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LETTER TO THE EDITOR

Suitable coordinates for the three-body problem in the adiabatic representation

E A Soloviev† and S I Vinitsky

Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, 141 980 Head Post Office, PO Box 79, 101 000 Moscow, USSR

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Abstract. A set of coordinates suitable for the three-body problem is introduced. In this case the three-body wavefunction possesses the remarkable property of being compatible with the physical boundary conditions in the adiabatic representation.

The adiabatic representation of the three-body problem is widely used in research on slow atomic and mesonic atomic collisions (Bates and Reid 1968, Komarov *et al* 1976, Delos 1981, Vinitsky and Ponomarev 1982, Ponomarev 1983). However, for a correct solution of the scattering problem in this approach it is necessary to use a large number of basis adiabatic wavefunctions even if the number of opened channels is small (Ponomarev and Vinitsky 1979, Ponomarev *et al* 1981). For the case of slow mesonic atomic collisions this complicated problem was solved straightforwardly by specially constructed algorithms (Melezhik *et al* 1983, 1984, Melezhik 1984). A more conventional approach consists in the construction of the adiabatic basis which is as compatible as possible with the physical boundary conditions corresponding to an infinite distance between scattering fragments. Usually this construction is made by some modification of the traditional basis of the Coulomb two-centre problem (Ponomarev *et al* 1980, Delos 1981). One may also try to find the compatible adiabatic basis (CAB) directly. This promising approach was adopted by Matveenko (1983, 1984), but his procedure of regrouping the total Hamiltonian into fast and slow parts was rather cumbersome.

In this letter we would like to propose some new coordinates for the three-body problem, which facilitate the construction of the CAB. These coordinates can be considered as suitable as they asymptotically transform into standard Jacobi coordinates of all three corresponding channels in terms of which the physical boundary conditions are normally formulated (see figure 1).

Let us consider a system of three particles a, b and c with masses M_a, M_b and M_c, respectively, and in addition let $M_{a,b} > M_c = 1$ (e.g. the heavy particles a, b are nuclei and the light particle c is a muon or electron). For simplicity we shall assume that the total angular momentum of the system $J = 0$. However, the results will be valid in the general case as well. In the adiabatic representation of the three-body problem the independent variables are usually the vectors $\boldsymbol{R}$ connecting nuclei a and b and

$$\boldsymbol{r}' = \boldsymbol{r}/R \tag{1}$$

† Permanent address: Department of Theoretical Physics, Institute of Physics, Leningrad State University, 198904, Leningrad, USSR.

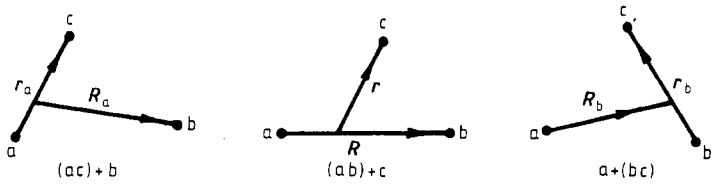

Figure 1. Three Jacobi coordinate systems for relative coordinates of two heavy particles a, b and a light particle c.

where the vector $\boldsymbol{r}$ connects the centre of mass of the nuclei (CMN) with the light particle c. The components of $\boldsymbol{r}'$ are defined in the body-fixed frame with Z' axis directed along the internuclear vector $\boldsymbol{R}$. The origin of such a frame may be placed at any point of R, e.g. at the CMN, at the geometrical centre, or at nuclei. This translational freedom is due to the scale transformation (1) and will be used in the analysis of the boundary conditions.

In the coordinates $\boldsymbol{R}$, $\boldsymbol{r}'$ the Schrödinger equation for the three-body system, after separation of the motion of the centre of mass of the whole system, takes the form (Vinitsky and Ponomarev 1974, 1982) in the units $M_c = \hbar = 1$:

$$\left[-\frac{1}{2M}\frac{1}{R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R}+\frac{1}{MR^2}(\boldsymbol{r}'\cdot\nabla_{\boldsymbol{r}'})\left(1+R\frac{\partial}{\partial R}\right)-\frac{1}{2m}\frac{\rho}{R^2}\Delta_{\boldsymbol{r}'}+V\right]\Psi = E\Psi \tag{2}$$

where $M^{-1} = M_a^{-1}M_b^{-1}$, $m^{-1} = 1+(M_a+M_b)^{-1}$, $\rho = 1+mr'^2/M$, $V = V_{ac}+V_{bc}+V_{ab}$, V_{ij} being the pair interaction energy. Equation (2) contains the cross derivative with respect to $\boldsymbol{r}'$ and R, which for $R\to\infty$ gives a constant component of the non-diagonal matrix elements of the total Hamiltonian in the traditional adiabatic basis (Faifman *et al* 1976). This leads to intertwining of a large number of basis functions even in the asymptotic regions of the configuration space and thus to the artificial extension of the R-integration region.

Instead of R let us introduce the new variable

$$\mathcal{R} = \sqrt{\rho}\,R \tag{3}$$

and represent the wavefunction in the form

$$\Psi = \mathcal{R}^{-3/2}\sqrt{\rho}\,\chi. \tag{4}$$

The normalisation of Ψ to unity in the initial coordinates $\boldsymbol{R}$, $\boldsymbol{r}$ leads to the same normalisation of χ in the new coordinates $\mathcal{R}$, $\boldsymbol{r}'$ with the volume element

$$\mathrm{d}\tau = 4\pi\mathcal{R}^2\,\mathrm{d}\mathcal{R}\,\rho^{-2}\,\mathrm{d}\boldsymbol{r}'.$$

After the transformations (3) and (4) the Schrödinger equation (2) takes the form

$$\mathcal{H}\chi = E\chi \qquad \mathcal{H} = -\frac{1}{2M}\frac{1}{\mathcal{R}^2}\frac{\partial}{\partial\mathcal{R}}\mathcal{R}^2\frac{\partial}{\partial\mathcal{R}}-\frac{1}{2m}\frac{\rho^2}{\mathcal{R}^2}\Delta_{\boldsymbol{r}'}+\frac{3}{8M\mathcal{R}^2}+V. \tag{5}$$

This equation has no cross derivative, but contains all those specific properties of the initial equation (2), which make the adiabatic separation of variables in the coordinates $\mathcal{R}$, $\boldsymbol{r}'$ justifiable. Indeed, in this case we have the new slow variable $\mathcal{R}$, whereas the

changed Hamiltonian of the fast subsystem may be written as follows

$$h = -\frac{1}{2m}\frac{\rho^2}{\mathcal{R}^2}\Delta_{r'} + V. \tag{6}$$

The CAB is defined by the total set of the eigenfunctions f_k of the new two-centre problem

$$hf_k(\boldsymbol{r}', \mathcal{R}) = E_k(\mathcal{R})f_k(\boldsymbol{r}', \mathcal{R}) \tag{7}$$

where $E_k(\mathcal{R})$ are the energy terms of the fast subsystem characterised by a set of quantum numbers k for the fixed $\mathcal{R}$. After averaging the total Hamiltonian $\mathcal{H}$ over the basis functions f_k the terms $E_k(\mathcal{R})$ play the role of new effective potentials. It is clear that the above mentioned intertwining problem does not arise in this approach.

Now let us consider the properties of the coordinates $\mathcal{R}$, $\boldsymbol{r}'$ in asymptotic regions of the configuration space corresponding to different reaction channels. We shall examine the case when the particle b goes to infinity, while the particles a and c remain in a bound state, i.e. the channel (ac)+b (for the channel a+(bc) indices a and b should be interchanged). Let us place the origin of the body-fixed frame for $\boldsymbol{r}'$ at the nucleus a and factorise into two parts the factor $m^{-1}\rho^2/\mathcal{R}^2$ of the Laplace operator $\Delta_{r'}$ in the Hamiltonian h of the fast subsystem (6), namely, $m^{-1}\rho^2/\mathcal{R}^2 = (1/m\rho^{-1})(\rho/\mathcal{R}^2)$. The factor $\rho/\mathcal{R}^2 = R^{-2}$ combined with the variable $\boldsymbol{r}'$ of $\Delta_{r'}$ gives the initial scale of length (1) and so permits the change from $\boldsymbol{r}'$ to the Jacobi vector $\boldsymbol{r}_a$ connecting nucleus a and light particle c. The remaining factor $m\rho^{-1}$ gives the correct reduced mass of the atomic complex (ac):

$$m\rho^{-1} \xrightarrow[Rr_a^{-1}\to\infty]{} (1+M_a^{-1})^{-1} = m_a.$$

The variable $\mathcal{R}$ in this limit becomes proportional to the modulus of the Jacobi vector $\boldsymbol{R}_a$ connecting the centre of mass of the atomic complex (ac) with the nucleus b:

$$\mathcal{R} \xrightarrow[Rr_a^{-1}\to\infty]{} \alpha|\boldsymbol{R} - (1+M_a)^{-1}\boldsymbol{r}_a| = \alpha R_a \tag{8}$$

where $\alpha = (m/m_a)^{1/2}$. Then in the Hamiltonian (5) we obtain the correct reduced mass of the complex (ac)+b:

$$\mu_a = M\alpha^2 = M_b(1+M_a)/(1+M_a+M_b)$$

as the reciprocal factor of the second derivative with respect to R_a. It can be easily verified that at finite R and $r\to\infty$ the coordinates $\mathcal{R}$, $\boldsymbol{r}'$ turn into the Jacobi coordinates r, $\boldsymbol{R}$ of the corresponding third channel (ab)+c. Thus, in all three asymptotic regions of the configuration space the coordinates $\mathcal{R}$, $\boldsymbol{r}'$ transform into corresponding standard Jacobi coordinates.

At first glance the Hamiltonian (5) almost exactly coincides with that obtained by Matveenko (1983, 1984), a slight discrepancy is explained by a different wavefunction normalisation. However, in those papers the new variable $\mathcal{R}$ was erroneously identified with the old variable R, thus making interpretation of the results obtained there impossible.

The approach developed here is a quantum analogue of the method of non-stationary scale of length (MNSL) elaborated for the case of the classical treatment of the nuclear motion. This method was used by Soloviev (1976) for a thorough study of the exactly solvable model of a particle in a field of two uniformly moving δ potentials, and also by the same author (Soloviev 1982) for establishing a simple

relation between non-stationary wavefunctions of a free particle and of an oscillator. To make this analogy more evident, let us call the basic points of the MNSL.

When the motion of the nuclei is treated classically, for the light particle the non-stationary Schrödinger equation in the CMN ($m = \hbar = 1$) holds:

$$[-\tfrac{1}{2}\Delta_{r'} + V_{ac}(|\boldsymbol{r} + \gamma_a \boldsymbol{R}|) + V_{bc}(|\boldsymbol{r} + \gamma_b \boldsymbol{R}|)]\psi = i\,\partial\psi/\partial t \tag{9}$$

where $\gamma_a = M_b/(M_a + M_b)$, $\gamma_b = -M_a/(M_a + M_b)$, $R(t) \equiv R$ is the distance between nuclei a and b, which is assumed to be a given function of time. For the case considered here ($J = 0$) we shall assume that the nuclei are moving along a straight line, e.g., along the Z axis. Introducing the variable

$$\boldsymbol{r}' = \boldsymbol{r}/R(t) \tag{10}$$

we rewrite the Schrödinger equation (9) in the form

$$[-\tfrac{1}{2}R^{-2}\Delta_{r'} + V_{ac}(R|\boldsymbol{r}' + \gamma_a \boldsymbol{k}|) + V_{bc}(R|\boldsymbol{r}' + \gamma_b \boldsymbol{k}|) + iR^{-1}\dot{R}(\boldsymbol{r}' \cdot \nabla_{r'})]\psi = i\,\partial\psi/\partial t \tag{11}$$

where $\boldsymbol{k}$ is the unit vector of the Z axis, and the dot means the time derivative. As a consequence of using the moving body-fixed frame (10) in equation (11) there appears the product of the relative momentum of nuclei and that of a light particle (cf equation (2)). To eliminate this product, one should explicitly separate, in the wavefunction, the general translation factor that takes into account the change of kinematics (10)

$$\psi = R^{-3/2}\exp(\tfrac{1}{2}ir^2R^{-1}(t)\dot{R}(t))\chi(\boldsymbol{r}', t) = R^{-3/2}\exp(\tfrac{1}{2}ir'^2R(t)\dot{R}(t))\chi(\boldsymbol{r}', t) \tag{12}$$

this factorisation being suggested by analogy with the Galilean transformation (see, e.g. Delos 1981). The factor $R^{-3/2}$ in (12) provides the normalisation of the wavefunction χ in the new coordinates r' (cf equation (4)). Substituting (12) into (11) we get for the function χ the following equation

$$\begin{aligned} &h_{cl}\chi = i\,\partial\chi/\partial t \\ &h_{cl} = -\tfrac{1}{2}R^{-2}\Delta_{r'} + V_{ac}(R|\boldsymbol{r}' + \gamma_a \boldsymbol{k}|) + V_{bc}(R|\boldsymbol{r}' + \gamma_b \boldsymbol{k}|) + \tfrac{1}{2}R\ddot{R}r'^2. \end{aligned} \tag{13}$$

The reduction of ψ to χ is analogous to introducing in the quantum case the variable $\mathscr{R}$ instead of R. In both the cases there occurs a partial extraction of the motion of a light particle from the Hamiltonian of the fast subsystem, leading to the elimination of the product of momenta.

When the adiabatic basis is used for solving equation (9), there also appear difficulties due to incompatibility of the asymptotic behaviour of the adiabatic wavefunction with the exact boundary conditions at $R \to \infty$ (Bates and McCarroll 1958). The reason is that the adiabatic wavefunctions do not contain the Galilean translation factor that takes account of the motion of the potential centres. The transformations (10) and (12) remove this drawback. In the modified Schrödinger equation (13) the centres are fixed, therefore, here we have the CAB. Indeed, in the asymptotic region the general translational factor which relates χ to ψ becomes the standard Galilean translation factor, namely, near the i centre i = a, b as $R \to \infty$ we have

$$\exp(\tfrac{1}{2}ir^2R^{-1}\dot{R}) \xrightarrow[R|r+\gamma_i R|^{-1}\to\infty]{} \exp[i(\boldsymbol{v}_i\boldsymbol{r} - \tfrac{1}{2}v_i^2 t)] \tag{14}$$

where $\boldsymbol{v}_i = -\gamma_i\dot{R}\boldsymbol{k}$ is the velocity of the i centre. Equation (14) has been derived under the assumptions that at $R \to \infty$ the value of v_i tends to be constant and $|\gamma_i|R \simeq v_i t$.

Note that the Hamiltonian h_{cl} (13) has only a discrete spectrum when $\ddot{R} > 0$. As will be seen later, in a quantum case the Hamiltonian of the fast subsystem (6) also possesses this useful property. The coordinates $\mathcal{R}$, r' introduced above are connected with other coordinates used in the three-body problem. The slow coordinate $\mathcal{R}$ is related by $\sqrt{M}\,\mathcal{R} = \mathcal{R}_G$ with the hyperradius $\mathcal{R}_G$ of the sphere on a four-dimensional space, in which the three-body problem may be treated (Demiralp and Suhubi 1977). From our variables one may pass to the hyperspherical coordinates by introducing angular variables α, ϑ, φ:

$$\cot \alpha/2 = (m/M)^{1/2} r' \qquad \cos \vartheta = z'/r' \qquad \tan \varphi = y'/x'$$

and returning to the initial wavefunction Ψ. Then the Schrödinger equation for Ψ acquires the form (Fock 1954)

$$\left(-\frac{1}{2}\frac{1}{\mathcal{R}_G^5}\frac{\partial}{\partial \mathcal{R}_G}\mathcal{R}_G^5\frac{\partial}{\partial \mathcal{R}_G} - \frac{2}{\mathcal{R}_G^2}\square^* + V\right)\Psi = E\Psi$$

where

$$\square^* = \frac{1}{\sin^2 \alpha}\left(\frac{\partial}{\partial \alpha}\sin^2 \alpha \frac{\partial}{\partial \alpha} + \frac{1}{\sin \vartheta}\frac{\partial}{\partial \vartheta}\sin \vartheta \frac{\partial}{\partial \vartheta} + \frac{1}{\sin^2 \vartheta}\frac{\partial^2}{\partial \varphi^2}\right)$$

is the angular part of the Laplace operator in the four-dimensional space $\{\mathcal{R}_G, \alpha, \vartheta, \varphi\}$. In general, to construct the adiabatic representation of the three-body problem one may use a wide set of coordinates on the four-dimensional sphere: spherical, toroidal, elliptic-cylindrical, generalised elliptic coordinates (Klein 1966, Kalnins *et al* 1976), allowing the separation of variables in the kinetic-energy operator, i.e. in $\square^*$ of the fast subsystem Hamiltonian $h_G = -2R_G^{-2}\square^* + V$. Then the adiabatic wavefunctions depend on these angular variables for any fixed value of $\mathcal{R}_G$ and the Hamiltonian h_G has only a discrete spectrum. For systems of type e^+H, e^-H, $e^-e^-e^+$ the adiabatic basis is usually formed in hyperspherical coordinates (Macek 1968, Fano 1976, Pelikan and Klar 1983). However, for the systems like mesonic molecules $dd\mu$, $dt\mu$ or molecular ions HD^+ it is more natural to use the spheroidal coordinates $\{\xi, \eta, \varphi\}$ (Komarov *et al* 1976) connected with $r' = \{x', y', z'\}$ by relations

$$x' = \tfrac{1}{2}[(\xi^2 - 1)(1 - \eta^2)]^{1/2} \cos \varphi \qquad y' = \tfrac{1}{2}[(\xi^2 - 1)(1 - \eta^2)]^{1/2} \sin \varphi$$
$$z' = \tfrac{1}{2}[\xi\eta - (M_b - M_a)/(M_b + M_a)].$$

In the given case the coordinates $\{\xi, \eta, \varphi\}$ are preferable, since due to the smallness of parameter m/M the Hamiltonian (6) differs slightly from that of the Coulomb two-centre problem, and as a result, nodal surfaces of the adiabatic wavefunctions f_k tend to the coordinate surfaces $\xi = \text{constant}$, $\eta = \text{constant}$, $\varphi = \text{constant}$.

The logarithmic singularities in the three-body problem are well known at the point of triple collision (Fock 1954) and are related only with the motion over $\mathcal{R}_G$. Therefore in the adiabatic separation of variables in (5) these singularities cannot influence the CAB itself and will be described by the wavefunction of the slow subsystem in terms of the variable $\mathcal{R}$.

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