

Definition of an appropriate free dynamics and the physical S -matrix in multichannel hyperradial adiabatic scattering

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Abstract. In the hyperradial adiabatic (HA) treatment of the three-body problem the total wave function is expanded as $\Psi_{HA}(\mathcal{R}, \xi, \eta) = \mathcal{R}^{-5/2} \sum_i \chi_i(\mathcal{R}) \varphi_i(\mathcal{R}|\xi, \eta)$, where \mathcal{R} denotes the hyperradius and (ξ, η) are internal hyperangles. Integration over ξ and η converts the Schrödinger equation into a system of coupled hyperradial equations. It is a well-known fact that, within the HA approach, the non-adiabatic corrections that couple channels converging to the same asymptotic configuration can show an unphysical long-range behavior $\sim 1/\mathcal{R}$. Though the latter is of purely kinematic origin and arises from the use of the hyperradius instead of the pertinent Jacobi variables, it is nevertheless the source of the considerable difficulties inherent in this approach. Here we propose, following the analysis of [1,2], to define appropriate hyperradial-distorted free incoming and outgoing waves ($HDFW$) that incorporate these unphysical long-range effects. Using them the physical S -matrix can be found in a straightforward manner.

1 Introduction

The standard approach to nonrelativistic scattering consists in solving the Schrödinger equation and comparing its solution with that of the corresponding free equation (incoming and outgoing plane or spherical waves, respectively). This allows extraction of the S -matrix and with it the interpretation of experimental data.

As is well known such a straightforward procedure is ill-suited if long-range correlations are present. One way out consists in taking resort to a distorted-wave picture. Herein, the intended comparison is made with the solution, not of the free, but of an appropriate "distorted-free" Schrödinger equation. In order that this approach be of practical use the latter must take care of the undesired long-range correlations, and its solution must either be analytically known or at least be easily calculable.

In the hyperradial adiabatic treatment of the three-body problem the hyperradius \mathcal{R} and two internal hyperangles (ξ, η) are chosen as the basic variables. Then the total wave function is expanded as

$$\Psi_{HA}(\mathcal{R}, \xi, \eta) = \mathcal{R}^{-5/2} \sum_i^N \chi_i(\mathcal{R}) \varphi_i(\mathcal{R}|\xi, \eta). \quad (1)$$

After integration over ξ and η one arrives at a system of coupled hyperradial equations which in matrix form reads

as

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

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

$$Q_{ij}(\mathcal{R}) = -\frac{1}{2M} \left\langle \varphi_i(\mathcal{R}|\xi, \eta) \left| \frac{d}{d\mathcal{R}} \varphi_j(\mathcal{R}|\xi, \eta) \right. \right\rangle \quad (3)$$

and

$$W_{ij}(\mathcal{R}) = -\frac{1}{2M} \left\langle \varphi_i(\mathcal{R}|\xi, \eta) \left| \frac{d^2}{d\mathcal{R}^2} \varphi_j(\mathcal{R}|\xi, \eta) \right. \right\rangle. \quad (4)$$

Moreover, $\boldsymbol{\epsilon}(\mathcal{R})$ denotes the diagonal matrix of the adiabatic eigenvalues and $\boldsymbol{\chi}(\mathcal{R})$ the column vector solution. It is a wellknown fact that, within the HA approach, the non-adiabatic corrections that couple channels converging to the same asymptotic configuration can show an unphysical long-range behavior $\sim 1/\mathcal{R}$ [1–3]. Its occurrence is a purely kinematic effect, arising from the use of the hyperradius instead of the appropriate Jacobi variables.

Traditionally the asymptotic form of the scattering solution of (2) is then searched in the form [4,5]

$$\boldsymbol{\chi}(\mathcal{R}) \sim \left[e^{-iK\mathcal{R}} \mathbf{1} - e^{iK\mathcal{R}} \mathbf{S} \right] \mathbf{B}, \quad \text{for } \mathcal{R} \rightarrow \infty, \quad (5)$$

yielding the S -matrix \mathbf{S} (\mathbf{B} represents suitable normalization factors). Because of the above mentioned long-range

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correlations such a procedure represents, however, an ill-posed problem and is the origin of the considerable difficulties encountered in practical applications.

To enhance the usefulness of this approach we propose the following strategy which is inspired by the classical distorted-wave picture outlined at the beginning of the section.

- **First find an appropriate auxiliary (“distorted-free”) scattering equation corresponding to (2) but with the property that its solutions account for the long-range correlations and are readily accessible.**
- **When the full equation (2) is solved subsequently, in order to define the physical S -matrix the asymptotic comparison is then made with the solutions of the above auxiliary equation instead of with the standard incoming and outgoing spherical waves as in (5).**

In more detail, following the analysis of [1, 2], we first have to find from the auxiliary scattering equation so-called hyperradial-distorted free incoming and outgoing waves

$$e^{-iK\mathcal{R}}\bar{\mathbf{S}}^{-1/2} \text{ and } e^{iK\mathcal{R}}\bar{\mathbf{S}}^{1/2} \quad (6)$$

(see below) that incorporate the above mentioned unphysical long-range effects and include an auxiliary scattering matrix $\bar{\mathbf{S}}$. The latter then allows to calculate the physical scattering matrix S as

$$S = \bar{\mathbf{S}}^{-1/2} \mathbf{S} \bar{\mathbf{S}}^{-1/2}, \quad (7)$$

which can strongly differ from the standard S -matrix (5).

Thus, in a first step a procedure to define and then to calculate the auxiliary S -matrix $\bar{\mathbf{S}}$ has to be outlined.

2 Hyperspheroidal Hamiltonian

We consider three charged particles having masses m_i , position vectors \mathbf{x}_i , ($i = 1, 2, 3$), and charges $Z_1 Z_2 > 0, Z_1 Z_3 < 0$. Units $\mu = e = \hbar = 1$ are chosen. Introduction of the familiar prolate spheroidal coordinates $\xi \in [1, \infty)$ and $\eta \in [-1, 1]$, defined by

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

with

$$R = |\mathbf{x}_2 - \mathbf{x}_3|, \quad r_1 = |\mathbf{x}_1 - \mathbf{x}_3|, \quad r_2 = |\mathbf{x}_2 - \mathbf{x}_3|, \quad (9)$$

and of the hyperradius

$$\mathcal{R} = R \sqrt{\rho(\xi, \eta)} = R \sqrt{1 + (r/R)^2 \mu/M} \quad (10)$$

yields (for non-rotational states) the hyperradial Hamiltonian depending on three variables

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

$$h(\mathcal{R}|\xi, \eta) = -\frac{\rho^2(\xi, \eta)}{2\mu\mathcal{R}^2} \hat{a} + \sqrt{\rho(\xi, \eta)} V(\mathcal{R}|\xi, \eta), \quad (12)$$

$$V(\mathcal{R}|\xi, \eta) = \frac{1}{\mathcal{R}} \left[Z_1 Z_2 - \frac{2Z_1 Z_3}{\xi + \eta} - \frac{2Z_2 Z_3}{\xi - \eta} \right]. \quad (13)$$

The volume element is $d\tau = (\xi^2 - \eta^2) d\xi d\eta / \rho^2(\xi, \eta)$. Here, the following abbreviations have been used:

$$\hat{a} = \frac{1}{\xi^2 - \eta^2} \left[\frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} \right],$$

$$\hat{q} = \frac{1}{\xi^2 - \eta^2} \left[(\xi - \kappa\eta)(\xi^2 - 1) \frac{\partial}{\partial \xi} + (\eta - \kappa\xi)(1 - \eta^2) \frac{\partial}{\partial \eta} \right], \quad (14)$$

$$\begin{aligned} \rho(\xi, \eta) &= 1 + \tilde{\alpha}(\xi^2 + \eta^2 - 2\kappa\xi\eta + \kappa^2 - 1), \\ \tilde{\alpha} &= \mu/(4M), \\ \kappa &= (m_2 - m_1)/(m_2 + m_1), \\ 1/M &= 1/m_1 + 1/m_2, \\ 1/\mu &= 1/m_3 + 1/(m_1 + m_2). \end{aligned} \quad (15)$$

The hyperradial adiabatic eigenvalue equation

$$h(\mathcal{R}|\xi, \eta) \varphi_i(\mathcal{R}|\xi, \eta) = \varepsilon_i(\mathcal{R}) \varphi_i(\mathcal{R}|\xi, \eta) \quad (16)$$

can be interpreted as describing 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 $h(\mathcal{R}|\xi, \eta)$ depends parametrically on the hyperradius \mathcal{R} resulting in a $1/\mathcal{R}$ -behavior of the eigenvalues $\varepsilon_i(\mathcal{R})$ for large \mathcal{R} , a fact established both numerically and analytically [3]. Moreover, as \mathcal{R} tends to infinity implying the disintegration of the system into atom plus nucleus, $\rho(\xi, \eta)$ approaches appropriate constant values such that the spectra with the proper values of the atomic energies are recovered.

3 Asymptotic behavior

In order to assess the efficiency of the *HA* approach it is of importance study the asymptotic behavior of the various quantities occurring in (2) for large \mathcal{R} [3] (in contrast to the opinion advanced in [7]). This is illustrated in detail at the example of the specific physical three-charged particle system consisting of antiproton, electron and proton in Fig. 1 (see also [8]). There we show our calculated hyperradial-adiabatic potential $\varepsilon_{11}(\mathcal{R})$ (i.e., the 11-th eigenvalue) and the corresponding effective potential $\varepsilon_{11}(\mathcal{R}) + W_{11,11}(\mathcal{R})$ which includes the diagonal nonadiabatic corrections, cf. (4).

Indeed, both curves tend asymptotically to the proper energy level of antiprotonium $(p\bar{p})_{n=5}$. But the speed of approach is dramatically different. The reason is that while $\varepsilon_{11}(\mathcal{R})$ clearly displays the unphysical attractive $1/\mathcal{R}$ -like tail the latter is, however, for a large region of \mathcal{R} -values compensated with sufficient accuracy by that of the diagonal matrix element $W_{11,11}(\mathcal{R})$ of the non-adiabatic corrections. Obviously, for this particular system the size of the corrections is substantial and is thus expected to strongly influence the convergence rate of the scattering observables (see, e.g. [5]). But it is important to keep in mind the established 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 a similar long-range behavior $\sim O(1/\mathcal{R})$.

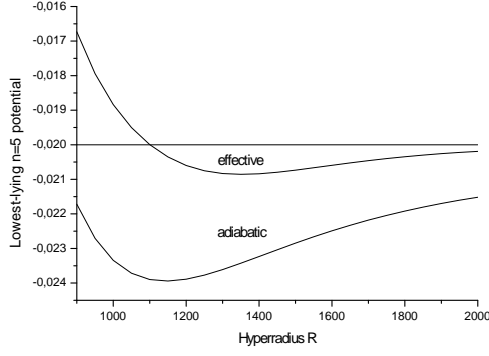
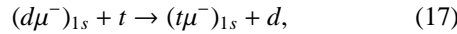


Fig. 1. Lowest adiabatic potential of the ($n=5$)-subset without ("adiabatic") and with ("effective") nonadiabatic correction. Both curves approach the proper energy of the ($p\bar{p}$) atom (in units $\mu = 1$), shown as a horizontal line, but at distinctly different values of the hyperradius \mathcal{R} .

4 Example of hyperradius-distorted free waves (HDFW)

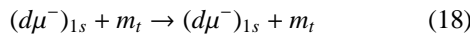
In order to enhance the convergence and to minimize the range of \mathcal{R} that should be used in the numerical solution of the hyperradial scattering equation (2), the following robust procedure is suggested.

To be specific consider the physical reaction



which has been thoroughly investigated in earlier days, see e.g. [4–6]. The asymptotic form of the solution of (2), if searched in the traditional way according to (5), includes the standard incoming ($\exp\{-iK\mathcal{R}\}$) and outgoing ($\exp\{iK\mathcal{R}\}$) spherical waves and an S -matrix \mathbf{S} (together with a column matrix \mathbf{B} of arbitrary coefficients). Clearly, the S -matrix defined in this way must be expected to be rather sensitive to the long-range kinematic effects introduced by using the hyperradius instead of the appropriate Jacobi variables.

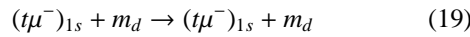
This fact suggests to first solve two auxiliary HA problems that physically represent the motion of the corresponding atoms with respect to a neutral "particle" with mass of the remaining third particle, namely



with

$$V = V_{d\mu^-}, V_{dt} = V_{\mu^-} = 0,$$

and



with

$$V = V_{t\mu^-}, V_{dt} = V_{d\mu^-} = 0.$$

These processes are trivial in the appropriate Jacobi variables since the corresponding wave functions are just products of hydrogen-like functions and plane waves. But when studied in the HA approach they suffer from the same kinematic inadequacy as the original reaction (17).

For these two reactions the HA ansatz (1) leads to a system of equations similar to (2). Asymptotically the solution for the reaction (18) behaves as

$$\chi^{d\mu^-}(\mathcal{R}) \sim [e^{-iK\mathcal{R}} - e^{iK\mathcal{R}}\mathbf{S}^{d\mu^-}] \mathbf{B}^{d\mu^-}, \quad \text{for } \mathcal{R} \rightarrow \infty, \quad (20)$$

and for (19) as

$$\chi^{t\mu^-}(\mathcal{R}) \sim [e^{-iK\mathcal{R}} - e^{iK\mathcal{R}}\mathbf{S}^{t\mu^-}] \mathbf{B}^{t\mu^-}, \quad \text{for } \mathcal{R} \rightarrow \infty. \quad (21)$$

As was demonstrated in [1], the "eigenvalues" and "non-adiabatic corrections" for these auxiliary reactions closely resemble those of the physical problem (17) 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 $\mathbf{W}^{t\mu^-}$ reproduces that for the corresponding quantities of the original physical problem (17). That is, in the HA approach these two free-motion problems look like a multichannel scattering problem where two different fragmentation channels are described using the same hyperradius \mathcal{R} .

Thus, the basic idea is to construct incoming and outgoing spherical waves that produce a unit S -matrix for the auxiliary problems shown above, and use them in the physical problem (17). In a first step we combine the solutions $\chi^{d\mu^-}$ and $\chi^{t\mu^-}$ into a common wave function, taking care of the energetic ordering of the asymptotic states,

$$\bar{\chi} = \begin{pmatrix} \chi^{d\mu^-} \\ \chi^{t\mu^-} \end{pmatrix}, \quad (22)$$

which asymptotically behaves as

$$\bar{\chi}(\mathcal{R}) \sim [e^{-iK\mathcal{R}}\mathbf{1} - e^{iK\mathcal{R}}\bar{\mathbf{S}}] \bar{\mathbf{A}}, \quad (23)$$

with the S -matrix

$$\bar{\mathbf{S}} = \begin{pmatrix} \mathbf{S}^{d\mu^-} & 0 \\ 0 & \mathbf{S}^{t\mu^-} \end{pmatrix}. \quad (24)$$

Let us rewrite (23) as

$$\bar{\chi}(\mathcal{R}) \sim [e^{-iK\mathcal{R}}\bar{\mathbf{S}}^{-1/2} - e^{iK\mathcal{R}}\bar{\mathbf{S}}^{1/2}] \bar{\mathbf{S}}^{1/2} \bar{\mathbf{A}} \quad (25)$$

$$=: [\bar{\chi}^{(-)}(\mathcal{R}) - \bar{\chi}^{(+)}(\mathcal{R})] \bar{\mathbf{A}}. \quad (26)$$

Then all unphysical couplings inherent in the HA approach are seen to have been incorporated in the distorted incoming and outgoing waves $\bar{\chi}^{(-)}(\mathcal{R})$ and $\bar{\chi}^{(+)}(\mathcal{R})$. We call them hyperradius-distorted free waves (HDFW), cf. (6). And we have arrived at a unit S -matrix as required for physical reasons.

5 Definition of the physical S -matrix

For the physical problem (17) we rewrite the asymptotic solution (5), introducing now the hyperradius-distorted free waves $\bar{\chi}^{(\pm)}$, as

$$\begin{aligned} \chi(\mathcal{R}) &\sim [e^{-iK\mathcal{R}}\bar{\mathbf{S}}^{-1/2}\bar{\mathbf{S}}^{1/2} - e^{iK\mathcal{R}}\bar{\mathbf{S}}^{1/2}\bar{\mathbf{S}}^{-1/2}] \mathbf{S} \mathbf{B} \\ &= [\bar{\chi}^{(-)}(\mathcal{R})\bar{\mathbf{S}}^{1/2} - \bar{\chi}^{(+)}(\mathcal{R})\bar{\mathbf{S}}^{-1/2}] \mathbf{S} \mathbf{B} \\ &= [\bar{\chi}^{(-)}(\mathcal{R}) - \bar{\chi}^{(+)}(\mathcal{R})\bar{\mathbf{S}}^{-1/2}\bar{\mathbf{S}}\bar{\mathbf{S}}^{-1/2}] \bar{\mathbf{S}}^{-1/2} \mathbf{B} \\ &=: [\bar{\chi}^{(-)}(\mathcal{R}) - \bar{\chi}^{(+)}(\mathcal{R})\mathbf{S}] \bar{\mathbf{B}}, \end{aligned} \quad (27)$$

so that for the physical scattering matrix \mathbf{S} we find the result (7).

Table 1. Elastic cross-section (in units of 10^{-20}cm^2) for $(d\mu^-)_{1s} + t \rightarrow (t\mu^-)_{1s} + d$ collisions. The center-of-mass incident energy is $E = 10^{-2} \text{eV}$. Various two-state approximations are compared.

Elastic cross-section	
BA [6]	2.13
HDFW (7)	2.21
HA [5]	2.39

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 much simpler auxiliary problems (18) and (19). Consequently, the physical values of scattering observables for the interesting reaction (17) are expected to be reached at much lower values of the hyperradius than in the original version of the method which is, of course, a very desirable feature.

This expectation is borne out by calculations of the elastic cross-section for the reaction (17) for the energy $E = 10^{-2} \text{eV}$. In Table 1 we compare three available two-state results. The best adiabatic (*BA*) calculations of [6] utilized an adiabatic expansion in which molecular states are constructed in (appropriate) Jacobi coordinates. Our result (second line of the Table 1) demonstrates the noticeable improvement over the traditional *HA* approach (third line of the Table 1). We mention that the multi-state *HA* approximation of [5] produced the value $2.15 \times 10^{-20} \text{cm}^2$.

6 Conclusions

The hyperradial-adiabatic approach is extensively used in solving various three body scattering problems, see for example [4,5]. Though convergence of the scattering results is usually claimed, it is not always as clear-cut as desirable. Here we propose for the first time to substitute the traditional way of calculating the scattering matrix using (5) by the following more elaborate but much more reliably looking procedure:

- **As a first step solve the appropriate hyperradial-distorted free scattering equation yielding the auxiliary \tilde{S} -matrix \tilde{S} .**
- **After that the conventional scattering matrix S is to be calculated using (5).**
- **The true physical scattering matrix \mathcal{S} is then found via expression (7).**

We mention that a related problem arises in the Born-Oppenheimer (*BO*) adiabatic approximation. In [9] boundary conditions for the radial multichannel Schrödinger equation were discussed, with the suggestion that the corresponding scattering theory "requires serious investigation". The reason for this warning is that here some matrix elements of the non-adiabatic couplings asymptotically approach even non-zero constant values. Clearly standard scattering theory is not applicable in such a case since free-motion states can not be introduced.

In contrast, in the *HA* approach matrix elements of the nonadiabatic corrections (3) and (4) and the adiabatic

eigenvalues $\epsilon_i(\mathcal{R})$ may behave asymptotically like $1/\mathcal{R}$. This at least allows one to follow the distorted-wave strategy of formal scattering theory presented here, which is distinctly different from the usual practice [4,5]. A first application has now been provided for the physical problem (17).

Here it should be noted that the matrix elements of angular couplings which are not discussed here are of a similarly long range, both in *HA* and in the *BO* approaches, i.e., untractable by conventional methods. In [2] we discuss two methods of how to circumvent this problem and give references.

In conclusion we expect that the *HA* approach, supplemented with the elimination of long-range parts of the unphysical couplings along the lines developed in this paper, i.e., using *HDFW*, will turn out to be rather effective. The numerical example from the previous section supports this conjecture.

Finally, we note the following two features of our main result (7)

$$S = \tilde{S}^{-1/2} \mathbb{S} \tilde{S}^{-1/2} ;$$

- **If the system of coupled hyperradial equations (2) is not large enough, both S and \mathbb{S} represent for the same number N of equations different approximations.**
- **On the other hand, if N is so large as to yield a converged physical \mathbb{S} -matrix, the auxiliary matrix \tilde{S} will approximately reduce to a unit matrix, resulting in**

$$S \approx \mathbb{S}.$$

Thus, a result $\tilde{S} \approx \mathbf{1}$ provides an easily obtainable independent and critical check of the convergence of the calculated scattering observables with respect to the number N of states taken into account, without having to solve the full physical scattering equation (2).

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