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ON BETWEEN THE BORN - OPPENHEIMER AND HYPERSPHERICAL COORDINATE METHODS IN A THREE - BODY PROBLEM

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1. INTRODUCTION

It has recently been experienced that rather different three-body pure Coulombic systems H_2^+ or HD^+ (molecular type)[1,2], He (atomic type)[3], and eee^+ ("nuclear" type)[4,5] can be treated on the same footing. The method is based on the old adiabatic idea of Born and Oppenheimer[6] of molecular physics. The details of their argumentation do not matter here, we shall simply suppose that the Schrödinger equation of a system should approximately be separable though we do not yet know in which coordinates. In order to find those coordinates we start with the pure molecular system HD^+, where the adiabatic idea works excellently and try to extend it to the others. As far as it is now believed[7] that the Born-Oppenheimer description is also applied to the physical problems with short interaction our analysis should actually be applicable also in that case. In a more general context, we are looking for the most convenient form of the kinetic energy operator for a three-particle system from both the physical and numerical points of view.

2. LANGUAGE
## 2.1. Nonrotational Three-Body States with HD⁺-Ion as an Example

We use m_a and m_b for the masses of heavier particles and m_c for that of a valence particle. Figure 1 shows the triangle of the particles with τ_a, τ_b, R being the interparticle distances. These are in turn used to define the prolate spheroidal coordinates[8]

$$\xi = \frac{\tau_a + \tau_b}{R} \quad , \quad \eta = \frac{\tau_a - \tau_b}{R}. \tag{1}$$

The molecular Jacobi reduced masses are

$$M = m_a \cdot m_b / (m_a + m_b), \quad m = m_c (m_a + m_b)/(m_a + m_b + m_c) \tag{2}$$

So, three coordinates ξ, η, R are enough to describe the deformation of the triangle from Figure 1 due to the Schrödinger equation
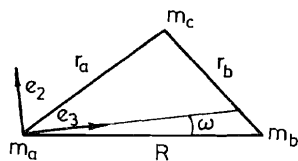
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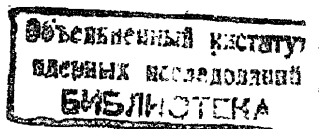
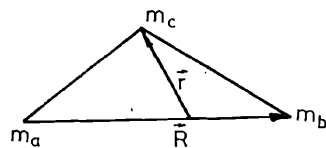Fig.1. Three-body triangle. Principal axes of the inertia tensor are indicated.

Fig.2. Molecular Jakobi coordinates for a three-body description.

$$H_{BO}^{J=0} \Psi(R,\xi,\eta) = E \Psi(R,\xi,\eta). \qquad (3)$$

The precise form of $H_{BO}^{J=0}$ can be found elsewhere[8]; it includes the Hamiltonian of the fast subsystem

$$\hbar = -\frac{1}{2m} \Delta_{\xi\eta} + V \qquad (4)$$

where $\Delta_{\xi\eta}$ is a $\{\xi,\eta\}$ part of the Laplace operator and $V = v_a(z_a) + v_b(z_b) + v_c(R)$, as usual. The standard procedure of the Born-Oppenheimer method is to approximate the wave function from (3) by the form

$$\Psi(R,\xi,\eta) = \Upsilon(\xi,\eta;R)\psi(R), \qquad (5)$$

where $\Upsilon(\xi,\eta;R)$ is the solution of the two-center problem

$$\hbar \Upsilon = \mathcal{E}(R)\Upsilon \qquad (6)$$

for the ground state with $\mathcal{E}(R)$ being its eigenvalue. After calculating $\mathcal{E}(R)$ and $\Upsilon(\xi,\eta;R)$ the molecular vibrational spectrum is defined from

$$\left[-\frac{1}{2M}\left(\frac{1}{R} + \frac{d}{dR} \right)^2 + \langle \Upsilon | H_{BO}^{J=0} | \Upsilon \rangle \right] \psi(R) = E^{\nu} \psi(R). \qquad (7)$$

Here the matrix element of $H_{BO}^{J=0}$ contains the adiabatic potential

$\mathcal{E}(R)$ from (6) and the adiabatic corrections to it. One can easily imagine a formal procedure in which the solution of the total Schroedinger equation (3) is searched in a form of the expansion over the total set of solutions of the two-center problem (6). In that case the operators from $H_{BO}^{J=0}$ generate matrix elements and equation (7) turns into the system of Schroedinger equations. These matrix elements exibit an unphysical asymptotic behaviour as $R \to \infty$, the so-called long-ranged radial and angular couplings. The operators forcing these couplings include cross derivatives of the type $\frac{\partial}{\partial R}\frac{\partial}{\partial \xi}$ and $\frac{\partial}{\partial R}\frac{\partial}{\partial \eta}$, thus mixing the fast $\{\xi,\eta\}$, and slow $\{R\}$ degrees of freedom.

Here, we introduce the inertia tensor components

$$I_1 = MR^2 \rho \quad , \quad I_2 + I_3 = I_1 \qquad (8)$$

with the principal axes $\vec{e}_2$ and $\vec{e}_3$, being given in Figure 1. The function of coordinates and masses of the system ρ from (7) has recently[8] been used in order to get rid of the cross-derivative terms in $H_{BO}^{J=0}$ by the transformation

$$H_{\Lambda} = exp(-\Lambda) H_{BO}^{J=0} exp(\Lambda) \qquad (9)$$

with the generator $\Lambda = \ln(\sqrt{\rho})R\left(\frac{1}{R} + \frac{\partial}{\partial R}\right)$. The Hamiltonian H_{Λ} is of a rather simple form

$$H_{\Lambda} = \hbar_{\Lambda} - \frac{1}{2M}\left(\frac{\partial^2}{\partial R^2} + \frac{5}{R}\frac{\partial}{\partial R} \right) - \frac{3}{2}\frac{1}{MR^2} \cdot \qquad (10)$$

where the redefined Hamiltonian of the fast subsystem $\hbar_{\Lambda}$ is given by

$$\hbar_{\Lambda} = -\frac{\rho^2}{2m}\Delta_{\xi\eta} + \sqrt{\rho}\,V . \qquad (11)$$

The formal simplicity of H_{Λ} is related with an important physical feature of $\hbar_{\Lambda}$, providing the exact dissociation limit of the molecule. That was not the case for the operator (4).

2.2. Rotational States

When the particles from Figure 1 are allowed to rotate (Figure 2) we need six coordinates R, Θ, Φ, ξ, η, γ to describe the system. Here $\{\Theta,\Phi\}$ are the polar angles of vector $\vec{R}$ and γ measures the angle of the rotation of the plane of the triangle, $\vec{R}$ being the axis of rotation. The original Born-Oppenheimer (molecular) Schroedinger equation takes the form

$$H_{BO}\Psi(R,\xi,\eta,\Theta,\Phi,\gamma) = E\,\Psi(R,\xi,\eta,\Theta,\Phi,\gamma),\qquad(12)$$

where[10]

$$H_{BO} = H_{BO}^{\gamma=0} + \frac{\vec{J}^2 - 2\vec{J}\cdot\vec{\ell}}{2MR^2}.\qquad(13)$$

The Λ-transformation commutes with both $\vec{J}^2$ and $\vec{J}\cdot\vec{\ell}$ so that the experience of the previous section can be used without any change but an additional attention should be paid to the long-ranged angular coupling term $\vec{J}\cdot\vec{\ell}$ that contains $\frac{\partial}{\partial\Theta}\frac{\partial}{\partial\xi}$, $\frac{\partial}{\partial\Phi}\frac{\partial}{\partial\eta}$ cross derivatives. This coupling was transformed[10] in order to make it zero in the fragmentation regions ($R\to\infty$, $\xi\to 1$, $\eta\to\pm 1$), where a molecule dissociates into an atom and a core. The resulting Hamiltonian $H_{\Lambda\Omega}$ is obtained by

$$H_{\Lambda\Omega} = e^{-\Omega}\,e^{-\Lambda}\,H_{BO}\,e^{\Lambda}\,e^{\Omega},\qquad(14)$$

where a new generator $\Omega = -i\omega J_1$ was introduced with J_1 being the projection of the total angular momentum onto the normal to the plane of the particle triangle, ω giving the angle between vector $\vec{R}$ and the nearest principal axis of the inertia tensor, which is known to be in the plane of the triangle. The transformed Hamiltonian can be written in the form

$$H_{\Lambda\Omega} = h_{\Lambda\Omega} - \frac{1}{2M}\left(\frac{\partial^2}{\partial R^2} + \frac{5}{R}\frac{\partial}{\partial R}\right) - \frac{3}{2MR^2},\qquad(15)$$

where $h_{\Lambda\Omega}$ should be referred to as the dynamical two-center operator for the rotational states. One further step of notation was proposed for practical purposes[11] (see also[12])

$$h_{\Lambda\Omega} = h_{\Lambda} + T_R + T_{Coriolis},\qquad(16)$$

where

$$T_R = \frac{1}{2}\left(\frac{J_1^2}{I_1} + \frac{J_2^2}{I_2} + \frac{J_3^2}{I_3}\right)\qquad(17)$$

is the operator of the classical rotator of the problem. By comparing the Born-Oppenheimer total Hamiltonian (13) with the transformed $H_{\Lambda\Omega}$, we note the important features of the resemblence and repudiation. Both utilize the idea of quasiseparation of the degrees of freedom. In the case of $H_{\Lambda\Omega}$ this quasiseparation turns into an exact separation in the fragmentation regions. The operator of radial coupling was diagonalized exactly while that of the angular coupling only asymptotically. The main rotational part was changed from that of a spherical rotator to an asymmetric top operator. The natural behaviour of $H_{\Lambda\Omega}$ in the fragmentation regions can be utilized[13] in producing the formal molecular-state scattering theory without unphysical difficulties of the traditional molecular-state approach[14].

2.3. Change of the Language

The effect of Λ and Ω transformation is equivalent to the change of slow variable R to $R_{\Lambda} = \sqrt{\rho}\,R$ and of the angular variables $\{\Theta,\Phi,\gamma\}$ to $\{\alpha,\beta,\gamma\}$ that are the Euler angles of the rotation putting the original laboratory axes $\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$ into the principal axes (body-fixed) of the inertia tensor of the system[10]. The Λ-transformation also changes the Hilbert space, where Hamiltonian acts.[13]. The change of the molecular Jacobi coordinates is accompanied by the change of the Jacobi reduced masses M and m to the effective coordinate dependent masses $M\rho$ and m/ρ having the property of reproducing the reduced masses of fragments in the fragmentation regions[8].

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The Born-Oppenheimer method was transformed into a hyper-spherical coordinates way of treating a three-body problem[16,17].

2.4. Backspace

In order to restore the Born-Oppenheimer description on a new level, we introduce the partial wave decomposition of the eigenfunction of $H_{\Lambda\Omega}$ by

$$\psi_M^{Jp} = \sum_{k=0}^{J} B_{MK}^{Jp}(\alpha,\beta,\gamma)\, \psi_K^{Jp}(R_\Lambda,\xi,\zeta) \qquad (18)$$

with the angular part B_{MK}^{Jp} producing the exact quantum numbers of total angular momentum J and parity p

$$B_{MK}^{Jp} = \mathcal{D}_{-M-K}^{J}(\alpha,\beta,\gamma) + P(-1)^J \mathcal{D}_{-MK}^{J}(\alpha,\beta,\gamma). \quad (19)$$

After projecting onto B_{MK}^{Jp}, $H_{\Lambda\Omega}$ is brought into the matrix Hamiltonian

$$H_{\Lambda\Omega}^{Jp} = h_{\Lambda\Omega}^{Jp} - \frac{1}{2M}\left(\frac{\partial^2}{\partial R_\Lambda^2} + \frac{5}{R_\Lambda}\frac{\partial}{\partial R_\Lambda}\right) - \frac{3}{2MR_\Lambda^2} \quad (20)$$

that contains the other matrix operator $h_{\Lambda\Omega}^{Jp}$ - the Hamiltonian of the dynamical two-center problem with exact quantum numbers. The eigenfunctions of $h_{\Lambda\Omega}^{Jp}$ are to be used in the Born-Oppenheimer like decomposition of $\psi_K^{Jp}(R_\Lambda,\xi,\zeta)$ from (18).

3. ILLUSTRATIVE MATERIAL

3.1. Exact Shroedinger Molecular-Like Equation for (J = 1, p =-1) State of (dtμ)$^+$ Ion

We materialize the ideas given above using a weakly bound state of (dtμ)$^+$ ion that have become very popular lately[18-20] due to its role in the μ-catalyzed fusion[21]. We are sure that the equations sketched below are nicely suited for a precise calculation of this state.

With $m_a = m_d$, $m_b = m_t$ and $m_c = m_\mu$ and leaving J, p, M indices out, we have in this case

$$B_0 = 2\mathcal{D}_{-M0}^{1}(\alpha,\beta,\gamma);\ B_1 = \mathcal{D}_{-M-1}^{1}(\alpha,\beta,\gamma) + \mathcal{D}_{-M1}^{1}(\alpha,\beta,\gamma) \quad (21)$$

for non-normalized B_{MK}^{Jp} from (18). The exact wave function looks like

$$\overline{\Psi} = B_0\, \psi_0(R_\Lambda,\xi,\zeta) + B_1\, \psi_1(R_\Lambda,\xi,\zeta). \quad (22)$$

The nontrivial part $h_{\Lambda\Omega}^{Jp}$ of projected $H_{\Lambda\Omega}^{Jp}$ (20) has the form

$$h_{\Lambda\Omega} = \begin{pmatrix} t & t_{12} \\ t_{12} & t \end{pmatrix} + \begin{pmatrix} v_0 & 0 \\ 0 & v_1 \end{pmatrix} \quad (23)$$

with the precise form of t, t_{12}, v_0 and v_1 being easily extracted[10,13]. The three-dimensional system of Schroedinger equations will be

$$\left(H_{\Lambda\Omega} - E\right)\begin{pmatrix} \psi_0(R_\Lambda,\xi,\zeta) \\ \psi_1(R_\Lambda,\xi,\zeta) \end{pmatrix} = 0. \quad (24)$$

After specifying the boundary conditions ($0 \le R_\Lambda < \infty$, $1 \le \xi < \infty$, $-1 \le \zeta \le 1$), the system (24) can be solved if a 3d code is available. If not, we can simplify the task.

3.2. Improved Born-Oppenheimer Description

A 2d code should be used to provide the eigenvalues and eigenfunctions of the problem

$$\left[h_{\Lambda\Omega} - \varepsilon(R_\Lambda)\right]\begin{pmatrix} \psi_0(\xi,\zeta;R_\Lambda) \\ \psi_1(\xi,\zeta;R_\Lambda) \end{pmatrix} = 0. \quad (25)$$

After that the adiabatic decomposition of the type

$$\Psi_K\left(R_\Lambda, \xi, \gamma\right) = \sum_n \Upsilon_K^{(n)}(\xi, \gamma, R_\Lambda) \chi_K^{(n)}(R_\Lambda), \quad K = 0, 1 \qquad (26)$$

can be introduced for the exact wave function of the state. The number of states in (26) should be limited, which is an approximation. On the other hand, the minimal physically meaningful decomposition (26) should include two states of the problem (25), which are to be chosen by their asymptotic behaviour as $R_\Lambda \to \infty$; $\varphi^{(a)}$ and $\varphi^{(\beta)}$ are such that

$$\mathcal{E}^{(a)} \xrightarrow[R_\Lambda \to \infty]{} -\frac{1}{2}\frac{m_t \cdot m_\mu}{m_t + m_\mu},$$

$$\mathcal{E}^{(\beta)} \xrightarrow[R_\Lambda \to \infty]{} -\frac{1}{2}\frac{m_d \cdot m_\mu}{m_d + m_\mu}. \qquad (27)$$

This choice is due to the quasidegeneracy of (27) and to the experience gained in earlier calculations[9].

3.3. Classical Rotator Model

A further simplification of the numerical task is achieved if we adopt the classical rotator model[11], in that case $h_{\Lambda\Omega}$ is substituted by

$$h_{\Lambda\Omega}^R = h_\Lambda + T_R \qquad (28)$$

from (16) with $T_{Coriolis}$ being omitted. The justification of this step can be found in ref.[12].

4. RESULTS

With two eigenstates of the operator (28) classified by the conditions (27), we have tried the improved Born-Oppenheimer decomposition (26) of the total wave function ($K = 0, n = a, \beta$).

Thus we have got $E_R = 0.44$ eV for the binding energy of the weakly bound state of $(dt\mu)^+$ ion, which should be compared with $E = 0.656 \pm 0.001$ eV from 844 -state approximation[18] of the usual Born-Oppenheimer scheme. In that case they have no binding at all if the number of states is less than eight. The important feature of the new basis should be mentioned. The spectrum of the operator (25) is discrete[22].

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и метода гиперсферических функций в задаче трех тел

В работе предложен новый метод расчета трехчастичных систем, который является объединением двух старых и хорошо известных подходов: метода Борна-Оппенгеймера и метода гиперсферических функций. Слабосвязанное состояние $(dt\mu)^+$ иона используется для демонстрации достоинств этого метода.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Matveenko A.V.   E4-86-568

On between the Born-Oppenheimer and Hypersperical
Coordinate Methods in a Three-Body Problem

An original method for the calculation of three-body systems is given which is also a combination of two old and well-khown approaches. The weakly bound state of $(dt\mu)^+$ ion is used to demonstrate the merits of the new way.

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