OPTICAL MODEL FOR THE SCATTERING OF INDISTINGUISHABLE MOLECULES*

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The optical and transition potentials are introduced for the scattering of indistinguishable molecules. A self-consistent renormalised perturbation scheme is proposed and used to obtain approximate expressions for these two operators. A close relation to the results of the field-theoretical approach is pointed out.

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1. Introduction

The optical potential method appeared an elegant and useful way to describe molecular collisions. In our previous papers [1, 2] we have shown how to introduce the optical and transition potential (for elastic and inelastic scattering respectively) in the formalism of first quantization and how to obtain the approximate formulae for these two operators using a renormalised self-consistent perturbation scheme. This has proved to be equivalent to the field-theoretical approach of Ficocelli Varracchio ([3–5] and the references therein).

Originally neither of the two approaches was adapted to describe collisions of identical molecules. This problem was later discussed by Ficocelli Varracchio [5] as far as the field-theoretical formulation is concerned. However, it is natural to expect that using such a sophisticated technique to handle such simple systems is not necessary. In the present paper we give the corresponding first-quantization optical model description of a collision of two identical molecules. This is a continuation of what has been presented in an earlier paper [1], though the method of introducing the optical and transition potential differs somewhat from that of [1] (the methods can be easily proved to be equivalent).

In the first section we define the optical potential of the elastic scattering and propose a method to derive approximations to this operator. The same method is used in the next

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section to obtain approximate formulae for the transition potential of inelastic scattering. Finally we show the close relation of our approach to the field-theoretical treatment of Ficocelli Varracchio [5] and also make some comments on the two approaches.

2. *Elastic scattering*

Consider a system of two colliding identical boson molecules (the case of fermions can be considered in an analogous way). The hamiltonian of the system is

$$H = T_R + h(r_1) + h(r_2) + V(R, r_1, r_2) = H_0 + V, \tag{1}$$

T_R being the kinetic energy of the relative motion, h — the internal hamiltonian of each molecule and V — the interaction potential.

Let $\phi_k(R)$ be a normalized plane wave and $\langle r_1, r_2 | \alpha_s \alpha_s' \rangle = \langle r_1 | \alpha_s \rangle \langle r_2 \alpha_s' \rangle$ an unsymmetrized internal state of the two molecules. Here α_s denotes a set of internal quantum numbers of a molecule and $\{\alpha_s\}$ is assumed to be ordered. Introduce the corresponding symmetric and antisymmetric states

$$\begin{aligned} \phi_k^{\pm}(R) &= 1/\sqrt{2}\,(\phi_k(R) \pm \phi_k(-R)) = 1/\sqrt{2}\,(\phi_k(R) \pm \phi_{-k}(R)), \\ |n_s^{\pm}\rangle &= 1/\sqrt{2}\,(|\alpha_s \alpha_s'\rangle \pm |\alpha_s' \alpha_s\rangle) \quad \text{for} \quad \alpha_s < \alpha_s', \\ |n_s^{+}\rangle &= |\alpha_s \alpha_s\rangle \quad \text{for} \quad \alpha_s = \alpha_s'. \end{aligned} \tag{2}$$

The S-matrix for the elastic scattering $k_i \alpha_i \alpha_i' \to k_f \alpha_i \alpha_i' (\alpha_i < \alpha_i')$ is given by the following expression [6, 7] (with all singularities in the inverse operators treated as usual in the scattering theory)

$$\begin{aligned} S_{fi} = &\lim_{\substack{t \to \infty \\ t' \to -\infty}} \langle \phi_{k_f}(t)| \langle \alpha_i \alpha_i'(t)| i\left(i\frac{\partial}{\partial t} - H\right)^{-1} \delta(t-t')\, |\alpha_i \alpha_i'(t')\rangle\, |\phi_{k_i}(t')\rangle \\ &+ \langle \phi_{-k_f}(t)| \langle \alpha_i' \alpha_i(t)| i\left(i\frac{\partial}{\partial t} - H\right)^{-1} \delta(t-t')\, |\alpha_i \alpha_i'(t')\rangle\, |\phi_{k_i}(t')\rangle \\ = &\lim_{\substack{t \to \infty \\ t' \to -\infty}} 1/2 \langle \phi_{k_f}^{\varrho}(t)\, \langle n_i^{\varrho}(t)| i\left(i\frac{\partial}{\partial t} - H\right)^{-1} \delta(t-t')\, |n_i^{\tau}(t')\rangle\, |\phi_{k_i}^{\tau}(t')\rangle. \end{aligned} \tag{3}$$

Summation is performed over repeating Greek indices which take the values $+$, $-$. We have taken $\phi_{k_i}^{\pm} = 1/\sqrt{2}(\phi_{k_i} \pm \phi_{-k_i})$. Depending on the definition of ϕ_{k_f} for a given k_f (we could have $\phi_{k_f}^{-} = 1/\sqrt{2}(\phi_{k_f} - \phi_{-k_f})$ or $\phi_{k_f} = 1/\sqrt{2}(\phi_{-k_f} - \phi_{k_f})$) the element of the sum in (3) corresponding to $\varrho = -$ may have the opposite sign. The optical potential can be introduced in the following way. First let us use in (3) the identity

$$\left(i\frac{\partial}{\partial t} - H\right)^{-1} = \left(i\frac{\partial}{\partial t} - H_0\right)^{-1} + \left(i\frac{\partial}{\partial t} - H_0\right)^{-1} V \left(i\frac{\partial}{\partial t} - H\right)^{-1}, \tag{4}$$

with $\left(i\frac{\partial}{\partial t}-H_0\right)^{-1}$ being a propagator of a free system. We get then the following expression for the $\mathscr{T}$-matrix ($S = I-\mathscr{T}$)

$$\mathscr{T}_{fi} = \lim_{t'\to-\infty}(-1/2)\int dt_1\langle\phi^{\varrho}_{k_f}(t_1)|\,\langle n^{\varrho}_i(t_1)|V\left(i\frac{\partial}{\partial t}-H\right)^{-1}\delta(t_1-t')\,|n^{\tau}_i(t')\rangle\,|\phi^{\tau}_{k_i}(t')\rangle. \tag{5}$$

If we now set

$$G^{\mu\nu}(t,t') = \langle n^{\mu}_i(t)|\left(i\frac{\partial}{\partial t}-H\right)^{-1}\delta(t-t')\,|n^{\nu}_i(t')\rangle, \tag{6}$$

$$|f^{\sigma(+)}_k(t)\rangle = i\lim_{t'\to-\infty}G^{\sigma\tau}(t,t')\,|\phi^{\tau}_k(t')\rangle. \tag{7}$$

$$\langle n^{\varrho}_i(t)|V\left(i\frac{\partial}{\partial t}-H\right)^{-1}\delta(t-t')\,|n^{\tau}_i(t')\rangle = \int dt_1\Sigma^{\varrho\sigma}(t,t_1)G^{\sigma\tau}(t_1,t') \tag{8}$$

we have

$$\begin{aligned}\mathscr{T}_{fi} &= i/2\int dt_1dt_2\langle\phi^{\varrho}_{k_f}(t_1)|\Sigma^{\varrho\sigma}(t_1,t_2)\,|f^{\sigma(+)}_{k_i}(t_2)\rangle\\ &= 2\pi i\cdot 1/2\delta(\varepsilon_{k_f}-\varepsilon_{k_i})\,\langle\phi^{\varrho}_{k_f}|\Sigma^{\varrho\sigma}(\varepsilon_{k_i})\,|f^{\sigma(+)}_{ki}\rangle,\end{aligned} \tag{9}$$

where we have also used the fact that $f^{\sigma(+)}_k(t) = f^{\sigma(+)}_k\exp(-i\varepsilon_k t)$.

The equalities (6) and (7) become after a Fourier transform

$$G^{\mu\nu}(\omega) = \langle n^{\mu}_i|\,(\omega+E_{n_i}-H)^{-1}|n^{\nu}_i\rangle, \tag{10}$$

$$\Sigma^{\varrho\sigma}(\omega)G^{\sigma\tau}(\omega) = \langle n^{\varrho}_i|V(\omega+E_{n_i}-H)^{-1}|n^{\tau}_i\rangle. \tag{11}$$

By the standard perturbation expansion of the inverse operator in the r.h.s. of (11) and introducing the projection operators $P = |n^{+}_i\rangle\langle n^{+}_i|+|n^{-}_i\rangle\langle n^{-}_i|$, $Q = I-P$, one can prove that the optical potential $\Sigma^{\varrho\sigma}$ defined through (11) exists and is identical to the Feshbach optical potential $\langle n^{\varrho}_i|PVP+PVQ(E-QHQ)^{-1}QVP|n^{\sigma}_i\rangle$. The function $f^{\nu(+)}_{k_i}$ can be considered as a projection of the total wave function of the system onto the internal state $|n^{\nu}_i\rangle$.

Since $|f^{\mu(+)}_{k_i}\rangle$ satisfies the Dyson equation with the potential Σ

$$|f^{\mu(+)}_{k_i}\rangle = |\phi^{\mu}_{k_i}\rangle+G^{\mu\varrho}_0(\varepsilon_{k_i})\Sigma^{\varrho\nu}(\varepsilon_{k_i})\,|f^{\nu(+)}_{k_i}\rangle, \tag{12}$$

with $G^{\mu\varrho}_0(\omega) = \langle n^{\mu}_i|(\omega+E_{n_i}-H_0)^{-1}|n^{\varrho}_i\rangle = \delta_{\mu\varrho}(\omega-T)^{-1}$, our approximation necessary to calculate the transition amplitudes in (9) will consist in using approximate expressions for Σ. We will use a renormalised self-consistent perturbation scheme.

We have

$$\begin{aligned}(\omega+E_{n_i}-H)^{-1} &= (\omega+E_{n_i}-H_0-W)^{-1}\\ &+(\omega+E_{n_i}-H_0-W)^{-1}\,(V-W)\,(\omega+E_{n_i}-H)^{-1}\end{aligned} \tag{13}$$

with

$$W = W(\omega+E_{n_i}) \equiv \sum_{n_j}|n^{u}_j\rangle\Sigma^{\mu\nu}(\omega-\omega_{ji})\,\langle n^{\nu}_j|, \qquad \omega_{ji} = E_{n_j}-E_{n_i}. \tag{14}$$

If we iterate (13) in the r.h.s. of (11) we shall obtain a series of approximations to Σ. The iteration scheme is somewhat complicated in the sense that to get an approximation of the n-th order, we need Σ in approximations of orders lower than n. The only criterion of order is the power of V. E.g. we obtain in the first and second order

$$^1\Sigma^{\varrho\sigma}(\omega) = V(n_i^\varrho, n_i^\sigma) \; - \text{ the matrix element of } V \text{ taken with unperturbed internal states,} \tag{15}$$

$$^2\Sigma^{\varrho\sigma}(\omega) = {}^1\Sigma^{\varrho\sigma}(\omega) + \sum_{n_j \neq n_i} V(n_i^\varrho, n_j^\mu) \langle n_j^\mu | (\omega + E_{n_i} - H_0 - W)^{-1} | n_j^\nu \rangle V(n_j^\nu, n_i^\sigma). \tag{16}$$

The operator in the second term in (16) is $G^{\mu\nu}(\omega - \omega_{ji})$ for the internal virtual states of the form

$$|n_j^\pm\rangle = 1/\sqrt{2}\,(|\alpha_j\alpha_j'\rangle \pm |\alpha_j'\alpha_j\rangle)$$

but not for those of the form $|n_j^+\rangle = |\alpha_j\alpha_j\rangle$. In the latter case it is equal to another Green's function $\tilde{G}^{++}$ which satisfies the equation

$$(\omega - T)\tilde{G}^{++}(\omega) - \Sigma^{++}(\omega)\tilde{G}^{++}(\omega) = I. \tag{17}$$

To have in our formulae only the function G, we have to apply an extra iteration scheme, namely that based on the relations

$$(\omega - T)\tilde{G}^{\alpha\beta} - \Sigma_1^{\alpha\gamma}\tilde{G}^{\gamma\beta} = \delta_{\alpha\beta}, \quad \hat{\Sigma}_1 = \begin{pmatrix} \Sigma^{++} & 0 \\ 0 & 0 \end{pmatrix},$$

$$(\omega - T)G^{\alpha\beta} - (\Sigma_1^{\alpha\gamma} + \Sigma_2^{\alpha\gamma})G^{\gamma\beta} = \delta_{\alpha\beta}, \quad \hat{\Sigma}_2 = \begin{pmatrix} 0 & \Sigma^{+-} \\ \Sigma^{-+} & \Sigma^{--} \end{pmatrix},$$

$$\hat{\tilde{G}} = \hat{G} - \hat{G}\hat{\Sigma}_2\hat{\tilde{G}}, \tag{18}$$

in particular

$$G^{++} = G^{++} - G^{++}\Sigma^{+-}G^{-+} - G^{+-}\Sigma^{-\beta}G^{\beta+} + \ldots . \tag{19}$$

Thus we can write

$$^2\Sigma^{\varrho\sigma}(\omega) = {}^1\Sigma^{\varrho\sigma}(\omega) + \sum_{n_j \neq n_i} V(n_i^\varrho, n_j^\mu) G^{\mu\nu}(\omega - \omega_{ji}) V(n_j^\nu, n_i^\sigma), \tag{20}$$

with further terms of (19) modifying $^3\Sigma$ etc.

The first term of (20) corresponds to the interaction of the molecules with their internal structure being undisturbed, the second describes the influence of internal distortion of the molecules (by taking into account internal virtual excitations). Further terms will represent multiple virtual excitations and corrections following from the fact that the propagator $\langle n_j^\mu | (\omega + E_{n_i} - H)^{-1} | n_j^\nu \rangle$ has been replaced by $G^{\mu\nu}(\omega - \omega_{ji})$. A more detailed discussion of the optical potentials of such a general form can be found in [1–5].

For $\alpha_i = \alpha_i'$ we have instead of (3)

$$S_{fi} \sim \lim_{\substack{t \to \infty \\ t' \to -\infty}} \langle \phi_{k_f}^+(t) | \langle n_i^+(t) | i \left(i \frac{\partial}{\partial t} - H \right)^{-1} \delta(t - t') \, | n_i^+(t') \rangle \, | \phi_{k_i}^+(t') \rangle. \tag{21}$$

We are able to define only the function G^{++} and the optical potential Σ^{++} corresponding to the one-dimensional projection $P = |n_i^+\rangle \langle n_i^+|$. The operator W is to be built as

$$W = \sum_{n_j} |n_j^\mu\rangle \Sigma^{++}(\omega - \omega_{ji}) \langle n_j^\mu|,$$

and the function G^{++} will be used to describe the evolution of the system during virtual excitations but not to switch from n_j^μ to n_j^ν.

This case is similar to that of distinguishable molecules [1–4] because of the one--dimensional projection.

There is also a possibility of choosing a reference state (state in which G is defined) different from the initial state n_i [4]. This would lead to a 2×2 Green function but also to an extra distorted-wave term in the final formula.

3. *Inelastic scattering*

The S-matrix for the inelastic process $\boldsymbol{k}_i\alpha_i\alpha_i' \to \boldsymbol{k}_f\alpha_f\alpha_f'$ ($\alpha_f \neq \alpha_f'$, $\alpha_i < \alpha_i'$) has the following form

$$S_{fi} = 1/2 \lim_{\substack{t\to\infty \\ t'\to-\infty}} \langle \phi_{\boldsymbol{k}_f}^\varrho(t)\, |\langle n_f^\varrho(t)| i\left(i\frac{\partial}{\partial t} - H\right)^{-1} \delta(t-t')\, |n_i^\tau(t')\rangle\, |\phi_{\boldsymbol{k}_i}^\tau(t')\rangle. \tag{22}$$

Depending on the definition of $\phi_{\boldsymbol{k}_f}$ for a given $\boldsymbol{k}_f$ and on whether $\alpha_f < \alpha_f'$ or $\alpha_f > \alpha_f'$ the term in (22) for $\varrho = -$ may have the opposite sign. Our aim is to introduce the transition potential $V(n_f \leftarrow n_i)$ i.e. to write the operator in (22) as

$$\langle n_f^\varrho(t)|\left(i\frac{\partial}{\partial t} - H\right)^{-1} \delta(t-t')\, |n_i^\tau(t')\rangle = \int G^{\varrho\mu}(t, t_1) V(n_f^\mu \leftarrow n_i^\nu)\,(t_1, t_2) G^{\nu\tau}(t_2, t')\, dt_1 dt_2 \tag{23}$$

or, after a Fourier transform

$$\langle n_f^\varrho|\,(\omega + (E_{n_f} + E_{n_i})/2 - H)^{-1}\, |n_i^\tau\rangle = G^{\varrho\mu}(\omega - \omega_{fi}/2) V(n_f^\mu \leftarrow n_i^\nu)\,(\omega) G^{\nu\tau}(\omega + \omega_{fi}/2). \tag{24}$$

Now let us introduce the vector $\langle f_{\boldsymbol{k}_f}^{\nu(-)}|$ as

$$\langle f_{\boldsymbol{k}_f}^{\nu(-)}(t)| = i \lim_{t'\to\infty} \langle \phi_{\boldsymbol{k}_f}^\mu(t')|G^{\mu\nu}(t', t), \tag{25}$$

which satisfies the equation

$$\langle f_{\boldsymbol{k}_f}^{\mu(-)}| = \langle \phi_{\boldsymbol{k}_f}^\mu| + \langle f_{\boldsymbol{k}_f}^{\nu(-)}|\Sigma^{\nu\varrho}(\varepsilon_{\boldsymbol{k}_f}) G_0^{\varrho\mu}(\varepsilon_{\boldsymbol{k}_f}). \tag{26}$$

The mentioned change of sign of some terms of (22) would lead to a change of sign in (25) and in the free term of (26) of terms for $\mu = -$.

After using the above equalities we get

$$S_{fi} = -2\pi i \cdot 1/2\delta(\varepsilon_{\boldsymbol{k}_f} + E_{n_f} - \varepsilon_{\boldsymbol{k}_i} - E_{n_i}) \langle f_{\boldsymbol{k}_f}^{\mu(-)}|V(n_f^\mu \leftarrow n_i^\nu)\,((\varepsilon_{\boldsymbol{k}_f} + \varepsilon_{\boldsymbol{k}_i})/2)\, |f_{\boldsymbol{k}_i}^{\nu(+)}\rangle. \tag{27}$$

To calculate the S-matrix elements we need an approximate form of two operators: the optical potential Σ (to solve the equations (12) and (26)) and the transition potential

$V(n_f \leftarrow n_i)$ (to calculate the matrix element (27)). Also the latter operator can be approximated with the help of the iteration scheme (13). Namely, if we iterate (13) in the l.h.s. of (24) we will get the corresponding formulae for $V(n_f \leftarrow n_i)$ in the required order of approximation e.g.

$$^1V(n_f^\mu \leftarrow n_i^\nu)(\omega) = V(n_f^\mu, n_i^\nu), \tag{28}$$

$$^2V(n_f^\mu \leftarrow n_i^\nu)(\omega) = {}^1V(n_f^\mu \leftarrow n_i^\nu) + \sum_{n_j \neq n_i, n_f} V(n_f^\mu, n_j^\varrho) G^{\varrho\tau}(\omega + (E_{n_f} + E_{n_i})/2 - E_{n_j})$$
$$\times V(n_j^\tau, n_i^\nu) + [V(n_f^\mu, n_f^\varrho) - V(n_i^\mu, n_i^\varrho)] G^{\varrho\tau}(\omega - \omega_{fi}/2)\, V(n_f^\tau, n_i^\nu). \tag{29}$$

For virtual states of the type $|\alpha_j \alpha_j\rangle$, the function $\tilde{G}^{++}$ has again been replaced by G^{++} according to (19).

In (29) we recognize the term corresponding to the direct transition, terms describing transitions through intermediate virtual states and the final-state correction. Terms of higher orders would again describe multiple virtual transitions and some more complicated corrections. The main formal difference between the corresponding expressions for the case of different and identical molecules is a 2×2 matrix character of operators in the latter case. However, general features of the discussion of those operators remain valid [1, 2, 4].

For $\alpha_f = \alpha_f'$ our formalism differs somewhat from the above. The corresponding S-matrix is

$$S_{fi} = 1/\sqrt{2} \lim_{\substack{t \to \infty \\ t' \to -\infty}} \langle \phi_{k_f}^+(t)| \langle n_f^+(t)| i \left(i \frac{\partial}{\partial t} - H \right)^{-1} \delta(t - t')\, |n_i^\tau(t')\rangle\, |\phi_{k_i}^\tau(t')\rangle. \tag{30}$$

Our iteration scheme based on (13) would lead to an expression analogous to (24) but with $G^{\varrho\mu}$ replaced by $\tilde{G}^{\varrho\mu}$, $\varrho = \mu = +1$. In consequence the final-state distorted wave would be propagated by $\tilde{G}^{++}$

Thus we have instead of (25), (26)

$$\langle f_{k_f}^{+(-)}(t)| = i \lim_{t' \to \infty} \langle \phi_{k_f}^+(t')| \tilde{G}^{++}(t', t), \tag{31}$$

$$\langle f_{k_f}^{+(-)}| = \langle \phi_{k_f}^+| + \langle f_{k_f}^{+(-)}| \Sigma^{++}(\varepsilon_{k_f}) G_0^{++}(\varepsilon_{k_f}). \tag{32}$$

Finally we obtain the S-matrix of the form

$$S_{fi} = -2\pi i \delta(\varepsilon_{k_f} + E_{n_f} - \varepsilon_{k_i} - E_{n_i}) 1/\sqrt{2}\, \langle f_{k_f}^{+(-)}| V(n_f^+ \leftarrow n_i^\nu)((\varepsilon_{k_f} + \varepsilon_{k_i})/2))\, |f_{k_i}^{\nu(+)}\rangle \tag{33}$$

with the transition potential having in the second order the following form

$$^2V(n_f^+ \leftarrow n_i^\nu)(\omega) = V(n_f^+, n_i^\nu) + \sum_{n_j \neq n_i, n_f} V(n_f^+, n_j^\varrho) G^{\varrho\tau}(\omega + (E_{n_f} + E_{n_i})/2 - E_{n_j}) V(n_j^\tau, n_i^\nu)$$
$$+ [V(n_f^+, n_f^+) - V(n_i^+, n_i^+)] \tilde{G}^{++}(\omega - \omega_{fi}/2) V(n_f^+, n_i^\nu). \tag{34}$$

$\tilde{G}$ can again be replaced by G, their difference modifying terms of higher orders.

For symmetry reasons (though, as we believe, not for practical ones) it would be good to have the corresponding formulae with the final-state distorted wave propagated not by $\tilde{G}$ but by G that is to use

$$\langle {}_1 f_{k_f}^{\mu(-)}(t)| = i \lim_{t' \to \infty} \langle \phi_{k_f}^{+}(t') G^{+\mu}(t', t), \tag{35}$$

$$\langle {}_1 f_{k_f}^{\mu(-)}| = \langle \phi_{k_f}^{+}|\delta_{\mu +} + \langle {}_1 f_{k_f}^{\nu(-)}|\Sigma^{\nu\varrho}(\varepsilon_{k_f}) G_0^{\varrho\mu}(\varepsilon_{k_f}). \tag{36}$$

This leads to the S-matrix

$$S_{fi} = -2\pi i \delta(\varepsilon_{k_f} + E_{n_f} - \varepsilon_{k_i} - E_{n_i}) 1/\sqrt{2}\, \langle {}_1 f_{k_f}^{\mu(-)}|_1 V(n_f^{\mu} \leftarrow n_i^{\nu})\, ((\varepsilon_{k_f} + \varepsilon_{k_i})/2)\, |f_{k_i}^{\nu(+)}\rangle \tag{37}$$

with

$$\begin{aligned} {}_1^2 V(n_f^{+} \leftarrow n_i^{\nu})\,(\omega) &= {}^2 V(n_f^{+} \leftarrow n_i^{\nu})\,(\omega) - V(n_i^{+}, n_i^{-}) G^{-+}(\omega - \omega_{fi}/2) V(n_f^{+}, n_i^{\nu}), \\ {}_1^2 V(n_f^{-} \leftarrow n_i^{\nu})\,(\omega) &= -V(n_i^{-}, n_i^{\varrho}) G^{\varrho +}(\omega - \omega_{fi}/2) V(n_f^{+}, n_i^{\nu}). \end{aligned} \tag{38}$$

For $\alpha_i = \alpha_i'$ a 1×1 operator G^{++} would be used to describe the distorted waves in both the initial and final state as well as the virtual transitions (see the final part of the preceding section).

4. *Discussion*

In the preceding sections we have introduced the optical model description of the scattering of identical molecules. We have given the explicit formulae for the optical and transition potential in the first and second order and presented the method of obtaining approximations of higher orders. Our results clearly exhibit a similarity to those of the field-theoretical approach [1–5].

In the framework of field theory a propagator for the elastic scattering has the following form

$$G^{\varrho\tau}(\boldsymbol{R}, t, \boldsymbol{R}', t') = -i \langle n_i^{\varrho}|T \psi_{\varrho}(\boldsymbol{R}, t) \psi_{\tau}^{+}(\boldsymbol{R}', t')\, |n_i^{\tau}\rangle, \tag{39}$$

ψ being the field operators for the translational degrees of freedom (see [5] for details). This propagator and our operator (6) in the position representation should be identical. Indeed, it can be shown by an analysis of the equations of motion (following from the Heisenberg equation) for G and for the Bethe–Salpeter amplitude

$$X(n_j^{\varrho}, n_i^{\tau})\,(\boldsymbol{R}, t, \boldsymbol{R}', t') = \langle n_j^{\varrho}|T \psi_{\varrho}(\boldsymbol{R}, t) \psi_{\tau}^{+}(\boldsymbol{R}', t')\, |n_i^{\tau}\rangle, \qquad n_j \neq n_i, \tag{40}$$

that (6) and (39) have the same optical potential of the form (15), (16) etc. The amplitude (40) is identical to the operator (23) multiplied by i (again in the position representation) and one can show that the two operators have the same transition potential (28), (29) etc.

The field-theoretical approach to our problem has been the subject of the paper of Ficocelli Varracchio [5] who used the state $|n_i^{+}\rangle + |n_i^{-}\rangle = \sqrt{2}|\alpha_i \alpha_i'\rangle$ as a reference state (which should in fact be normalised). With the field-theoretical hamiltonian as in [5]

(the interaction terms should in fact be divided by 2) his Green function g is related to ours by

$$g^{\varrho\tau} = -i\langle\alpha_i\alpha_i'|T\psi_\varrho\psi_\tau^+|\alpha_i\alpha_i'\rangle = 1/2(G^{\varrho\tau}+G_0^{\varrho\tau}) \quad \text{for} \quad \alpha_i \neq \alpha_i'$$

$$\text{and } g^{++} = G^{++}, \quad g^{--} = g_0^{--} = g_0^{++} = G_0^{++},$$

$$g^{+-} = g^{-+} = G^{+-} = G^{-+} = G^{--} = 0 \quad \text{for} \quad \alpha_i = \alpha_i'. \tag{41}$$

Of course g also contains full information about the elastic process. However, repeating our calculations of the preceding sections for the function g with the help of (41) is more complicated. It requires an extra renormalisation procedure because in every step there will appear the function g_0 which is to be replaced by g minus terms of higher orders.

In [5] the author used another decoupling technique, namely that based on the Martin-Schwinger identity. Results yielded by this method are similar to those which can be obtained for g from our formalism developed for G and the extra renormalisation. A difference between the two results is that the former leads to an additional change of sign of some of the renormalised terms. Differences of this type appear when we examine the renormalised equations of motion for g and the amplitudes $\langle\alpha_p\alpha_p'|T\psi_\mu\psi_\nu^+|\alpha_n\alpha_n'\rangle$. The sign in the final expressions depends on whether we deal separately with the amplitudes $\langle\alpha_p\alpha_p'|T\psi_\mu\psi_\nu^+(\alpha_n\alpha_n'\rangle$ and $\langle\alpha_p'\alpha_p|T\psi_\mu\psi_\nu^+|\alpha_n\alpha_n'\rangle$ or use the exact fact that they differ by the factor (± 1) for $\mu = \pm$respectively.

A comparison of two such different renormalisation procedures can be performed only on the level of non-renormalised formulae.

In our equations for the function g (in any approach) the virtual process $\alpha_s\alpha_s' \to \alpha_i'\alpha_i \to \alpha_i\alpha_i'$ must be taken into account which reflects in the appearing of the terms of the type $V(n_s^\varrho, n_i^\mu)G^{\mu\nu}V(n_i^\nu, n_i^\tau)$ in the second-order approximation for the optical potential ($s = i$) and the transition potential ($s = f$). Such terms are missing from the corresponding formulae of [5] while some of them should remain also in the "diagonal approximation".

Connected with the lack of normalisation of the reference state in [5] are also inappropriate numerical factors in the formulae for Σ and $V(n_f \leftarrow n_i)$[1].

We believe that our first-quantization approach is simpler and more natural than the sophisticated field-theoretical formalism. Our renormalisation procedure seems also more consistent. It also seems that the functions $\tilde{G}^{++}$ describe the evolution of the system in the virtual state $|\alpha_j\alpha_j\rangle$ better than the non-diagonal $G^{\mu\nu}$. For $\alpha_f = \alpha_f'$ where the final-state distorted wave is naturally one dimensional ($|f_{k_f}^{+(-)}\rangle$), introducing the other component ($|{}_1f_{k_f}^{-(-)}\rangle$) and then the operator ${}_1V(n_f^- \leftarrow n_i^\mu)$, while $|n_f^-\rangle \equiv 0$, is rather artificial. It is also easier to solve a one-dimensional equation (32) than two coupled equations (36). The last two problems appear in the field-theoretical approach which leads to final results of the type (35)–(38).

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[1] They are, in fact, suitable for the function G but not for g.

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