A Multichannel "Potential Curves Hopping" Model for Inelastic Collisions

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We introduce a multichannel "potential curves hopping" model and obtain the exact quantum mechanical S-matrix by solving the associated set of coupled second-order ordinary differential equations that describes the inelastic collisions between atomic particles. The only assumption is that the interaction matrix element between each pair of channels (say, γ and β) is of the form $U_{\gamma\beta}(r) = U_{\beta\gamma}(r) =: U_{\gamma\beta}\delta(r - r_{\gamma\beta})$, where $\delta(x)$ is the Dirac deltafunction, and $r_{\gamma\beta}$ and $U_{\gamma\beta}$ are parameters which can be chosen freely.

Semiclassical techniques can be incorporated directly in the theory if the Schrödinger equations for the uncoupled channels allow this treatment. The formulation is particularized to the two-channel problem and illustrated with a semiclassical example the $He^+ + Ne$ problem at 70.9 eV.

1. Introduction

In this paper we shall be concerned with an N-channel model for the study of inelastic collision processes between a pair of atomic particles, the motion of which can be described by one-dimensional potential energy curves. We shall label the possible two-particle states, called channels, by α, β and γ. The N-channel system is governed by a set of coupled equations for each angular momentum l:

$$(d^2/dr^2 + k_\beta^2 - l(l+1)/r^2 - U_{\beta\beta}(r))\,\Psi_{\beta\alpha}(l;r) = \sum_{\gamma=1}^{N} (1-\delta_{\beta\gamma})\,U_{\beta\gamma}(r)\,\Psi_{\gamma\alpha}(l;r)\,,$$
$$\alpha,\beta,\gamma = 1,2,\ldots,N\,. \qquad (1)$$

In this equations α is the initial channel

$$(\alpha = 1,2,\ldots,N)\,, \quad U_{\beta\gamma}(r) = (2\mu/\hbar^2)\,V_{\beta\gamma}(r)$$

are certain matrix elements, and k_β denotes the wavenumber corresponding to channel β when the total energy is E, that is

$$k_\beta^2 = (2\mu/\hbar^2)\,(E - \varepsilon_\beta)\,, \qquad (2)$$

where ε_β is the threshold of channel β and μ is the reduced mass of the system. The threshold of the initial channel α is, of course, zero.

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At present there is a real possibility of treating the scattering problem by solving (1) by means of electronic computers. However, since a direct solution is a very time consuming process, it is important to develop simple models in order to gain insight into the physical picture of the collision process. The present paper will deal with a model for which the only assumption is that the interaction matrix element between each pair of channels (say, γ and β) is of the form

$$U_{\beta\gamma}(r) = U_{\gamma\beta}(r) = U_{\beta\gamma}\delta(r - r_{\gamma\beta})\,, \qquad (3)$$

where $\delta(y)$ is the Dirac deltafunction. This model involves for each pair of channels two independent parameters: the point $r_{\gamma\beta}$ where the coupling between channels and the transition takes place, and the amplitude $U_{\gamma\beta}$ of the interaction. We will find an analytical expression for the **S**-matrix and will obtain from its knowledge all information concerning elastic and inelastic cross sections, via expressions for the scattering amplitudes. This model will then be combined with the well-known uniform semiclassical approximation to treat two-channel ion-atom scattering.

The interest in two-state models began in 1932 when Landau [1], Zener [2] and Stückelberg [3] independently proposed a model to treat potential-curve-crossing problems. Since then, the model has been analyzed, critized or extended by various authors [4–16].

The so-called Landau-Zener (LZ) model uses the fact first pointed out by Mott [17] that, when the

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interacting particles are atomic systems, the theory is greatly simplified by the assumption that the nuclei move like classical particles, which leads immediately to the impact parameter treatment [18–20]. The LZ-model uses also the assumption that transitions are restricted to a small region around the point r_0 of the intersection of the diabatic curves $U_{11}(r)$ and $U_{22}(r)$, which leads to following simplifying equations [12, 14]:

$$U_{11}(r) = \bar{U}(r_0) - F_1(r - r_0)\,,$$
$$U_{22}(r) = \bar{U}(r_0) - F_2(r - r_0)\,, \quad U_{12}(r) = a\,, \quad (4)$$

where $\bar{U}(r_0) =: U_{11}(r_0) = U_{22}(r_0)$ and, a, F_1, and F_2 are constants. The equation of the trajectory in the vicinity of r_0 is also approximated by a linear function of time: $r - r_0 = v_0 t$.

The two-state curve-crossing problem was attacked by Stückelberg [3] by employing the same LZ-model assumptions of (4), but instead of the impact parameter method he used a WKB-type of treatment in order to solve a single fourth-order differential equation derived from the set of two coupled radial Schrödinger equations. The method was later clarified by Crothers [4] and Thorson et al. [21]. At this point we remark that, different from the LZ-model, the Stückelberg method (denoted as LZS method) allows for nuclear interference, that is, interference between particles following different collision paths, but arriving at the same scattering angle. The interference results then in the so-called Stückelberg oscillations of the cross sections.

The introduction in the present paper of a Dirac deltafunction coupling, (3), for each pair of channels is related to the idea of Tully and Preston [22] implemented in the so called "Surface-Hopping Trajectory" (SHT) theory. In this approach the nuclear motion is treated completely classically like in the LZ-model; a nonadiabatic transition is represented as a hop from one adiabatic potential surface to another, and it is assumed that such hops can occur at only a finite number of distinct points along any trajectory. In the SHT approach the classical trajectories propagate on the initial potential surface until the point of large interaction is reached, then a probability P of switching to another surface is computed and the trajectories are continued on both surfaces, each weighted by the appropriate probability: the weights $(1 - P)$ and P are assigned to the branches on the old and the new potential surfaces, respectively.

Contrary to the SHT approach, the "Potential-Curves-Hopping" (PCH) model developed in the present paper is a fully quantum-mechanical one in which electronic and nuclear degrees of freedom are treated on the same dynamical footing. So there is one important difference between the SHT and the PCH models: the first one adds probabilities and the quantum-mechanical behaviour of the colliding particles is not taken into consideration while the second one adds probability amplitudes and allows for nuclear interference, like the LZS model. In other words, the Dirac deltafunction, introduced in the present paper to represent the hops between potential curves, leads to a mathematical treatment of phase coherence contrary to the STH model which assumes that the phase can be neglected.

At this point it is also to note that the technique of adding probabilities rather than amplitudes has also been used by Gershtein [23] and Salop and Olson [24] to modify the usual two-state LZ-theory for applications to a multistate system. They and Janev et al. [25] have studied with this theory collisions between hydrogen atoms and several fully stripped heavy ions.

The N-channel PCH model of the present paper is probably crude for realistic applications. However, since it is an exact quantum-mechanical one and there is no restriction about the energy range or the number of channels, it can be useful for comparisons to study realistic systems or approximation methods.

To end this section it is worth to mention other works concerning the multichannel problem of atom(ion)-atom scattering: Wooley [26], McLafferty and George [27], Hwang and Pechukas [28], Cho and Eu [29], Laing and George [30], Korsch [31]. The list is, however, not complete and the reader is referred to the cited articles and references therein for further information and references on this subject.

2. Review of the formalism

In an earlier work one of us [32] concerning inelastic collisions, a method was formulated to treat coupled radial Schrödinger equations. In the present paper we will use this method to treat with the PCH model, defined by arbitrary diabatic potentials $U_{\beta\beta}(r)$ and the interaction matrix elements $U_{\gamma\beta}(r)$ given by (3). The notation will be the same as in [32].

Let us begin with a briefly review of the four steps involved in the general formalism.

Pure elastic case

That is, solution of the elastic scattering problem for each channel in the absence of coupling between channels ($U_{\gamma\beta}(r) = 0, \gamma \neq \beta$). In this step we have to find for each channel (say, β) the incoming Jost solution $\Phi_\beta^-(k_\beta, l; r)$ of the homogeneous equation

$$(\mathrm{d}^2/\mathrm{d}r^2 + k_\beta^2 - l(l+1)/r^2 - U_{\beta\beta}(r))\, \Phi_\beta^-(k_\beta, l; r) = 0 \tag{5}$$

and the corresponding scattering matrix element

$$s_\beta(k_\beta, l) = \exp[2i\eta_\beta(k_\beta, l)], \tag{6}$$

where η_β is the phaseshift associated with the channel β, the angular momentum l and the wavenumber k_β.

For later convenience we note that the incoming Jost solution of (5) is defined by the boundary condition

$$\Phi_\beta^-(k_\beta, l; r) = \exp[-\mathrm{i}(k_\beta r - \tfrac{1}{2} l\pi)], \quad r \to \infty . \tag{7}$$

Φ_β^-, like any complex number, can be written as a product of modulus and phase:

$$\Phi_\beta^-(k_\beta, l; r) = |\Phi_\beta^-(k_\beta, l; r)| \exp[-\mathrm{i}\Delta_\beta(k_\beta, l; r)]. \tag{8}$$

In the appendix we will show that for a real potential $U_{\beta\beta}(r)$ the following relation is valid:

$$\Delta_\beta(0) =: \lim_{r \to 0} \Delta_\beta(k_\beta, l; r) = -\eta_\beta(k_\beta, l) . \tag{9}$$

In the following we will abbreviate the notation by dropping the dependence of the variables l and k_β; so we will write $\Delta_\beta(r)$ instead of $\Delta_\beta(k_\beta, l; r)$.

Evolution matrix

The second step deals with the effect of the coupling between channels. Our task is to express $\Psi_{\beta\alpha}(l; r)$ in terms of the "comparison" function $\Phi_\beta^-(k_\beta, l; r)$. The set (1) of coupled radial equations is reduced to an equivalent system of coupled first-order differential equations by introducing for each channel (say, β) new unknowns, $Y_{\beta\alpha}(r)$ and $Z_{\beta\alpha}(r)$, defined by

$$\Psi_{\beta\alpha} = \Phi_\beta^- Y_{\beta\alpha} ,$$
$$Z_{\beta\alpha} =: \Phi_\beta^-(\mathrm{d}\Psi_{\beta\alpha}/\mathrm{d}r) - \Psi_{\beta\alpha}(\mathrm{d}\Phi_\beta^-/\mathrm{d}r) .$$

By using Φ_β^- as comparison function, the obtained set of differential equations describes only the effect of the coupling between channels and, therefore, is completely specified by the amplitude $Y_{\beta\alpha}(r)$ and the Wronskian $Z_{\beta\alpha}(r)$.

From the mathematical point of view, in the second step we have to find the $2N \times 2N$ "evolution matrix" associated with the set of $2N$ first-order differential equations. This matrix, called $\mathbf{W}(r, r_0)$, satisfies the differential equation

$$(\mathrm{d}/\mathrm{d}r)\, \mathbf{W}(r, r_0) = \mathbf{A}(r)\, \mathbf{W}(r, r_0) ,$$
$$\mathbf{W}(r_0, r_0) = \mathbf{I} , \tag{10}$$

where

$$\mathbf{A}(r) =: \begin{bmatrix} \mathbf{0} & \mathbf{A}_1(r) \\ \mathbf{A}_2(r) & \mathbf{0} \end{bmatrix} \tag{11a}$$

with

$$\mathbf{A}_1(r) =: \mathbf{\Phi}^{-1}(r)\, \mathbf{\Phi}^{-1}(r) ,$$
$$\mathbf{A}_2(r) =: \mathbf{\Phi}(r)\, \mathbf{U}(r)\, \mathbf{\Phi}(r) . \tag{11b}$$

Here we have introduced the $N \times N$ square matrices

$$\mathbf{\Phi}(r) =: [\Phi_\beta^-(r)\, \delta_{\beta\alpha}] ,$$
$$\mathbf{U}(r) =: [U_{\beta\alpha}(r)\, (1 - \delta_{\beta\alpha})] ; \tag{12}$$

$\mathbf{\Phi}^{-1}(r)$ denotes the inverse of the diagonal matrix $\mathbf{\Phi}(r)$; $\mathbf{0}$ and $\mathbf{1}$ are the $N \times N$ zero and the $2N \times 2N$ unit matrices, respectively. At this point let us also note that the evolution matrix $\mathbf{W}(r, r_0)$ can be decomposed into the form

$$\mathbf{W}(r, r_0) =: \begin{bmatrix} \mathbf{W}_{11}(r, r_0) & \mathbf{W}_{12}(r, r_0) \\ \mathbf{W}_{21}(r, r_0) & \mathbf{W}_{22}(r, r_0) \end{bmatrix} . \tag{13}$$

Scattering matrix elements

In the third step we calculate the $N \times N$ scattering matrix $\mathbf{S}$ associated with the coupled equations (1) and the angular momentum l, via the relation

$$\mathbf{S} = (\mathbf{K}^{-1/2}\, \mathbf{W}_{22}(\infty, 0)\, \mathbf{M}^{-1}\, \mathbf{K}^{1/2})\, \mathbf{s} , \tag{14}$$

where $\mathbf{s} =: [s_\beta \delta_{\beta\alpha}]$, $\mathbf{K} =: [k_\beta \delta_{\beta\alpha}]$ and

$$\mathbf{M} =: \mathbf{1} + \mathbf{s} \int_0^\infty \mathrm{d}r'\, \mathbf{\Phi}^*(r')\, \mathbf{U}(r')\, \mathbf{\Phi}(r')\, \mathbf{W}_{12}(r', 0) , \tag{15}$$

$\mathbf{1}$ being the $N \times N$ unit matrix and * denoting the complex conjugate.

Cross sections

Let now $S_{\beta\alpha}$ be the element of the $\mathbf{S}$-matrix corresponding to the transition $\beta \leftarrow \alpha$, and l the angular

momentum. The multichannel partial-wave amplitude and the partial-wave series are given by (e.g. Taylor [31])

$$f_{\beta\alpha}^{(l)} =: (S_{\beta\alpha} - \delta_{\beta\alpha})/(2i)\,(k_\alpha k_\beta)^{1/2},$$
$$f_{\beta\alpha}(\theta) = \sum (2l+1)\, f_{\beta\alpha}^{(l)}\, \mathbf{P}_l(\cos\theta). \tag{16a}$$

The differential, $\sigma_{\beta\alpha}(\theta)$, and the total, $Q_{\beta\alpha}$, cross sections for the process $\beta \leftarrow \alpha$ are calculated via the usual relations

$$\sigma_{\beta\alpha}(\theta) = (k_\beta/k_\alpha)\,|f_{\beta\alpha}(\theta)|^2,$$
$$Q_{\beta\alpha} = (\pi/k_\alpha^2) \sum (2l+1)\,|S_{\beta\alpha} - \delta_{\beta\alpha}|^2. \tag{16b}$$

3. *Exact solution of the PCH model*

We begin by defining an $N \times N$ matrix $\mathbf{P}_{\gamma\beta}$ whose elements are all zero safe the elements $(\gamma\beta)$ and $(\beta\gamma)$ which are unity. Having the set of matrices $\{\mathbf{P}_{\gamma\beta};\ \gamma, \beta = 1, 2, \ldots, N\}$ we can decompose the coupling matrix $\mathbf{U}(r)$ into the form

$$\mathbf{U}(r) = \sum_{\gamma<\beta}\sum U_{\gamma\beta}(r)\, \mathbf{P}_{\gamma\beta}, \tag{17}$$

where we assume $U_{\gamma\beta}(r) = U_{\beta\gamma}(r)$ and the sums run from 1 to N with the restriction $\gamma < \beta$. The decomposition (17) shows explicitly the coupling between each pair of channels (say, γ and β), which hereafter is assumed to have the Dirac delta-function dependence given by (3).

At this point we note that the delta-function has meaning only so long as an integration over its argument is carried out. Thus it is convenient to rewrite (10) and (11) in an integral form, from which we obtain the coupled integral equations

$$\mathbf{W}_{22}(r, r_0) = \mathbf{1} + \int_0^r \mathrm{d}r'\, \mathbf{A}_2(r')\, \mathbf{W}_{12}(r', 0), \tag{18a}$$

$$\mathbf{W}_{12}(r, r_0) = \int_0^r \mathrm{d}r'\, \mathbf{A}_1(r')\, \mathbf{W}_{22}(r', 0) \tag{18b}$$

whose solution is required in order to calculate the **S**-matrix via (14) and (15). Returning to the definition of the matrix $\mathbf{A}_2(r)$, (11b), and using (17) and (3), we see that

$$\mathbf{A}_2(r) = \sum_{\gamma<\beta}\sum \mathbf{\Phi}(r)\, U_{\gamma\beta}\, \mathbf{P}_{\gamma\beta}\, \mathbf{\Phi}(r)\, \delta(r - r_{\gamma\beta}). \tag{19}$$

For later convenience we introduce the Heaviside step function

$$\theta(r - r') = 1 \quad \text{if} \quad r > r' \quad \text{and}$$
$$\theta(r - r') = 0 \quad \text{if} \quad r \leqq r' \tag{20a}$$

and note following identities:

$$\int_0^r \mathrm{d}r'\, g(r')\, \delta(r' - r_x) = \int_0^\infty \mathrm{d}r'\, g(r')\, \theta(r - r')\, \delta(r' - r_x)$$
$$= g(r_x)\, \theta(r - r_x), \tag{20b}$$

$$\int_0^r \mathrm{d}r'\, g(r')\, \theta(r' - r_x) = \left(\int_{r_x}^r \mathrm{d}r'\, g(r')\right) \theta(r - r_x). \tag{20c}$$

Let us now return to the solution of the coupled integral equations (18). After substitution of (19) into (18a) we get

$$\mathbf{W}_{22}(r, 0) = \mathbf{1} + \sum_{\gamma<\beta}\sum \tilde{\mathbf{\Omega}}_{\gamma\beta}(r)\, \mathbf{W}_{12}(r_{\gamma\beta}, 0)\, \theta(r - r_{\gamma\beta}), \tag{21}$$

where we have defined the $N \times N$ matrix

$$\tilde{\mathbf{\Omega}}_{\gamma\beta}(r) =: \mathbf{\Phi}(r_{\gamma\beta})\, U_{\gamma\beta}\, \mathbf{\Phi}(r_{\gamma\beta}) \tag{22}$$

whose elements are all zero safe the elements $(\gamma\beta)$ and $(\beta\gamma)$, which are

$$\tilde{\omega}_{\gamma\beta} =: \Phi_\gamma^-(r_{\gamma\beta})\, U_{\gamma\beta}\, \Phi_\beta^-(r_{\gamma\beta}) \tag{23a}$$
$$= a_{\gamma\beta} \exp[-i(\Delta_\gamma(r_{\gamma\beta}) + \Delta_\beta(r_{\gamma\beta})] \tag{23b}$$

with

$$a_{\gamma\beta} =: U_{\gamma\beta}\,|\,\Phi_\gamma^-(r_{\gamma\beta})\,|\,|\,\Phi_\beta^-(r_{\gamma\beta})\,|. \tag{23c}$$

Now, introducing (21) into (18b) and defining the diagonal matrix

$$\mathbf{B}_1(r, r_0) = \int_{r_0}^r \mathrm{d}r'\, \mathbf{A}_1(r') \tag{24}$$

we obtain

$$\mathbf{W}_{12}(r, 0) = \mathbf{B}_1(r, 0) + \sum_{\gamma<\beta}\sum \tilde{\mathbf{\Omega}}_{\gamma\beta}(r)\, \mathbf{W}_{12}(r_{\gamma\beta}, 0)$$
$$\cdot\, \mathbf{B}_1(r, r_{\gamma\beta})\, \theta(r - r_{\gamma\beta}). \tag{25}$$

At this point we emphasize that the relations (21) and (25) will be useful if we can evaluate the matrix $\mathbf{W}_{12}(r, 0)$ in the transition points $\{r_{\gamma\beta}\}$. We now will do this.

In the present PCH model two channels couple only in a point, so that the N-channel system has $n =: N(N-1)/2$ transition points $\{r_{12}, r_{13}, \ldots, r_{N,N-1}\}$ which can be ordered increasingly and named $\{r_1, r_2, \ldots, r_n\}$, so that $r_1 \leqq r_2 \leqq \ldots \leqq r_n$. Associated with the change $r_{\gamma\beta} \to r_j$ we introduce also the following notation: $\tilde{\mathbf{\Omega}}_{\gamma\beta} \to \tilde{\mathbf{\Omega}}_j$, $\mathbf{P}_{\gamma\beta} \to \mathbf{P}_j$, etc.

In this way (25) can be rewritten as

$$\mathbf{W}_{12}(r, 0) = \mathbf{B}_1(r, 0) + \sum_{j=1}^N \tilde{\mathbf{\Omega}}_j(r)\, \mathbf{W}_{12}(r_j, 0)$$
$$\cdot\, \mathbf{B}_1(r, r_j)\, \theta(r - r_j) \tag{26}$$

and, according to the definition (20a) of the step function, we obtain from this relation and (24) the equations

$$\mathbf{W}_{12}(r_1, 0) = \mathbf{B}_1(r_1, 0)\,, \tag{27}$$

$$\mathbf{W}_{12}(r_{i+1}, 0) = \mathbf{W}_{12}(r_i, 0) + \left(\mathbf{1} + \sum_{j=1}^{N} \tilde{\mathbf{\Omega}}_j \mathbf{W}_{12}(r_j, 0)\right) \cdot \mathbf{B}_1(r_{i+1}, r_i)\,, \tag{28}$$

which allow us to propagate the matrix $\mathbf{W}_{12}(r, 0)$ on the mesh of points $\{r_1, r_2, \ldots, r_n\}$.

In what follows we shall be interested in obtaining the matrices $\mathbf{W}_{22}(\infty, 0)$ and $\mathbf{M}$ required for the calculation of the **S**-matrix via (14). Returning to (21) we see that

$$\mathbf{W}_{22}(r_1, 0) = \mathbf{1}\,, \tag{29}$$

$$\mathbf{W}_{22}(r_{i+1}, 0) = \mathbf{1} + \sum_{j=1}^{i} \tilde{\mathbf{\Omega}}_j \mathbf{W}_{12}(r_j, 0)\,, \tag{30}$$

$$\mathbf{W}_{22}(\infty, 0) \quad = \mathbf{1} + \sum_{j=1}^{n} \tilde{\mathbf{\Omega}}_j \mathbf{W}_{12}(r_j, 0)\,. \tag{31}$$

The matrix $\mathbf{M}$ is also computed by setting (17) and (3) into (15), which with suitable change of notation yields

$$\mathbf{M} = \mathbf{1} + \mathbf{s} \sum_{j=1}^{n} \mathbf{\Omega}_j \mathbf{W}_{12}(r_j, 0) \tag{32}$$

where, in analogy with (22), we introduce an $N \times N$ matrix $\mathbf{\Omega}_{\gamma\beta} \to \mathbf{\Omega}_j$ defined by

$$\mathbf{\Omega}_j =: \mathbf{\Phi}^*(r_j)\, U_j \mathbf{P}_j \mathbf{\Phi}(r_j)\,, \tag{33}$$

whose elements are all zero safe the element $(\gamma\beta)$, which is

$$\omega_{\gamma\beta} =: \Phi_\gamma^{-*}(r_{\gamma\beta})\, U_{\gamma\beta} \Phi_\beta^-(r_{\gamma\beta}) \tag{34a}$$

$$= a_{\gamma\beta} \exp[i(\Delta_\gamma(r_{\gamma\beta}) - \Delta_\beta(r_{\gamma\beta})]\,, \tag{34b}$$

and the element $(\beta\gamma)$, which takes the value $(\omega_{\gamma\beta})^*$.

At this stage we have all information required to calculate the **S**-matrix, all equations being exact within the PCH model. The utility of these equations (see (27) and (28) can be increased in practice by an analytical evaluation of the integrals involved in the definition of the diagonal matrix $\mathbf{B}_1(r, r_0)$, which according to (24) and (11) is given by

$$\mathbf{B}_1(r, r_0) = [b_\beta(r, r_0)\, \delta_{\gamma\beta}]\,, \tag{35}$$

where

$$b_\beta(r, r_0) =: \int_{r_0}^{r} \mathrm{d}r' [\Phi_\beta^-(r')]^{-2} \tag{36a}$$

$$= |\, b_\beta(r, r_0)\,| \exp[i(\Delta_\beta(r) + \Delta_\beta(r_0))] \tag{36b}$$

with

$$k_\beta |\, b_\beta(r, r_0)\,| = |\sin(\Delta_\beta(r) - \Delta_\beta(r_0))\,|\,. \tag{36c}$$

In the appendix we will show that (36b) is valid for a real potential $U_{\beta\beta}(r)$. At this point let us also remind (9), which establishes that at the origin $\Delta_\beta(0) = -\eta_\beta$.

Since the potential matrix of the PCH model is real and symmetric, and the model has been solved exactly, the **S**-matrix is unitary and symmetric (e.g. Child [34], Section 6.2) and the following relations are valid:

$$\mathbf{S}^+\mathbf{S} = \mathbf{S}\mathbf{S}^+ = \mathbf{1}\,, \quad \hat{\mathbf{S}} = \mathbf{S}\,, \tag{37}$$

where $\hat{\mathbf{S}}$ and $\mathbf{S}^+$ are the transpose and the hermitian conjugate of **S**, respectively.

4. Two-Channel Problem

For the purpose of an illustration of the general theory, we discuss in the present section the two-channel problem. In this case the coupling between channels 1 and 2 takes place at only one point, called r_{12} or simply r_1, and the basic matrices involved in the calculations are:

$$\mathbf{K} = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix}, \quad \mathbf{\Phi}(r) = \begin{bmatrix} \Phi_1^-(k_1, l; r) & 0 \\ 0 & \Phi_2^-(k_2, l; r) \end{bmatrix},$$

$$\mathbf{s} = \begin{bmatrix} s_1 & 0 \\ 0 & s_2 \end{bmatrix}, \quad \mathbf{P}_{12} = \mathbf{P}_1 =: \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

$$\tilde{\mathbf{\Omega}}_{12} =: \tilde{\mathbf{\Omega}}_1 = \begin{bmatrix} 0 & \tilde{\omega}_{12} \\ \tilde{\omega}_{12} & 0 \end{bmatrix}, \quad \mathbf{\Omega}_{12} =: \mathbf{\Omega}_1 = \begin{bmatrix} 0 & \omega_{12} \\ \omega_{12}^* & 0 \end{bmatrix},$$

where $\tilde{\omega}_{12}$ and ω_{12} are given by (23) and (34), respectively. On the other hand, (27), (31) and (32) lead to

$$\mathbf{W}_{12}(r_1, 0) = \begin{bmatrix} b_1(r_1, 0) & 0 \\ 0 & b_2(r_1, 0) \end{bmatrix},$$

$$\mathbf{W}_{22}(\infty, 0) = \mathbf{1} + \tilde{\mathbf{\Omega}}_1 \mathbf{W}_{12}(r_1, 0) = \begin{bmatrix} 1 & \tilde{\omega}_{12} b_2(r_1, 0) \\ \tilde{\omega}_{12} b_1(r_1, 0) & 1 \end{bmatrix},$$

$$\mathbf{M} = \mathbf{1} + \mathbf{s}\,\boldsymbol{\Omega}_1\,\mathbf{W}_{12}(r_1, 0)$$
$$= \begin{bmatrix} 1 & s_1\omega_{12}b_2(r_1,0) \\ s_2\omega_{12}^* b_1(r_1,0) & 1 \end{bmatrix},$$

and we note that the determinant of $\mathbf{M}$ is

$$M_+ =: \det(\mathbf{M})$$
$$= 1 - s_1 s_2 |\omega_{12}|^2 b_1(r_1,0)\, b_2(r_1,0). \quad (38)$$

Finally, we evaluate the **S**-matrix via (14) and find

$$\mathbf{S} = \frac{1}{M_+}\begin{bmatrix} (1-\tilde{\omega}_{12}\omega_{12}^* b_1 b_2 s_2)\, s_1 & \\ (k_1/k_2)^{1/2}(\tilde{\omega}_{12} - \omega_{12}^* s_2)\, b_1 s_1 & \\ & \cdot (k_2/k_1)^{1/2}(\tilde{\omega}_{12} - \omega_{12} s_1)\, b_2 s_2 \\ & (1-\tilde{\omega}_{12}\omega_{12} b_1 b_2 s_1)\, s_2 \end{bmatrix}. \quad (39)$$

Here and in the following we use the abbreviations $b_\beta =: b_\beta(r_1, 0)$, $\Delta_\beta =: \Delta_\beta(r_1)$.

The **S**-matrix can be expressed most conveniently by using (23 b), (34 b) and (36). In particular, we calculate the determinant M_+ defined by (38) and introduce also a new quantity M_- so that:

$$M_\pm =: 1 - M_0 \exp[i((\Delta_2 + \eta_2) \pm (\Delta_1 + \eta_1))] \quad (40\,a)$$
$$= |M_\pm| \exp(-i\lambda_\pm), \quad (40\,b)$$

where

$$M_0 =: ((a_{12})^2/k_1 k_2) \cdot |\sin(\Delta_1 + \eta_1)\sin(\Delta_2 + \eta_2)|, \quad (40\,c)$$
$$|M_\pm| = \{1 + M_0^2 - 2M_0\cos((\Delta_2 + \eta_2) \pm (\Delta_1 + \eta_1))\}^{1/2}, \quad (40\,d)$$
$$\mathrm{tg}(\lambda_\pm) = M_0 \sin((\Delta_2 + \eta_2) \pm (\Delta_1 + \eta_1))/ \cdot \{1 - M_0\cos((\Delta_2 + \eta_2) \pm (\Delta_1 + \eta_1))\}. \quad (40\,e)$$

In this way we rewrite the elements of the **S**-matrix, (39), as

$$S_{11} = (M_-/M_+)\exp(2i\eta_1) = (M_-/M_+) \cdot \exp[i(2\eta_1 + \lambda_+ - \lambda_-)],$$
$$S_{22} = (M^*/M_+)\exp(2i\eta_2) = (|M_-|/|M_+|) \cdot \exp[i(2\eta_2 + \lambda_+ + \lambda_-)],$$
$$S_{12} = -iQ\exp[i(\eta_1 + \eta_2 + \lambda_+)],$$
$$S_{12} = S_{21},$$

where we have defined

$$Q =: (k_1 k_2)^{-1/2}(2a_{12}/|M_+|) \cdot |\sin(\Delta_1 + \eta_1)\sin(\Delta_2 + \eta_2)|. \quad (41)$$

Finally, noting the identity

$$1 - (|M_-|/|M_+|)^2 = Q^2,$$

the elements of the **S**-matrix can be written symmetrically:

$$S_{11} = (1-Q^2)^{1/2}\exp[i(2\eta_1 + \lambda_+ - \lambda_-)], \quad (42\,a)$$
$$S_{22} = (1-Q^2)^{1/2}\exp[i(2\eta_2 + \lambda_+ + \lambda_-)], \quad (42\,b)$$
$$S_{12} = S_{21} = -iQ\exp[i(\eta_1 + \eta_2 + \lambda_+)], \quad (42\,c)$$

in concordance with (37).

5. Semiclassical approximation

Let us begin this section by remarking that the formulae for the **S**-matrix derived in the last two sections are exact for the PCH model, and that a practical application of the procedure requires to solve the Schrödinger equation (5) for each channel ($\beta = 1, 2, \ldots, N$). In real situations the diagonal potentials are complicated functions of the independent variable r and, therefore, such equations can not be solved exactly. At the present time, however, there is a very fully developed semiclassical theory of purely elastic scattering, which allows us to obtain analytical approximations for the wavefunctions $\Phi_\beta^-(k_\beta, l; r)$. By using this approximations in the theory developed in the present paper we will have an N-channel semiclassical model to describe inelastic collisions in systems such as atom-atom or ion-atom, where the masses and energies usually involved justify the use of semiclassical approximations. This not only reduces computation time, but also can give valuable physical insight into the phenomenon under study.

Surveys of semiclassical methods for obtaining approximate solutions of the Schrödinger equation (5) are given by Berry and Mount [33], Child [34, 35], Connor [36]. The attention has been directed not only to the WKB method but also to the so-called uniform semiclassical approximation, which began with the work of Miller and Good [37]. Since the simple WKB wavefunction "blows up" in the region around the semiclassical turning point, in the present paper we will use for each channel (see (5)) the uniform WKB wavefunction, which is valid both close to and far from the classical turning point.

Let us consider the Schrödinger equation (5) for a given channel (say, β), define a "local wavenumber" by

$$K_\beta(k_\beta, l; r) =: [k_\beta^2 - U_{\beta\beta}(r) - l + \tfrac{1}{2})^2/r^2]^{1/2} \quad (43)$$

and denote the classical turning point by R_β; it satisfies $K_\beta(k_\beta, l; R_\beta) = 0$. The uniform approximation to (5) involves a variable transformation $r \rightleftharpoons Z_\beta(r)$ defined by (e.g. Child (35))

$$Z_\beta(r) = q\,|\,(3/2)\int_{R_\beta}^{r} \mathrm{d}r'\,K_\beta(r')\,|^{2/3} \quad (44)$$

with

$$q =: \begin{cases} +1 \text{ in the classical region } (r > R_\beta,\ K_\beta^2 > 0)\,, \\ -1 \text{ in the nonclassical region } (r < R_\beta,\ K_\beta^2 < 0)\,, \end{cases}$$

and leads to a phaseshift given by

$$\eta_\beta = \lim_{r\to\infty} \{(2/3)\,Z_\beta(r)^{3/2} - k_\beta r\} + (l + \tfrac{1}{2})\,\tfrac{1}{2}\,\pi\,. \quad (45)$$

It can also be verified that the uniform approximation to the incoming Jost solution of (5) takes the form

$$\Phi_\beta^-(r) = H_\beta(r)\,[\mathrm{Bi}\,(-Z_\beta(r)) - i\,\mathrm{Ai}\,(-Z_\beta(r))]\exp(i\,\eta_\beta) \quad (46)$$

with

$$H_\beta(r) =: (\pi k_\beta)^{1/2}[Z_\beta(r)/K_\beta(r)^2]^{1/4}\,, \quad (47)$$

where $\mathrm{Ai}\,(-Z)$ and $\mathrm{Bi}\,(-Z)$ are the usual pair of linearly solutions of the Airy equation (Abramowitz and Stegun [38]).

To use the uniform expression for $\Phi_\beta^-(r)$ in the formulas obtained in Sects. 3 and 4 of the present paper, we need expressions for the amplitude (modulus) and phase of the incoming Jost solution

$$|\,\Phi_\beta^-(r)\,| = |\,H_\beta(r)\,|\,\{[\mathrm{Ai}\,(-Z_\beta(r))]^2 + [\mathrm{Bi}\,(-Z_\beta(r))]^2\}^{1/2}\,, \quad (48\,a)$$

$$\Delta_\beta(r) = -\eta_\beta + \arctan[\mathrm{Ai}\,(-Z_\beta(r))/\mathrm{Bi}\,(-Z_\beta(r))]\,. \quad (48\,b)$$

Here, $\arctan(x)$ is the usual inverse-tangent function with range between $-\pi/2$ and $\pi/2$.

By using the asymptotic forms (Abramowitz and Stegun [38])

$$\mathrm{Ai}\,(-Z) = \pi^{-1/2}Z^{-1/4}\sin((2/3)\,Z^{3/2} + \pi/4)\,, \quad (49\,a)$$

$$\mathrm{Bi}\,(-Z) = \pi^{-1/2}Z^{-1/4}\cos((2/3)\,Z^{3/2} + \pi/4)\,, \quad (49\,b)$$

valid when $Z \to \infty$, we can verify that at large r the modulus of $\Phi_\beta^-(r)$ goes to one and that the phase $\Delta_\beta(r)$ goes to $k_\beta r - \frac{1}{2}\,l\,\pi$, as required by (7).

At this point it is also worth noting that the equalities (9) and (36) employed in the last sections and derived in the appendix for the exact wavefunction, $\Phi_\beta^-(r)$, are also valid for the approximate uniform wavefunction (46). In fact: On one side, when $r < R_\beta$, Z_β is negative (classically inaccessible) and when $r \to 0$, $Z_\beta \to -\infty$. In this case the asymptotic forms are (Abramowitz and Stegun [38], Child [35])

$$\mathrm{Ai}\,(-Z) = (1/2)\,\pi^{-1/2}\,|\,Z\,|^{-1/4}\exp(-(2/3)\,|\,Z\,|^{3/2})\,, \quad (50\,a)$$

$$\mathrm{Bi}\,(-Z) = \pi^{-1/2}\,|\,Z\,|^{-1/4}\exp((2/3)\,|\,Z\,|^{3/2}) \quad (50\,b)$$

which together with (48 b) produce at the origin the relation (9) between the phase of the incoming Jost solution and the phaseshift. On the other side, from (48) and by using the relation

$$(\mathrm{d}/\mathrm{d}r)\,Z_\beta(r) = |\,K_\beta(r)\,|/(q\,Z_\beta(r))^{1/2} \quad (51)$$

derived from (44), we obtain the identity

$$(\mathrm{d}/\mathrm{d}r)\exp(2\,i\,\Delta_\beta(r)) = 2\,i\,k_\beta(\Phi_\beta^-(r))^{-2}\,, \quad (52)$$

which by direct integration leads to (36). In order to obtain the above relations we have used the fact that the Wronskian between $\mathrm{Ai}\,(x)$ and $\mathrm{Bi}\,(x)$ is equal to $1/\pi$, and for $r < R_\beta$ employed also the identities

$$K_\beta(r) = i\,|\,K_\beta(r)\,|\,,$$

$$\left|\int_{R_\beta}^{r} \mathrm{d}r'\,K_\beta(r')\right| = -\int_{R_\beta}^{r} \mathrm{d}r'\,|\,K_\beta(r')\,|\,.$$

6. A semiclassical two-channel example

It is the purpose of the present section to illustrate the theory of sections 4 and 5, for which we choose as example the $He^+ + Ne$ problem [39–42] at 70.9 eV. This system may be adequately described by a two-channel approximation. The energy, E, and the reduced mass of the system, μ, take the values $E = 70.9$ eV $= 2.606$ a.u, $\mu = 6099$ a.u.

For the diagonal elements of the effective potential matrix we adopt the model parameter values of Eu and Tsien [40],

$$U_{11}(r) = 2\mu\,(22.1/r)\exp(-r/0.678)\,, \quad (53)$$

$$U_{22}(r) = 2\mu\,((21.1/r - 12.1)\exp(-r/0.678) + \varepsilon_2)\,,$$

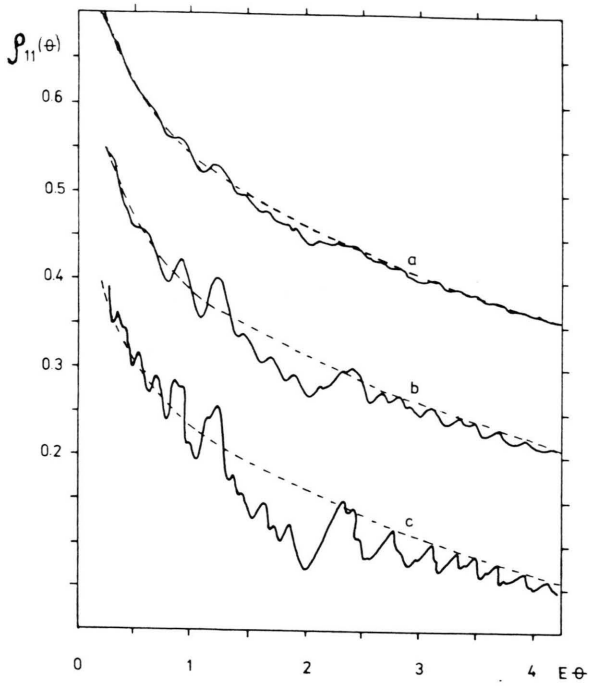

Fig. 1. 70.9 eV reduced elastic differential cross section $\varrho_{11}(\theta) = \theta(\sin\theta)\,\sigma_{11}(\theta)$ vs. $E\theta$, calculated by setting (in atomic units) $r_1 = 2.02$ and using for U_{12} the values 10.06 (curve a), 13.12 (curve b) and 15.24 (curve c). The indicated vertical scale corresponds to curve b; for the sake of comparison, curves a and c have been shifted by 1.5 and -1.5 units, respectively, $\varrho_{11}(\theta)$ is in units of $10^{-16}\,\mathrm{cm}^2$ and $E\theta$ in units of 10^3 eV-degrees. The dashed lines represent the pure elastic case.

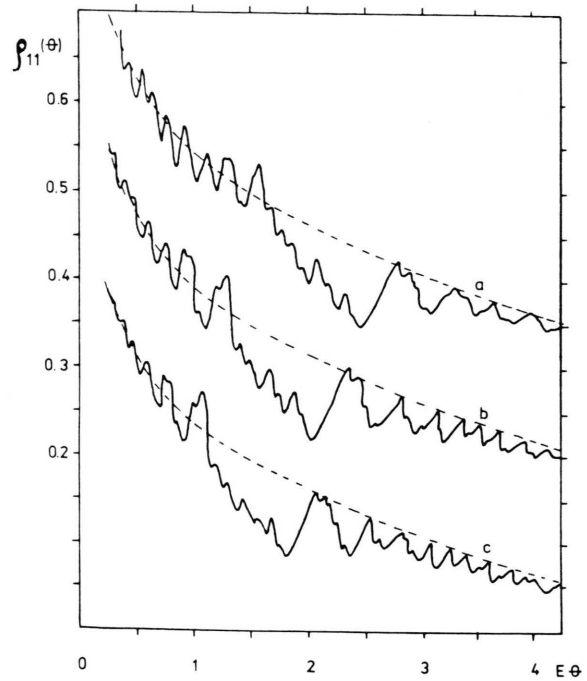

Fig. 2. 70.9 eV reduced elastic differential cross section $\varrho_{11}(\theta) = \theta(\sin\theta)\,\sigma_{11}(\theta)$ vs. $E\theta$, calculated by setting (in atomic units) $U_{12} = 15.24$ and using for r_1 the values 1.92 (curve a), 2.02 (curve b) and 2.12 (curve c). The scale, the units and the dashed lines are as in Figure 1.

where the potentials are written in atomic units and the threshold of channel 2 is $\varepsilon_2 = 16.8$ eV $= 0.6174$ a.u. As noted in previous sections, the coupling matrix element $U_{12}(r)$ is of the form $U_{12}(r) = U_{12}\,\delta(r - r_1)$ and involves two arbitrary parameters (r_1 and U_{12}) to be chosen suitably.

In order to investigate the effect of the parameters r_1 and U_{12} on the cross sections and related quantities, we have systematically scanned and tried various sets of parameters. We report the calculations obtained by keeping fixed either r_1 or U_{12} and changing the other parameter, within the following set of values in atomic units

$$r_1 = 1.92,\ 2.02,\ 2.19\,, \quad U_{12} = 10.06,\ 13.12,\ 15.24\,.$$

For the calculations and the discussion we take as "reference parameters" the values $r_1 = 2.02$ a.u. and $U_{12} = 13.12$ a.u. The first one represents the point where the intersection of the diabatic curves $U_{11}(r)$ y $U_{22}(r)$ takes place; the choice of this value is, therefore, in the spirit of the LZS model. The chosen reference value of U_{12} reproduces approximately the $He^+ + Ne$ inelastic total cross section (0.729 a.u.) obtained by Olson and Smith [39] by using a distorted-wave-Born approximation. With these reference parameters we obtain for Q_{21} the value 0.73 a.u.

Figures 1 and 2 show with solid lines the quantity $\varrho_{11}(\theta) = \theta(\sin\theta)\,\sigma_{11}(\theta)$ calculated for several values of r_1 and U_{12} (curves a, b and c), $\sigma_{11}(\theta)$ being the elastic differential cross section. The vertical scale of these figures corresponds to curve b; for a better comparison the curves a and c have been shifted by 1.5 and -1.5 atomic units, respectively. The curves a, b and c include also dashed lines representing $\tilde{\varrho}_{11}(\theta) = \theta(\sin\theta)\,\tilde{\sigma}_{11}(\theta)$, $\tilde{\sigma}_{11}(\theta)$ being the elastic differential cross section in *absence* of coupling between channels (the so-called pure elastic case).

Figures 1 and 2 clearly demonstrate that the coupling between channels produces in $\varrho_{11}(\theta)$ an oscillatory structure with respect to the pure elastic

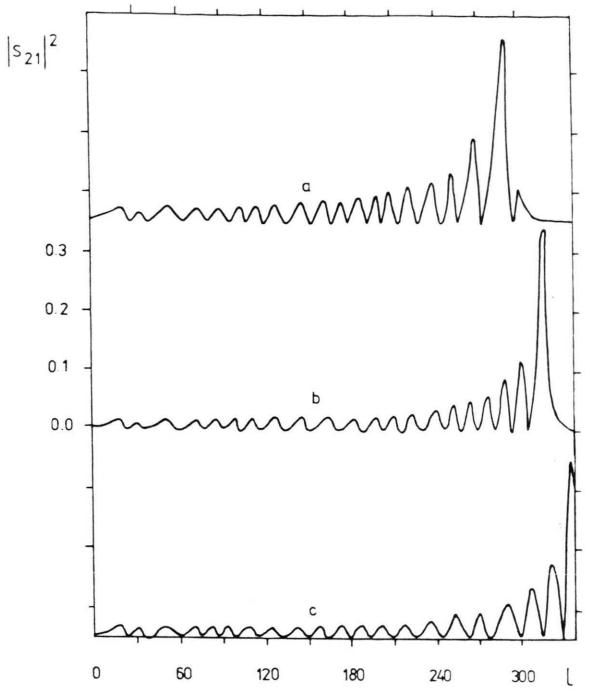

Fig. 3. Transition probabilities $|s_{21}|^2$ at 70.9 eV, calculated by setting (in atomic units) $U_{12} = 13.12$ and using for r_1 the values 1.92 (curve a), 2.02 (curve b) and 2.12 (curve c). The indicated vertical scale corresponds to curve b; for the sake of comparison, curves a and c have been shifted by 3.5 and -3.5 units, respectively.

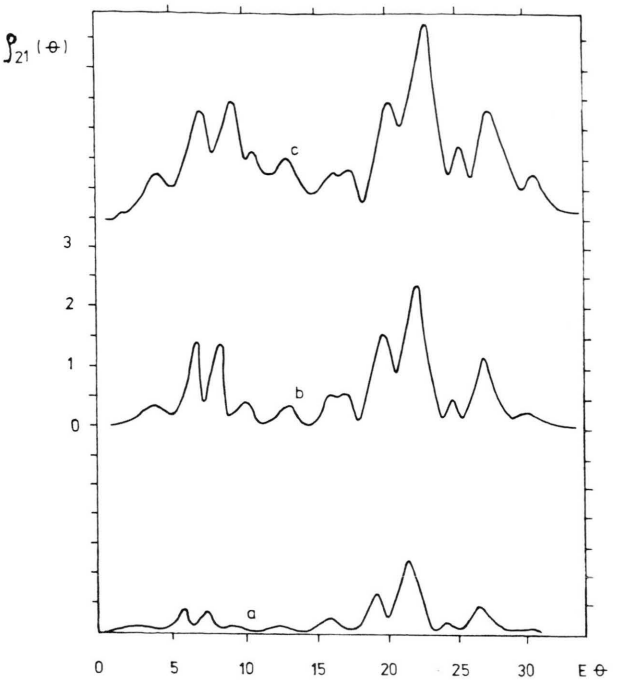

Fig. 4. 70.9 eV reduced inelastic differential cross section $\varrho_{21}(\theta) = \theta(\sin\theta)\,\sigma_{21}(\theta)$ vs. $E\theta$, calculated by setting (in atomic units) $r_1 = 1.92$ and using for U_{12} the values 10.06 (curve a), 13.12 (curve b) and 15.24 (curve c). The indicated vertical scale corresponds to curve b; curves c and a have been shifted by 3.5 and -3.5 units, respectively. $\varrho_{21}(\theta)$ is in units of 10^{-18} cm^2 and $E\theta$ in units of 10^2 eV-degrees.

case. The amplitude of the oscillations is determined essentially by the intensity of the coupling U_{12} (see Fig. 1), while the parameter r_1 generates a shift in the position of the oscillatory structure: when r_1 is increased, the position of the minima of $\varrho_{11}(\theta)$ is shifted to smaller scattering angles (see Figure 2).

In Fig. 3 are plotted the transition probability $|S_{21}|^2$ versus the angular momentum l, for fixed U_{12} and several values of r_1 (curves a, b and c). The vertical scale for this figure corresponds to curve b; the curves a and c have been shifted by 3.5 and -3.5 units, respectively. The probability $|S_{21}|^2$ has an oscillatory behaviour and reaches a maximum at a large value of l (say, l_{max}). We see that l_{max} increases when the parameter r_1 becomes greater and, therefore, by increasing r_1 the small-angle elastic differential cross section is affected, as noted previously. We note also that for $l > l_{max}$, the probability function becomes very small and, therefore, partial waves greater l_{max} do not change the inelastic cross sections significantly. At this point we remark also that the value of U_{12} affects the amplitude of the oscillations of $|S_{21}|^2$ versus l, which rebounds into the structure of the differential elastic and inelastic cross sections.

To end this section we plot in Figs. 4 and 5 the quantity $\varrho_{21}(\theta) = \theta(\sin\theta)\,\sigma_{21}(\theta)$ calculated for several values of r_1 and U_{12} (curves a, b and c), $\sigma_{21}(\theta)$ being the differential inelastic cross section. The indicated vertical scale of these figures corresponds to curve b; for sake of comparison the curves a and c have been shifted by 3.5 and -3.5 atomic units, respectively. From Fig. 4, in which r_1 is fixed, we conclude that the peak positions of $\varrho_{21}(\theta)$ remain unmodified by changing U_{12}; however, the value of this parameter determines essentially the amplitude of the peaks. On the other hand, from Fig. 5, where U_{12} is fixed, we conclude that a change of r_1 generates a new oscillatory structure of $\varrho_{21}(\theta)$: the number of peaks, their position and amplitudes are changed significantly.

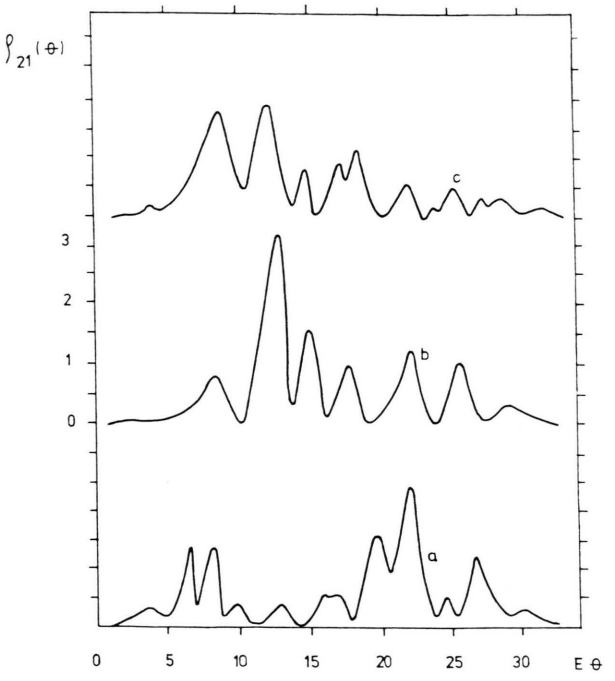

Fig. 5. Reduced inelastic differential cross sections corresponding to the transition probabilities of Figure 3. The vertical scale and the units are as in Figure 4.

A qualitative comparison with the results obtained by other methods (compare e.g. Fig. 5 of Olson and Smith [39] with Fig. 1 of the present work) indicates that with a suitable choice of parameters the features of the cross sections are well reproduced by the simple PCH model.

7. Concluding Remarks

We have presented a full multichannel quantum-mechanical model to treat inelastic collisions, which from the physical point of view follows the spirit of the LZS and the SHT models.

The present PCH model is, however, free from some difficulties and restrictions of the LZS-method [21]:

a) The shapes for the diagonal potentials $U_{\beta\beta}(r)$ can be chosen freely, contrary to the LZS method which uses a linear model (see (4)).
b) The parameters $r_{\gamma\beta}$ and $U_{\gamma\beta}$ can be chosen arbitrarily, e.g. by comparison of the theoretical cross sections and the experimental cross sections, while the applicability of the LZS-theory is restricted to the weak coupling regime and the fulfillment of restrictions about the distance between the crossing point and the classical turning points [8, 21].
c) The theory developed in the present paper is valid for N channels, contrary to the LZS formula whose derivation requires the use of a two-state model and cannot be easily extended to multichannel problems.
d) An encouraging property of the PCH model is the symmetry and unitarity of the **S**-matrix.

Contrary to the LZS method, a difficulty of the PCH model is the fact that at present we have no direct way to determine the parameters $r_{\gamma\beta}$ and $U_{\gamma\beta}$ for a given system. However, the advantage of being able to choose them freely is that they can be used as fitting parameters to reproduce approximately the elastic and inelastic data. The fitting procedure is not strange in physics: e.g. the potentials (53) and the coupling element $U_{12(r)} = 2\mu a_4 \exp(-r/0.667)$ for the $He^+ + Ne$ problem were determined by Olson and Smith [39] and Eu and Tsien [40] by using a fitting procedure; Crothers [42] have also studied the transition probabilities $|S_{21}|^2$ as a function of the parameter a_4 previously mentioned.

Appendix

Starting from the definition (36 a) of the integral $b_\beta(r, r_0)$ we want first to prove the relations (36 b, c). As in an earlier work [32], we begin by introducing for the channel β the regular solution $\Phi^{\times}_{\beta}(k_\beta, l; r)$ and the Jost solutions, $\Phi^{\pm}_{\beta}(k_\beta, l; r)$, of the Schrödinger equation (5). Next we define the auxiliar function

$$\Gamma_\beta(r) =: \Phi^{-}_{\beta}(r)\, b_\beta(r, 0)\,, \tag{A.1}$$

and by direct differentiation, using (36 a) and (5), we find that $\Gamma_\beta(r)$ satisfies the differential equation

$$(\mathrm{d}^2/\mathrm{d}r^2 + k^2_\beta - U_{\beta\beta}(r) - l(l+1)/r^2)\,\Gamma_\beta(r) = 0\,. \tag{A.2}$$

From this equation and the fact that

$$\lim_{r \to 0} \Gamma_\beta(r) = 0\,, \tag{A.3}$$

as can be seen from (A.1) and (36 a), we conclude that $\Gamma_\beta(r)$ is the regular solution of (5), that is

$$\Gamma_\beta(r) = C_\beta \Phi^{\times}_{\beta}(r)\,, \tag{A.4}$$

where C_β is a constant, independent of r, to be determined by the boundary conditions.

Let us now assume that $U_{\beta\beta}(r)$ is real and remind the well-known relations (e.g. Taylor [42])

$$\Phi_\beta^{\times}(r) = \tfrac{1}{2} i[F_\beta \Phi_\beta^-(r) - F_\beta{}^* \Phi_\beta^+(r)], \quad (A.5)$$

$$\Phi_\beta^+(r) = (\Phi_\beta^-(r))^*, \quad (A.6)$$

where $F_\beta(k_\beta, l)$ is the Jost function given by

$$F_\beta = |F_\beta| \exp(-i\eta_\beta), \quad (A.7)$$

which is related to the scattering matrix element s_β by

$$s_\beta = F_\beta^*/F_\beta = \exp(2i\eta_\beta). \quad (A.8)$$

By combining the above equations with (A.4) and (8) we obtain from (A.1) the relation

$$b_\beta(r, 0) = \tfrac{1}{2} i C_\beta F_\beta^* [\exp(-2i\eta_\beta) - \exp(2i\Delta_\beta(r))], \quad (A.9)$$

which still involves the unknown parameter C_β.

To determine C_β we consider two arbitrary points, r_1 and r_2, large enough, that is such that they are lieing in the asymptotic region where the phase $\Delta_\beta(r)$ is given by (see (7))

$$\Delta_\beta(r) = k_\beta r - \tfrac{1}{2} l\pi, \quad r \to \infty. \quad (A.10)$$

Next we evaluate the quantities

$$b_\beta(r_2, 0) - b_\beta(r_1, 0) = \int_{r_1}^{r_2} (\Phi_\beta^-(r))^{-2} \mathrm{d}r,$$

the term on the left hand side by employing (A.9) and (A.10); the other one by direct integration and using (7). In this way we obtain $C_\beta F_\beta^* = 1/k_\beta$.

Finally, by noting that $\lim_{r \to 0} b_\beta(r, 0) = 0$, (9) is obtained from (A.9). On the other side, by using the identity $b_\beta(r, r_0) = b_\beta(r, 0) - b_\beta(r_0, 0)$ we deduce (36) from (A.9).

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