# NEW ON-SHELL $S$-MATRIX RELATIONS FOR POTENTIAL SCATTERING

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Some identities for on-shell $S$-matrices in consecutive scattering on two potentials are derived. As a straightforward consequence, the first order formula for the perturbed on-shell $S$-matrix is obtained. Finally, a new derivation of equations of variable phase method is proposed.

## *1. Introduction*

Questions related to the potential scattering from a sum of two potentials have been extensively discussed in the literature, see e. g. [1, 2]. We present here an alternative approach to the problem. The kinetic energy operator and two consecutive potentials are used to construct three on-shell $S$-matrices. A simple multiplication rule for them is the main result of Section 2. As a consequence, the additivity of phase shifts is established in cases where these are sufficient for the parametrization of the $S$-matrix.

In Section 3 we give the identities which relate a derivative of the on-shell $S$-matrix to the matrix elements of the derivative of the potential (with respect to the parameter). A special case of these relations is already known [3]; besides generality our derivation seems to be extremely simple and transparent because of the new formalism used.

Section 4 is devoted to a new formal derivation of the phase equation [4]. The procedure described there may be easily generalized to obtain similar equations in any case of interest (e. g. coupled channels).

## *2. Additive interaction*

In this section we shall derive some formal relations in the problem of the elastic scattering of a particle by a sum of two potentials $V_1$ and $V_2$. In that case there are two basic possibilities of decomposing the total Hamiltonian $H_t$

$$H_t = H_0 + V_1 + V_2$$

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into an unperturbed part and a perturbation. As the unperturbed part we may take either the kinetic energy operator $H_0$ or the operator

$$H_1 = H_0 + V_1.$$

The different decompositions of the Hamiltonian into a "free" and a perturbation part lead to the construction of three on-shell $S$-matrices. The $S$-matrices are related by a multiplication rule as will be shown below.

We first introduce three auxiliary operators depending on a real parameter $\eta > 0$. These are

$$U_{01}(E) = \frac{E-H_0+i\eta}{E-H_0-i\eta} \cdot \frac{E-H_1-i\eta}{E-H_1+i\eta}, \tag{1a}$$

$$U_{1t}(E) = \frac{E-H_1+i\eta}{E-H_1-i\eta} \cdot \frac{E-H_t-i\eta}{E-H_t+i\eta}, \tag{1b}$$

and

$$U_{0t}(E) = \frac{E-H_0+i\eta}{E-H_0-i\eta} \cdot \frac{E-H_t-i\eta}{E-H_t+i\eta}. \tag{1c}$$

From these definitions we infer

$$U_{0t}(E) = U_{01}(E) \cdot U_{1t}(E). \tag{2}$$

As is obvious from Eq. (1), all three operators $U$ are unitary. However, it should be kept in mind that these operators are not equal to the usual $S$-matrices. After some purely algebraic calculations we find that

$$U_{01}(E) = 1-2i\eta \frac{1}{E-H_0-i\eta} t_{01}(E+i\eta) \frac{1}{E-H_0+i\eta}, \tag{3a}$$

$$U_{1t}(E) = 1-2i\eta \frac{1}{E-H_1-i\eta} t_{1t}(E+i\eta) \frac{1}{E-H_1+i\eta}, \tag{3b}$$

$$U_{0t}(E) = 1-2i\eta \frac{1}{E-H_0-i\eta} t_{0t}(E+i\eta) \frac{1}{E-H_0+i\eta}, \tag{3c}$$

where the operators $t_{01}$, $t_{1t}$ and $t_{0t}$ are defined as follows:

$$t_{01}(E+i\eta) = V_1 + V_1 \frac{1}{E-H_1+i\eta} V_1, \tag{4a}$$

$$t_{1t}(E+i\eta) = V_2 + V_2 \frac{1}{E-H_t+i\eta} V_2, \tag{4b}$$

$$t_{0t}(E+i\eta) = V_1+V_2+(V_1+V_2) \frac{1}{E-H_t+i\eta} (V_1+V_2). \tag{4c}$$

Here $t_{01}$ and $t_{0t}$ are the well-known scattering operators, whereas the definition of $t_{1t}$ is slightly unusual since the unperturbed part $t_{1t}$ differs from the pure kinetic energy operator. A similar definition of the scattering operator is used, e. g. in the distorted wave calculations where the potential $V_1$ represents pure Coulomb interaction.

Insering Eq. (3) into Eq. (2), we obtain a relation between the operators $t_{01}$, $t_{1t}$ and $t_{0t}$. Now we multiply this relation by $i\eta$. Thus we arrive at the equation:

$$\begin{aligned}
&\frac{-i\eta}{E-H_0-i\eta}\, t_{01}(E+i\eta)\, \frac{i\eta}{E-H_0+i\eta} \\
&\quad + \frac{-i\eta}{E-H_1-i\eta}\, t_{1t}(E+i\eta)\, \frac{i\eta}{E-H_1+i\eta} \\
&+ \frac{-i\eta}{E-H_0-i\eta}\, t_{01}(E+i\eta)\, \frac{1}{E-H_0+i\eta} \times(-2i\eta) \\
&\quad \times \frac{1}{E-H_1-i\eta}\, t_{1t}(E+i\eta)\, \frac{i\eta}{E-H_1+i\eta} \\
&\quad = \frac{-i\eta}{E-H_0-i\eta}\, t_{0t}(E+i\eta)\, \frac{i\eta}{E-H_0+i\eta}\,. \qquad (5)
\end{aligned}$$

We now introduce a complete orthonormal set of free-particle states $|\chi_E^c\rangle$ corresponding to $H_0$, where the index $c$ describes a proper set of discrete quantum numbers. These states obey the relations

$$\langle \chi_{E'}^{c'} | \chi_E^c \rangle = \delta_{c'c}\delta(E'-E), \qquad (6a)$$

$$\sum_c \int dE |\chi_E^c\rangle \langle \chi_E^c| = 1, \qquad (6b)$$

and the Hamiltonian $H_0$ is diagonal in this basis.

In order to arrive at the on-shell relation among operators $t_{01}$, $t_{1t}$ and $t_{0t}$, we take the matrix element of Eq. (5) between the states $|\chi_E^{c'}\rangle$ and $|\chi_E^c\rangle$. It yields the equation:

$$\begin{aligned}
&\langle \chi_E^{c'} | t_{01}(E+i\eta)\, |\chi_E^c\rangle + \langle \psi_{1E}^{c'+} | t_{1t}(E+i\eta)\, |\psi_{1E}^{c+}\rangle \\
&-2\pi i \sum_{c''} \langle \chi_E^{c'} | t_{01}(E+i\eta)\, |\chi_E^{c''}\rangle \langle \psi_{1E}^{c''+} | t_{1t}(E+i\eta)\, |\psi_{1E}^{c+}\rangle = \langle \chi_E^{c'} | t_{0t}(E+i\eta)\, |\chi_E^c\rangle, \qquad (7)
\end{aligned}$$

where the limit $\eta \to 0^+$ is understood. Therefore the state

$$|\psi_{1E}^{c+}\rangle = \lim_{\eta\to 0^+} \frac{i\eta}{E-H_1+i\eta}\, |\chi_E^c\rangle, \qquad (8)$$

being the eigenstate of the Hamiltonian $H_1$, corresponds to the superposition of free and outgoing waves. Moreover, in order to obtain the equation (7) we have used the identities

$$V_1 \frac{1}{E-H_1+i\eta} = t_{01}(E+i\eta)\, \frac{1}{E-H_0+i\eta}, \qquad (9a)$$

$$V_1 |\psi_{1E}^{c+}\rangle = t_{01}(E+i\eta)\, |\chi_E^c\rangle, \qquad (9b)$$

and spectral representation of the unit operator based on the set of states (8). In general, this set of states is not complete. Nevertheless, the bound states of the Hamiltonian $H_1$, if any, are unimportant here because the energy $E$ is chosen to be real and positive.

Finally, the equation (7) can be simplified. For this purpose we introduce three unitary on-shell $S$-matrices:

$$S_{01}^{c'c}(E) = \delta_{c'c} - 2\pi i \langle \chi_E^{c'} | t_{01}(E+i\eta) \, | \chi_E^c \rangle, \tag{10a}$$

$$S_{1t}^{c'c}(E) = \delta_{c'c} - 2\pi i \langle \psi_{1E}^{c'+} | t_{1t}(E+i\eta) \, | \psi_{1E}^{c+} \rangle, \tag{10b}$$

$$S_{0t}^{c'c}(E) = \delta_{c'c} - 2\pi i \langle \chi_E^{c'} | t_{0t}(E+i\eta) \, | \chi_E^c \rangle. \tag{10c}$$

The unitarity of these matrices is a well-known fact, we do not prove it here. By means of Eq. (10), equation (7) can be rewritten and this leads to the following equation:

$$S_{0t}(E) = S_{01}(E) \cdot S_{1t}(E). \tag{11}$$

This equation is the goal of considerations in this section. It should be noted that the time evolution operators of a quantum system are related in a manner similar to that of the operators in Eq. (11).

We end this section by presenting a special case of Eq. (11). We shall assume the $S$-matrices (10) to be diagonal (e. g. for central potentials $V_1$ and $V_2$), then the phase shifts are sufficient for their parametrization:

$$S_{01}^{c'c}(E) = \delta_{c'c} e^{2i\delta_{01}{}^c(E)}, \tag{12a}$$

$$S_{1t}^{c'c}(E) = \delta_{c'c} e^{2i\delta_{1t}{}^c(E)}, \tag{12b}$$

$$S_{0t}^{c'c}(E) = \delta_{c'c} e^{2i\delta_{0t}{}^c(E)}. \tag{12c}$$

Inserting Eq. (12) into Eq. (11), we obtain the phase shifts additivity rule

$$\delta_{0t}^c(E) = \delta_{01}^c(E) + \delta_{1t}^c(E), \tag{13}$$

as was stated in the introduction.

### *3. The first order formula*

On the basis of the results obtained in the previous section we may now derive the relations which express a change of the on-shell $S$-matrix elements caused by a change of the potential. A special case of these relations has already been derived [3] in various contexts and may be obtained as a simple consequence of Eq. (16) below.

Suppose $V_\lambda$ is a potential in which $\lambda$ is a parameter and $S_\lambda$ is the corresponding on-shell $S$-matrix depending on the parameter $\lambda$ too. Suppose the potential is altered by changing $\lambda$ to $\lambda+\Delta\lambda$. We may define the increments $\Delta V$ and $\Delta S$ of the potential and of the $S$-matrix, respectively. These definitions are

$$V_{\lambda+\Delta\lambda} = V_\lambda + \Delta V, \tag{14a}$$

and

$$S_{\lambda+\Delta\lambda} = S_\lambda + \Delta S. \tag{14b}$$

The problem considered here may be reduced to the one described in the previous section. From Eq. (14a) we see that for this purpose it is sufficient to replace $V_\lambda$, $\Delta V$, $S_\lambda$, $S_{\lambda+\Delta\lambda}$ by $V_1$, $V_2$, $S_{01}$, $S_{02}$, respectively, in all the formulas to be used.

From Eq. (11) we now infer

$$S_{\lambda+\Delta\lambda} = S_\lambda \cdot S_{\Delta\lambda}, \tag{15}$$

where the on-shell $S$-matrix $S_{\Delta\lambda}$ corresponds to $\Delta V$ by means of Eq. (10b) and Eq. (4b). Therefore, inserting Eq. (15) into Eq. (14b), we get a relation between $\Delta S$ and $\Delta V$. Both the increments $\Delta S$ and $\Delta V$ may be expanded as a Taylor series in $\Delta\lambda$. Taking the first terms only in these series ($\Delta\lambda \to 0$) we finally obtain the equation

$$\frac{\partial}{\partial\lambda} S_\lambda^{c'c}(E) = -2\pi i \sum_{c''} S_\lambda^{c'c''}(E) \langle \psi_{\lambda E}^{c''+} | \frac{\partial V_\lambda}{\partial\lambda} | \psi_{\lambda E}^{c+} \rangle. \tag{16}$$

This equation is the desired one, and expresses the change of the $S$-matrix caused by the change of the potential.

We now give a special case of Eq. (16), mentioned above. Suppose the $S$-matrix to be diagonal for all the values of the parameter $\lambda$ lying in an interval $(\lambda_1, \lambda_2)$. Using the parametrization (12), we obtain the following equation

$$\frac{\partial}{\partial\lambda} \delta_\lambda^c(E) = -\pi \langle \psi_{\lambda E}^{c+} | \frac{\partial V_\lambda}{\partial\lambda} | \psi_{\lambda E}^{c+} \rangle \tag{17}$$

holding in this special case.

### *4. Phase equations*

As is well known, the so-called variable phase method represents a useful approach to the problem of the potential scattering. Several papers and textbooks have been written on this subject [4]. The usual treatment of the equations of this method is based on the general connection between second-order linear differential equations and first order equations of the Riccati type.

We shall show here that there is a close connection between our formula (16) and the method of a variable phase. First, we confine ourselves to the case of a local potential $V$. We define a projector $P_\lambda$ on the interior of a sphere $\Omega_\lambda$ with the radius $\lambda$ in the configuration space. Further, we define the potential

$$V_1 = V_\lambda = P_\lambda V \tag{18}$$

and insert it into Eq. (16). Differentiation of $V_\lambda$ with respect to $\lambda$ transforms the radial matrix elements of the projector $\langle r|P_\lambda|r'\rangle = \delta(r-r')\,\vartheta(\lambda-r)$ into delta function, $\langle r|\partial_\lambda P_\lambda|r'\rangle = \delta(r-r')\,\delta(\lambda-r)$. We see that only the surface values of the exact wave function $|\psi_{\lambda E}^{c+}\rangle$ will be needed in the coordinate representation. Potential acting in the region outside of the sphere $\Omega_\lambda$ is equal to zero and the value of the wave function at the distance $\lambda$ from the origin may be simply continued into the asymptotic region. At the

same time, the asymptotic behaviour of the wave function may be expressed using the on-shell $S$-matrix elements $S_\lambda^{c'c}(E)$. Matrix elements $\langle \psi_{\lambda E}^{c''+} | \dfrac{\partial V_\lambda}{\partial \lambda} | \psi_{\lambda E}^{c+} \rangle$ may therefore be calculated in terms of $S_\lambda^{c'c}(E)$.

Let us analyze the situation in more detail. Let the particle of the mass $\mu$ be scattered by the central potential $V(r)$. As is usual in such a case, we choose the following set of free particle states

$$\langle \vec{r} | \chi_E^{lm} \rangle = \sqrt{\frac{2\mu}{\pi k}} \frac{j_l(kr)}{r} Y_{lm}(\Omega), \tag{19}$$

that satisfy the relations (6). In the definition (19) $(r, \Omega)$ are spherical coordinates of the vector $\vec{r}$ and $k = \sqrt{2\mu E}$ is an impulse of the particle. The spherical Bessel and Neumann functions $j_l$ and $n_l$, respectively, are defined in accordance with Ref. [4].

Wave functions $\langle \vec{r} | \psi_{\lambda E}^{lm} \rangle$ defined by the relation (8) are exact solutions of the problem with the potential $V_\lambda(r) = V_\lambda(r)\, \vartheta(\lambda - r)$ and in the region $r \geqslant \lambda$ they have the form

$$\langle \vec{r} | \psi_{\lambda E}^{lm} \rangle = \sqrt{\frac{2\mu}{\pi k}} \frac{e^{i\delta_\lambda^{lm}(E)}}{r} (j_l(kr) \cos \delta_\lambda^{lm}(E) + n_l(kr) \sin \delta_\lambda^{lm}(E)) \cdot Y_{lm}(\Omega). \tag{20}$$

Since the on-shell $S$-matrix is diagonal in the quantum numbers $l$, $m$, it is possible to use the equation (17) foı the calculation of the phase shifts $\delta_\lambda^{lm}(E)$. Inserting the potential into this equation and performing the radial integration in configuration space, we get

$$\frac{\partial}{\partial \lambda} \delta_\lambda^{lm}(E) = -\pi \lambda^2 V(\lambda) \oint d\Omega |\langle \lambda, \Omega | \psi_{\lambda E}^{lm} \rangle|^2. \tag{21}$$

Inserting Eq. (20) into this integral we finally get the well-known phase equations

$$\frac{\partial}{\partial \lambda} \delta_\lambda^{lm}(E) = -\frac{2\mu}{k} V(\lambda) [j_l(k\lambda) \cos \delta_\lambda^{lm}(E) + n_l(k\lambda) \sin \delta_\lambda^{lm}(E)]^2, \tag{22}$$

that are valid in our special case.

The variable phase method refers not only to the phase shifts. In the more general case (e. g. coupled channels, distorted waves etc.), this method is represented by a system of the first order nonlinear differential equations, where all the on-shell $S$-matrix elements are taken into account. The particular form of these equations depends entirely on the particular choice in the $S$-matrix parametrization, dimension of the configuration space, form of the potential, etc. Our method may be applied as well.

The equations (16) are used as a starting point. In all cases that allow to calculate the matrix elements $\langle \psi_\lambda^{c''+}(E) | \dfrac{\partial V_\lambda}{\partial \lambda} | \psi_{\lambda E}^{c+} \rangle$ in terms of the functions $S_\lambda^{c'c}(E)$, Eq. (16) may be looked upon as the generalized phase equation. One of the possibilities for $\lambda$ chosen as a radial cutoff in a configuration space, is given just by the definition (18) of the $\lambda$-dependent potential $V_\lambda$.

## REFERENCES

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