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# On the evaluation of transition matrices for rearrangement in atom–antiatom scattering

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## Abstract

We examine a method used by Zygelman *B et al* (2004 *Phys. Rev. A* **69** 042715) to evaluate the transition matrix for rearrangement in atom–antihydrogen scattering. We make a small change to the expression used previously and generalize it to all kinds of rearrangement processes.

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## 1. Introduction

The recent production of low-temperature antihydrogen in the ATHENA [1] and ATRAP [2] experiments at CERN has stimulated considerable interest in atom–antiatom interactions. The low-temperature scattering of atoms and antiatoms offers several challenges that are qualitatively new compared to atom–atom scattering. One such is the strong nuclear force, which not only causes annihilation, but also changes the elastic scattering cross sections [3–6].

Another challenge is rearrangement processes, i.e. processes where the nucleus, antinucleus and in some cases a number of electrons form one bound system, while the positron from the antihydrogen and the remaining electrons form another bound system. In what follows, we shall refer to these as the *heavy* and *light* subsystems. Rearrangement processes are particularly difficult to treat theoretically for atom–antiatom systems having a *critical distance*, i.e. an internuclear distance below which the leptons are no longer bound to the nuclei. This is for instance the case for the hydrogen–antihydrogen system. For systems with a critical distance the rearrangement cross section cannot be calculated accurately within the Born–Oppenheimer approximation [5, 7]. Instead non-adiabatic methods such as close-coupling [8], Kohn variational [9] or optical potential [10] must be used.

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Helium–antihydrogen is an example of a system that does not suffer from this complication. While the validity of the Born–Oppenheimer approximation still cannot be taken for granted, it is reasonable that it will give a fair approximation to the correct rearrangement cross section. Moreover, it can be systematically improved by including non-adiabatic couplings to other Born–Oppenheimer states. In this case, the distorted wave Born approximation may be invoked to derive a  $T$ -matrix method [10, 11] to evaluate the rearrangement cross section. The rearrangement cross section is then given by the expression

$$\sigma^{\text{rearr}} = \frac{(2\pi)^4}{k_i^2} |T_{fi}|^2, \quad (1)$$

where  $k_i$  is the collision wave vector and  $T_{fi}$  is the transition matrix ( $T$ -matrix). In [10], a particularly useful expression for the  $T$ -matrix in the form of an energy difference multiplied by an overlap matrix element was used. This form, which we shall call the *overlap approximation*, considerably simplifies the numerical evaluation of the  $T$ -matrix. It is important to give it a firm theoretical foundation. Thus, in this paper we make a formal derivation of the overlap approximation and consider its possible generalizations.

Atomic units are used throughout the paper.

## 2. Coordinates

We consider antihydrogen ( $\bar{\text{H}}$ ) colliding with an atom with  $N$  electrons. The system rearranges into a light system consisting of the positron and  $n$  electrons (for  $n = 0$  only a positron,  $n = 1$  positronium and  $n = 2$   $e^+e^-e^-$ ) and a heavy system consisting of the atomic nucleus, the antiproton and  $N - n$  electrons. Suppose that the atomic nucleus has mass  $m_A$  and charge  $Z_A$  and the mass of the antiproton is  $m_p$ . Let  $\mathbf{R}_A$  and  $\mathbf{R}_B$  be the coordinates of the nucleus and the antiproton, respectively, with respect to the non-rotating coordinate axes in an inertial frame which can most conveniently be taken to be the centre-of-mass frame. Let the coordinates of the  $N$  electrons and positron with respect to these axes be  $\tilde{\mathbf{r}}_i$  ( $i = 1, \dots, N$ ) and  $\tilde{\mathbf{r}}_{N+1}$ . We assume that the centre-of-mass motion has been separated out and introduce internal coordinates of Jacobi type:

$$\mathbf{R} = \mathbf{R}_A - \mathbf{R}_B \quad (2)$$

$$\mathbf{r}_i = \tilde{\mathbf{r}}_i - \frac{1}{m_p + m_A + i - 1} \left( m_A \mathbf{R}_A + m_p \mathbf{R}_B + \sum_{j=1}^{i-1} \tilde{\mathbf{r}}_j \right) \quad i = 1, \dots, N - n \quad (3)$$

$$\boldsymbol{\rho} = \frac{1}{n + 1} \sum_{i=N-n+1}^{N+1} \tilde{\mathbf{r}}_i - \frac{1}{m_A + m_p + N - n} \left( m_A \mathbf{R}_A + m_p \mathbf{R}_B + \sum_{j=1}^{N-n} \tilde{\mathbf{r}}_j \right) \quad (4)$$

$$\mathbf{s}_i = \tilde{\mathbf{r}}_{i+N-n+1} - \frac{1}{i} \sum_{j=N-n+1}^{i+N-n} \tilde{\mathbf{r}}_j \quad i = 1, \dots, n. \quad (5)$$

Here,  $\mathbf{R}$  is the internuclear separation,  $\mathbf{r}_i$  are Jacobi coordinates of the electrons in the heavy subsystem,  $\boldsymbol{\rho}$  connects the centres of mass of the heavy and light systems and  $\mathbf{s}_i$  are Jacobi coordinates of the electrons and the positron in the light subsystem. We denote this set of internal coordinates collectively as  $\mathcal{S} = \{\mathbf{R}, \mathbf{r}_i, \boldsymbol{\rho}, \mathbf{s}_i\}$ . In terms of these coordinates, the kinetic energy operator takes the simple form

$$\hat{T} = -\frac{1}{2\mu_N} \Delta_R - \sum_{i=1}^{N-n} \frac{1}{2\mu_i} \Delta_{r_i} - \frac{1}{2\mu_f} \Delta_{\boldsymbol{\rho}} - \sum_{i=1}^n \frac{1}{2\nu_i} \Delta_{s_i}. \quad (6)$$

Here, the different reduced masses are  $\mu_N = m_p m_A / (m_p + m_A)$ ,  $\mu_i = (m_A + m_p + i - 1) / (m_A + m_p + i)$ ,  $\mu_f = (m_A + m_p + N - n)(n + 1) / (m_A + m_p + N + 1)$  and  $\nu_i = i / (i + 1)$ .

The coordinates  $\mathcal{S}$  are with respect to the non-rotating axes. We next make the transformation into the reference frame following the rotation of the atom–antiatom system,  $\mathcal{S} \rightarrow \bar{\mathcal{S}} = \{\mathbf{R}, \bar{\mathbf{r}}_i, \bar{\boldsymbol{\rho}}, \bar{\mathbf{s}}_i\}$ . This transformation is carried out by applying a proper orthogonal transformation to the Cartesian components of  $\mathbf{r}_i$ ,  $\mathbf{s}_i$  and  $\boldsymbol{\rho}$ ,

$$\begin{pmatrix} \bar{x} \\ \bar{y} \\ \bar{z} \end{pmatrix} = U \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \tag{7}$$

where  $\{\bar{x}, \bar{y}, \bar{z}\}$  and  $\{x, y, z\}$  are the Cartesian components of the coordinates of any lepton in the rotating and non-rotating frame, respectively. Following Kołos and Wolniewicz [12] we chose the following form for this transformation:

$$U = \begin{pmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{pmatrix}, \tag{8}$$

where  $\theta$  and  $\phi$  are the spherical polar angles of  $\mathbf{R}$ , with respect to the non-rotating axes. This gives a coordinate system rotating with the nuclei and with the  $\bar{z}$  axis in the direction of  $\mathbf{R}$ . The terms in (6) involving  $\Delta_{r_i}$ ,  $\Delta_{s_i}$  and  $\Delta_{\boldsymbol{\rho}}$  are the same irrespective of whether the partial derivatives are in terms of members of  $\mathcal{S}$  or  $\bar{\mathcal{S}}$ . This is because the transformation (7) is orthogonal and the nuclear coordinates are the same in  $\mathcal{S}$  and  $\bar{\mathcal{S}}$ . However, extra terms occur in the partial derivatives with respect to the nuclear coordinates  $\theta$  and  $\phi$ , keeping the other members of  $\mathcal{S}$  constant, when these derivatives are expressed in terms of partial derivatives with respect to members of the set  $\bar{\mathcal{S}}$ . This is because a different set of variables is kept constant in each differentiation. Under the transformation from  $\mathcal{S}$  to  $\bar{\mathcal{S}}$ , partial derivatives with respect to  $R$ ,  $\theta$  and  $\phi$  transform as

$$\frac{\partial}{\partial R} \rightarrow \frac{\partial}{\partial R}, \tag{9}$$

$$\frac{\partial}{\partial \theta} \rightarrow \frac{\partial}{\partial \theta} - i \hat{L}_y, \tag{10}$$

$$\frac{\partial}{\partial \phi} \rightarrow \frac{\partial}{\partial \phi} - i \cos \theta \hat{L}_z + i \sin \theta \hat{L}_x. \tag{11}$$

Here,  $\hat{L}_\alpha$  is the total angular momentum along the  $\alpha$  axis of all leptons in terms of the relative coordinates introduced in (3)–(5) and transformed to the rotating system, i.e.,

$$\hat{\mathbf{L}} = -i \sum_{i=1}^{N-n} \bar{\mathbf{r}}_i \times \nabla_{\bar{\mathbf{r}}_i} - i \bar{\boldsymbol{\rho}} \times \nabla_{\bar{\boldsymbol{\rho}}} - i \sum_{i=1}^n \bar{\mathbf{s}}_i \times \nabla_{\bar{\mathbf{s}}_i}. \tag{12}$$

The first term on the right-hand side of (6) then becomes in the set of coordinates  $\bar{\mathcal{S}}$

$$\begin{aligned} & -\frac{1}{2\mu_N} \left\{ \frac{\partial^2}{\partial R^2} + \frac{2}{R} \frac{\partial}{\partial R} - \frac{\hat{\mathbf{J}}^2}{R^2} - \frac{1}{R^2} \left( \hat{L}_x^2 + \hat{L}_y^2 + \cot^2 \theta \hat{L}_z^2 + 2i \frac{\cot \theta}{\sin \theta} \hat{L}_z \frac{\partial}{\partial \phi} \right) \right. \\ & \left. + \hat{L}_+ \frac{1}{R^2} \left( -\frac{\partial}{\partial \theta} + \cot \theta \hat{L}_z + \frac{i}{\sin \theta} \frac{\partial}{\partial \phi} \right) + \hat{L}_- \frac{1}{R^2} \left( \frac{\partial}{\partial \theta} + \cot \theta \hat{L}_z + \frac{i}{\sin \theta} \frac{\partial}{\partial \phi} \right) \right\}, \tag{13} \end{aligned}$$

where  $\hat{\mathbf{J}}$  is the orbital angular momentum operator of the nuclei and  $\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$ . The extra terms are centrifugal and Coriolis terms resulting from the transformation to axes that rotate with the nuclei.

The Jacobi set of coordinates introduced above has the advantage that the kinetic energy operator contains no mass polarization terms, i.e. terms which couple derivatives with respect to coordinates of different particles. These are, however, usually not the coordinates used in molecular calculations based on the Born–Oppenheimer approximation. We now introduce a different set of coordinates  $\mathcal{T} = \{\mathbf{R}, \mathbf{t}_i\}$ , ( $i = 1, \dots, N+1$ ), more suitable for the molecule-like entrance channel. The  $N+1$  leptonic coordinates  $\mathbf{t}_i$  are with respect to non-rotating axes but with origin at the geometrical centre of the nucleus and antinucleus,

$$\begin{aligned} \mathbf{t}_i &= \tilde{\mathbf{r}}_i - \frac{1}{2}(\mathbf{R}_A + \mathbf{R}_B) \\ &= \begin{cases} \mathbf{r}_i + \sum_{j=1}^{i-1} \frac{1}{m_A + m_p + j} \mathbf{r}_j - \frac{1}{2} \frac{m_p - m_A}{m_p + m_A} \mathbf{R} & \text{for } i \leq N-n \\ \boldsymbol{\rho} + \sum_{j=1}^{N-n} \frac{1}{m_A + m_p + j} \mathbf{r}_j + \frac{i - N + n - 1}{i - N + n} \mathbf{s}_{i-N+n-1} \\ - \sum_{j=i-N+n}^n \frac{1}{j+1} \mathbf{s}_j - \frac{1}{2} \frac{m_p - m_A}{m_p + m_A} \mathbf{R} & \text{for } i > N-n. \end{cases} \end{aligned} \quad (14)$$

Inverting these relations one obtains

$$\mathbf{r}_i = \mathbf{t}_i - \frac{1}{m_A + m_p + i - 1} \left( \frac{m_A - m_p}{2} \mathbf{R} + \sum_{j=1}^{i-1} \mathbf{t}_j \right), \quad i = 1, \dots, N-n, \quad (15)$$

$$\boldsymbol{\rho} = \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbf{t}_{i+N-n} - \frac{1}{m_A + m_p + N-n} \left( \frac{m_A - m_p}{2} \mathbf{R} + \sum_{i=1}^{N-n} \mathbf{t}_i \right), \quad (16)$$

$$\mathbf{s}_i = \mathbf{t}_{i+N-n+1} - \frac{1}{i} \sum_{j=1}^i \mathbf{t}_{j+N-n}, \quad i = 1, \dots, n. \quad (17)$$

We can also express the kinetic energy operators in the set of coordinates  $\mathcal{T}$ ,

$$\hat{T} = -\frac{1}{2\mu_N} \Delta_{\mathbf{R}} - \frac{1}{2\mu_a} \sum_{i=1}^{N+1} \nabla_{\mathbf{R}} \cdot \nabla_{\mathbf{t}_i} - \frac{1}{8\mu_N} \sum_{i=1}^{N+1} \Delta_{\mathbf{t}_i} - \frac{1}{4\mu_N} \sum_{i=1}^{N+1} \sum_{j=i+1}^{N+1} \nabla_{\mathbf{t}_i} \cdot \nabla_{\mathbf{t}_j} - \frac{1}{2} \sum_{i=1}^{N+1} \Delta_{\mathbf{t}_i} \quad (18)$$

where  $\mu_a = m_A m_p / (m_p - m_A)$ . The coordinates  $\mathcal{T}$  can be transformed to coordinates  $\tilde{\mathcal{T}}$  with respect to the rotating axes through the transformation given by (8). The first term on the right-hand side of (18) will be transformed into a form similar to (13), while the second term in (18) will give rise to additional terms.

In order to describe the rearrangement channel we require a set of coordinates  $\mathcal{U} = \{\mathbf{R}, \mathbf{t}_i, \boldsymbol{\rho}, \mathbf{s}_j\}$  ( $i = 1, \dots, N-n$ ,  $j = 1, \dots, n$ ), i.e., with the coordinates of the electrons in the heavy subsystem centred at the geometrical centre of the nucleus and antinucleus, while

Jacobi coordinates are used for the light subsystem. In  $\mathcal{U}$ , the kinetic energy operator is

$$\begin{aligned} \hat{T} = & -\frac{1}{2\mu_N}\Delta_R - \frac{1}{2\mu_a}\sum_{i=1}^{N-n}\nabla_R\cdot\nabla_{t_i} - \frac{1}{8\mu_N}\sum_{i=1}^{N-n}\Delta_{t_i} \\ & - \frac{1}{4\mu_N}\sum_{i=1}^{N-n}\sum_{j=i+1}^{N-n}\nabla_{t_i}\cdot\nabla_{t_j} - \frac{1}{2}\sum_{i=1}^{N-n}\Delta_{t_i} - \frac{1}{2\mu_f}\Delta_\rho - \sum_{i=1}^n\frac{1}{2v_i}\Delta_{s_i}. \end{aligned} \quad (19)$$

Similarly to above, a rotating system  $\bar{\mathcal{U}}$  can be defined by the transformation (8). It is important to realize that even though the coordinates  $t_i$  ( $i = 1, \dots, N - n$ ) represent the same vectors in the sets of coordinates  $\mathcal{T}$  and  $\mathcal{U}$ , their partial derivatives are different, since they are taken with different sets of coordinates held constant. Below we shall use the notation  $|_{\mathcal{U}}$  or  $|_{\mathcal{T}}$  to indicate in which set of coordinates a given partial derivative is evaluated. Using the chain rule we then obtain the relations

$$\sum_{i=1}^{N-n}\Delta_{t_i}|_{\mathcal{T}} = \sum_{i=1}^{N-n}\Delta_{t_i}|_{\mathcal{U}} + \frac{N-n}{(m_A+m_p+N-n)^2}\Delta_\rho|_{\mathcal{U}} - \frac{2}{m_A+m_p+N-n}\sum_{i=1}^{N-n}\nabla_{t_i}\cdot\nabla_\rho|_{\mathcal{U}}, \quad (20)$$

$$\sum_{i=N-n+1}^{N+1}\Delta_{t_i}|_{\mathcal{T}} = \frac{1}{n+1}\Delta_\rho|_{\mathcal{U}} + \sum_{i=1}^n\frac{1}{v_i}\Delta_{s_i}|_{\mathcal{U}}. \quad (21)$$

This equation gives a relation between the kinetic energy terms of the leptons in the initial and final states. The same relations hold between the rotating systems  $\bar{\mathcal{T}}$  and  $\bar{\mathcal{U}}$ .

### 3. Application to the $T$ -matrix elements

We now derive a formula for the rearrangement  $T$ -matrix. The total Hamiltonian of the system is

$$\hat{H} = \hat{T} + V_{\text{heavy}} + V_{\text{light}} + V_{\text{ex}}, \quad (22)$$

where the kinetic energy operator may be expressed in any of the sets of coordinates introduced in the previous section. The potentials internal to the heavy and light systems are

$$V_{\text{heavy}} = \sum_{i=1}^{N-n}\frac{Z_A}{|\tilde{\mathbf{r}}_i - \mathbf{R}_A|} - \sum_{i=1}^{N-n}\frac{1}{|\tilde{\mathbf{r}}_i - \mathbf{R}_B|} + \sum_{i=1}^{N-n}\sum_{j=i+1}^{N-n}\frac{1}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|} \quad (23)$$

$$V_{\text{light}} = -\sum_{i=N-n+1}^N\frac{1}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_{N+1}|} + \sum_{i=N-n+1}^N\sum_{j=i+1}^N\frac{1}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|}. \quad (24)$$

The potential connecting the fragments is

$$\begin{aligned} V_{\text{ex}} = & \sum_{i=N-n+1}^N\frac{Z_A}{|\tilde{\mathbf{r}}_i - \mathbf{R}_A|} - \sum_{i=N-n+1}^N\frac{1}{|\tilde{\mathbf{r}}_i - \mathbf{R}_B|} + \sum_{i=1}^{N-n}\sum_{j=N-n+1}^N\frac{1}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|} \\ & - \frac{Z_A}{|\tilde{\mathbf{r}}_{N+1} - \mathbf{R}_A|} + \frac{1}{|\tilde{\mathbf{r}}_{N+1} - \mathbf{R}_B|} - \sum_{i=1}^{N-n}\frac{1}{|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_{N+1}|}. \end{aligned} \quad (25)$$

We assume that the wavefunctions of the atom in the initial state, as well as the wavefunctions of the fragments in the final state, are antisymmetrized with respect to the

internal coordinates of the electrons they contain. It still remains to antisymmetrize the final-state wavefunction with respect to electrons in different fragments. Allowing for this antisymmetrization, the  $T$ -matrix for rearrangement takes the form [13]

$$T_{\text{fi}} = \sqrt{\frac{N!}{n!(N-n)!}} \frac{1}{N!} \sum_{\hat{P}} p \langle \hat{P} \Phi_f | \hat{P} (V_{\text{ex}} - V_{\text{Coul}}) \hat{P}^{-1} | \Psi_{k_i} \rangle, \quad (26)$$

where  $\Psi_{k_i}$  is the exact scattering wavefunction for the scattering of  $\bar{H}$  by the atom under consideration and  $\Phi_f$  is the wavefunction representing the rearrangement channel we are considering. The sum runs over all permutations  $\hat{P}$  of the electrons, and  $p = \pm 1$  according to whether  $\hat{P}$  is an even or odd permutation. The wavefunction  $\Phi_f$  is an eigenfunction of  $\hat{H}_0 = \hat{H} - V_{\text{ex}} + V_{\text{Coul}}$ , with outgoing wave boundary condition.  $V_{\text{Coul}}$  is of the form

$$V_{\text{Coul}} = \frac{(1-n)(Z_A - 1 - N + n)}{\rho}. \quad (27)$$

It is the Coulombic potential for charges  $Z_A - 1 - N + n$  and  $1 - n$ , a distance  $\rho$  apart.  $V_{\text{Coul}}$  is included in  $\hat{H}_0$  so that if the charges on the fragments are both non-zero the continuum part of  $\Phi_f$  has the asymptotic form of the appropriate Coulomb wave, as in the Coulomb–Born approximation.

Using the properties of the permutation operator  $\hat{P}$ , the expression (26) can be rewritten as

$$T_{\text{fi}} = \sqrt{\frac{N!}{n!(N-n)!}} \frac{1}{N!} \sum_{\hat{P}} p \langle \Phi_f | (V_{\text{ex}} - V_{\text{Coul}}) \hat{P} | \Psi_{k_i} \rangle. \quad (28)$$

Furthermore, since  $\hat{P} \Psi_{k_i} = p \Psi_{k_i}$ , we obtain

$$T_{\text{fi}} = \sqrt{\frac{N!}{n!(N-n)!}} \langle \Phi_f | V_{\text{ex}} - V_{\text{Coul}} | \Psi_{k_i} \rangle. \quad (29)$$

Thus, antisymmetrization of the electrons just leads to multiplication by a numerical factor, and no additional matrix elements need to be evaluated.

We choose to use the set of coordinates  $\bar{T}$  for the initial state,  $\Psi_{k_i}$ , and the set of coordinates  $\bar{U}$  for the rearrangement state  $\Phi_f$ . The exact wavefunctions for initial and final states have to be calculated using all terms of the kinetic energy operator in the forms (18) and (19), respectively, along with the additional terms introduced by transformation into the rotating system. This is a very complicated task even for small systems. The problem is considerably simplified by using the distorted wave Born approximation, in which the  $T$ -matrix may be evaluated using the Born–Oppenheimer approximation to the initial state  $\Psi_{k_i}$  [10, 11]. To this end, we introduce the Born–Oppenheimer Hamiltonians of the initial and the final states, expressed in the sets of coordinates  $\bar{T}$  and  $\bar{U}$  respectively,

$$\hat{H}_i^{\text{BO}} = -\frac{1}{2} \sum_{i=1}^{N+1} \Delta_{\bar{t}_i} \Big|_{\bar{T}} + V_{\text{heavy}} + V_{\text{light}} + V_{\text{ex}}, \quad (30)$$

$$\hat{H}_f^{\text{BO}} = -\frac{1}{2} \sum_{i=1}^{N-n} \Delta_{\bar{u}_i} \Big|_{\bar{U}} + V_{\text{heavy}}. \quad (31)$$

We define the usual eigenfunctions and eigenvalues of the Born–Oppenheimer Hamiltonians with a parametric dependence on the nuclear coordinates. If the coordinates of the leptons are considered in the rotating system, these eigenfunctions and eigenvalues depend only on  $R$ ,

$$\hat{H}_i^{\text{BO}} \psi_\alpha^{\text{BO}}(R; \bar{t}_1, \dots, \bar{t}_{N+1}) = \varepsilon_i^\alpha(R) \psi_\alpha^{\text{BO}}(R; \bar{t}_1, \dots, \bar{t}_{N+1}), \quad (32)$$

$$\hat{H}_f^{\text{BO}} \omega_\alpha^{\text{BO}}(R; \bar{t}_1, \dots, \bar{t}_{N-n}) = \varepsilon_f^\alpha(R) \omega_\alpha^{\text{BO}}(R; \bar{t}_1, \dots, \bar{t}_{N-n}). \quad (33)$$

The Born–Oppenheimer Hamiltonians can be used to rewrite the  $T$ -matrix,

$$T_{\text{fi}} = \sqrt{\frac{N!}{n!(N-n)!}} \langle \Phi_f | \hat{H}_i^{\text{BO}} + \frac{1}{2} \sum_{i=1}^{N+1} \Delta_{\bar{t}_i} | \bar{\tau} - V_{\text{light}} - \hat{H}_f^{\text{BO}} + \frac{1}{2} \sum_{i=1}^{N-n} \Delta_{\bar{t}_i} | \bar{u} - V_{\text{Coul}} | \Psi_{k_i} \rangle. \quad (34)$$

Using relations (20) and (21) for the kinetic terms this becomes

$$\begin{aligned} T_{\text{fi}} = & \sqrt{\frac{N!}{n!(N-n)!}} \langle \Phi_f | \hat{H}_i^{\text{BO}} + \sum_{i=1}^n \frac{1}{2\nu_i} \Delta_{\bar{s}_i} | \bar{u} - V_{\text{light}} \\ & + \frac{1}{2} \left( \frac{1}{n+1} + \frac{N-n}{(m_A + m_p + N-n)^2} \right) \Delta_{\bar{\rho}} | \bar{u} \\ & - \frac{1}{m_A + m_p + N-n} \sum_{i=1}^{N-n} \nabla_{\bar{t}_i} \cdot \nabla_{\bar{\rho}} | \bar{u} - \hat{H}_f^{\text{BO}} - V_{\text{Coul}} | \Psi_{k_i} \rangle. \end{aligned} \quad (35)$$

Note that even though the Born–Oppenheimer Hamiltonians are used in this expression, we still have not invoked the Born–Oppenheimer approximation, and (35) is therefore exact. We can, still without invoking any approximation, simplify this expression by noting that  $\hat{H}_0$  separates into two parts,

$$\hat{H}_0 = \hat{H}_{\text{heavy}} + \hat{H}_{\text{light}}, \quad (36)$$

where in the set of coordinates  $\mathcal{U}$ , using (19),

$$\begin{aligned} \hat{H}_{\text{heavy}} = & \hat{H}_f^{\text{BO}} - \frac{1}{2\mu_N} \Delta_{\mathbf{R}} | \mathcal{U} - \frac{1}{2\mu_a} \sum_{i=1}^{N-n} \nabla_{\mathbf{R}} \cdot \nabla_{\mathbf{t}_i} | \mathcal{U} - \frac{1}{8\mu_N} \sum_{i=1}^{N-n} \Delta_{\mathbf{t}_i} | \mathcal{U} \\ & - \frac{1}{4\mu_N} \sum_{i=1}^{N-n} \sum_{j=i+1}^{N-n} \nabla_{\mathbf{t}_i} \cdot \nabla_{\mathbf{t}_j} | \mathcal{U}, \end{aligned} \quad (37)$$

$$\hat{H}_{\text{light}} = -\frac{1}{2\mu_f} \Delta_{\bar{\rho}} | \mathcal{U} - \sum_{i=1}^n \frac{1}{2\nu_i} \Delta_{s_i} | \mathcal{U} + V_{\text{light}} + V_{\text{Coul}}. \quad (38)$$

Since  $V_{\text{light}}$  depends only on the coordinates  $s_i$ , the final-state wavefunction separates as

$$\Phi_f(\mathbf{R}, \bar{t}_1, \dots, \bar{t}_{N-n}, \mathbf{s}_i, \boldsymbol{\rho}) = \phi_{n_f}(s_i) F_{l_f}(k_f \rho) Y_{l_f m_f}(\Omega_\rho) \Upsilon_{v_f, J_f, M_f}(\mathbf{R}, \bar{t}_1, \dots, \bar{t}_{N-n}). \quad (39)$$

Here,  $\phi_{n_f}$  is the wavefunction of the light subsystem in internal state,  $n_f$  with energy  $\mathcal{E}_{n_f}$ . The relative momentum of the light and heavy subsystems is  $k_f$ , and  $l_f, m_f$  their relative angular momentum.  $F_{l_f}$  is a spherical Bessel function unless  $V_{\text{Coul}} \neq 0$ , in which case it is a Coulomb function. The wavefunction  $\Upsilon_{v_f, J_f, M_f}$  represents the final state of the heavy system with total orbital angular momentum  $J_f, M_f$ , with energy  $\mathcal{E}_{v_f, J_f}$ . Note that we have expressed the light subsystem in terms of the non-rotating coordinates  $s_i$  and  $\boldsymbol{\rho}$ , while the coordinates of the electrons in the heavy subsystem are expressed in the rotating reference frame. This poses no problem since the Laplacians in (31), (35) and (38) are unchanged by the transformation between the non-rotating and rotating reference frames. On the other hand, the term proportional to  $\sum_{i=1}^{N-n} \nabla_{\bar{t}_i} \cdot \nabla_{\bar{\rho}}$  in (35) will change when  $\boldsymbol{\rho}$ , but not  $\bar{t}_i$ , is expressed



in the non-rotating reference frame. We now introduce an approximation by omitting this term, which is always small since the nuclear and proton masses are very large compared to the electron mass, and vanishes if  $N = n$ , as, for example, in the case of protonium formation in hydrogen–antihydrogen scattering. With these considerations, the  $T$ -matrix becomes

$$T_{\bar{n}} = \sqrt{\frac{N!}{n!(N-n)!}} \langle \Phi_f | \hat{H}_1^{\text{BO}} - \mathcal{E}_{n_f} - \left( \frac{1}{n+1} + \frac{N-n}{(m_A + m_p + N-n)^2} \right) \frac{k_f^2}{2} - \hat{H}_f^{\text{BO}} | \Psi_{k_i} \rangle. \quad (40)$$

The full spectrum of Born–Oppenheimer eigenfunctions given by (30) and (31) forms a complete set of states for the leptonic part of the problem. It is therefore, in principle, possible to expand the exact molecular eigenfunctions in terms of the Born–Oppenheimer states as [14]

$$\Psi_{k_i}(\mathbf{R}, \bar{\mathbf{t}}_i) = \sum_{\alpha} \chi_{k_i, J_i, M_i}^{\alpha}(\mathbf{R}) \psi_{\alpha}^{\text{BO}}(\mathbf{R}; \bar{\mathbf{t}}_i), \quad (41)$$

where  $k_i$  is the relative momentum, and  $J_i, M_i$  the relative angular momentum, of the colliding atom and antiatom in the initial state. The functions  $\chi_{k_i, J_i, M_i}^{\alpha}$  are solutions to an infinite set of Schrödinger equations for nuclear motion coupled by the non-diagonal matrix elements of the operator in (18). Similarly, the wavefunction of the heavy subsystem of the final state can be written as

$$\Upsilon_{v_f, J_f, M_f}(\mathbf{R}, \bar{\mathbf{t}}_1, \dots, \bar{\mathbf{t}}_{N-n}) = \sum_{\alpha} \xi_{v_f, J_f, M_f}^{\alpha}(\mathbf{R}) \omega_{\alpha}^{\text{BO}}(\mathbf{R}; \bar{\mathbf{t}}_1, \dots, \bar{\mathbf{t}}_{N-n}), \quad (42)$$

where  $\xi_{v_f, J_f, M_f}^{\alpha}$  are solutions to a set of coupled equations for the motion of nucleus and antinucleus in the final state. If we now insert the wavefunctions defined in (39) and (41), we can rewrite the  $T$ -matrix as a sum of overlap integrals multiplied by an energy difference,

$$T_{\bar{n}} = \sqrt{\frac{N!}{n!(N-n)!}} \sum_{\alpha, \beta} \int d\mathbf{R} \left[ \varepsilon_1^{\alpha}(\mathbf{R}) - \varepsilon_f^{\beta}(\mathbf{R}) - \left( \frac{1}{n+1} + \frac{N-n}{(m_A + m_p + N+n)^2} \right) \frac{k_f^2}{2} - \mathcal{E}_{n_f} \right] \\ \times \langle \phi_{n_f}(\mathbf{s}_i) F_{l_f}(k_f \rho) Y_{l_f m_f}(\Omega_{\rho}) \xi_{v_f, J_f, M_f}^{\beta}(\mathbf{R}) \omega_{\beta}^{\text{BO}}(\mathbf{R}; \bar{\mathbf{t}}_i) | \chi_{k_i, J_i, M_i}^{\alpha}(\mathbf{R}) \psi_{\alpha}^{\text{BO}}(\mathbf{R}; \bar{\mathbf{t}}_i) \rangle. \quad (43)$$

In this and the following expressions  $\langle \dots \rangle$  signifies integration over the leptonic coordinates only.

In the Born–Oppenheimer approximation, the couplings between different Born–Oppenheimer states are neglected, and hence the sums in (41) and (42) reduce to single terms, for instance scattering between the lowest adiabatic states  $\alpha = \beta = 0$ , which gives

$$T_{\bar{n}} = \sqrt{\frac{N!}{n!(N-n)!}} \int \xi_{v_f, J_f, M_f}^0(\mathbf{R}) t_{\bar{n}}(\mathbf{R}) \chi_{k_i, J_i, M_i}^0(\mathbf{R}) d\mathbf{R}, \quad (44)$$

$$t_{\bar{n}}(\mathbf{R}) = \left[ \varepsilon_1^0(\mathbf{R}) - \varepsilon_f^0(\mathbf{R}) - \left( \frac{1}{n+1} + \frac{N-n}{(m_A + m_p + N+n)^2} \right) \frac{k_f^2}{2} - \mathcal{E}_{n_f} \right] \\ \times \langle \phi_{n_f}(\mathbf{s}_i) F_{l_f}(k_f \rho) Y_{l_f m_f}(\Omega_{\rho}) \omega_0^{\text{BO}}(\mathbf{R}; \bar{\mathbf{t}}_i) | \psi_0^{\text{BO}}(\mathbf{R}; \bar{\mathbf{t}}_i) \rangle. \quad (45)$$

This is our final expression for the rearrangement  $T$ -matrix. The matrix element (45) is considerably easier than the original expression (29) to evaluate numerically since it does not involve any Coulombic terms. Thus, if the eigenfunctions and eigenvalues of the Born–Oppenheimer approximation (32) and (33) have been calculated, it is relatively easy to obtain the corresponding  $T$ -matrix. When the matrix element (45) or (29) is evaluated numerically, the

initial and final states must be represented in the same coordinate system. This requires that the final state is expressed in rotating coordinates, which creates additional complications if  $l_f \neq 0$  or if the light fragment has non-zero internal angular momentum. In this case, the angular variables will include dependences on the nuclear coordinates through the transformation (8). Normally, one will also take the origin of  $\rho$  to be the centre of mass of the nuclei, rather than the centre of mass of the entire heavy subsystem including  $N - n$  electrons. If  $N \neq n$ , this introduces an error, which, however, should be small.

#### 4. Discussion

In this paper, we have expressed the kinetic operator,  $\hat{T}$ , in terms of several systems of coordinates. One would like to be able to write it in a form that applies in all coordinate systems, in accordance with Einstein's principle of general covariance. This can be done by expressing  $\hat{T}$  in the form

$$\hat{T} = -(1/2)h^{ab}D_aD_b. \quad (46)$$

By the Einstein summation convention,  $a$  and  $b$  are summed over all the  $3N + 6$  coordinates used to describe the internal motion of the system.  $h^{ab}$  are the components of a type  $(2, 0)$  tensor field. If the coordinates  $S$  are all Cartesian,  $h^{ab}$  is diagonal with diagonal elements associated with  $R$ ,  $1/\mu_N$ , with  $r_i$ ,  $1/\mu_i$ , etc.  $D_a$  is the covariant derivative with respect to the  $a$ th coordinate.

We did make use of  $\hat{T}$  in this form but found the associated transformation operations between coordinates more cumbersome than using the chain rule. It is possible that this difficulty could be avoided by making use of a suitable mathematics software package.

We have provided a rigorous derivation and generalization of the expression for the leptonic  $T$ -matrix used in [10]. If equation (43) is used to calculate  $T_{fi}$  for hydrogen–antihydrogen scattering for which  $N = n = 1$ , the third term in the square brackets is  $-\frac{1}{4}k_f^2$ . This differs slightly from the corresponding term in the treatment in [10] which is  $-\frac{k_f^2}{2\mu_f}$ , where  $\mu_f = \frac{2m_p}{(m_p+1)}$  as  $m_A = m_p$  in this case.

The reason for this difference is as follows. If the kinetic energy operator in  $\hat{H}_i^{\text{BO}}$  is taken to include the extra terms

$$-\frac{1}{4m_p} \sum_{i=1}^2 \Delta_{\bar{e}_i} |_{\bar{T}} - \frac{1}{2m_p} \nabla_{\bar{e}_1} \cdot \nabla_{\bar{e}_2} |_{\bar{T}}, \quad (47)$$

from equation (18), in addition to the kinetic energy term in equation (30), the coefficient of the term in  $\Delta_{\bar{p}} |_{\bar{u}}$  in equation (35) becomes  $\frac{1}{2\mu_f}$ . As a consequence of this the term in equation (43) involving  $k_f$  becomes  $-\frac{k_f^2}{2\mu_f}$  instead of  $-\frac{k_f^2}{4}$ .

The difference between these terms is very small,  $\sim 0.05\%$ . If  $T_{fi}$  is evaluated using equations (44) and (45), the inclusion of the terms in (47) in  $\hat{H}_i^{\text{BO}}$  results in a slight improvement in accuracy as the effect of these terms is incorporated directly into the eigenvalues and eigenfunctions in equation (32). They thus do not have to be included in the terms that couple the eigenfunctions when evaluating  $T_{fi}$  using equation (43). However, the terms in (47) are not normally included in the Hamiltonian in the Born–Oppenheimer approximation [11, 12].

We have shown that the overlap approximation can be generalized to all kinds of rearrangement processes, including those in which the interaction between the final fragments is of the Coulomb form asymptotically. The only further approximations introduced beyond the distorted wave Born approximation are the application of the Born–Oppenheimer approximation to the description of the fragment in the final channel that contains the nuclei

and the location of the centre of mass of the other fragment at the centre of mass of the nuclei. The effect of these approximations can be expected to be small.

Moreover, equation (43) makes it possible to evaluate the  $T$ -matrix when the distorted wave Born approximation has been extended to include coupled Born–Oppenheimer states of the atom + antihydrogen in the elastic channel and the fragment that contains the nuclei in the rearrangement channel. We are examining the accuracy of the overlap approximation by evaluating cross sections for a number of rearrangement processes in helium–antihydrogen scattering [15] using both equation (29) and equations (44) and (45).

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