QUASI-CLASSICAL APPROXIMATION FOR MULTI-CHANNEL SCATTERING

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We suggest a quasi-classical method to determine the multi-channel S-matrix for an arbitrary number of channels considered. We discuss the role of turning points in multi-channel scattering and methods to take them into account when constructing the S-matrix. We find an analytical expression for the S-matrix by using phase integrals for the case of binary "pseudo-intersections" of electron levels, which is suitable for actual calculations.

INTRODUCTION

THE quasi-classical method for solving the one-dimensional scalar Schrödinger equation

$$\alpha^2\Psi''(x) + p^2(x)\Psi(x) = 0, \quad \alpha \ll 1 \tag{1}$$

($x = r/r_0$ is the dimensionless length, $p(x) = [1 - V(x)/E]^{1/2}$ the classical momentum, $\lambda\!\!\!^{-} = \hbar/\sqrt{(2mE)}$ the de Broglie wavelength, $\alpha = \lambda\!\!\!^{-}/r_0$ the quasi-classical parameter, r_0 the range of the potential $V(r)$) is rather well developed and reduces to a series of well-known manipulations with two WKB solutions (see, e.g.,[1]):

$$\Psi_\pm(x) = \frac{1}{\sqrt{p(x)}}\exp\left(\pm\frac{i}{\alpha}\int^x p(x)\,dx\right). \tag{2}$$

In a number of physical problems in quantum mechanics (multi-channel scattering), hydrodynamics, physical kinetics, the theory of the propagation of waves in various media, and so on, it is necessary to generalize the method to apply to a set of differential equations of the same kind as (1). In particular, for multi-channel scattering which we shall study the initial set has the form[1)]

$$\alpha^2\Psi''(x) + P(x)\Psi(x) = 0, \quad \alpha \ll 1, \quad 0 \leqslant x < \infty, \tag{3}$$

where

$$P(x) = 1 - \frac{\mathscr{E}}{E} - \frac{\mu^2}{x^2} - \frac{U(x)}{E}, \qquad \mu = \alpha\left(l + \frac{1}{2}\right),$$

$\mathscr{E} = \{\mathscr{E}_1, \ldots, \mathscr{E}_n\}$ is the diagonal threshold matrix, $U(x)$ the symmetric n-th order perturbation matrix which is real on the real axis and analytical in a sufficiently wide region of the complex x-plane adjoining the real axis. $\psi(x)$ is a vector function of dimension n which must be regular at zero and as $x \to \infty$ must asymptotically have the form

$$\Psi(x) \sim k^{-1/2}\exp\left[-\frac{i}{\alpha}\left(kx - \frac{\mu\pi}{2} + \frac{\pi\alpha}{4}\right)\right]\mathbf{d} - k^{-1/2}\exp\left[+\frac{i}{\alpha}\left(kx - \frac{\mu\pi}{2} + \frac{\pi\alpha}{4}\right)\right]\mathbf{D}, \tag{4}$$

where $k = P^{1/2}(\infty) = \{(1 - \mathscr{E}_1/E)^{1/2}, \ldots, (1 - \mathscr{E}_n/E)^{1/2}\}$ is the diagonal channel momentum matrix, d and D are constant vectors connected by the relation

$$\mathbf{D} = S\mathbf{d}, \tag{5}$$

and S is the scattering matrix defined in the quasi-classical case ($\alpha \ll 1$).

This problem has earlier been solved only for the special case of two states in a form which did not admit a generalization[2]; there are no analytical results at all in the physical literature for an arbitrary number of states.[2)]

We give in the present paper a strict analysis of the quasi-classical approach to find a solution of Eq. (3) as a function of the canonical structure of the $P(x)$ matrix and we find a general formula for the scattering matrix S, which shows the role of the turning points (TP) in multi-channel scattering and makes it possible to use a parametric method to determine it. We discuss the possibility to take TP into account to all orders in the parameter α and also develop a phase integral method to match the principal terms of the asymptotic form. We obtain an explicit analytical expression for the scattering matrix S in the case of binary intersections of electron terms which can be used for actual calculations.

1. FORM OF THE QUASI-CLASSICAL APPROACH TO EQ. (3) IN THE CASE OF SIMPLE EIGENVALUES OF THE P(x) MATRIX

We shall assume that $P(x)$ is a quadratic matrix of order n, analytical in the region considered and not having multiple eigenvalues in it. We look for a solution of (3) in the form of a formal expansion

$$\Psi(x) = \exp\left(\frac{i}{\alpha}\int^x s(x)\,dx\right)\sum_{l=0}^{\infty}\mathbf{y}^{(l)}(x)\,\alpha^l \tag{6}$$

Substituting (6) into (3) and equating terms with the same power of α we get a set of equations to determine the scalar function $s(x)$ and the vectors $\mathbf{y}^{(l)}(x)$:

$$P\mathbf{y}^{(l)} - \lambda\mathbf{y}^{(l)} = \mathbf{L}^{(l)}; \tag{7}$$

$$\mathbf{L}^{(l)}(x) = i(1 - \delta_{l0})\left[-s'\mathbf{y}^{(l-1)} - 2s\mathbf{y}^{(l-1)\prime} + i\mathbf{y}^{(l-2)\prime\prime}(1 - \delta_{l0} - \delta_{l1})\right], \tag{8}$$

$\lambda(x) = s^2(x)$, δ_{lm} is the Kronecker symbol.

Equations (7) allow us to solve successively all unknown functions. Indeed, we find for $l = 0$ that the

[1)]The set of partial wave equations in the total angular momentum representation.

[2)]The quasi-classical approach was used in [3,4] as an auxiliary tool to perform numerical calculations.

$\lambda_m (m = 1, 2, \ldots, n)$ are the eigenvalues and the $y_m^{(0)}$ the corresponding eigenvectors of the P matrix. We find the remaining terms for the solutions $\psi_{m\pm}$ from the set of equations

$$P y_{m\pm}^{(l)} - \lambda_m y_{m\pm}^{(l)} = \mathbf{L}_{m\pm}^{(l)}, \qquad l \geqslant 1. \tag{9}$$

The condition that this set can be solved can, as is well known[5], be stated in the form

$$(y_m^{(0)} \mathbf{L}_{m\pm}^{(l)}) = 0, \qquad l = 1, 2 \ldots, \tag{10}$$

and the solution has the form

$$y_{m\pm}^{(l)} = \sum_{j=1}^{n} \frac{(y_j^{(0)} \mathbf{L}_{m\pm}^{(l)})}{\lambda_j - \lambda_m} y_j^{(0)}, \qquad m = 1, 2, \ldots, n, \tag{11}$$

where the ± signs correspond to two values of the function $s(x) = \pm\sqrt{\lambda(x)}$. One can show[6] that the series (6) constructed in this way is an asymptotic expansion for the exact solutions $\psi_\pm(x)$ which is valid in regions which do not contain TP, as is immediately clear from (11). One sees easily from (8), (9), (11) that on the real axis $\psi_{m+} = \psi_{m-}^*$ as in the case of the one-dimensional equation.[7] It is well known that the eigenvectors $y_m^{(0)}$ are determined unambiguously, apart from an arbitrary function f_m. One can remove this arbitrarity by imposing the condition

$$\Psi_{m\pm} \xrightarrow[x\to\infty]{} (\lambda_m)^{-1/4} \exp\left(\pm\frac{i}{\alpha}\int^x \sqrt{\lambda_m}\, dx\right) \mathbf{e}_m, \tag{12}$$

where the vector column $\mathbf{e}_m$ has only one non-vanishing m-th component. The form (12) corresponds to the usual WKB approximation for channels between which there are no transitions.

For the sake of simplicity we shall in what follows be interested only in the principal terms of the expansion (6) and write then the general solution of Eq. (3) in the form

$$\Psi(x) = \sum_{m=1}^{n} y_m^{(0)} \left[a_{m-} (\lambda_m)^{-1/4} \exp\left(-\frac{i}{\alpha}\int^x \sqrt{\lambda_m}\, dx\right) - a_{m+} (\lambda_m)^{-1/4} \exp\left(+\frac{i}{\alpha}\int^x \sqrt{\lambda_m}\, dx\right)\right], \tag{13}$$

where the $a_{m\pm}$ are arbitrary constants and the factor $\lambda_m^{-1/4}$ is split off from the vectors $y_m^{(0)}$. For instance, for two levels a simple calculation gives

$$y_{1,2}^{(0)} = 2^{-1/2} \exp\left(-\frac{1}{2}\int_0^q \frac{q\, dq}{1+q^2}\right) \begin{pmatrix} \pm\mathscr{E}_\pm \\ \mathscr{E}_\mp \end{pmatrix}, \quad \mathscr{E}_\pm = \exp\left(\pm\frac{1}{2}\int_0^q \frac{dq}{\sqrt{1+q^2}}\right) \tag{14}$$

$$q = \frac{P_{11} - P_{22}}{2P_{12}}, \qquad \lambda_{1,2} = \frac{P_{11} + P_{22}}{2} \pm \sqrt{\frac{(P_{11} - P_{22})^2}{4} + P_{12}^2}. \tag{15}$$

We introduce the quasi-classical scattering phase defined by the equation

$$\eta_m = \lim_{x\to\infty} \left(\frac{1}{\alpha}\int_{x_m}^{x} \sqrt{\lambda_m}\, dx - \frac{1}{\alpha}\int_{x_m^0}^{x} \sqrt{\lambda_m^0}\, dx\right), \tag{16}$$

where x_m is the classical turning point $(\lambda_m(x_m) = 0)$, $\lambda_m^0 = P_{mm} \mid U_{mm} = 0$, and also the diagonal phase matrix $\eta = \{\eta_1, \eta_2, \ldots, \eta_n\}$ and the vectors $\mathbf{a}_-$ and $\mathbf{a}_+$ with components a_{m-} and a_{m+}. We shall assume that $\mathbf{a}_+$ and $\mathbf{a}_-$ are connected with one another through a T-matrix

$$\mathbf{a}_+ = T\mathbf{a}_-. \tag{17}$$

We can then write the solution (13) as $x \to \infty$ in the form

$$\Psi \sim k^{-1/2} \exp\left(-\frac{i}{\alpha}\left(kx - \frac{\mu\pi}{2} + \frac{\pi\alpha}{4}\right)\right] e^{-i\eta} \mathbf{a}_- - k^{-1/2} \exp\left[+\frac{i}{\alpha}\left(kx - \frac{\mu\pi}{2} + \frac{\pi\alpha}{4}\right)\right] e^{+i\eta} \mathbf{a}_+. \tag{18}$$

Comparing this equation with (4) and (5) and using (17), we get for the scattering matrix S the following general expression

$$S = e^{i\eta} T e^{i\eta}. \tag{19}$$

Now $S^+S = 1$, provided $T^+T = 1$, i.e., the T matrix must be unitary.

When there is no intersection of the eigenvalues λ_m the expansion (13) is inapplicable only in the classical turning points; however, they can easily be taken into account (vide infra) and give $T = 1$ and $S = e^{2i\eta}$, i.e., we obtain a well-known expression which indicates the absence of inelastic transitions to all orders in α.

Another case when we assume η to be a scalar matrix and $S = e^{2i\eta}T$ corresponds to separating the elastic scattering from the inelastic and indicates a transition to the equations of the parametric method which determine the T matrix. In that case the differential cross-section for inelastic scattering $\sigma_{mj}(\theta)$ for the simplest case of spinless particles and a spherically symmetric interaction[3)] can be written in the form

$$\sigma_{mj}(\theta) = \sigma_0(\theta)\, |T_{mj}|^2,$$

$$\sigma_0(\theta) = \left|\frac{1}{2ik_1}\sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)\, e^{2i\eta_{l0}}\right|^2 \quad (k \sim k_1), \tag{20}$$

where $\sigma_0(\theta)$ is the quasi-classical cross-section for elastic scattering by an average potential $U_0(x)$ and the T matrix can be calculated for a well-defined impact parameter ρ corresponding to the angle θ.

2. PARAMETRIC METHOD

We establish the equation determining the T matrix for our case. To do this we rewrite (3) as follows

$$\alpha^2 \Psi''(x) + \varkappa^2(x) \Psi(x) = \frac{v(x)}{E} \Psi(x); \tag{21}$$

$$\varkappa^2(x) = 1 - \frac{\mu^2}{x^2} - \frac{U_0(x)}{E} - \frac{U_1(x)}{E}, \qquad v(x) = P(x) - \varkappa^2(x),$$

$$U_1(x) = \{\mathscr{E}_1 + U_{11}(x) - U_0(x), \ldots, \mathscr{E}_n + U_{nn}(x) - U_0(x)\}$$

where $U_0(x)$ is some average potential determining the elastic scattering. We shall look for a solution of (21) in the form

$$\Psi(x) = \Psi_-(x)\mathbf{a}_-(x) - \Psi_+(x)\mathbf{a}_+(x), \tag{22}$$

where

$$\Psi_\pm(x) = \varkappa^{-1/2} \exp\left(\pm\frac{i}{\alpha}\int^x \varkappa\, dx\right) \tag{23}$$

are two fundamental matrices of the homogeneous Eq. (21) and $\mathbf{a}_+(x)$ and $\mathbf{a}_-(x)$ are the required vectors. As $x \to \infty$ the expansion (22) is the same as (13) and thus the values $\mathbf{a}_+(\infty)$ and $\mathbf{a}_-(\infty)$ determine the required T matrix. One easily verifies that if we neglect small terms containing the factor $\alpha^2 \kappa^{-1/2}(\kappa^{-1/2})'' \ll 1$ and strongly oscillating terms containing factors such as

3) For particles with spin with an arbitrary interaction see [4].

$$\varkappa^{-1/2}\exp\left(\pm\frac{i}{\alpha}\int^x\varkappa\,dx\right)\frac{v}{E}\exp\left(\pm\frac{i}{\alpha}\int^x\varkappa\,dx\right)\varkappa^{-1/2},$$

we find for $\mathbf{a}_+(x)$

$$2i\frac{d\mathbf{a}_+(x)}{dx}=\varkappa^{-1/2}\exp\left(-\frac{i}{\alpha}\int^x\varkappa\,dx\right)\frac{v(x)}{E}\varkappa^{-1/2}\exp\left(+\frac{i}{\alpha}\int^x\varkappa\,dx\right)\mathbf{a}_+(x), \tag{24}$$

and the corresponding equation for $\mathbf{a}_-(x)$ is the complex conjugate of (24). Since $v(x)$ is Hermitean

$$|\mathbf{a}_\pm(x)|^2=\text{const} \tag{25}$$

and the $\mathbf{a}_\pm(x)$ can thus be normalized to unity; this corresponds to the law of conservation of particle flux.

When $\kappa^2(x)\gg U_1(x)/E$ we can write approximately

$$\varkappa(x)\approx\left(1-\frac{\mu^2}{x^2}-\frac{U_0(x)}{E}\right)^{1/2}-\frac{U_1(x)}{2E}\left(1-\frac{\mu^2}{x^2}-\frac{U_0(x)}{E}\right)^{-1/2}. \tag{26}$$

Changing to the variable r and also using the relations $\hbar^2 l^2\approx M^2$ (M is the classical angular momentum), and

$$\frac{dr(t)}{dt}=\pm\left[\frac{2}{m}\left(E-U_0-\frac{M^2}{m^2r^2}\right)\right]^{1/2},$$

we get

$$i\hbar\frac{d\mathbf{a}(t)}{dt}=\exp\left(\frac{i}{\hbar}\int^t U_1\,dt\right)v(t)\exp\left(-\frac{i}{\hbar}\int^t U_1\,dt\right)\mathbf{a}(t), \tag{27}$$
$$-\infty<t<+\infty,$$

where t is the classical time and one can combine the equations for $\mathbf{a}_-(x)$ and $\mathbf{a}_+(x)$ into one, and they correspond to the approach ($\mathbf{a}_-$) and departure ($\mathbf{a}_+$) of particles. Equation (27) is the time-dependent Schrödinger equation

$$i\hbar\frac{d\Phi}{dt}=[U_1(t)+v(t)]\Phi,\quad H(t)=U_1(t)+v(t), \tag{28}$$

written in the interaction representation while use has been made of the parametric method; the T matrix is then determined from the condition

$$\mathbf{a}(+\infty)=T\mathbf{a}(-\infty), \tag{29}$$

and the differential inelastic scattering cross-section is given by Eq. (20).

3. FORM OF THE QUASI-CLASSICAL EXPANSION FOR EQUATIONS SUCH AS (28) FOR THE CASE WHERE THE EIGENVALUES OF THE H(t) MATRIX COINCIDE

When analyzing the quasi-classical expansion in the case of coinciding eigenvalues of the matrix P it is convenient to start from an equation such as (28). We introduce instead of t a new dimensionless variable $\tau=\beta t$ where $\beta=1/t_0$ is a quantity which is the reciprocal of the characteristic time t_0 and we shall solve Eq. (28), rewritten in the form[4)]

$$\beta d\Phi(\tau)/d\tau=-iH(\tau)\Phi(\tau) \tag{30}$$

under adiabatic conditions ($\beta\ll 1$) which is equivalent to the quasi-classical situation for Eq. (3). The following results are based upon a number of mathematical theorems referring to the asymptotic splitting up of a set such as (30).[6] Therefore, omitting the proofs and restricting ourselves for the sake of simplicity to only the principal asymptotic expansions of the solution of Eq. (30) we give their form as a function of the behavior of the eigenvalues and elementary divisors of the matrix $H(\tau)$ in the complex τ-plane.

a) In the previously analyzed case of simple eigenvalues of the $H(\tau)$ matrix the general solution of Eq. (30) has the especially simple form

$$\Phi(\tau)=\sum_{j=1}^{n}C_j\exp\left(-\frac{i}{\beta}\int^\tau\lambda_j\,d\tau\right)\mathbf{y}_j(\tau), \tag{31}$$

where the $\lambda_j(\tau)$ are the roots of the equation $|H(\tau)-\lambda I|=0$, and the $\mathbf{y}_j(\tau)$ the columns of the matrix $Y(\tau)$ which diagonalizes $H(\tau)$:

$$Y^{-1}HY=\{\lambda_1,\lambda_2,\ldots,\lambda_n\}, \tag{32}$$

which are normalized by the condition

$$\mathbf{y}_j(\tau)\xrightarrow[|\tau|\to\infty]{}\mathbf{e}_j. \tag{33}$$

The expansion (31) is valid also in the case when there are in the region considered p different eigenvalues of the H matrix which in that region retain their multiplicities $n_1, n_2, \ldots, n_p$ ($\sum_{j=1}^{p} n_j=n$),[5)] and all elementary divisors of H are simple. The $\mathbf{y}_j(\tau)$ are then the columns of the matrix Y which diagonalizes $H(\tau)$ and each λ_j ($j=1,2,\ldots,p$) is counted as often as its multiplicity.

b) In the case of one simple elementary divisor of multiplicity n_j corresponding to one Jordan block of index j, $H(\tau)$ can be reduced to the form[9] [6)]

$$Y^{-1}HY=\{\lambda_1 I_1+H_1,\lambda_2 I_2+H_2,\ldots,\lambda_p I_p+H_p\}, \tag{34}$$

where $\lambda_j I_j+H_j$ is a Jordan block of index j and the main term in the expansion for $\Phi(\tau)$ has the form (31) where the $\mathbf{y}_j$ are the columns of the matrix Y of (34) and, very importantly, the further terms in the expansion of the j-th solution go in powers of the parameters β^{1/n_j} (or β^{1/n_j-1}).[6] To obtain a complete set of linearly independent solutions we must consider in (31) all columns of the matrix Y. We can write down the form of the expansion in the case of r_j ($1<r_j<n_j$) elementary divisors for each j; but we shall not discuss them.

c) From the point of view of physical applications, the most interesting and at the same time most difficult are the cases when in separate isolated points there may occur intersections of the eigenvalues λ_j of the matrix $H(\tau)$ or (when there are equal eigenvalues) a change in the multiplicity of the elementary divisors of the matrix $H(\tau)$. Commonly such points are called turning points (TP).[10] The main problem which occurs in different physical problems is then to connect the asymptotic expansions such as (13) and (31), which can not be applied in TP in order to obtain the quasi-classical representation of a well-defined solution along the whole of the real axis. General prescriptions for solving this problem in all orders of the quasi-classical expansions were discussed in[11] but more

4)One can easily generalize the theory to the case when $H(\tau,\beta)=\Sigma H_l(\tau)\beta^l$ (for instance, by using the dynamical perturbations when atoms collide).

5)Such a case is realized, for instance, in atomic collisions when doubly degenerate terms with non-vanishing angular momentum components along the intermolecular axis are split under the action of a dynamic perturbation (Λ-doubling). [8]

6)We are dealing with physical problems with a non-Hermitean matrix $H(\tau)$.

concrete results can be obtained only for well-defined sharply outlined problems.

4. PHASE INTEGRAL METHOD

The problem simplifies considerably when we are dealing with the matching of the principal terms of the asymptotic expansion of Eq. (3) when we can apply a method analogous to Zwaan's method[12] for Eq. (1) which is also called, following[13], the phase integral method. The power of the phase integral method for Eq. (1) is rather clearly elucidated in[1] and its application for the case $n = 2$ can be found in[2,14,15] and so on, so that we shall not go into details but refer the readers to the above-mentioned literature. We give the main results obtained by the phase integral method for $n = 2$ from the point of view of the general expansion (13) and in a form which is suitable for further generalizations, basing ourselves upon a more detailed analysis given in an earlier paper by us.[14]

The quasi-classical expansion of $\psi(x)$ for $n = 2$ has the form (13), (14) which is inapplicable, as already mentioned, in points where the roots of the characteristic equation $|H - sI| = 0$ (the matrix H in this case is obtained by changing from two second order equations to four first order equations) intersect. There are four of those roots ($s_1 = +\sqrt{\lambda_1}$, $s_2 = -\sqrt{\lambda_1}$, $s_3 = +\sqrt{\lambda_2}$, $s_4 = -\sqrt{\lambda_2}$) and, in principle, there can thus be six intersections; however, as the equation for the s is biquadratic, there remain only four intersections ($s_1 = s_2 = 0$, $s_3 = s_4 = 0$, $s_1 = s_3$, $s_2 = s_4$). The first two intersections are the classical turning points x_1, x_2 (see the figure) and the continuation of the expansion (13) with $n = 2$ compatible with $\psi(x)$ being finite as $x \to \infty$ ($a_{1+} = a_{2+} = 0$, if $\operatorname{Im}\sqrt{\lambda_{1,2}} > 0$ when $x < x_{1,2}$) through the TP $x_{1,2}$ along the contour shown in the figure gives for $x > x_{1,2}$ for the expansion coefficients

$$\mathbf{a}_+ = \mathbf{a}_- = e^{-i\pi/4}\mathbf{c}, \tag{35}$$

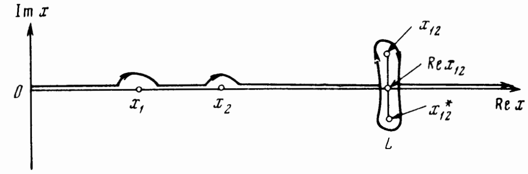
where $\mathbf{c} = \binom{c_1}{c_2}$ is an arbitrary vector. If there are no other TP near the real axis, $T = I$ and $S = e^{2i\eta}$ in agreement with what we said earlier. If, however, when moving along the x-axis we cross $\operatorname{Re} x_{12}$ where x_{12} and x_{12}^* are two complex conjugated TP[7)] the coefficients a_+, a_- change discontinuously, and $T \neq I$ and must be determined. The form or the T matrix is entirely determined by the nature, number, and relative position of the TP following the x_j. We consider different cases which are of practical interest.

1. From the physical point of view one of the most important ones is the case of "pseudo-intersecting" levels, when $(P_{11}(x) - P_{22}(x))|_{\operatorname{Re} x_{12}} = 0$; then $s_1 = s_3$ in the TP x_{12}, x_{12}^*; here x_{12}, x_{12}^* are the roots of the "adiabatic frequency" $\lambda_1 - \lambda_2$ of multiplicity $1/2$ and $\operatorname{Re} x_{12}$ lies sufficiently far from $x_{1,2}$ (see below for quantitative criteria). From[14] we have in this case

$$\mathbf{b}_\pm = M_\pm \mathbf{a}_\pm, \tag{36}$$

$$M_+ = M_-^* = \begin{pmatrix} e^{-\delta} & e^{i\gamma}\sqrt{1-e^{-2\delta}} \\ -e^{-i\gamma}\sqrt{1-e^{-2\delta}} & e^{-\delta} \end{pmatrix}, \tag{37}$$

7)Because the coefficients of the H(x) matrix are real on the real axis the TP lie in pairs symmetrically with respect to the real axis.



$a_+ = a_-$ and the coefficients b_+, b_- characterize the required expansion for $x > \operatorname{Re} x_{12}$. In equation (37)

$$\delta = \frac{i}{2\alpha}\oint_L (s_1 - s_3)\,dx, \quad \gamma = \frac{1}{\alpha}\int_{x_1}^{\operatorname{Re} x_{12}} s_1\,dx - \frac{1}{\alpha}\int_{x_2}^{\operatorname{Re} x_{12}} s_3\,dx, \tag{38}$$

where the integration in the expression for δ is along a contour L which encircles the TP x_{12}, x_{12}^* in a direction determined by the condition $\delta > 0$ (e.g., when $\lambda_1 - \lambda_2 > 0$ on the real axis for $x < \operatorname{Re} x_{12}$ the direction is clockwise). For T we get

$$T = M_+ M_-^{-1} = \begin{pmatrix} e^{-2\delta} + e^{2i\gamma}(1 - e^{-2\delta}) & 2i\sin\gamma\sqrt{1-e^{-2\delta}} \\ 2i\sin\gamma\sqrt{1-e^{-2\delta}} & e^{-2\delta} + e^{-2i\gamma}(1 - e^{-2\delta}) \end{pmatrix}, \tag{39}$$

and one easily checks that

$$T^+ T = 1 \tag{40}$$

and the scattering matrix S is unitary and asymmetric. It is necessary to note that the phases η_1, and η_2 are determined uniquely by Eq. (16) where the integrals

$$\int_{x_{1,2}}^{x} \sqrt{\lambda_{1,2}}\,dx$$

are taken bearing in mind the change in the root of $\lambda_1 - \lambda_2$ when passing through the cut (integration along intersecting terms). For the scattering matrix we have then the unique expression (19) with η and T determined by Eqs. (16), (38), and (39).

We can obtain a quantitative criterion that x_1 and x_2 are sufficiently far from $\operatorname{Re} x_{12}$ by comparing the expression obtained for S with the results obtained in[16] in the linear terms model. If we introduce the dimensionless parameters (in the earlier units)

$$\varepsilon = \frac{E|\Delta F|}{2a|F|}, \quad b = \frac{4a}{\hbar}\left(\frac{ma}{|F||\Delta F|}\right)^{1/2}, \tag{41}$$

where $\Delta F = F_1 - F_2$ is the difference in force in the intersection point, $F^2 = F_1F_2$, $a \equiv U_{12}(\operatorname{Re} r_{12})$ is the interaction matrix element in that point, one can easily check that the expression obtained for S is the same as the result of[16] provided

$$\varepsilon \gg 1, \quad b \gg 1, \tag{42}$$

and this is thus the quantitative criterion for the applicability of (38) and (39). In the case of a small splitting of the electron terms the T matrix can be evaluated using perturbation theory (in the linear terms model (38) and (39) are the same as perturbation theory when $\delta = \pi b/8\,|\epsilon^{1/2}| \ll 1$) and in intermediate cases we can use for its evaluation the results of numerical calculations.[17] For "subbarrier" transitions near pseudo-intersection points when x_1 and x_2 lie to the right of $\operatorname{Re} x_{12}$ we can for $\delta \ll 1$ find the T matrix from perturbation theory and for $\delta \gg 1$ by using the Pokrovskiĭ-Khalatnikov method.[18] 8) We may thus as-

8)In [16], an expression was obtained for S when $\delta \gg 1$, but the scattering matrix is then non-unitary.

sume that the T matrix is known for any relative position of the TP x_1, x_2 and x_{12}, x_{12}^* for the case of "pseudo-intersecting" electron levels. It is necessary to note that the results (38) and (39) are valid not only in the special case of "pseudo-intersection" of electron levels when $(P_{11}(x) - P_{22}(x))|_{\mathrm{Re}\, x_{12}} = 0$ but also in the more general case when the adiabatic frequency $\lambda_1 - \lambda_2$ has a minimum in some point Re x_{12} (such a case was considered for atomic collisions in[19]).

2) If apart from the TP x_1, x_2 and x_{12}, x_{12}^* there is yet a TP x_2' to the right of Re x_{12}, this corresponds to the physical picture of resonance scattering and leads to the following expression for the scattering matrix

$$S = e^{2i\eta_0}, \tag{43}$$

where the resonance phase η_0 was calculated in[14].

3) The case $s_1 = s_4$ (so that $s_1 - s_4$ has two complex-conjugate roots x_{12} and x_{12}^* of multiplicity $1/2$) is usually not considered although, in principle in collisions and also in a number of other physical problems it may occur (see, e.g.,[15]). Applying the phase integral method and performing calculations similar to case 1, we get

$$b_{1+} = e^{-\delta}a_{1+} + e^{i\gamma}\sqrt{1-e^{-2\delta}}a_{2-}, \quad b_{2+} = -e^{-i\gamma}\sqrt{1-e^{-2\delta}}a_{1-} + e^{-\delta}a_{2+}, \tag{44}$$

$$b_{1-} = e^{-\delta}a_{1-} + e^{-i\gamma}\sqrt{1-e^{-2\delta}}a_{2+}, \quad b_{2-} = -e^{i\gamma}\sqrt{1-e^{-2\delta}}a_{1+} + e^{-\delta}a_{2-}, \tag{45}$$

where

$$\gamma = \frac{1}{\alpha}\int_{x_1}^{\mathrm{Re}\, x_{12}} s_1\, dx - \frac{1}{\alpha}\int_{x_2}^{\mathrm{Re}\, x_{12}} s_4\, dx, \quad \delta = \frac{i}{2\alpha}\oint_L (s_1 - s_4)\, dx \tag{46}$$

and the way one goes around the contour L is determined from the condition $\delta > 0$. Bearing in mind that $a_+ = a_-$ we get for T the earlier Eq. (39) with γ and δ determined by Eqs. (46).

We now generalize the results obtained for any number of levels and an arbitrary number of binary "pseudo-intersections" between them (provided the "pseudo-intersection" points are sufficiently far from one another). To do this we introduce the vectors

$$A = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}, \quad B = \begin{pmatrix} b_+ \\ b_- \end{pmatrix}$$

and rewriting the results (36), (44), and (45), respectively, in the form

$$B = MA, \quad B = ZA, \tag{47}$$

where

$$M = \begin{pmatrix} M_+ & 0 \\ 0 & M_- \end{pmatrix},$$

$$Z = \begin{pmatrix} e^{-\delta} & 0 & 0 & e^{i\gamma}\sqrt{1-e^{-2\delta}} \\ 0 & e^{-\delta} & -e^{-i\gamma}\sqrt{1-e^{-2\delta}} & 0 \\ 0 & e^{-i\gamma}\sqrt{1-e^{-2\delta}} & e^{-\delta} & 0 \\ -e^{i\gamma}\sqrt{1-e^{-2\delta}} & 0 & 0 & e^{-\delta} \end{pmatrix} \tag{48}$$

and[9]

$$M^+M = Z^+Z = 1. \tag{49}$$

One then sees easily that for the general case considered the vectors B and A (of order 2n) are connected by the previous relation B = MA, where

$$M = \prod_{j,k} M_{jk}, \tag{50}$$

the matrix M_{jk} (of order 2n) corresponds to the "pseudo-intersection" of the levels j and k and all its elements $m_{\mu\nu}$ vanish except the following

$$m_{\alpha\alpha} = 1, \quad m_{jk} = -m_{kj}^* = e^{i\gamma_{kj}}\sqrt{1-e^{-2\delta_{kj}}} = m_{n+k,n+j} = -m_{n+j,n+k}^*,$$
$$m_{jj} = m_{kk} = m_{n+j,\,n+j} = m_{n+k,\,n+k} = e^{-\delta_{kj}}, \tag{51}$$

where

$$\gamma_{kj} = \frac{1}{\alpha}\int_{x_k}^{\mathrm{Re} x_{kj}} \sqrt{\lambda_k}\, dx - \frac{1}{\alpha}\int_{x_j}^{\mathrm{Re} x_{kj}} \sqrt{\lambda_j}\, dx, \quad \delta_{kj} = \frac{i}{2\alpha}\oint_{L_{kj}} (s_k - s_j)\, dx. \tag{52}$$

The integral for δ_{kj} is taken here along a contour L_{kj} encircling the TP x_{kj}, x_{kj}^* in a direction determined by the condition $\delta_{kj} > 0$.

The matrices M_{jk} multiply in the order in which the pseudo-intersection points (after going through the TP x_j) follow one another, and if there are TP with $\sqrt{\lambda_k} + \sqrt{\lambda_j} = 0$ they are replaced by the matrices Z_{jk} with matrix elements which can be determined from (48). One checks easily that $M^+M = 1$. Having found the matrix $M = \prod_{jk} M_{jk}$ we write the relation connecting the vectors B and A in the form

$$\begin{pmatrix} b_+ \\ b_- \end{pmatrix} = M \begin{pmatrix} a_+ \\ a_- \end{pmatrix}, \tag{53}$$

where $a_+ = a_-$ in agreement with what we said earlier. Solving the last n equations ($b_- = M_-a_-$) for the vector a_- ($a_- = M^{-1}b_-$) and substituting the result in the first n equations ($b_+ = M_+a_+$) we get a general expression for the scattering matrix S

$$S = e^{i\eta}M_+M_-^{-1}e^{i\eta}, \tag{54}$$

which completely solves the problem stated above.

We note that the phase integral method is applicable also in more complex cases of intersections in TP x_{jk} of an arbitrary number of eigenvalues of the matrix H(x) when the problem can be reduced to the case, considered before, of binary intersections.[20] In particular, one can thus consider the limiting case of a very close relative position of "pseudo-intersection" points of electron levels.[10] Exactly in the same way we can consider the effect of other analytical singularities of the H(x) matrix on the probabilities for inelastic transitions.

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[9] Because of this there exists for a system of coupled oscillators with slowly varying parameters an adiabatic invariant

$$J = \sum_{i=1}^{N} \frac{E_i}{s_i},$$

where E_i is the energy and s_i the normal frequency of the i-th mode. [20]

[10] We must note that in the physically important case of a system of parallel terms which intersect with the same slope, when such a situation may be realized, the problem can be solved exactly. [21]

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