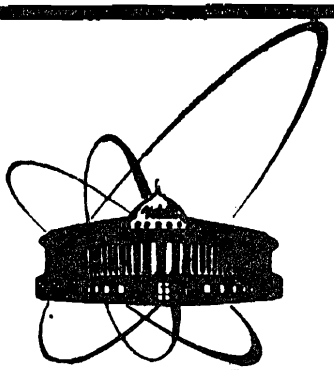

объединенный
институт
ядерных
исследований
дубна

E4-86-467

A.V.Matveenko, Y.Abe*

ASYMPTOTICALLY ADAPTED THREE-BODY MOLECULAR STATES

Submitted to "Few-Body Systems"

* Research Institute for Fundamental Physics, Kyoto University, Japan

1986

Introduction

The Born-Oppenheimer adiabatic or molecular state method has first appeared in atomic physics /1/ but now is widely used also in nuclear physics /2/. Most of the textbooks consider it to some extent /3/. Nevertheless the method is defective by itself what has not been so important at the beginning of the story in atomic physics but became apparent when muonic molecules started to be widely treated by the same approach /4/. Again, it was not so important in the nuclear physics as many other uncertainties were involved in that case. To understand the essence of the problem we should return to the simplest three-body molecular states with the well-defined interaction, without any additional complications like spin, etc.

So, we have for example HD^+ system consisting of three particles with Coulomb interaction, namely $p+d+e$ /5/. Much heavier nuclei are almost fixed at some stationary positions and a valence electron moving with rather a high velocity provides the binding of the system. This clear physical picture gives grounds for the usual adiabatic strategy for the solution of the problem. At first step the nuclei are considered infinitely heavy (fixed), so that a much simpler three-dimensional problem of the electron moving in the field of two fixed centers is to be solved at the beginning. For a particular case of the Coulomb interaction this two-center problem happens to be completely separable in prolate spheroidal coordinates thus providing a comparatively easy way to calculate the eigenvalues and eigenfunctions of the problem both depending on the internuclear distance as a parameter /6/. Next, this parameter should again be converted into a dynamic variable. In this treatment, the electronic motion (with fixed nuclei) appears in the zeroth order, the vibrational motion of the nuclei is of the second order, and the rotations are of the fourth order, The expansion parameter is $(m/M)^{1/4}$, where m and M are typical masses of the light and heavy particles respectively /7/. This approach results in a strongly coupled system of Schrödinger equations for the radial motion of nuclei, that persist to be coupled even in that part of the configurational space where two particles are bound forming an atom, one of the nuclei being far away. As a result of such a nonphysical asymptotic coupling the boundary conditions for the scattering problem in this

approach are not easy to meet. The situation is rather strange - in the zeroth order theory provides extremely good results but the slightest attempt to improve this simplest approximation kills the theory itself.

Several attempts were made to treat this disaster. In the most extensive calculations /8/ the authors used 52 bound and 792 continuum states of the two-center problem declaring that though the theory is defective they have used almost a complete set of solutions so that one could be sure of their results. The variational calculations from /9/ have disproved this assertion. In another approach /10/, see also ref. /11/, the authors are trying to treat the infinite system of coupled radial Schroedinger equations by transforming it to a more physically acceptable form. We shall mention here two more attempts to treat the boundary conditions in the molecular state framework, that imply the introduction of translational exponential factors or the so-called diabatic (i.e. opposite to molecular or adiabatic) states /12/. It is not an easy task to discuss these approaches because both things have never been clearly defined. Even more, when introducing them one usually supposes that some adiabatic states are already available to use them for those speculations. So, all the problems that appear when adiabatic states are introduced in the study of the three-body states, namely, the effect of proper mass, asymptotic radial and Coriolis coupling between slow and fast degrees of freedom, are still open to a direct treatment. In what follows we present a formal theory which is free of all those drawbacks but contains all the advantages of the usual Born-Oppenheimer approach. Due to that, our method should be very appropriate for studying the scattering problem and also weakly bound states in the framework of the molecular state approach.

Our strategy is rather different from the classical one, though the starting point is the same, i.e. three-body Hamiltonian in the rotational frame with Z -axis being the internuclear axis. We examine carefully the structure of different coupling terms which are parts of the total Hamiltonian and introduce two subsequent transformations of the coordinate system and also of the wave function and then arrive at the new much simpler expression for the total Hamiltonian. This new Hamiltonian allows one to redefine the partition of the physical system into its fast (originally electronic) part and rather slow (nuclear) part. A new two-center Hamiltonian appears, that exactly reproduces the spectrum of the associated atom when one of the nuclei is put to be infinitely far away. Next, the partial wave analysis is made, that provides the states with exact quantum

numbers of the total angular momentum $\mathcal{J}$ and parity p . After that the two-center Hamiltonian converts into the system of $(\mathcal{J}+1)$ or $\mathcal{J}$ coupled Schroedinger equations in two variables to account for the motion of a fast sybsystem. This program has partly been presented by one of the authors /13/. Here it will be reproduced in a more clear way with important physical details being stressed. After that we shall be able to construct a formal scattering theory with exact asymptotic states and provide formulae for the amplitude and scattering cross sections in the laboratory frame in terms of the molecular state S -matrix.

1. Molecular Description: Jacobi Coordinates, Recoil Operators

In order to describe in a simple way the asymptotic states for the transfer reaction

$$(a+c)_{\ell m} + b \longrightarrow (b+c)_{\ell' m'} + a \qquad (1)$$

we need two sets of relative Jacobi coordinates (Fig.1a, 1b).

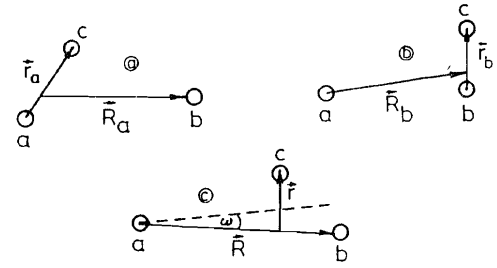

Fig.1.

Jacobi coordinates for the left (1a) and right-hand (1b) sides of the transfer reaction (1). In Fig. 1c the Jacobi coordinates one proceeds with in the molecular-like approach are given. Formula (18a) provides the value of ω .

Here are two cores a and b with masses m_a and m_b and a sort of a valence particle c with mass m_c which can provide binding of the total system. In that case for low relative velocities the process (1) should proceed through some molecular stage. That is why one usually writes down the internal Hamiltonian in terms of relative Jacobi coordinates (Fig. 1c). The motion of a valence particle

c is quantized onto the $\vec{R}$ -axis (rotating reference frame). Three sets of Jacobi coordinates (1a)-(1c) are connected with each other. For instance,

$$\begin{pmatrix} \vec{R}_a \\ \vec{\tau}_a \end{pmatrix} = \begin{pmatrix} 1 & f \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ e & 1 \end{pmatrix} \begin{pmatrix} \vec{R} \\ \vec{\tau} \end{pmatrix}. \tag{2}$$

The coefficients e and f depend on masses of the particles

$$e = \frac{m_\beta}{m_\alpha + m_\beta}, \qquad f = -\frac{m_c}{m_\alpha + m_c}. \tag{3}$$

The transformation matrix (2) is factorized into two matrices of the subsequent shifts.

Formula(2) provides the relevant formulae for the gradients

$$\begin{pmatrix} \nabla_{\vec{R}_a} \\ \nabla_{\vec{\tau}_a} \end{pmatrix} = \begin{pmatrix} 1 & -e \\ -f & 1+ef \end{pmatrix} \begin{pmatrix} \nabla_{\vec{R}} \\ \nabla_{\vec{\tau}} \end{pmatrix}. \tag{2a}$$

The change of variables (2) can be treated as the change of the representation if one introduces the operator

$$T_\alpha = exp\,(e\,\vec{R}\,\nabla_{\vec{\tau}})\; exp\,(f\,\vec{\tau}\,\nabla_{\vec{R}}) \tag{4}$$

so that for any operator H , say, Hamiltonian, it yields in the new representation

$$H_\alpha = T_\alpha\, H\, T_\alpha^{-1}.$$

The operator T_α has the properties

$$\begin{aligned} T_\alpha\, \vec{R}\, T_\alpha^{-1} &= \vec{R}_\alpha, \qquad T_\alpha\, \vec{\tau}\, T_\alpha^{-1} = \vec{\tau}_\alpha, \\ T_\alpha\, \nabla_{\vec{R}}\, T_\alpha^{-1} &= \nabla_{\vec{R}_\alpha}, \qquad T_\alpha\, \nabla_{\vec{\tau}}\, T_\alpha^{-1} = \nabla_{\vec{\tau}_\alpha}. \end{aligned} \tag{4a}$$

These formulae follow immediately from the operator identity

$$exp\,(Y)\,X\,exp\,(-Y) = X + [Y,X] + \frac{1}{2!}[Y,[Y,X]] + \dots \tag{5}$$

The translational operator (4) accounts for the recoil effect precisely /14/, though it can hardly be recommended for a practical use. Nevertheless, all numerous attempts /12/ to describe the asymptotic states in a molecular basis by incorporating some additional exponential factor in front of the molecular wave function are due to its peculiar form (4).

So, as it is usually done, we choose Jacobi coordinates (1c) with polar coordinates $\{R, \theta, \Phi\}$ being introduced for vector $\vec{R}$. Then, the Hamiltonian of the associated three-body problem will be

$$\tilde{H} = \frac{1}{2M}\left(\frac{1}{R} + \frac{\partial}{\partial R}\right)^2 - \frac{\vec{L}^2}{2MR^2} - \frac{1}{2m}\,\Delta_{\vec{\tau}} + V, \tag{6}$$

where the potential energy

$$V = V_\alpha(\tau_\alpha) + V_\beta(\tau_\beta) + V_c(R) \tag{6a}$$

and the square angular momentum operator

$$\vec{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\Phi^2}. \tag{6b}$$

The reduced masses M and m are given by

$$\begin{aligned} \frac{1}{M} &= \frac{1}{m_\alpha} + \frac{1}{m_\beta} \\ \frac{1}{m} &= \frac{1}{m_c} + \frac{1}{m_\alpha + m_\beta} \end{aligned} \tag{6c}$$

and $\varkappa = (m_\beta - m_\alpha)/(m_\alpha + m_\beta)$ for further use.

Next, the operator

$$\mathcal{D}(\Phi, \theta, 0) = e^{-i\Phi\ell_{z'}}\, e^{-i\theta\ell_{y'}}. \tag{7}$$

is applied so that the transformed Hamiltonian is given by

$$H = \mathcal{D}\tilde{H}\mathcal{D}^{-1}. \tag{8}$$

Now, $\vec{R}$ -vector is still referred to the initial laboratory frame but the motion of the valence particle is described in the rotating coordinate system with /7/

$$\vec{e}_{x'} = \vec{e}_\theta(\theta,\Phi), \quad \vec{e}_{y'} = \vec{e}_\Phi(\theta,\Phi), \quad \vec{e}_{z'} = \vec{e}_R(\theta,\Phi). \tag{7a}$$

This is due to a specific form of $\mathcal{D}$ -operator that depends on the angular momentum projections $\ell_{y'}$, $\ell_{z'}$ of c -particle in the (7a) frame. The transformation (8) is usually introduced as a simple coordinate transformation due to

$$\mathcal{D}\vec{\tau}\mathcal{D}^{-1} = \vec{\tau}', \qquad \mathcal{D}\vec{R}\mathcal{D}^{-1} = \vec{R}. \tag{9}$$

In order to receive the standard Born-Oppenheimer picture the prolate spheroidal coordinates /6/ should be used for the motion of

the light particle

$$\xi = \frac{r_a + r_b}{R} \quad , \quad \eta = \frac{r_a - r_b}{R} \quad , \quad \varphi = arctg\, y'/x' \tag{9a}$$

and after that we arrive at what can be called an original Born--Oppenheimer or adiabatic Hamiltonian /15/

$$H_{BO} = h - \frac{1}{2MR^2}\, r'^2 \Delta_{\vec{r}'} - \frac{1}{2M}\left(\frac{1}{R} + \frac{\partial}{\partial R}\right)^2 + \frac{\vec{J}^2}{2MR^2}$$
$$+ \frac{1}{MR}\left(\frac{1}{R} + \frac{\partial}{\partial R}\right)\hat{q} - \frac{\vec{J}\vec{\ell}}{MR^2} \,. \tag{10}$$

Here, the squared total angular momentum

$$\vec{J}^2 = -\frac{1}{\sin^2\theta}\left(\frac{\partial}{\partial \phi} - \cos\theta \frac{\partial}{\partial \varphi}\right)^2 - \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{\partial^2}{\partial\varphi^2} \tag{10a}$$

and the two-center Hamiltonian h for the motion of the valence particle (fast subsystem) is given as usual by

$$h = \frac{1}{2m}\Delta_{\vec{r}'} + V \quad , \tag{10b}$$

where the Laplace operator is now given by

$$\Delta_{\vec{r}'} = \Delta_{\xi\eta} + \Delta_{\varphi} \tag{10c}$$

with

$$\Delta_{\xi\eta} = \frac{4}{R^2(\xi^2-\eta^2)}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right]$$

and

$$\Delta_{\varphi} = \frac{4}{R^2 S^2}\,\frac{\partial^2}{\partial\varphi^2} \,.$$

Two last terms of (10) account for the radial and angular coupling of the motion of a valence particle with that described by $\vec{R}$ --coordinates. The precise form of the coupling operators follows from

$$\hat{q} = \frac{1}{\xi^2-\eta^2}\left\{(\xi - x\eta)(\xi^2-1)\frac{\partial}{\partial\xi} + (\eta - x\xi)(1-\eta^2)\frac{\partial}{\partial\eta}\right\} \,,$$
$$\ell_{x'} \pm i\ell_{y'} = exp(\pm i\varphi)\left\{\pm\frac{S^2}{\xi^2-\eta^2}\left[(\eta - x\xi)\frac{\partial}{\partial\xi} - (\xi - x\eta)\frac{\partial}{\partial\eta}\right] + \frac{\xi\eta - x}{S}\, i\,\frac{\partial}{\partial\varphi}\right\}$$
$$\ell_{z'} = -i\frac{\partial}{\partial\varphi} \,; \quad S = \left[(\xi^2-1)(1-\eta^2)\right]^{1/2}. \tag{10d}$$

The projections of $\vec{J}$ are given by

$$\vec{J} = \vec{\ell}_{x'}\left(\frac{i}{\sin\theta}\frac{\partial}{\partial\phi} - i\,ctg\,\theta\frac{\partial}{\partial\varphi}\right) + \vec{\ell}_{y'}\left(-i\frac{\partial}{\partial\theta}\right) + \vec{\ell}_{z'}\left(-i\frac{\partial}{\partial\varphi}\right). \tag{10e}$$

For the volume element we have

$$d\vec{R}\,d\vec{r}' = R^2\sin\theta\, dR\, d\theta\, d\Phi\, \frac{R^3}{8}(\xi^2-\eta^2)\, d\xi\, d\eta\, d\varphi \,. \tag{10f}$$

Quite formally the coupling terms survive as $R \to \infty$ and the two-center Hamiltonian (10b) does not reproduce the spectrum of $(a+c)$ or $(b+c)$ "atom" in the same limit. One can say that the recoil effect is not accounted for properly at this stage. The most impressive way to understand what it is all about would probably be to look at matrix elements of the coupling terms from (10) calculated between different eigenstates of (10b) for pure Coulombic interaction /4/. Almost all of them tend to some constant values as $R \to \infty$.

2. Elimination of the Radial Coupling: Hyperspheroidal Coordinates

It has recently been shown /16/ that the radial coupling is unphysical in the sense that it can be eliminated exactly by some isometric transformation of the total Hamiltonian (10)

$$H_\Lambda = e^{-\Lambda} H_{BO}\, e^{\Lambda} \tag{11}$$

with the generator Λ given by

$$\Lambda = ln\,(\sqrt{\rho})\, R\left(\frac{1}{R} + \frac{\partial}{\partial R}\right), \tag{11a}$$

where

$$\rho = 1 + \frac{m}{4M}\left(\xi^2 + \eta^2 - 1 - 2x\xi\eta + x^2\right) \tag{11b}$$

is the dimensionless function of relative coordinates. The direct use of the operator identity (5) produces for the transformed Hamiltonian and wave function

$$H_\Lambda = h_\Lambda - \frac{1}{2M}\left(\frac{\partial^2}{\partial R_\Lambda^2} + \frac{5}{R_\Lambda}\frac{\partial}{\partial R_\Lambda}\right) - \frac{3}{2MR_\Lambda^2} + \rho\,\frac{\vec{J}^2 - 2\vec{J}\vec{\ell}}{2MR_\Lambda^2} - \frac{\rho^2}{2m}\,\frac{R^2}{R_\Lambda^2}\,\Delta\varphi \tag{12}$$

and

$$\Psi_\Lambda = e^{-\Lambda}\,\psi(\vec{R},\vec{\tau}') = \frac{1}{\sqrt{\rho}}\,\psi(\sqrt{\rho}\,\vec{R},\vec{\tau}').$$

(12a)

The expression (12a) follows just from the known identity

$$exp[\ln(\alpha)\,\vec{\tau}\,\nabla_{\vec{\tau}}]\,f(\vec{\tau}) = f(\alpha\vec{\tau}).$$

(13)

So, both the coordinates and the wave function are changed by the transformation (11). The new slow radial variable R_Λ is given by /17/

$$R_\Lambda = \sqrt{\rho}\,R.$$

(12b)

The operator

$$h_\Lambda = -\frac{1}{2m}\,\rho^2\tilde{\Delta}_{\xi\eta} + V$$

(14)

is to be identified with the transformed Hamiltonian for the motion of a fast subsystem. Here

$$\tilde{\Delta}_{\xi\eta} = \frac{\dot{R}^2}{R_\Lambda^2}\,\Delta_{\xi\eta}.$$

(14a)

Now, one can see that the radial coupling term is missing in (12). Due to this fact the recoil effect is exactly described now as instead of the original Jacobi reduced masses m and M the coordinate dependent masses m/ρ and $M\rho$ are incorporated in the theory. In order to see this, R_Λ should be changed back to R by using (12b) in expressions (12) and (14). These variable reduced masses have the important properties

$$\rho/m \xrightarrow[(\xi\to 1,\,\eta\to -1)]{R\tau_a^{-1}\to\infty} \frac{1}{m_a} + \frac{1}{m_c} = m_{ac}^{-1} = \rho_a/m$$

$$(M\rho)^{-1} \xrightarrow[(\xi\to 1,\,\eta\to -1)]{R\tau_a^{-1}\to\infty} \frac{1}{m_\beta} + \frac{1}{m_a+m_c} = M_a^{-1} = (M\rho_a)^{-1}$$

(15)

just like it should be for the left-hand side of the reaction (1). In the case of $R\tau_\beta^{-1}\to\infty$ limit formulae like (15) hold with α and β being interchanged. As far as the transformation (11) leads to the change of the independent variable by (12a), a new collective radial variable R_Λ should be introduced, that has very useful asymptotic properties

$$R_\Lambda = \sqrt{\rho}\,R \to \begin{cases} \sqrt{\rho_\alpha}\,R = \sqrt{\frac{M_a}{M}}\,R_a, & R\tau_a^{-1}\to\infty\ (\xi\to 1,\,\eta\to -1) \\ \sqrt{\rho_\beta}\,R = \sqrt{\frac{M_\beta}{M}}\,R_\beta, & R\tau_\beta^{-1}\to\infty\ (\xi\to 1,\,\eta\to 1), \end{cases}$$

(15a)

where R_α and R_β are the Jacobi radii that correspond to τ_α and τ_β. Formulae (15) indicate that in the region of pair collisions the transformed Hamiltonian has the proper behaviour and the formula (15a) should be used for the matching the eigenfunctions of H_Λ with the asymptotic solutions that represent the channels of the reaction (1).

The singularity connected with the triple collision should also be considered in studying the general three-body system. It can easily be shown /17/ that R_Λ coincides with the hyperradius of the system which is the proper variable to treat Fock's singularity. So, while restoring the proper pair collision behaviour of the total three-body Hamiltonian, we have got the theory which is adequate for treating the region of the triple collision.

The result of this section can be summarized in a simple way. The R, ξ, η coordinates of the usual Born-Oppenheimer description should be changed to "hyperspheroidal" coordinates R_Λ, ξ, η. The change of the wave function (12a) is also desirable in order to simplify the resulting Hamiltonian.

One can also say that Λ-transformation simulates in its own way a "radial" part of the recoil operator (4) resulting in Hamiltonian (12) with good asymptotic behaviour in radial variables. The original Born-Oppenheimer quasiseparation of variables is subsituted by the new one.

3. Rotational Coupling: Inertia Tensor of a Three-Body System

The commutational relation $[\Lambda,\ \vec{J}\cdot\vec{\ell}\,] = 0$ holds so that the structure of the rotational coupling operator is not changed by Λ-transformation. This is an additional indica-

tion to that R_Λ is a good three-body generalized radial coordinate. On the other hand, the asymptotic properties of $\vec{\mathcal{J}}\cdot\vec{\ell}$ operator are still poor. Due to this fact we have solved the problem of the proper asymptotical behaviour of the theory only for the simplest case of $\vec{\mathcal{J}} = 0$ as yet. A further transformation is needed and it is almost evident that this should be a rotation. In order to simplify the presentation, this rotation should be accomplished in two steps. The first one is to restore the proper commutational relations of the components of $\vec{\mathcal{J}}$ that are until now more than abnormal. Indeed, using $\mathcal{J}_{x'}$, $\mathcal{J}_{y'}$ and $\mathcal{J}_{z'} = \ell_{z'}$ from (10e), we have

$$[\mathcal{J}_{x'}, \mathcal{J}_{y'}] = -i\,ctg\,\theta\,\mathcal{J}_{x'} - i\,\mathcal{J}_{z'};\ [\mathcal{J}_{x'}, \mathcal{J}_{z'}] = [\mathcal{J}_{y'}, \mathcal{J}_{z'}] = 0 \qquad (16a)$$

though providing (10a) for $\vec{\mathcal{J}}\cdot\vec{\mathcal{J}}$. To restore a usual algebra for the projections of $\vec{\mathcal{J}}$ we define anow the unit vectors $\vec{e}_1$, $\vec{e}_2$ and $\vec{e}_3$ by

$$\vec{e}_1 = \vec{e}_{x'}\sin\varphi - \vec{e}_{y'}\cos\varphi, \quad \vec{e}_3 = \vec{e}_R$$
$$\vec{e}_2 = \vec{e}_{x'}\cos\varphi + \vec{e}_{y'}\sin\varphi \qquad (17)$$

so that for the components of $\vec{\mathcal{J}} = \vec{e}_1\mathcal{J}_1 + \vec{e}_2\mathcal{J}_2 + \vec{e}_3\mathcal{J}_3$ we have $[\mathcal{J}_1, \mathcal{J}_2] = -i\,\mathcal{J}_3$ and so on. These properties happened to be useful /13/ to introduce one more transformation of the total Hamiltonian

$$H_{\Lambda\Omega} = e^{-\Omega} H_\Lambda e^{\Omega}, \qquad (18)$$

where $\Omega = -i\omega\mathcal{J}_1$ and ω defined by

$$\sin 2\omega = \frac{m}{2M}\,\frac{(\xi\eta - \varkappa)\cdot S}{\rho\sqrt{1-\Delta}}, \quad \Delta = \frac{m}{M}\,\frac{S^2}{\rho^2} \qquad (18a)$$

is the angle between the vector $\vec{R}$ and the principal axis of the

inertia tensor of the three-body system. So, (18) provides the new rotational reference frame in which by using (5) we arrive at

$$H_{\Lambda\Omega} = h_{\Lambda\Omega} - \frac{1}{2M}\left(\frac{\partial^2}{\partial R_\Lambda^2} + \frac{5}{R_\Lambda}\frac{\partial}{\partial R_\Lambda}\right) - \frac{3}{2MR_\Lambda^2}. \qquad (19)$$

The operator

$$h_{\Lambda\Omega} = h_\Lambda + T_R + \frac{1}{2MR_\Lambda^2}\,\frac{1}{1-\Delta}\left\{\Delta\cdot\mathcal{J}_1^2 + i\,\mathcal{J}_1\left[4\mathcal{L}_1 + 2\rho\Delta\left(\mathcal{L} + \frac{\xi\eta - \varkappa}{2S}\right)\right]\right\} \qquad (20)$$

with

$$\mathcal{L} = \frac{S}{\xi^2 - \eta^2}\left[(\eta - \varkappa\xi)\frac{\partial}{\partial\xi} - (\xi - \varkappa\eta)\frac{\partial}{\partial\eta}\right],$$
$$\mathcal{L}_1 = \frac{S}{\xi^2 - \eta^2}\left[\eta(\xi^2 - 1)\frac{\partial}{\partial\xi} + \xi(1 - \eta^2)\frac{\partial}{\partial\eta}\right] \qquad (20')$$

should be referred to as a rotational dynamic two-center Hamiltonian. It contains the operator

$$T_R = \frac{1}{2}\left(\frac{\mathcal{J}_1^2}{I_1} + \frac{\mathcal{J}_2^2}{I_2} + \frac{\mathcal{J}_3^2}{I_3}\right) \qquad (20a)$$

that is just the Hamiltonian of an asymmetric top with the classical expressions for the principal inertia moments

$$I_1 = I_2 + I_3 = MR^2\rho, \quad I_2 = \frac{1}{2}MR^2\rho\left(1 + \sqrt{1-\Delta}\right), \qquad (21)$$

so that ρ already given by (11b) is simply defined by I_1. The original long-armed Coriolis coupling term $\vec{\mathcal{J}}\vec{\ell}$ from (10d) is now transformed into the rotational coupling term that is given in the curly brackets of (20). Now it has a multiplier in front of it that makes it zero as $R z_{a,\beta}^{-1} \to \infty$. So, the transformed $H_{\Lambda\Omega}$ Hamiltonian is completely separable in that part of the configurational space that is defined by the channels of the transfer reaction (1).

Three subsequent rotations were involved to arrive at the resulting Hamiltonian (19) with its rotational part given by (20). Finally we give the expressions providing the Euler angles α, β, γ of the resulting rotation that puts original-space-fixed frame into that making the inertia tensor of the three-body system to be diagonal /13,18/

$$ctg\,(\alpha - \varphi) = \cos\theta\,ctg\,\varphi + ctg\,\omega\,\frac{\sin\theta}{\sin\varphi}$$
$$\cos\beta = \cos\theta\cos\omega - \sin\theta\sin\omega\cos\varphi$$
$$tg\,\gamma = -\cos\omega\,ctg\,\varphi - ctg\,\theta\,\frac{\sin\omega}{\sin\varphi}. \qquad (22)$$

This rotation depending on internal coordinates of the system again can be thought of as an angular part of the total recoil operator (4), but opposite to Λ -transformation it diagonalizes the rotational coupling only in the asymptotic region.

The sequence of the coordinate transformations used in this paper can be finally summarized at this place. The original Born-Oppenheimer three-body center-of-mass coordinates R , θ , Φ , ξ , η , φ were substituted by a special choice of the hyperspherical coordinates R_Λ , ξ , η , α , β , γ . There exists a number of papers in the fields of the nuclear, molecular and atomic physics where authors start by using hyperspherical coordinates in their investigations. We shall indicate here only representative references /19,20/, noting the papers by Johnson /21/, where there is an interesting discussion of different variants of the Hamiltonian in hyperspherical coordinates, and the papers by Macek who was probably the first to introduce the Born-Oppenheimer-type description of a three-body system in hyperspherical coordinates /5,22/.

4. Partial Wave Analysis of $H_{\Lambda\Omega}$: States with Good Quantum Numbers

The asymptotically adapted three-body molecular Hamiltonian (19) allows one to meet proper boundary conditions for the transfer process (1). In the usual Born-Oppenheimer description the two-center Hamiltonian (10b) is used to provide the molecular-type eigenfunctions as a basis to expand a total three-body wave function. In our case the operator (20) plays that role. The angular degrees of freedom should be separated at the first step. This procedure can be combined with an introduction into the theory of the states with good quantum numbers of total angular momentum $\mathcal{J}$ and total parity p by writing the expansion of a three-body wave function in the form

$$\Psi_M^{\mathcal{J}p}(\tilde{R}_\Lambda, \tilde{\tau}') = \sum_{K=0}^{\mathcal{J}} B_{MK}^{\mathcal{J}p}(\alpha,\beta,\gamma)\,\Psi_K^{\mathcal{J}p}(R_\Lambda, \xi, \eta)\,. \tag{23}$$

This function has to satisfy the Schroedinger equation

$$H_{\Lambda\Omega}\Psi = E\Psi\,. \tag{24}$$

In (23) the summation is over the values of the total angular momentum projection onto the rotating z' -axis. The quantum number M is the total angular momentum projection onto the original fixed

z -axis. The angular part of the wave function has the form

$$B_{MK}^{\mathcal{J}p}(\alpha,\beta,\gamma) = \mathcal{D}_{-M-K}^{\mathcal{J}}(\alpha,\beta,\gamma) + p(-1)^{\mathcal{J}}\mathcal{D}_{-M\,K}^{\mathcal{J}}(\alpha,\beta,\gamma)\,. \tag{23a}$$

It contains Wigner $\mathcal{D}$ -functions defined as in /18/ and provides good quantum numbers $\mathcal{J}$ and p . The number of terms in the expansion (23) is not higher than $\mathcal{J}+1$. Hence, the projection onto the states (23a) leads to the system of $\mathcal{J}+1$ or $\mathcal{J}$ Schroedinger equations with the matrix Hamiltonian

$$H_{\Lambda\Omega}^{\mathcal{J}p} = h_{\Lambda\Omega}^{\mathcal{J}p} - \frac{1}{2M}\left(\frac{\partial^2}{\partial R_\Lambda^2} + \frac{5}{R_\Lambda}\frac{\partial}{\partial R_\Lambda}\right) - \frac{3}{2MR_\Lambda^2} \tag{25}$$

which includes the matrix operator of the dynamic two-center problem for the rotational states $h_{\Lambda\Omega}^{\mathcal{J}p}$ that is just the operator (20) averaged over the angular states (23a). The operator of an assymetric rotator T_R couples the states (23a) for $K' = K \pm 2$ and the Coriolis-type operator from (20) includes also $K' = K \pm 1$ -type coupling. Both couplings disappear in the asymptotic region where $R\tau_\alpha^{-1}$ or $R\tau_\beta^{-1} \to \infty$ and then K starts to be a good quantum number which is not true in the general case. Again, only asymptotically the rotational part of the total wave function decouples into the (23a) form with arguments of $\mathcal{D}$ -function being converted into Φ , θ , $\varphi - \frac{\pi}{2}$ due to formulae (22) where ω should be put equal to zero.

The system of Schroedinger equations in three variables $\{R_\Lambda, \xi, \eta\}$ with Hamiltinian (25) that we rewrite

$$H^{\mathcal{J}p}\Psi^{\mathcal{J}p}(R_\Lambda, \xi, \eta) = E\Psi^{\mathcal{J}p}(R_\Lambda, \xi, \eta) \tag{26}$$

using $\Psi^{\mathcal{J}p}$ for column-vector $\Psi_K^{\mathcal{J}p}$ from (23) is ready for the solution. If a three-dimensional code is available, the solution of (26) is straightforward to provide the spectrum and eigenfunctions of a three-body system. The scattering problem is more complicated as it should be. In the next section we shall introduce the Born-Oppenheimer-like approximation for the solution of (26) that will be a tool for treating both the eigenvalue problem and the scattering problem (1).

5. Generalized Born-Oppenheimer Description: Two-Center Problem with Good Quantum Numbers

Now we are ready to make use of a rather general Born-Oppenheimer or adiabatic idea, i.e. to separate approximately the total dynamic system into its fast and slow parts. The starting Hamiltonian is given by (25) in our case, the collective "slow" variable will be R_Λ, so that a fast subsystem will depend on two intrinsic variables ξ, η with the generalized two-center rotational Hamiltonian $h^{J p}$ from (25) that is just the operator (20) projected onto rotational states (23a). The associated Schroedinger equation reads

$$h^{J p}\tilde{\varphi}_n^{J p}(\xi,\eta;R_\Lambda) = \mathcal{E}_n^{J p}(R_\Lambda)\,\tilde{\varphi}_n^{J p}(\xi,\eta;R_\Lambda). \qquad (27)$$

Its eigenvalues and eigenfunctions depend on R_Λ that is a parameter for the moment. The "vibrational" quantum number n can easily be interpreted by inspecting the $R\tau_{a,b}^{-1}\to\infty$ limit of the Schroedinger system (27). As it follows from expressions (20) and (20a)

$$h_{\Lambda\Omega} \xrightarrow[(\xi\to 1,\ \eta\to\pm 1)]{R\tau_{a,b}^{-1}\to\infty} h_\Lambda + \frac{1}{2}\frac{\mathcal{J}_3^2}{I_3} \qquad (27a)$$

so that the projection of $\bar{\mathcal{J}}$ onto the body-fixed z'-axis starts to be a good quantum number in this limit. For a general spherically symmetric pair potential the orbital momentum ℓ of $(a+c)$ subsystem will be the additional asymptotically good quantum number. Both can be used for the classification of the states. In order to distinguish between $(a+c)$ and $(b+c)$ asymptotic states the third quantum number $\alpha = a$ or b will be introduced. This specification allows one, for example, to consider $R_\Lambda\to\infty$ limit as $R\tau_a^{-1}\to\infty$ for $\alpha = a$ or as $R\tau_b^{-1}\to\infty$ for $\alpha = b$.

One can say that the solutions of (27) diagonalize the rotational coupling exactly but unfortunately only by some numerical procedure. Once equation (27) is solved, we can introduce the Born-Oppenheimer-like expansion for the solution of (26) ($\mathcal{J}, p$ indices for the solutions of (27) are omitted from now on)

$$\Psi^{J p}(R_\Lambda,\xi,\eta) = \sum_{\ell K\alpha}\tilde{\varphi}_{\ell K\alpha}(\xi,\eta;R_\Lambda)\,\chi_{\ell K\alpha}(R_\Lambda). \qquad (28)$$

Equation (26) projected onto the solutions of (27) provides the system of Schroedinger equations for $\chi_n(R_\Lambda)$. The index $n=\{\ell K\alpha\}$ enumerates a number of states that should be involved in a particular calculation. Those are chosen due to the following reasons. As far as we are interested in some specific two-body asymptotic states for reaction (1) these define at least two corresponding n. The simplest analysis of the $\mathcal{E}_n(R_\Lambda)$ behaviour supplies one with physical understanding of their particular role in the process involved. This is just due to the fact that $\mathcal{E}_n(R_\Lambda)$ are the generalized effective potentials that define molecular-like dynamics of the problem in question. Of course, we hope that only few of them are really important. This is a "definition" of a class of physical problems that should be treated in this way.

6. One Level Approximation: Classical Rotator Model

The success of the Born-Oppenheimer method is mainly due to a rather high accuracy of its simplest one-state approximation. The theory given in this paper should provide more accurate results also on that level of approximation as far as it incorporates additional operators into the generalized two-center operator (14). Its eigenfunctions should be chosen for the case of the zeroth total angular momentum $\bar{\mathcal{J}}$. If $\mathcal{J}\neq 0$ the generalized two-center Hamiltonian for the rotational states looks too much complicated. Recently, the one-level alternative was proposed for the states with normal parity $p = (-1)^{\mathcal{J}}$, $\mathcal{J} > 0$ /24/.

In that case the last term of the generalized two-center operator (20) is left out and in addition only $K = 0$ projection is used in the decomposition (24) of the total wave function. Under these simplifications the system of equations (27) is reduced to the only Schroedinger equation. The authors of /24/ have given no motivation for this approximation though σ -terms ($K = 0$) are known to be the most important in the Born-Oppenheimer method. The special choice of the rotational part of the total Hamiltonian in the form of (20a) can find justification in /25/, where the author declares that in two cases, where the Coriolis coupling can be eliminated with the help of redefinition of the body axes, the rotational part of the operator is transformed into the form (20a). The numerical example from /24/ also supports this model.

7. Scattering Amplitudes: Body Fixed to Laboratory Frame Transformation

The coupled system of Schroedinger radial-like equations for $X^{\mathcal{J}p}_{\ell K\alpha}(R_\Lambda)$ that follows from the Born-Oppenheimer ansatz (28) has the usual form

$$\left[-\frac{1}{2M}\left(\frac{1}{R_\Lambda}+\frac{d}{dR_\Lambda}\right)^2+\mathcal{E}^{\mathcal{J}p}(R_\Lambda)-\frac{3}{4MR_\Lambda^2}+\frac{1}{2M}\left(U^{\mathcal{J}p}+Q^{\mathcal{J}p}\frac{d}{dR_\Lambda}\right)\right]X^{\mathcal{J}p}=EX^{\mathcal{J}p}. \tag{29}$$

Here $\mathcal{E}^{\mathcal{J}p}(R_\Lambda)$ is the diagonal matrix from the generalized two-center problem (27). The matrix elements of $U^{\mathcal{J}p}$ and $Q^{\mathcal{J}p}$ are defined by

$$U^{\mathcal{J}p}_{ij}=\left\langle\frac{\partial\tilde{\varphi}_i}{\partial R_\Lambda}\,\middle|\,\frac{\partial\tilde{\varphi}_j}{\partial R_\Lambda}\right\rangle,\quad Q^{\mathcal{J}p}_{ij}=\left\langle\tilde{\varphi}_i\,\middle|\,\frac{\partial\tilde{\varphi}_j}{\partial R_\Lambda}\right\rangle,$$

$$Q_{ii}=0;\quad i,j=\{\ell,K,\alpha\}, \tag{30}$$

where $\tilde{\varphi}^{\mathcal{J}p}_i$ are the solutions of (27) corresponding to $\mathcal{E}^{\mathcal{J}p}_i$. In some way the matrices $U^{\mathcal{J}p}$ and $Q^{\mathcal{J}p}$ restore the radial coupling of the problem but this is an inherent feature of the Born-Oppenheimer scheme. It is rather straightforward to find the discrete spectrum of (29). It should be close to that of the total projected Hamiltonian (26) if our approximation is valid. In the case of the scattering process (1) we look for a body-frame solution $\Phi^{\ell m\alpha}$ with the initial relative motion to be in the direction of the laboratory z -axis

$$\Phi^{\ell m\alpha}(\vec{R}_\alpha,\vec{\tau}_\alpha)=exp(i\vec{K}_{\ell\alpha}\vec{R}_\alpha)\varphi_{\ell m}(\vec{\tau}_\alpha)$$
$$+\sum_{\ell'm'\alpha'}R^{-1}_{\alpha'}f^{\ell m\alpha}_{\ell'm'\alpha'}(\hat{R}_{\alpha'})\varphi_{\ell'm'}(\vec{\tau}_{\alpha'})exp(iK_{\ell'\alpha'}R_{\alpha'}), \tag{31}$$

where $\varphi_{\ell m}(\vec{\tau}_\alpha)=\tilde{\varphi}_\ell(\tau_\alpha)Y_{\ell m}(\hat{\tau}_\alpha)$ with $\alpha=a$ or b are the wave functions of the bound states for the scattering process (1) in the laboratory frame. The channel wave numbers are defined by

$$K^2_{\ell\alpha}=2M\rho_\alpha(E-\mathcal{E}^{\mathcal{J}p}_{\ell\alpha}(\infty)). \tag{32}$$

This equation follows from Schroedinger system (29) when the relation between R and R_Λ given by (15a) is used. Equations (29) had better to be solved in their original form with

$$(K^\Lambda_{\ell\alpha})^2=2M(E-\mathcal{E}^{\mathcal{J}p}_{\ell\alpha}(\infty))$$

so $K_{\ell\alpha}=K^\Lambda_{\ell\alpha}\rho^{1/2}_\alpha$ (32a). In the expressions for the channel wave

numbers $\mathcal{E}^{\mathcal{J}p}_{\ell\alpha}(\infty)$ provide the exact values of channel energies.

Our basic solutions $\Psi^{\mathcal{J}p\ell K\alpha}_M(\vec{R}_\Lambda,\vec{\tau}')$ with good quantum numbers $\mathcal{J}$ and p are now given by

$$\Psi^{\mathcal{J}p\ell K\alpha}_M(\vec{R}_\Lambda,\vec{\tau}')=\sum_{K'\ell'\alpha'}B^{\mathcal{J}p}_{MK'}(\alpha,\beta,\gamma)\tilde{\varphi}^{\mathcal{J}p}_{\ell'K'\alpha'}(\xi,\eta;R_\Lambda)X^{\mathcal{J}p\ell K\alpha}_{\ell'K'\alpha'}(R_\Lambda)R^{-1}_\Lambda, \tag{33}$$

where $\tilde{\varphi}^{\mathcal{J}p}(\xi,\eta;R_\Lambda)$ are the solutions of the generalized two-centern problem (27) and the expansion (28) was used. As $R_\Lambda\to\infty$ both $\tilde{\varphi}^{\mathcal{J}p}_{\ell K\alpha}$ and $B^{\mathcal{J}p}_{MK}$ are simplified:

$$\tilde{\varphi}^{\mathcal{J}p}_{\ell K\alpha}(\xi,\eta;R_\Lambda)\xrightarrow[R_\Lambda\to\infty]{}\tilde{\varphi}_\ell(\tau'_\alpha)Y_{\ell K}(\hat{\tau}'_\alpha)e^{-iK(\varphi-\pi/2)}$$
$$B^{\mathcal{J}p}_{MK}(\alpha,\beta,\gamma)\xrightarrow[R_\Lambda\to\infty]{}B^{\mathcal{J}p}_{MK}(\Phi,\theta,\varphi-\pi/2). \tag{33a}$$

For the functions $X^{\mathcal{J}p\ell K\alpha}_{\ell'K'\alpha'}(R_\Lambda)$ we have chosen the solution of (29) subject to the boundary conditions $X^{\mathcal{J}p\ell K\alpha}_{\ell'K'\alpha'}(0)=0$ and

$$X^{\mathcal{J}p\ell K\alpha}_{\ell'K'\alpha'}\xrightarrow[R_\Lambda\to\infty]{}\left(\frac{M}{K^\Lambda_{\ell'\alpha'}}\right)^{1/2}\left[\delta_{\ell\ell'}\delta_{KK'}\delta_{\alpha\alpha'}p(-1)^\ell e^{-iK^\Lambda_{\ell\alpha}R_\Lambda}\right.$$
$$\left.-S^{\mathcal{J}p}(\ell'K'\alpha'/\ell K\alpha)e^{iK^\Lambda_{\ell'\alpha'}R_\Lambda}\right] \tag{34}$$

The phase factor $p(-1)^\ell$ should be incorporated into the theory to simplify the presentation of the free motion term of (31) when it is transformed to the body-fixed system /26/. It is

$$exp(i\vec{K}_{\ell\alpha}\vec{R}_\alpha)\varphi_{\ell m}(\vec{\tau}_\alpha)\xrightarrow[R_\alpha\to\infty]{}$$
$$\frac{i}{2K_{\ell\alpha}R_\alpha}\sum_{p,L}(2L+1)\frac{1+p(-1)^{L+\ell}}{2}P_L(\cos\theta)\left[(-1)^Le^{-iK_{\ell\alpha}R_\alpha}-e^{iK_{\ell\alpha}R_\alpha}\right]\varphi_{\ell m}(\vec{\tau}_\alpha) \tag{35}$$
$$=\frac{i}{4K_{\ell\alpha}R_\alpha}\sum_{\mathcal{J}p}(2\mathcal{J}+1)\left[p(-1)^\ell e^{-iK_{\ell\alpha}R_\alpha}-e^{iK_{\ell\alpha}R_\alpha}\right]B^{\mathcal{J}p}_{mm}(\Phi,\theta,\varphi-\pi/2)\tilde{\varphi}_{\ell m\alpha}(\xi,\eta;\infty).$$

Now the scattering wave function $\Phi^{\ell m\alpha}(\vec{R}_\alpha,\vec{\tau}_\alpha)$ can be found by expansion

$$\Phi^{\ell m\alpha}(\vec{R}_\alpha,\vec{\tau}_\alpha)=\sum_{\mathcal{J},p,M}A(\mathcal{J},p,M,\ell,m,\alpha)\Psi^{\mathcal{J}p\ell K\alpha}_M(\vec{R}_\Lambda,\vec{\tau}'), \tag{36}$$

where $A(\mathcal{J},p,M,\ell,m,\alpha)$ should be given by

$$A(\mathcal{J},p,M,\ell,m,\alpha)=\frac{i}{4}(2\mathcal{J}+1)\delta_{mM}\delta_{|m|K}(M\cdot K^{\Lambda}_{\ell\alpha})^{-1/2} \qquad (37)$$

in order to provide the asymptotic form (31). A further body-fixed to space-fixed frame transformation should be applied /26/ to receive the expression for the scattering amplitude from (31)

$$f^{\ell m\alpha}_{\ell'm'\alpha'}(\theta,\Phi)=\frac{i}{4(K_{\ell\alpha}K_{\ell'\alpha'})^{1/2}}\left(\frac{M_\alpha}{M_{\alpha'}}\right)^{1/4}$$
$$\times\sum_{\mathcal{J}p\ell'\Omega\Omega'}\delta_{\Omega|m|}[1+p(-1)^{\ell-L'}](2\mathcal{J}+1)\,T^{\mathcal{J}p}(\alpha'\ell'\Omega'/\alpha\ell\Omega) \qquad (38)$$
$$\times C^{L'm'-m}_{\mathcal{J}-m\ell'm'}\,C^{L'0}_{\mathcal{J}-\Omega'\ell'\Omega'}\,\mathcal{D}^{L'}_{m'-m\,0}(\Phi,\theta,0).$$

In this expression the transition matrix

$$T^{\mathcal{J}p}=\delta_{\ell\ell'}\delta_{KK'}\delta_{\alpha\alpha'}-S^{\mathcal{J}p} \qquad (38a)$$

and the Clebsch-Gordon coefficients $C^{c\gamma}_{\alpha\alpha\beta\beta}$ are involved in summation.

The degeneracy-averaged scattered intensity is given by

$$I(\alpha'\ell'/\alpha\ell)=(2\ell+1)^{-1}K^{-1}_{\ell\alpha}K_{\ell'\alpha'}\sum_{m,m'}|f^{\ell m\alpha}_{\ell'm'\alpha'}(\theta,\Phi)|^2 \qquad (39)$$

and the integral cross section

$$\sigma(\alpha'\ell'/\alpha\ell)=\int_0^{2\pi}\int_0^{\pi}d\Phi\sin\theta d\theta\, I(\alpha'\ell'/\alpha\ell) \qquad (40)$$

is simplified to

$$\sigma(\alpha'\ell'/\alpha\ell)=\frac{\pi}{K^2_{\ell\alpha}}\sum_{\mathcal{J},p}(2\mathcal{J}+1)\,P^{\mathcal{J}p}(\alpha'\ell'/\alpha\ell), \qquad (41)$$

where average transition probabilities are defined by

$$P^{\mathcal{J}p}(\alpha'\ell'/\alpha\ell)=(2\ell+1)^{-1}\sum_{KK'}|T^{\mathcal{J}p}(\ell'K'\alpha'/\ell K\alpha)|^2\left(\frac{M_\alpha}{M_{\alpha'}}\right)^{1/2} \qquad (42)$$

The scattering amplitude from (38) is the main result of this paper. It was not possible to receive it without some or

other approximations involved in previous attempts /2,4,15/, because the asymptotically adequate two-center Hamiltonian was not available until now.

In the derivation of (38) we followed the paper by Pack /26/ where some important details can be found.

Summary

The formal theory for three-body rearrangement scattering processes in the molecular states approach was formulated for the first time without any difficulties with unphysical long-ranged couplings. The main idea used was to transform the traditional molecular three body Hamiltonian into the form that has neither radial nor angular coupling in the asymptotic region. Hence the wave function and the internal variables were to be changed.

The transformed Hamiltonian was projected onto the states with good quantum numbers of total angular momentum $\mathcal{J}$ and parity p, thus providing the system of Schroedinger equations in three variables. Two of these variables can be chosen to describe the fast subsystem. The relative Hamiltonian is to be reffered as dynamic two-center Hamiltonian for rotational states. Its eigenvalues and eigenvectors provide grounds for the Born-Oppenheimer like approach with original physical intuition but without tranditional asymptotic difficulties.

In this way the eigenvalues of the generalized adiabatic Hamiltonian (27) form the family of effective potentials for the radial-like system of the Schroedinger equations (29) in slow variable. The solution of this system for scattering states in the form (34) defines the body-fixed molecular state S-matrix $S^{\mathcal{J}p}$. The specific phase factor in (34) is chosen to simplify the matching of the general body-fixed solution (36) with the scattering solution of the usual form (31) given in the laboratory frame. The laboratory frame scattering amplitude (38) follows from this matching. If molecular states are really involved in the scattering process only those $\mathcal{E}^{\mathcal{J}p}_n(R_\Lambda)$ which are attractive and powerful enough to support the bound states are important for the scattering process. A further preliminary information is supplied by the general behaviour of the matrix elements of $U^{\mathcal{J}p}$ and $Q^{\mathcal{J}p}$ matrices which are sensitive to such specific phenomena as crossing and quasicrossing of $\mathcal{E}^{\mathcal{J}p}_n(R_\Lambda)$ that are very important for the dynamics of reaction (1).

As a result, only few matrix elements of $S^{J\rho}$ for a limited number of $\{J,\rho\}$ -pairs should be included into the summation (38) in order to derive the molecular state scattering amplitude. The important kinematical features are completely accounted for by the Clebsh-Gordon coefficients and the coefficients of the irreducible representations of the rotation group which are involved into summation. The angular distribution of the products of reaction (4) should be very sensitive to the particular form of the scattering amplitude (38) and we believe that it also can serve for parametrization of the accurate experimental differential cross-sections if the molecular description of process (1) is supposed to play a governing role.

Expression (38) for the scattering amplitude is a kind of the partial wave decomposition which is very close in structure to that of the usual theory of elastic two-particle scattering /3/. In our case partial amplitudes are much more complicated and the angular distribution of partial waves is accounted for by Wigner $\mathcal{D}$ -functions that depend on two angles which define the polar angles of the vector connecting the scattering products. From the formal point of view we have the case of multichannel scattering in a noncentral field. As usual, the partial wave representation of the scattering amplitude should be used in the low energy region where only few partial waves are really important.

The three-body Hamiltonian $H_{\Lambda\Omega}$ (19) was derived from the original Born-Oppenheimer adiabatic Hamiltonian (10) in order to describe exactly the effect of the pair collisions in a three-body system. The case of the triple collisions was not taken into account explicitly. Nevertheless, the R_Λ -part of $H_{\Lambda\Omega}$ coincides precisely with the hyperradial part of a three-body Laplacian which is a proper way to account for Fock's singularity /20/. It is clear that the rest of the Hamiltonian (19) can be given in the form of the "angular hyperspherical part" of a three-body Laplacian. Due to this fact one can say that we have established the connection between the Born-Oppenheimer and hyperspherical harmonics methods in a three-body problem.

At this point it should be mentioned that there exist recent calculations of the molecular-like systems in the hyperspherical basis /27/. The convergence of the method happened to be rather poor. In this paper we were going in the opposite direction. As the starting point the traditional molecular Hamiltonian was chosen and transformed to account better for the finite masses of the "centers".

The one-state Born-Oppenheimer-like calculations of the binding energies of ddd^* -system /23/ and the position of ($J=2$, $\rho=1$) resonance in $t\mu^- + t$ scattering proved that our approach describes the dynamics of a three-body system much better than the original Born-Oppenheimer method /24/.

In 1981 Fano /28/ put forward a program for a unified treatment of collisions in a system of few particles. In our paper this program is partially fulfilled.

Acknowledgements

The authors highly appreciate the useful comments of Prof. W.Sheid on reading the manuscript of this paper. The fruithful discussions with Dr.P.Fiziev were very helpful.

References:

1. Born M. and Oppenheimer J.R.: Ann.Phys. (Leipzig) 84, 457 (1927).
   Born M. and Huang K.: Dynamical Theory of Crystal Lattice. Oxford Univ.Press, London and New York, 1954.
2. Park J.Y., Scheid W., and Greiner W.: Phys.Rev. 20C, 188 (1979).
   Broglia R.A., Liotta R., Nilsson B.S. and Winther A.: Phys. Rep., 29C, 291 (1977).
3. Landau L.D. and Lifshitz E.M.: Quantum Mechanics. Pergamon, Oxford, 1965.
4. Vinitsky S.I. and Ponomarev L.I.: Sov.J.Part.Nucl., 13, 557 (1982).
5. Matveenko A.V.: JETP Lett., 40, 1329 (1984).
   Pack.R.T.: Phys.Rev., 32A, 2022 (1985).
   Macek J., Jerjian K.A.: Phys.Rev., 33A 233 (1986).
6. Power J.D.: Phys.Trans.Soc.Lond., A247, 663 (1973).
7. Judd B.E.: Angular Momentum Theory for Diatomic Molecules, Academic Press 1975.
8. Gocheva et al.: Phys.Lett., 153B, 349 (1985).
9. Frolov A.M., Efros V.D.: J.Phys. B18, L265 (1985).
10. Bunker P.R. and Moss R.E.: Mol.Phys., 33, 417 (1977).
11. Ponomarev L.I. Somov L.N. and Vukajlovic F.R.: J.Phys. B14, 591 (1981).
12. Smith F.T.: Phys.Rev. 179, 111 (1969).
    Delos J.B.: Rev.Mod.Phys.53, 287 (1981).
13. Matveenko A.V.: Proceedings of the X European Symposium on the Dynamics of Few-Body System, Balatonfured, Hungary (1985).

14. Matveenko A.V.: Proceedings of the 1983 RCNP International Symposium on Light Ion Reaction Mechanism, Osaka, 906 (1983).
15. Matveenko A.V. and Lovas I.: Nucl.Phys. A299, 333 (1978).
16. Matveenko A.V.: Phys.Lett. 129B, 11 (1983).
17. Soloviev E.A., Vinitsky S.I.: J.Phys. 18B L557 (1985).
18. Varshalovich D.A., Moskalev A.H., Khersonsky V.K.: Quantum Theory of the Angular Momentum, Nauka, Leningrad (1975).
19. Smirnov Yu.F., Shitikova K.V.: Sov.J.Part.Nucl., 8, 344 (1977). Ballot J.L., Fabre de la Ripelle M.: Ann.Phys. 127, 62 (1980).
20. Fock V: K.Norske Vidensk.Selsk.Forhandl. 31, 138 (1958). Klar H.: J.Phys. 18A, 1561 (1985).
21. Johnson B.R.: J.Chem.Phys.: 73, 5051 (1980); 79, 1906, 1916 (1983).
22. Macek J.H.: J.Phys.B1, 831 (1968).
23. Kaschiev M. and Matveenko A.V.: J.Phys., 18B, L645 (1985).
24. Kaschiev M., Matveenko A.V. and Revai J.: Phys.Lett. 162B (1985) 18.
25. Hori S.: Suppl.Prog.Theor.Phys.Extra Number (1968), 80.
26. Pack T.P.: Journ.Chem.Phys.: 60, 633 (1974).
27. Aquilanti V., Grossi G. and Lagana A.: Lett.Nuovo Cim., 41, 541 (1984). Green C.H.: Phys.Rev., 26A, 2974 (1982).
28. Fano U.: Phys.Rev. A24, 2402 (1981).

Received by Publishing Department
on July 10, 1986.

SUBJECT CATEGORIES OF THE JINR PUBLICATIONS

Index	Subject
1.	High energy experimental physics
2.	High energy thooretical physics
3.	Low energy experimental physics
4.	Low energy theoretical physics
5.	Mathematics
6.	Nuclear spectroscopy and radiochemistry
7.	Heavy ion physics
8.	Cryogenics
9.	Accelerators
10.	Automatization of data processing
11.	Computing mathematics and technique
12.	Chemistry
13.	Experimental techniques and methods
14.	Solid state physics. Liquids
15.	Experimental physics of nuclear reactions at low energies
16.	Health physics. Shieldings
17.	Theory of condenced matter
18.	Applied researches
19.	Biophysics

Матвеенко А.В., Абэ Я.

E4-86-467

Асимптотически корректные молекулярные состояния в задаче трех тел

В задаче трех тел впервые построена формальная теория рассеяния с перераспределением частиц. Рассеяние происходит через стадию образования квазимолекулы, для описания которой ранее использовался метод Борна - Оппенгеймера. Построено преобразование гамильтониана Борна - Оппенгеймера, приводящее к асимптотически корректной формулировке теории.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1986

Matveenko A.V., Abe Y.

E4-86-467

Asymptotically Adapted Three-Body Molecular States

For the first time formal theory for three-body rearrangement scattering processes in the molecular state approach was formulated encounting no difficulties with unphysical long-ranged couplings.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1986