Spheroidal and hyperspheroidal coordinates in the adiabatic representation of scattering states for the Coulomb three-body problem

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Abstract.

Recently, an involved approach has been used (2008 *Journal of Physics* B: *At. Mol. Opt. Phys.* **41** 175201) to introduce a separable adiabatic basis into the hyperradial adiabatic (HA) approximation. The aim was to combine the separability of the Born-Oppenheimer (BO) adiabatic basis and the better asymptotic properties of the HA approach. Generalizing this results we present here three more different separable bases of the same type by making use of a previously introduced adiabatic hamiltonian expressed in hyperspheroidal coordinates (1983 *Phys. Lett.* **B129** 11). In addition, we propose a robust procedure which accounts in a stepwise procedure for the unphysical couplings that are inherently present in the hyperradial adiabatic multichannel scattering approach. The advantages of the new approach are demonstrated on the example of the basic reaction in muon-catalyzed fusion physics $d\mu + t \rightarrow t\mu + d$.

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1. Introduction

For the investigation of the system of two protons and an electron, i.e. the hydrogen molecular ion H_+^2, the celebrated Born-Oppenheimer (BO) adiabatic approach has been popular from the very early days of quantum mechanics. Herein, the total wave function of the system is searched in the form of the adiabatic expansion (we restrict ourselves for simplicity to non-rotational states with $J = 0$ with the exception of Sec. 6)‡

$$\Psi_{BO}(R, \xi, \eta) = \sum_i \tilde{\chi}_i(R)\tilde{\phi}_i(R|\xi, \eta). \tag{1}$$

Here, R is the internuclear distance: the spheroidal coordinates ξ and η are famous since they allow for a separable representation of the adiabatic basis function (for fixed R)

$$\tilde{\phi}_i(R|\xi, \eta) = g_i(R|\xi)f_i(R|\eta). \tag{2}$$

Hence, with $\tilde{\phi}_i(R|\xi, \eta)$ available in simple form the multichannel Schrödinger equation for the components $\tilde{\chi}_i(R)$ which describe the internuclear motion are easily obtained. This system is, however, unfortunately also notorious for its unphysical large-R behavior.

In the hyperradial adiabatic (HA) approach a similar adiabatic expansion of the total wave function is applied,

$$\Psi_{HA}(\mathcal{R}, \xi, \eta) = \mathcal{R}^{-5/2} \sum_i \chi_i(\mathcal{R})\varphi_i(\mathcal{R}|\xi, \eta). \tag{3}$$

Here, $\mathcal{R}$ denotes the hyperradius of the system. One advantage of this method is that the asymptotic behavior, although not unproblematic, is not so severe as in the BO case. On the other hand, the useful separability of the adiabatic basis is lost in the HA approach.

In [1] the declared aim was to have the combination of these two approaches. For this purpose the separable Coulomb two-center problem solutions of the BO adiabatic approach were introduced into the hyperradial-adiabatic analysis by making use of hyperspheroidal coordinates $(\mathcal{R}, \xi, \eta)$. We note that earlier theoretical [2, 3, 4, 5, 7, 8, 9, 10] and numerical work [11, 12, 13] in which these coordinates had already been introduced and applied has been completely ignored.

We start by recalling that the spheroidal ($H(R, \xi, \eta)$) and the hyperspheroidal ($\mathcal{H}(\mathcal{R}, \xi, \eta)$) hamiltonians are related by a similarity transformation[2, 10]. Then, by using $H(R, \xi, \eta)$ we discuss chances for improving the asymptotic behavior of the BO adiabatic basis. Next, we consider $\mathcal{H}(\mathcal{R}, \xi, \eta)$ and its adiabatic part in order to introduce three different separable adiabatic hamiltonians for fixed hyperradius $\mathcal{R}$ which, following [1], have a proper large-$\mathcal{R}$ pair energy behavior. Finally, we sum up the critical analysis of the hyperradial adiabatic method [4] and present a novel way for overcoming its defects in multichannel scattering applications.

2. Spheroidal and hyperspheroidal coordinates

We consider three charged particles having masses m_i, position vectors $\mathbf{x}_i$, $(i = 1, 2, 3)$, and charges $Z_1Z_2 > 0, Z_1Z_3 < 0$. The familiar separable Coulomb two-center solutions that form the basis of the BO adiabatic approach (1), solve the eigenvalue equation

$$\tilde{h}(R|\xi, \eta)\tilde{\phi}_i(R|\xi, \eta) = \tilde{\epsilon}_i(R)\tilde{\phi}_i(R|\xi, \eta), \tag{4}$$

with the adiabatic Hamiltonian

$$\tilde{h}(R|\xi, \eta) = -\frac{2}{\mu R^2}\hat{a} + V, \quad V = \frac{Z_1Z_2}{R} - \frac{2Z_1Z_3}{R(\xi + \eta)} - \frac{2Z_2Z_3}{R(\xi - \eta)}, \tag{5}$$

and volume element

$$\widetilde{d\tau} = (\,\xi^2 - \eta^2)\; d\xi d\eta. \tag{6}$$

Here, $\tilde{h}(R|\xi, \eta)$ is part of the total hamiltonian

$$\tilde{H} = -\frac{2\rho(\xi, \eta)}{\mu R^2}\hat{a} - \frac{1}{2M}\left(\frac{1}{R} + \frac{\partial}{\partial R}\right)^2 + \frac{1}{MR}\hat{q}\left(\frac{1}{R} + \frac{\partial}{\partial R}\right) + V \tag{7}$$

which, for simplicity, is written down here for non-rotational states only.

‡ In the overall CM system we need only three internal coordinates to characterize any three-body state.

As is well-known, introduction of prolate spheroidal coordinates $\xi \in [1,\infty)$ and $\eta \in [-1,1]$, defined by

$$r_1 = R(\xi+\eta)/2,\ r_2 = R(\xi-\eta)/2, \tag{8}$$

with $R = |\mathbf{x}_2 - \mathbf{x}_3|$, $r_1 = |\mathbf{x}_1 - \mathbf{x}_3|$, and $r_2 = |\mathbf{x}_2 - \mathbf{x}_3|$, renders the eigenvalue problem (4) separable (cf. (2)) and, thus, greatly simplifies the analysis. The following abbreviations are used:

$$\begin{array}{lcl}
\hat{a} & = & \dfrac{1}{\xi^2-\eta^2}\left[\dfrac{\partial}{\partial\xi}(\xi^2-1)\dfrac{\partial}{\partial\xi} + \dfrac{\partial}{\partial\eta}(1-\eta^2)\dfrac{\partial}{\partial\eta}\right], \\
\hat{q} & = & \dfrac{1}{\xi^2-\eta^2}\left[(\xi-\kappa\eta)(\xi^2-1)\dfrac{\partial}{\partial\xi} + (\eta-\kappa\xi)(1-\eta^2)\dfrac{\partial}{\partial\eta}\right], \\
\rho(\xi,\eta) & = & 1+\tilde{\alpha}(\xi^2+\eta^2-2\kappa\xi\eta+\kappa^2-1), \\
\tilde{\alpha} & = & \mu/(4M), \\
\kappa & = & (m_2-m_1)/(m_2+m_1), \\
1/M & = & 1/m_1+1/m_2, \\
1/\mu & = & 1/m_3+1/(m_1+m_2).
\end{array} \tag{9}$$

Units $\mu = e = \hbar = 1$ are chosen.

The hyperradial counterpart of the total hamiltonian (7) can be derived by the similarity transformation [2, 10],

$$\mathcal{H} = \exp(-\Lambda)\tilde{H}\exp\Lambda, \quad \Lambda = \ln\sqrt{\rho(\xi,\eta)}\ \left(1+R\frac{\partial}{\partial R}\right), \tag{10}$$

yielding§

$$\mathcal{H} = h(\mathcal{R}|\xi,\eta) - \frac{1}{2M}\frac{1}{\mathcal{R}^5}\frac{\partial}{\partial\mathcal{R}}\mathcal{R}^5\frac{\partial}{\partial\mathcal{R}}, \tag{11}$$

$$h(\mathcal{R}|\xi,\eta) = -\frac{\rho^2(\xi,\eta)}{2\mu\mathcal{R}^2}\hat{a} + \frac{\sqrt{\rho(\xi,\eta)}}{\mathcal{R}}\left[Z_1Z_2 - \frac{2Z_1Z_3}{\xi+\eta} - \frac{2Z_2Z_3}{\xi-\eta}\right], \tag{12}$$

with hyperradius

$$\mathcal{R} = R\sqrt{\rho(\xi,\eta)} = R\sqrt{1+(r/R)^2\mu/M} \tag{13}$$

and volume element

$$d\tau = \widetilde{d\tau}/\rho^2(\xi,\eta). \tag{14}$$

We point out that in [1] an alternative introduction of the hyperspherical coordinates $(\mathcal{R},\xi,\eta)$ is given via non-trivial geometric considerations. But the corresponding adiabatic hamiltonian (12) could not be derived.

3. Exact atomic energies and adiabatic hamiltonians

The standard *BO* adiabatic hamiltonian (5) is well-known to lead in the pair collision limits $R\to\infty, \xi\to 1, \eta\to\pm1$, to inaccurate atomic energies

$$\tilde{\epsilon}_{i,n}(\infty) = \frac{Z_i^2Z_3^2}{2n^2}\mu, \quad i=1,2, \tag{15}$$

since μ, as given by (9), does not coincide with any one of the exact reduced atomic masses $\mu_1 = m_1m_3/(m_1+m_3)$ or $\mu_2 = m_2m_3/(m_2+m_3)$. One obvious remedy consists in incorporating the mass polarization term occurring in (7) into the kinetic energy operator part of (5),

$$\tilde{h}_1(R|\xi,\eta) = -\frac{2\rho(\xi,\eta)}{\mu R^2}\hat{a} + V. \tag{16}$$

The result is that the new effective mass $\mu/\rho(\xi,\eta)$ is found to reproduce in the pair collision limits the appropriate reduced masses

$$\mu_1 := \mu/\rho_-, \quad \mu_2 := \mu/\rho_+, \text{ with } \rho_\pm := \rho(1,\pm1), \tag{17}$$

§ The Λ-transformation (10) results in a change of the variables and of the functional form [11, 10].

for the two available channels. But the welcome separability of the *BO* hamiltonian (5) is lost. In addition, (16) is no longer self-adjoint. This latter defect can, however, be easily cured by including one more operator from the total hamiltonian (7), leading to

$$\begin{aligned}\tilde{h}_2 &= \tilde{h}_1 + \hat{q}/(MR^2) \\ &= -\frac{2}{\mu R^2}\frac{1}{\xi^2-\eta^2}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\rho(\xi,\eta)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\rho(\xi,\eta)\frac{\partial}{\partial\eta}\right] + V.\end{aligned} \tag{18}$$

This hamiltonian has been discussed in [14].

Of course, if one insists in a *BO* treatment of having a two-center hamiltonian which is separable and has eigenvalues possessing an exact large-R behavior, the standard trick

$$\tilde{h} = \tilde{h}_{AS} + (\tilde{h} - \tilde{h}_{AS}) \tag{19}$$

always works where $\tilde{h}_{AS}$ is chosen separable and asymptotically good. In this case an extra operator $(\tilde{h} - \tilde{h}_{AS})$ is to be moved into the matrix elements of non-adiabatic corrections.

The hyperradial adiabatic eigenvalue equation

$$h(\mathcal{R}|\xi,\eta)\varphi_i(\mathcal{R}|\xi,\eta) = \varepsilon_i(\mathcal{R})\varphi_i(\mathcal{R}|\xi,\eta) \tag{20}$$

describes the motion of a quasi-particle with mass $\mu/\rho^2(\xi,\eta)$ in a renormalised interaction potential $\sqrt{\rho(\xi,\eta)}V$ (cf. (12)). As indicated, the hamiltonian depends parametrically on the hyperradius $\mathcal{R}$. As $\mathcal{R}\to\infty$ and the system disintegrates into atom plus nucleus, $\rho(\xi,\eta)$ approaches asymptotically constant values, leading to spectra of the type (15) but with the proper values of the reduced masses μ_i for the two channels (17).

With (20) at hand and using a decomposition of the type (19) we can easily produce three replicas of the main results from [1], i.e., separable hyperradial adiabatic hamiltonians $h_{AS}(\mathcal{R}|\xi,\eta)$ each with a renormalised constant mass μ^{ren} and renormalised charges Z_i^{ren}. They are separable (for fixed $\mathcal{R}$) similar

Table 1.

μ^{ren}	Z_i^{ren}	Z_2^{ren}
$\mu/(\rho_-\rho_+)$	$Z_1\sqrt{\rho_+}$	$Z_2\sqrt{\rho_-}$
μ/ρ_-^2	$Z_1\sqrt{\rho_-}$	$Z_2(\rho_-/\sqrt{\rho_+})$
μ/ρ_+^2	$Z_1(\rho_+/\sqrt{\rho_-})$	$Z_2\sqrt{\rho_+}$

to the *BO* hamiltonian (5), but with the interparticle distance R replaced by the hyperradius $\mathcal{R}$. Note that the first one is symmetric with respect to the two nuclei while for identical nuclei all three cases coincide.

In [1] possible advantages of a separable hyperradial adiabatic approach are discussed in detail so that we just mention its serious drawbacks. Firstly, the matrix elements of the rather complicated operator $h(\mathcal{R}|\xi,\eta) - h_{AS}(\mathcal{R}|\xi,\eta)$ that appears as non-adiabatic correction of the hamiltonian require for their evaluation 2-dimensional quadratures which in general is a heavy numerical task. Secondly, the separable hamiltonian is Hermitian with the volume element (6) while the volume element of the total hamiltonian (11) is $\mathcal{R}^5 d\mathcal{R} d\tau$ with $d\tau$ given by (14) which also entails severe numerical complications‖. Consequently, the enthusiasm with respect to any separable hyperradial adiabatic approach such as the one displayed in [1] requires thorough substantiation by numerical work.

But it should be kept in mind that even the *HA* approach by itself is not free of defects. The next section aims at curing its unphysical features.

4. Definition of free dynamics in the multichannel *HA* scattering

In the *HA* approach, starting from the hamiltonians (11) and (12) and the eigenvalue equation (20) leads to a representation of the total wave function of the three-body system in the form (3). After integration over the variables ξ and η (or any other pair of internal hyperspherical angles) one arrives at the following system of coupled hyperradial equations which in matrix form read as

$$\left[-\frac{1}{2M}\frac{d^2}{d\mathcal{R}^2}\mathbf{1} + \boldsymbol{\varepsilon}(\mathcal{R}) + 2\mathbf{Q}(\mathcal{R})\frac{d}{d\mathcal{R}} + \mathbf{W}(\mathcal{R})\right]\boldsymbol{\chi}(\mathcal{R}) = E\boldsymbol{\chi}(\mathcal{R}). \tag{21}$$

‖ This complication was not addressed in [1]. We also note that the content of the very last paragraph of [1] should be clarified. Contrary to what is stated there, also standard *HA* variational bases can be constructed with states that generate eigenvalues converging to the three-body break-up limit as, e.g., those shown in Eq. (6) of [20].

The elements of the matrices $\mathbf{Q}(\mathcal{R})$ and $\mathbf{W}(\mathcal{R})$ that constitute the non-adiabatic corrections are given as usual by

$$Q_{ij}(\mathcal{R}) = -\frac{1}{2M}\left\langle \varphi_i(\mathcal{R}|\xi,\eta)\left|\frac{d}{d\mathcal{R}}\varphi_j(\mathcal{R}|\xi,\eta)\right.\right\rangle \tag{22}$$

and

$$W_{ij}(\mathcal{R}) = -\frac{1}{2M}\left\langle \varphi_i(\mathcal{R}|\xi,\eta)\left|\frac{d^2}{d\mathcal{R}^2}\varphi_j(\mathcal{R}|\xi,\eta)\right.\right\rangle. \tag{23}$$

$\boldsymbol{\varepsilon}(\mathcal{R})$ denotes the diagonal matrix of eigenvalues and $\boldsymbol{\chi}(\mathcal{R})$ the column vector solution.

In contrast to [1] where it is written that 'We did not study the asymptotics of the matrix elements at large $\mathcal{R}$ in detail as it is not necessary for the statement of the scattering problem' we consider this question as being of fundamental importance. This our contrarian opinion is illustrated by a study of the asymptotic behavior of the corresponding matrix elements for the physical three-charged particle system consisting of antiproton, electron and proton (see also [15]). Fig. 1 shows our calculated hyperradial-adiabatic potential $\epsilon_{11}(\mathcal{R})$ (i.e., the 11th eigenvalue) and the corresponding effective potential $\varepsilon_{11}(\mathcal{R}) + W_{11,11}(\mathcal{R})$ which includes the nonadiabatic corrections calculated with (20). Although both

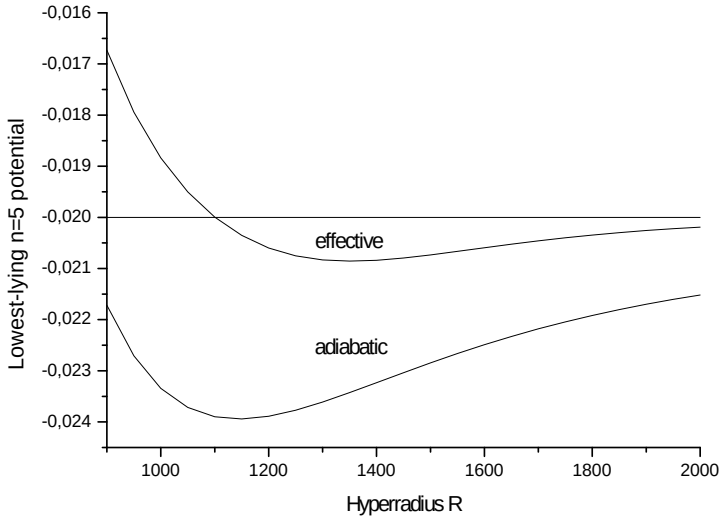

Figure 1. Lowest adiabatic potential of the (n=5)-subset without (adiabatic) and with (effective) nonadiabatic correction. Both curves approach the proper energy of the $(p\bar{p})$ atom (in units $\mu = 1$), shown as a horizontal line.

curves tend asymptotically to the proper $(p\bar{p})_{n=5}$ energy level the speed is drastically different. The reason is that the former contains an unphysical attractive $1/\mathcal{R}-$like tail which, however, is sufficiently accurately compensated for a large region of $\mathcal{R}$-values by the diagonal matrix element $W_{11,11}(\mathcal{R})$ of the non-adiabatic corrections. Obviously, for this particular system the size of corrections is enormous and thus is expected to strongly influence the convergence rate of the scattering observables (see, e.g. [17]). In this context we would like to point to the universal fact that within the HA approach also non-diagonal corrections that couple channels converging to the same configuration but containing different states of the atom can show the same long-range behavior $\sim O(1/\mathcal{R})$ (see the discussion in [11, 12, 16]).

In order to enhance the convergence and to minimize the range of $\mathcal{R}$ that should be used in the numerical solution of the scattering problem (21) the following robust procedure is suggested. To be specific consider the physical reaction

$$(d\mu^-)_{1s} + t \to (t\mu^-)_{1s} + d, \tag{24}$$

which has been thoroughly investigated in earlier days [16]. The asymptotic form of the solution of (21) we search in the usual form

$$\boldsymbol{\chi}(\mathcal{R}) \sim \left[e^{-iK\mathcal{R}} - e^{iK\mathcal{R}}\mathbf{S}\right]\mathbf{B}, \text{ for } \mathcal{R}\to\infty, \tag{25}$$

that includes the incoming ($\exp\{-iK\mathcal{R}\}$) and outgoing ($\exp\{iK\mathcal{R}\}$) spherical waves, the $S-$matrix and a matrix $\mathbf{B}$ of arbitrary coefficients. Clearly, the S-matrix includes the kinematic effects of using the hyperradius instead of the appropriate Jacobi variables.

This fact suggests to first solve two auxiliary HA problems that physically represent the motion of the corresponding atoms with respect to a neutral "particle" with mass of the remaining third particle,

$$(d\mu^-)_{1s} + m_t \to (d\mu^-)_{1s} + m_t, \text{ with } V = V_{d\mu^-}, V_{dt} = V_{t\mu^-} = 0, \tag{26}$$

and

$$(t\mu^-)_{1s} + m_d \to (t\mu^-)_{1s} + m_d, \text{ with } V = V_{t\mu^-}, V_{dt} = V_{d\mu^-} = 0. \tag{27}$$

These processes are trivial in the appropriate Jacobi variables since the corresponding eigenfunctions are just products of hydrogen-like functions and plane waves. But when studying them in the HA approach they incorporate the same kinematic inadequacy as the original reaction (24).

The HA ansatz (3) leads to the system of equations like (21). Asymptotically the solution for the reaction (26) behaves as

$$\boldsymbol{\chi}^{d\mu^-}(\mathcal{R}) \sim \left[e^{-iK\mathcal{R}} - e^{iK\mathcal{R}}\mathbf{S}^{d\mu^-}\right]\mathbf{B}^{d\mu^-}, \text{ for } \mathcal{R} \to \infty, \tag{28}$$

and for (27) as

$$\boldsymbol{\chi}^{t\mu^-}(\mathcal{R}) \sim \left[e^{-iK\mathcal{R}} - e^{iK\mathcal{R}}\mathbf{S}^{t\mu^-}\right]\mathbf{B}^{t\mu^-}, \text{ for } \mathcal{R} \to \infty. \tag{29}$$

As was demonstrated in [4] the "eigenvalues" and "non-adiabatic corrections" for these auxiliary "reactions" look very much alike those of the physical problem (24) and, what is to be particularly stressed here, the large-$\mathcal{R}$ behavior of the corresponding matrices $\mathbf{Q}^{d\mu^-}, \mathbf{Q}^{t\mu^-}, \mathbf{W}^{d\mu^-}$, and $\mathbf{W}^{t\mu^-}$ reproduce those for the corresponding quantities of the original physical problem (24). That is, these two free-motion problems look like a multichannel scattering problem in the HA approach where two different fragmentation channels are described using the same hyperradius $\mathcal{R}$.

Thus, the basic idea is to construct incoming and outgoing waves that produce a unit S-matrix for the auxiliary problems shown above, and use them in the physical problem (24). In a first step we combine the solutions $\boldsymbol{\chi}^{d\mu^-}$ and $\boldsymbol{\chi}^{t\mu^-}$ into a common wave function

$$\bar{\boldsymbol{\chi}} = \begin{pmatrix} \boldsymbol{\chi}^{d\mu^-} \\ \boldsymbol{\chi}^{t\mu^-} \end{pmatrix}, \tag{30}$$

which asymptotically behaves as

$$\bar{\boldsymbol{\chi}}(\mathcal{R}) \sim \left[e^{-iK\mathcal{R}} - e^{iK\mathcal{R}}\bar{\mathbf{S}}\right]\mathbf{A}, \tag{31}$$

with the S-matrix

$$\bar{\mathbf{S}} = \begin{pmatrix} \mathbf{S}^{d\mu^-} & 0 \\ 0 & \mathbf{S}^{t\mu^-} \end{pmatrix}. \tag{32}$$

Let us rewrite (31) as

$$\bar{\boldsymbol{\chi}}(\mathcal{R}) \sim \left[e^{-iK\mathcal{R}}\bar{\mathbf{S}}^{-1/2} - e^{iK\mathcal{R}}\bar{\mathbf{S}}^{1/2}\right]\bar{\mathbf{S}}^{1/2}\mathbf{A} \tag{33}$$

$$=: \left[\bar{\boldsymbol{\chi}}^{(-)}(\mathcal{R}) - \bar{\boldsymbol{\chi}}^{(+)}(\mathcal{R})\right]\bar{\mathbf{A}}. \tag{34}$$

Then all unphysical couplings inherent in the HA approach are seen to have been incorporated in the distorted free incoming and outgoing waves $\bar{\boldsymbol{\chi}}^{(-)}(\mathcal{R})$ and $\bar{\boldsymbol{\chi}}^{(+)}(\mathcal{R})$. We call them hyperradius- distorted free waves ($HDFW$).

For the physical problem (24) we rewrite the asymptotic solution (25), making use of the distorted free waves $\bar{\boldsymbol{\chi}}^{(\pm)}$,

$$\begin{aligned} \boldsymbol{\chi}(\mathcal{R}) &\sim [e^{-iK\mathcal{R}}\bar{\mathbf{S}}^{-1/2}\bar{\mathbf{S}}^{1/2} - e^{iK\mathcal{R}}\bar{\mathbf{S}}^{1/2}\bar{\mathbf{S}}^{-1/2}\mathbf{S}]\mathbf{B} \\ &= [\bar{\boldsymbol{\chi}}^{(-)}(\mathcal{R})\bar{\mathbf{S}}^{1/2} - \bar{\boldsymbol{\chi}}^{(+)}(\mathcal{R})\bar{\mathbf{S}}^{-1/2}\mathbf{S}]\mathbf{B} \\ &= [\bar{\boldsymbol{\chi}}^{(-)}(\mathcal{R}) - \bar{\boldsymbol{\chi}}^{(+)}(\mathcal{R})\bar{\mathbf{S}}^{-1/2}\mathbf{S}\bar{\mathbf{S}}^{-1/2}]\bar{\mathbf{S}}^{-1/2}\mathbf{B} \\ &=: [\bar{\boldsymbol{\chi}}^{(-)}(\mathcal{R}) - \bar{\boldsymbol{\chi}}^{(+)}(\mathcal{R})\mathcal{S}]\bar{\mathbf{B}}, \end{aligned} \tag{35}$$

so that we get for the physical scattering matrix

$$\mathcal{S} = \bar{\mathbf{S}}^{-1/2}\mathbf{S}\bar{\mathbf{S}}^{-1/2}. \tag{36}$$

The advantage of such an approach is evident: all unphysical long-range effects of the HA approach have been incorporated in the similar but numerically simpler auxiliary problems (26) and (27).

Consequently, the final calculation of the scattering observables for the physically interesting reaction (24) is expected to show a much faster convergence in reaching their asymptotic values than in the original version of the method.

This expectation is borne out by the calculations of the elastic cross-section of the reaction (24). The multistate HA approximation of [17] produced $2.15 * 10^{-20} cm^2$ for this value ($E = 10^{-2}$ eV), which is here compared with available two state results from the Table 2. The best adiabatic (BA) calculations [22] utilized an adiabatic expansion in which molecular states are constructed in Jacobi coordinates. Our result (second line of the Table 2) demonstrates the noticeable improvement over the traditional HA approach (first line of the Table 2).

Table 2. Elastic cross-section (in units of $10^{-20} cm^2$) for $(d\mu^-)_{1s} + t \to (t\mu^-)_{1s} + d$ collisions. The center-of-mass incident energy $E = 10^{-2}$ eV . Two state approximations have been utilized.

	Elastic cross-section
HA [17]	2.39
HDFW (36)	2.21
BA [22]	2.13

5. Angular couplings in the adiabatic approach

Till now we have limited our discussion to the case of total angular momentum $J = 0$. The general total hamiltonian in the coordinates (R, ξ, η) or $(\mathcal{R}, \xi, \eta)$ can be found in [4] where we commented on the fact that the Λ-transformation (10) commutes with the angular part of the total BO hamiltonian thus leaving it identical in both adiabatic approaches. This means that the unphysical long-range angular coupling of the BO approach survive in the HA case and, thus, render the scattering equation (21) difficult to tackle. Earlier we suggested two ways to handle this difficulty. First, some time ago it has been shown that a suitable choice of the body-fixed quantization axis allows minimization of these unphysical long-range rotational couplings [3]. Secondly, within the HA approach they even can be eliminated exactly [5, 13]. This latter proposal has already been used in [13] in a rotationally invariant calculation of the eigenvalue for $(J = 31, \pi = -1)$-symmetry states of H_2^+.

6. Conclusions

Boundary conditions for the radial multichannel Schrödinger equation that arises in the BO adiabatic approximation were discussed in [19], with the suggestion that the corresponding scattering theory "requires serious investigation". Note that here some matrix elements of the non-adiabatic couplings asymptotically approach non-zero constant values. We think that no scattering theory is possible in such a case.

In the HA approach the matrix elements of (22) and (23) behave asymptotically like $1/\mathcal{R}$ which simplifies the problem but the matrix elements of angular couplings are as long-range as they were in the BO case, i.e., untractable. In previous section we have referred to two methods of how to circumvent this problem.

Finally, the separable basis in the HA treatment of the scattering problem can be easily calculated using standard codes but introduces, as discussed at the end of Sec. 3, additional numerical complications in the corresponding multichannel scattering theory. We think that the original HA basis is much more adequate even numerically since in this case only two additional matrices (22) and (23) must be calculated. In this case an analytic analysis of asymptotic couplings is also possible [16, 21].

In conclusion we expect that the HA approach supplemented with the elimination of the unphysical couplings along the lines developed in this paper, i.e., using $HDFW$, should be effective. The numerical example from the previous section supports our conjecture.

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References

[1] Abramov D I 2008 *Journal of Physics* B: *At. Mol. Opt. Phys.* **41** 175201
[2] Matveenko A V 1983 *Phys. Lett.* **B129** 11
[3] Matveenko A V and Abe Y 1987 Few-Body Syst. **2** 127
[4] Matveenko A V and Fukuda H 1996 *Journal of Physics* B: *At. Mol. Opt. Phys.* **B29** 1575
[5] Matveenko A V 2001 *Journal of Physics* B: *At. Mol. Opt. Phys.* **34** L87
[6] Matveenko A V 2001 *Phys. Rev. Lett.* **86** 746
[7] Bunker P R and Moss R E 1977 *Mol. Phys.* **33** 425
[8] Moss R E and Sadler I A 1988 *Mol. Phys.* **64** 165
[9] Moss R E 1993 *Mol. Phys.* **78** 371
[10] Moss R E and Sadler I A 1989 *Mol. Phys.* **66** 591
[11] Hara S, Fukuda H, Ishihara T and Matveenko A V 1988 *Phys. Lett.* **A130** 22
[12] Hara S, Fukuda H and Ishihara T 1989 *Phys. Rev.* **A39** 35
[13] Matveenko A V, Alt E O and Fukuda 2001 *Few-Body Syst. Suppl.* **13** 140
[14] Kaschiev M and Matveenko A V 1985 *Journal of Physics* B: *At. Mol. Opt. Phys.* **18** L645
[15] Esry B D and Sadeghpour H R 2003 *Phys. Rev.* **A67** 012704
[16] Fukuda H, Ishihara T and Hara S 1990 *Phys. Rev.* **A41** 145
[17] Igarashi A, Toshima N and Shirai T 1994 *Phys. Rev.* **A50** 4951
[18] Fukuda H and Ishihara T 1992 *Phys. Rev.* **A46** 5531
[19] Korobov V I 1994 *Journal of Physics* B: *At. Mol. Opt. Phys.* **27** 733
[20] Rost J M and Briggs J S 1988 *Journal of Physics* B: *At. Mol. Opt. Phys.* **21** L233
[21] Klar H 1985 *Journal of Physics* A:*Math. and General* **A18** 1561
[22] Kobayashi K, Ishihara T and Toshima N 1988 *Muon Catalyzed Fusion* **2** 191