ by laying a cut along the positive real axis, we have $\exp[i\alpha \sqrt{\varsigma^2}] = \exp[i\alpha \varsigma]$ which remains bounded in the upper halfplane. We can now close the contour in (3.4) and pick up the residue in $\sqrt{\varsigma}$ with the result

\[ X_\alpha(z) = -i \exp[i\alpha \sqrt{\varsigma}] < k_1 | M_j \tilde{K}(z) N_h | k_2 > = \exp[i\alpha \sqrt{\varsigma}] X_0(z), \]
\[ Y_\alpha(z) = \exp[i\alpha(\sqrt{\varsigma} - k_0)] X_0(z). \]  

(3.6)

One has

\[ a^{-1} \int_0^a d\alpha Y_\alpha(k_0^2 + i0) = X_0(k_0^2 + i0). \]

(3.7)

On the other hand

\[ a^{-1} \int_0^a d\alpha Y_\alpha(k_0^2 + i0) = \]
\[ \int < k_1 | a^{-1} \int_0^a d\alpha \exp[-i\alpha \sqrt{H_0}] t_j(k_0^2 + i0) \exp[i\alpha \sqrt{H_0}] | k > < k_1 | R_0(z) t_h(z) | k_2 > dk. \]  

(3.8)

But

\[ < k_1 | a^{-1} \int_0^a d\alpha \exp[-i\alpha \sqrt{H_0}] t_j(z) \exp[i\alpha \sqrt{H_0}] | k > \exp[i\alpha(k - k_0)] - 1 \]
\[ \frac{1}{i\alpha(k - k_0)} < k_1 | t_j(z) | k > , \]

(3.9)

which vanishes for large $a$ unless $k = k_0$ indicating that only the on-shell part of $t_j(k_0^2 + i0)$ contributes to $X_0(k_0^2 + i0) = \lim_{\varepsilon \to 0} < k_1 | t_j(z) R_0(z) t_h(z) | k_2 >$. Since $R_0(z)$ is diagonal in momentum representation, the same is also true for $t_h$, i.e., only the on-shell part of $t_h$ contributes to $X_0(k_0^2 + i0)$. Further insight is provided by considering two nonoverlapping spherically symmetric (muffin tin) potentials $V_j$ and $V_h$, one centered at the origin and the second at the point $\mathbf{R}$. Then, in terms of spherical Bessel functions and spherical harmonics, one has for $x \in A_j$ and $y \in A_h$

\[ - \frac{\exp[ik_0|x - y|]}{4\pi |x - y|} = ik_0 \sum_{lm} k_0 j_l(k_0 x) h_l^{(+)}(k_0 y) Y_l^m(x) Y_l^m(y) = \sum_{lml'm'} j_l(k_0 x) g_{lm;l'm'}(k_0, R) j_{l'}(k_0 |y - R|) Y_{l'm'}(y - R), \]  

(3.10)

where $g_{lm;l'm'}(k_0, R)$ are the so-called structure constant (see, for example, [7]). Then

\[ < k_1 | t_j(k_0^2 + i0) R_0(k_0^2 + i0) t_h(k_0^2 + i0) | k_2 > |k_1| = |k_2| = k_0 \]
\[ = \sum_{lml'm'} g_{lm;l'm'}(k_0, R) t_{lm}(k_0) t_{l'm'}(k_0), \]

(3.11)
where \( t_{lm}(k_0) = -\sin \eta_l \exp(i\eta_l)/k_0 \) and \( \eta_l = \eta_l(k_0) \) is the corresponding phase-shift.

We can repeat the procedure for \( \langle k_1|t_j(z)R_0(z)t_h(z)R_0(z)t_k(z)|k_2 \rangle \), \( j \neq h \neq k \), and higher terms in the multiple-scattering expansion (2.4) with the result that only the on-shell parts of the individual T-matrices contribute. Apart from a change in the free Green’s functions \( \langle x|R_0(z)|y \rangle \), the same procedure can be followed in the one and two-dimensional cases.

### IV. OVERLAPPING POTENTIALS

The crucial point in the derivation of the previous section is the behaviour of the operator \( \tilde{K}(z) \) defined in (3.5). The class of potentials, called Rollnik potentials, for which \( \tilde{K}(z) \) makes sense has been profoundly studied in the literature [4] [6]. The absolutely and square integrable potentials are members of this class. Here we need some subtle properties of \( \tilde{K}(z) \), which were obtained by Blauw and Tip [8], who started off from its time-dependent counterpart \( K(t) = \varphi_j \exp[-iH_0 t] \varphi_h \). In the present situation (for the three-dimensionsional case) it was found that \( \tilde{K}(z) \) is analytic outside the positive real axis and that \( \tilde{K}(k_0^2 \pm i\varepsilon), \ k > 0 \), have the limits \( \tilde{K}(k_0^2 \pm i0) \):

\[
\langle x|\tilde{K}(k_0^2 \pm i0)|y \rangle = \varphi_j(x) \frac{\exp[\pm i k|x - y|]}{4\pi i|x - y|} \varphi_h(y). \tag{4.1}
\]

In addition,

\[
||\tilde{K}(z)||_4 = [\text{tr}\{\tilde{K}(z)^*\tilde{K}(z)\}^2]^{1/4} \leq c < \infty, \quad \forall z \in \mathbb{C},
\]

\[
\int_0^\infty dk^2||\tilde{K}(k^2 \pm i0)||^r_4 < \infty, \quad r > 4,
\]

\[
||\tilde{K}(k^2 \pm i0)||_4 \to 0, \quad (k \to \infty). \tag{4.2}
\]

The first of these statements implies that \( \tilde{K}(z) \) is a compact operator. Using Hölder’s inequality, it follows from the second that \( X_\alpha(z) \) exists and, translating the above properties to those of \( L(k) \) defined earlier, we conclude once more that the contour can be closed. Now the remainder of the derivation in section III can be repeated without change. However, (3.11) looses its meaning. Also the results of [8], are not available in the one and two-dimensional cases. On the other hand one expects that the conditions on the potentials can be relaxed.

### V. DISCUSSION

Using an analytic continuation argument, we have shown that for a large class of potentials the single scatterer T-matrices in a multiple scattering expansion can be evaluated on the energy shell. For the individual potential \( V_j \) it suffices that it is both integrable and square integrable. This allows local Coulomb singularities and a behaviour at infinity \( \sim x^{-\alpha}, \ \alpha > 3 \) (if there is an infinity of potentials such as on a lattice, further requirements are needed to avoid a catastrophic building up of tail contributions). An earlier result on overlapping potentials is that of Faulkner and Stocks [9], who considered overlapping muffin
tin potentials. Note further that the present result strongly depends on the dimension of the system through the specific form of the free resolvent entering into the definition of the operator $\tilde{K}(z)$.

Turning back to Peierls’ discussion, we conclude that quite generally it is impossible to abstract off-shell T-matrix information from multiple scattering. The situation is different if off-shell matrix elements of the density operator are observed. Then off-shell T-matrix elements link the on-shell part of the density operator at the initial time with off-shell ones at later times. Second, if we consider three identical particles interacting through identical pair potentials, the Fadeev equations come into play and also here off-shell elements of the individual T-operators appear.

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