Cold collisions of atomic hydrogen with antihydrogen atoms: An optical potential approach

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We present a theory that describes the interaction of hydrogen atoms with antihydrogen at subkelvin temperatures. The formalism includes a nonlocal complex optical potential, whose imaginary component describes the breakup of the H-$\bar{\text{H}}$ complex into positronium and protonium fragments. Using *ab inito* methods, we construct the imaginary part of the optical potential and calculate the cross sections for fragmentation in ultracold collisions of H and $\bar{\text{H}}$. We find a 35% reduction in the value of the scattering length from that obtained in the Born-Oppenheimer approximation. We estimate the lifetimes for quasibound states of this complex to fragment into a protonium-positronium pair.

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I. INTRODUCTION

Recent advances [1–3] in the laboratory realization of low-energy antihydrogen allow the prospect for high-precision spectroscopic study of neutral antimatter. For precise measurements that may herald new bounds for *CPT* violation and the weak equivalence principle [4], it is desirable to trap the antihydrogen in a cold or ultracold environment [5]. Following suggestions [6] that ultracold hydrogen atoms may be useful as a buffer gas to cool trapped antihydrogen, we undertook [7–10] an investigation of hydrogen-antihydrogen atom collisions at low energies. Our studies revealed that elastic collisions drive and favor cooling at gas temperatures above 0.1 K. However, at colder temperatures, inelastic processes, in particular, the rearrangement reaction

$$\text{H} + \bar{\text{H}} \rightarrow p\bar{p} + e^+e^-, \tag{1}$$

and proton-antiproton in-flight annihilation dominate [8] and may limit the utility of the sympathetic cooling of $\bar{\text{H}}$ by cold H atoms. Other inelastic processes, such as lepton-antilepton annihilation in flight [10], and the association process [9]

$$\text{H} + \bar{\text{H}} \rightarrow \text{H}\bar{\text{H}} + h\nu, \tag{2}$$

also occur at very cold temperatures. Here H$\bar{\text{H}}$ is a quasibound state of the hydrogen-antihydrogen molecule and $h\nu$ is the energy of an emitted photon during radiative association. Though the rate for process (2) is small [9], the emitted radiation resulting from association could be exploited as a diagnostic. Unlike the H_2 system, in which dipole radiations resulting from transitions between vibrational levels of the ground electronic state are forbidden, the H$\bar{\text{H}}$ complex does possess an electric dipole moment. This property of the system may allow for the spectroscopic study of this novel four-body matter-antimatter complex.

The main goal of this paper is to develop a theory that provides a full quantum-mechanical description of the processes itemized above. Though our previous work incorporated a state-of-the-art molecular Born-Oppenheimer (BO) potential for the H-$\bar{\text{H}}$ system, as well as a Schrödinger description of atom dynamics, it is limited by the assumption of a single channel Born-Oppenheimer approximation. In this paper we address these limitations and develop a theory that includes multichannel effects through the introduction of a nonlocal optical potential [11]. It describes both the fragmentation dynamics for process (1) and gives the leading-order correction to the BO potential. The theory provides a framework for the calculation of collision cross sections as well as lifetimes and level shifts of the quasibound levels of the H$\bar{\text{H}}$ molecule.

Estimates [12–15] for elastic and inelastic cross sections, at collision energies corresponding to room temperatures and higher, were based on a semiclassical description of the heavy particle dynamics. At low collision energies a Schrödinger description, used in several recent studies [16–18], is necessary. The theory presented here provides a multichannel description within the framework of a Born-Oppenheimer separation of leptonic and baryonic motion.

In Sec. II we review the coordinate systems corresponding to the various rearrangement channels that are used in

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setting up the relevant coupled equations. In Sec. III we outline the basic coupled-channel approach that we use to construct the optical potential. We derive an expression for the imaginary part of the complex scattering length and use it to calculate fragmentation cross sections. We compare the procedure used here with that given in a previous formulation [7,8] based on a post-prior treatment of fragmentation. We show that the two formulations are equivalent within a distorted-wave approximation but that the former involves the use of a renormalized interaction.

In Sec. IV we present the results of *ab initio* calculations for the parameters that characterize the optical potential. We calculate the values of the BO coupling coefficients that determine fragmentation rates, and calculate the cross sections for process (1) at ultracold collision energies. We compare the results obtained using the optical potential with those obtained in a previous theoretical treatment [8]. We show that the imaginary part of the optical potential leads to a 35% reduction in the value of scattering length from that obtained in the Born-Oppenheimer approximation. We use the optical potential to calculate the lifetimes for quasibound levels of the $H\bar{H}$ complex to fragment into protonium-positronium pairs. Atomic units will be used, unless otherwise stated, throughout.

II. COORDINATE SYSTEMS

The nonrelativistic Hamiltonian for a hydrogen-antihydrogen atom pair is

$$H = \frac{\mathbf{P}_1^2}{2M} + \frac{\mathbf{P}_2^2}{2M} + \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} - \frac{1}{|\mathbf{r}_1 - \mathbf{R}_1|} - \frac{1}{|\mathbf{r}_2 - \mathbf{R}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{R}_2|} + \frac{1}{|\mathbf{r}_2 - \mathbf{R}_1|} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} - \frac{1}{|\mathbf{R}_1 - \mathbf{R}_2|}, \quad (3)$$

where $\mathbf{R}_1, \mathbf{R}_2, \mathbf{r}_1,$ and $\mathbf{r}_2$ are the proton, antiproton, electron, and positron position vectors, expressed in an arbitrary inertial coordinate system, respectively. $\mathbf{P}_1, \mathbf{P}_2, \mathbf{p}_1, \mathbf{p}_2$ are the corresponding conjugate momenta, M is the baryon and m the leptonic mass. We introduce the column vector $\mathbf{Y} \equiv (\mathbf{R}_1, \mathbf{R}_2, \mathbf{r}_1, \mathbf{r}_2)^\dagger$ and use the symbol $\mathbf{Y}$ to label this coordinate system. Because of the possibility for different arrangements, we employ the Jacobi coordinate systems and we label $\mathbf{X}_a, \mathbf{X}_b, \mathbf{X}_c$, defined as follows; $\mathbf{X}_a \equiv (\mathbf{R}_{cm}, \mathbf{R}_a, \mathbf{x}_{1a}, \mathbf{x}_{2a})^\dagger$, where

$$\mathbf{X}_a = W_a \mathbf{Y}, \quad (4)$$

$$W_a \equiv \begin{pmatrix} \frac{M}{2(M+m)} & \frac{M}{2(M+m)} & \frac{m}{2(M+m)} & \frac{m}{2(M+m)} \\ -1 & 1 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 1 \end{pmatrix}. \quad (5)$$

$\mathbf{x}_{1a}, \mathbf{x}_{2a}$ are the leptonic position vectors whose origin is located at the baryon center of mass, momenta $\mathbf{P}_a$ are conjugate to $\mathbf{X}_a$ and are related to momenta $\mathbf{P}$, conjugate to $\mathbf{Y}$, according to

$$\mathbf{P}_a = W_a^{-T} \mathbf{P}, \quad (6)$$

where W_a^{-T} is the transpose of the inverse of W_a. We call $\mathbf{X}_a$ the molecular coordinate system, since it is the system in which the BO approximation for the leptonic eigenstates is made. The Jacobi system $\mathbf{X}_b = (\mathbf{R}_{cm}, \mathbf{R}_b, \mathbf{x}_{1b}, \mathbf{x}_{2b})^\dagger$ is useful for describing the asymptotic eigenstates of the hydrogen-antihydrogen fragment. It is related to $\mathbf{Y}$ according to $\mathbf{X}_b = W_b \mathbf{Y}$, where

$$W_b \equiv \begin{pmatrix} \frac{M}{2(M+m)} & \frac{M}{2(M+m)} & \frac{m}{2(M+m)} & \frac{m}{2(M+m)} \\ -\frac{M}{M+m} & \frac{M}{M+m} & -\frac{m}{M+m} & \frac{m}{M+m} \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}. \quad (7)$$

The systems $\mathbf{X}_a$ and $\mathbf{X}_b$ differ in that $\mathbf{R}_a$ represents the internuclear separation vector, whereas $\mathbf{R}_b$ is the vector that joins the hydrogen center of mass to the antihydrogen center of mass and the position vectors $\mathbf{x}_{1b}, \mathbf{x}_{2b}$, are defined with respect to origins located at the parent baryon of the respective lepton. Both systems include a common total center-of-mass position vector $\mathbf{R}_{c.m.}$. Finally, we introduce the system $\mathbf{X}_c = (\mathbf{R}_{c.m.}, \mathbf{R}_c, \mathbf{u}_{pn}, \mathbf{u}_{ps})^\dagger$, where $\mathbf{X}_c = W_c \mathbf{Y}$ and

$$W_c \equiv \begin{pmatrix} \frac{M}{2(M+m)} & \frac{M}{2(M+m)} & \frac{m}{2(M+m)} & \frac{m}{2(M+m)} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}. \quad (8)$$

$\mathbf{R}_c$ is the vector that joins the center of mass of the $p\bar{p}$, protonium, fragment to the center of mass of the $e^- e^+$, positronium, fragment. $\mathbf{u}_{pn}$ is the $p\bar{p}$ separation vector and $\mathbf{u}_{ps}$ the leptonic separation vector. It is useful to partition Hamiltonian (3) into terms involving fragment Hamiltonians and to rewrite Eq. (3) in the form

$$H = H_{0\mathrm{b}} + H'_{\mathrm{b}}$$
$$H_{0\mathrm{b}} \equiv \frac{\mathbf{P}_{c.m.}{}^2}{4(M+m)} + \frac{\mathbf{P}_b{}^2}{2\mu_i} + \frac{\mathbf{p}_{1b}{}^2}{2\mu} + \frac{\mathbf{p}_{2b}{}^2}{2\mu} - \frac{1}{|\mathbf{x}_{1b}|} - \frac{1}{|\mathbf{x}_{2b}|}, \quad (9)$$

where $\mathbf{P}_{c.m.}, \mathbf{P}_b$, are momenta conjugate to $\mathbf{R}_{c.m.}$ and $\mathbf{R}_b$, respectively, and $\mathbf{p}_{1b}, \mathbf{p}_{2b}$ are the leptonic momenta conjugate to $\mathbf{x}_{1b}, \mathbf{x}_{2b}$, respectively. The interaction H'_{b} contains all terms in Eq. (3) that are not included in $H_{0\mathrm{b}}$, $\mu = mM/(M+m)$ is the reduced mass of the hydrogen (antihydrogen) atom, and $\mu_i \equiv (m+M)/2 \approx M/2$. The eigenstates of $H_{0\mathrm{b}}$ are asymptotic eigenstates of H and represent the fragment corresponding to a free hydrogen and antihydrogen atom pair. In the $\mathbf{X}_b$ Jacobi

system, they have the form, apart from a normalization factor,

$$\langle \mathbf{X}_b|\Psi_b\rangle \simeq \exp(i\mathbf{K}_{c.m.}\cdot\mathbf{R}_{c.m.})\exp(i\mathbf{K}_b\cdot\mathbf{R}_b)\phi_{1s}(\mathbf{x}_{1b})\phi_{1s}(\mathbf{x}_{2b}), \tag{10}$$

where $\mathbf{K}_{c.m.}$ is the total momentum of the $H\bar{H}$ fragment, and since $\mathbf{P}_{c.m.}$ commutes with H, it is conserved under rearrangement. In the remaining discussion we will work in an inertial frame where $\mathbf{K}_{c.m.}=0$. In Eq. (10), $\mathbf{K}_b$ is the relative momentum of the atom-antiatom pair and ϕ_{1s} is a $1s$ hydrogenic orbital. The eigenenergy E, for eigenstate $|\Psi_b\rangle$, is

$$E = \frac{\mathbf{K}_b{}^2}{2\mu_i} + \epsilon(1s) + \epsilon(1s), \tag{11}$$

where $\epsilon(1s)$ is the ground-state energy of the hydrogen atom. Throughout, we will specialize to low collision energies so that for an incoming state $|\Psi_b\rangle$, only the ground $1s$ states of the atom-antiatom are occupied.

If we assume a collision of atoms initially prepared in $|\Psi_b\rangle$ we must allow for the possibility of a rearrangement to a positronium-protonium fragment that is best described in the $\mathbf{X}_c$ Jacobi system. For this fragment we define

$$\begin{aligned} H &= H_{0c} + V_f, \\ H_{0c} &\equiv \frac{\mathbf{P}_{c.m.}{}^2}{4(M+m)} + \frac{\mathbf{P}_c{}^2}{2\mu_f} + \frac{\mathbf{p}_{pn}{}^2}{M} + \frac{\mathbf{p}_{ps}{}^2}{m} - \frac{1}{|\mathbf{u}_{pn}|} - \frac{1}{|\mathbf{u}_{ps}|}, \end{aligned} \tag{12}$$

where $\mathbf{P}_c$ are momenta conjugate to $\mathbf{R}_c$, $\mathbf{p}_{pn}$ is the momentum for the relative motion of the baryons in the protonium system, $\mathbf{p}_{ps}$ the momentum for the relative leptonic motion in the positronium system, and $\mu_f=2\ mM/(m+M)$. V_f includes all terms in Eq. (3) not contained in H_{0c}. The eigenstates of H_{0c} are asymptotic eigenstates of the Hamiltonian H and represent the fragment corresponding to a free protonium and positronium pair. In the $\mathbf{X}_c$ Jacobi system, they have the form

$$\langle \mathbf{X}_c|\Psi_c\rangle \simeq \exp(i\mathbf{K}_\mathbf{c}\cdot\mathbf{R}_c)\psi_{nl}(\mathbf{u}_{pn})\varphi_{n'l'}(\mathbf{u}_{ps}), \tag{13}$$

where $\mathbf{K}_c$ is the momentum for the relative motion of the protonium and positronium pair and ψ_{nl}, $\varphi_{n'l'}$ are hydrogenic orbitals for the protonium and positronium systems, respectively. In this discussion we limit the quantum numbers for the positronium atom to have the values $n'=1, l'=0$, but relax this constraint in the latter sections. According to Eq. (12), the energy eigenvalue for state $|\Psi_c\rangle$ is

$$E = \frac{\mathbf{K}_c{}^2}{2\mu_f} + \epsilon_{pn}(nl) + \epsilon_{ps}(1s). \tag{14}$$

Conservation of energy requires that the energy eigenvalue E, corresponding to an incoming eigenstate $|\Psi_b\rangle$, must satisfy the equality

$$E = \frac{\mathbf{K}_b{}^2}{2\mu_i} + \epsilon(1s) + \epsilon(1s) = \frac{\mathbf{K}_c{}^2}{2\mu_f} + \epsilon_{pn}(nl) + \epsilon_{ps}(1s). \tag{15}$$

For molecular calculations we choose to work in the $\mathbf{X}_a$ coordinate system, and we express the fragment states $|\Psi_b\rangle$ and $|\Psi_c\rangle$, defined in Eqs. (10) and (13), respectively, using the coordinates defined in the $\mathbf{X}_a$ system. Thus,

$$\begin{aligned} \Psi_b(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a}) &\equiv \langle \mathbf{X}_a|\Psi_b\rangle \\ &\simeq \exp\left(i\frac{m\mathbf{K}_b\cdot(\mathbf{x}_{1a}-\mathbf{x}_{2a})}{M+m}\right)\phi_{1s}(\mathbf{x}_{1a}+\mathbf{R}_a/2) \\ &\quad\times\phi_{1s}(\mathbf{x}_{2a}-\mathbf{R}_a/2) \end{aligned} \tag{16}$$

and

$$\begin{aligned} \Psi_c(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a}) &\equiv \langle \mathbf{X}_a|\Psi_c\rangle \\ &\simeq \exp\left[i\mathbf{K}_c\cdot(\mathbf{x}_{1a}+\mathbf{x}_{2a})/2\right] \\ &\quad\times\psi_{nl}(\mathbf{R}_a)\varphi_{1s}(\mathbf{x}_{2a}-\mathbf{x}_{1a}). \end{aligned} \tag{17}$$

III. CLOSE-COUPLING EQUATIONS

Motivated by the discussion leading to Eqs. (16) and (17), we introduce a close-coupling ansatz for the system wave function $|\Psi\rangle$ that describes the collision of H with $\bar{H}$ and allows for fragmentation into $p\bar{p}+e^+e^-$. We define

$$\begin{aligned} \langle \mathbf{X}_a|\Psi\rangle &\equiv F_b(\mathbf{R}_a)\langle \mathbf{X}_a|b\rangle + \sum_c F_c(\mathbf{R}_a)\langle \mathbf{X}_a|c\rangle, \\ \langle \mathbf{X}_a|b\rangle &\equiv u_b(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a}), \\ \langle \mathbf{X}_a|c\rangle &\equiv u_c(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a}), \end{aligned} \tag{18}$$

where the index c refers to positronium fragments with center-of-mass energy $\kappa_c^2/2\mu_f$ and according to relations (16) and (17), we require that $|b\rangle$ and $|c\rangle$ tend to the asymptotic limits,

$$\begin{aligned} u_b(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a}) &\to \exp\left(i\frac{m\mathbf{K}_b\cdot(\mathbf{x}_{1a}-\mathbf{x}_{2a})}{M+m}\right) \\ &\quad\times\phi_{1s}(\mathbf{x}_{1a}+\mathbf{R}_a/2)\phi_{1s}(\mathbf{x}_{2a}-\mathbf{R}_a/2) \\ &\approx \phi_{1s}(\mathbf{x}_{1a}+\mathbf{R}_a/2)\phi_{1s}(\mathbf{x}_{2a}-\mathbf{R}_a/2), \end{aligned} \tag{19}$$

$$u_c(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a}) \to \frac{\exp(i\kappa_c|\mathbf{x}_{1a}+\mathbf{x}_{2a}|/2)}{|\mathbf{x}_{1a}+\mathbf{x}_{2a}|/2}\varphi_{1s}(\mathbf{x}_{2a}-\mathbf{x}_{1a}). \tag{20}$$

Up to a normalization factor, Eq. (20) represents the outgoing wave, with radial momentum κ_c, for a positronium atom in its $1s$ state.

In the remaining discussion we work exclusively in the $\mathbf{X}_a$ frame and henceforth drop all frame subscripts. For the sake of economy in notation we represent all amplitudes as ket vectors. For example, in this notation the amplitude $u_b(\mathbf{R}_a,\mathbf{x}_{1a},\mathbf{x}_{2a})$ defined in Eq. (18) is equivalently written as $u_b(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)$ or simply $|b\rangle$. In the asymptotic limit $\mathbf{R}\to\infty$,

$u_b(\mathbf{R}_a, \mathbf{x}_{1a}\mathbf{x}_{2a})$ approaches the ground asymptotic eigenstate of the leptonic adiabatic, or Born-Oppenheimer, Hamiltonian

$$H_{e^-e^+} \equiv \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{2M} - \frac{1}{\left|\mathbf{x}_1 + \frac{\mathbf{R}}{2}\right|} - \frac{1}{\left|\mathbf{x}_2 - \frac{\mathbf{R}}{2}\right|} + \frac{1}{\left|\mathbf{x}_1 - \frac{\mathbf{R}}{2}\right|} + \frac{1}{\left|\mathbf{x}_2 + \frac{\mathbf{R}}{2}\right|} - \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} - \frac{1}{|\mathbf{R}|}, \quad (21)$$

provided that we ignore the lepton translation factor. The summation in Eq. (18) over positronium fragments involves a continuum but since we are interested in low-energy *s*-wave collisions we are allowed [8] to restrict the continuum functions in expansion (18) to *s* waves. It is useful to introduce cavity normalized states according to the prescription

$$|\kappa_n\rangle \equiv \frac{1}{\sqrt{2\pi R_0}} \frac{\sin(\kappa_n R_c)}{R_c} \varphi_{1s}(\xi),$$

$$\kappa_n = \frac{\pi n}{R_0},$$

$$R_c \equiv |\mathbf{R}_c| = |(\mathbf{x}_1 + \mathbf{x}_2)|/2, \quad (22)$$

$$\xi \equiv \mathbf{u}_{ps} = (\mathbf{x}_1 - \mathbf{x}_2),$$

where n is an integer and R_0 is the cutoff radius for the spherical cavity. The ket $|\kappa_n\rangle$ is a direct product of the positronium continuum function, which is regular at the origin, φ_{1s} is state function that represents the relative motion of the constituent positronium leptons, and R_c is the distance between the positronium atom and the center of mass of the protonium system. The kets have the property

$$\langle \kappa_n | \kappa_m \rangle = \delta_{nm}, \quad (23)$$

where the bracket notation implies integration over all lepton coordinates, $\langle | \rangle \rightarrow \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2$. In the continuum limit, a sum over κ_n of an arbitrary function $f(\kappa_n)$ is equal to the integral

$$\sum_n f(\kappa_n) \rightarrow \frac{R_0}{\pi} \int_0^\infty dk f(k) \quad (24)$$

as $R_0 \rightarrow \infty$. In this notation, ansatz (18) is rewritten as

$$|\Psi\rangle = F(\mathbf{R})|\tilde{a}\rangle + \sum_n f_{\kappa_n}(\mathbf{R})|\kappa_n\rangle, \quad (25)$$

where

$$|\tilde{a}\rangle \equiv \frac{P|a\rangle}{\sqrt{\langle a|P|a\rangle}},$$

$$P \equiv 1 - \sum_n |\kappa_n\rangle\langle\kappa_n|, \quad (26)$$

$$H_{e^-e^+}|a\rangle = e(R)|a\rangle$$

and $e(R)$ is the BO potential for the Born-Oppenheimer eigenstate $|a\rangle$ that correlates to the ground atomic eigenstate of the $H(1s)+\bar{H}(1s)$ fragment. It follows from definitions (26) and (23) that $P^2=P$ is a projection operator. We define $Q=1-P=\Sigma_n |\kappa_n\rangle\langle\kappa_n|$ and note that $Q|\kappa_n\rangle=|\kappa_n\rangle$ and $\langle a|P|\kappa_n\rangle=0$. In the limit $R\rightarrow\infty$ the free positronium amplitudes $|\kappa_n\rangle$ are orthogonal to the ground-Born Oppenheimer state $|a\rangle$, and $|\tilde{a}\rangle \rightarrow |a\rangle$ in this limit. Therefore ansatz (25) has the desired properties; (i) in the limit $R\rightarrow\infty$ it correlates to the approximate asymptotic state for the $H(1s)+\bar{H}(1s)$ fragment, (ii) it accounts for the possibility of fragmentation into the asymptotic positronium states that are described by the channel functions $|\kappa_n\rangle$. We have included the projection operator P in ansatz (25) in order that the channel states $|\tilde{a}\rangle$ and $|\kappa_n\rangle$ remain orthogonal at all internuclear distances. Because we limit the projection operator sum in Eq. (26) to fragment channels that are orthogonal to the BO ground state $|a\rangle$ in the asymptotic region, we satisfy the relation $P|a\rangle \rightarrow |a\rangle$, as $R \rightarrow \infty$. The choice for projection operator P is not unique, but we also require that $\langle a|P|a\rangle \neq 0$, for if $\langle a|P|a\rangle \rightarrow 0$ in some region of $\mathbf{R}$, ansatz (25) describes an expansion of an overcomplete set of states in that region. If that is the case, ansatz (25) should be replaced by an alternative description.

We obtain an effective Schrödinger equation for amplitude $F(\mathbf{R})$ by requiring that

$$\langle \tilde{a}|H_{e^-e^+}|\Psi\rangle = E\langle\tilde{a}|\Psi\rangle,$$
$$\langle \kappa_n|H_{e^-e^+}|\Psi\rangle = E\langle\kappa_n|\Psi\rangle, \quad (27)$$

where H is given by Eq. (3) expressed in the $\mathbf{X}_a$ system and E is the collision energy in the center-of-mass frame. Using ansatz (25), recognizing that $\langle\tilde{a}|\tilde{a}\rangle=1$ and $\langle\kappa_n|\kappa_m\rangle=\delta_{nm}$, we find that, if we neglect nonadiabatic couplings [19], Eqs. (27) are equivalent to

$$\frac{\mathbf{P}^2}{2\mu_i}F(\mathbf{R}) + \langle\tilde{a}|PH_{e^-e^+}P|\tilde{a}\rangle F(\mathbf{R}) - EF(\mathbf{R}) + \sum_n \langle\tilde{a}|PH_{e^-e^+}Q|\kappa_n\rangle f_{\kappa_n}(\mathbf{R}) = 0,$$
$$\frac{\mathbf{P}^2}{2\mu_i}f_{\kappa_n}(\mathbf{R}) + \sum_m \langle\kappa_n|QH_{e^-e^+}Q|\kappa_m\rangle f_{\kappa_m}(\mathbf{R}) - Ef_{\kappa_n}(\mathbf{R}) = -\langle\kappa_n|QH_{e^-e^+}P|a\rangle F(\mathbf{R}). \quad (28)$$

We evaluate the matrix element

$$\langle\kappa_n|QH_{e^-e^+}Q|\kappa_m\rangle \approx \delta_{mn}\left(\frac{\kappa_n^2}{2\mu_f} + \epsilon_{ps}(1s)\right) + \delta_{mn}V_{p\bar{p}}(\mathbf{R}),$$

$$V_{p\bar{p}}(\mathbf{R}) \equiv -\frac{1}{R} + \langle\kappa_n|V_f|\kappa_n\rangle, \quad (29)$$

$$V_f \equiv -\frac{1}{\left|\mathbf{x}_1+\frac{\mathbf{R}}{2}\right|}-\frac{1}{\left|\mathbf{x}_2-\frac{\mathbf{R}}{2}\right|}+\frac{1}{\left|\mathbf{x}_1-\frac{\mathbf{R}}{2}\right|}+\frac{1}{\left|\mathbf{x}_2+\frac{\mathbf{R}}{2}\right|},$$

where we have neglected the off-diagonal elements that contribute to $V_{p\bar{p}}(\mathbf{R})$. The integrand in Eq. (29) is odd under the interchange of lepton coordinates and since, according to definition (22), $|\kappa_n\rangle$ is invariant under this symmetry operation, the matrix element of the operator V_f vanishes. Thus, in the approximation where off-diagonal elements in Eq. (29) are ignored, $V_{p\bar{p}}(\mathbf{R})=-1/R$.

We define the eigenfunctions $\phi_m(\mathbf{R})$ that are solutions of the equation

$$\frac{\mathbf{P}^2}{2\mu_i}\phi_m(\mathbf{R})+V_{p\bar{p}}(\mathbf{R})\phi_m(\mathbf{R})-e_m\phi_m(\mathbf{R})=0, \tag{30}$$

where e_m is the mth eigenvalue. Using Eq. (30), we can rewrite Eq. (28) in integral form

$$\begin{aligned}&\frac{\mathbf{P}^2}{2\mu_i}F(\mathbf{R})+\tilde{V}_{aa}F(\mathbf{R})-EF(\mathbf{R})+\sum_n \tilde{V}_{a\kappa_n}f_{\kappa_n}(\mathbf{R})=0,\\ &f_{\kappa_n}(\mathbf{R})=\int d^3\mathbf{R}'\sum_m \frac{\phi_m(\mathbf{R})\phi_m^\dagger(\mathbf{R}')}{E-e_m-\frac{\kappa_n^2}{2\mu_f}-\epsilon_{ps}(1s)}\tilde{V}_{\kappa_n a}F(\mathbf{R}'),\end{aligned} \tag{31}$$

where

$$\begin{aligned}\tilde{V}_{aa}(\mathbf{R})&\equiv\frac{\langle a|PH_{e^-e^+}P|a\rangle}{\langle a|P|a\rangle},\\ \tilde{V}_{\kappa_n a}(\mathbf{R})&\equiv\frac{\langle\kappa_n|QH_{e^-e^+}P|a\rangle}{\sqrt{\langle a|P|a\rangle}},\\ \tilde{V}_{a\kappa_n}(\mathbf{R})&\equiv\frac{\langle a|PH_{e^-e^+}Q|\kappa_n\rangle}{\sqrt{\langle a|P|a\rangle}}.\end{aligned} \tag{32}$$

The above expression for the amplitude $f_{\kappa_n}(\mathbf{R})$ contains a sum over discrete values for quantum index m as well as a continuum contribution. We use the summation symbol to represent both. In the limit of cold collisions, energy conservation [8] requires that $f_{\kappa_n}(\mathbf{R})\to 0$ in the limit $R\to 0$, that is, only bound protonium fragments are allowed in the exit channels.

Combining the two terms in Eq. (31), we obtain

$$\begin{aligned}&\frac{\mathbf{P}^2}{2\mu_i}F(\mathbf{R})+\tilde{V}_{aa}(\mathbf{R})F(\mathbf{R})-EF(\mathbf{R})\\ &\quad+\int d^3\mathbf{R}'\sum_m\sum_n\frac{\phi_m(\mathbf{R})\phi_m^\dagger(\mathbf{R}')}{E-e_m-\frac{\kappa_n^2}{2\mu_f}-\epsilon_{ps}(1s)}\tilde{V}_{a\kappa_n}(\mathbf{R})\\ &\quad\times\tilde{V}_{\kappa_n a}(\mathbf{R}')F(\mathbf{R}')=0.\end{aligned} \tag{33}$$

The optical potential

From the above definition we note that

$$\begin{aligned}\tilde{V}_{aa}(\mathbf{R})=\frac{1}{\det S}(&\langle a|H_{e^-e^+}|a\rangle-\sum_n(\langle a|H_{e^-e^+}|\kappa_n\rangle S_{\kappa_n a}\\ &+S_{a\kappa_n}\langle\kappa_n|H_{e^-e^+}|a\rangle)+\sum_n\sum_m\langle\kappa_n|H_{e^-e^+}|\kappa_m\rangle S_{a\kappa_n}S_{\kappa_m a}),\end{aligned} \tag{34}$$

where we define the overlap matrix

$$\begin{aligned}S_{a\kappa_n}&\equiv\langle a|\kappa_n\rangle,\\ \langle a|P|a\rangle&=1-\sum_n|\langle a|\kappa_n\rangle|^2=1-\sum_n|S_{a\kappa_n}|^2\equiv\det S.\end{aligned} \tag{35}$$

Since $H_{e^-e^+}|a\rangle=e(R)|a\rangle$, we find using Eq. (29),

$$\begin{aligned}\tilde{V}_{aa}(\mathbf{R}&=\frac{1}{\det S}\left[e(R)\left(1-2\sum_n|S_{a\kappa_n}|^2\right)\right.\\ &\left.+\sum_n\left(\frac{\kappa_n^2}{2\mu_f}+\epsilon_{ps}(1s)+V_{p\bar{p}}(\mathbf{R})\right)|S_{a\kappa_n}|^2\right]\\ &=e(R)+\sum_n\frac{|S_{a\kappa_n}|^2\Delta\epsilon(\mathbf{R})_{\kappa_n}}{\det S},\end{aligned}$$

$$\Delta\epsilon(\mathbf{R})_{\kappa_n}\equiv\frac{\kappa_n^2}{2\mu_f}+\epsilon_{ps}(1s)+V_{p\bar{p}}(\mathbf{R})-e(R), \tag{36}$$

and

$$\tilde{V}_{a\kappa_n}(\mathbf{R})=\tilde{V}^*_{\kappa_n a}(\mathbf{R})=\frac{-\Delta\epsilon(\mathbf{R})_{\kappa_n}S_{a\kappa_n}}{\sqrt{\det S}}. \tag{37}$$

We reexpress this matrix element by noting that

$$\begin{aligned}\Delta\epsilon(\mathbf{R})_{\kappa_n}S_{a\kappa_n}&=\langle a|\Delta\epsilon(\mathbf{R})_{\kappa_n}|\kappa_n\rangle\\ &=\langle a|\frac{\kappa_n^2}{2\mu_f}+\epsilon_{ps}(1s)+V_{p\bar{p}}(\mathbf{R})-e(R)|\kappa_n\rangle\\ &=-\langle a|V_f|\kappa_n\rangle\end{aligned} \tag{38}$$

or

$$\tilde{V}_{a\kappa_n}(\mathbf{R})=\tilde{V}^*_{\kappa_n a}(\mathbf{R})=\frac{\langle a|V_f|\kappa_n\rangle}{\sqrt{\det S}}. \tag{39}$$

Also

$$\tilde{V}_{aa}(\mathbf{R})=e(R)+\sum_n\frac{|\tilde{V}_{a\kappa_n}(\mathbf{R})|^2}{\Delta\epsilon(\mathbf{R})_{\kappa_n}}. \tag{40}$$

Combining the above results, we rewrite Eq. (33) in the form

$$\frac{\mathbf{P}^2}{2\mu_i}F(\mathbf{R}) + e(R)F(\mathbf{R}) - EF(\mathbf{R}) + \int d^3\mathbf{R}' V_{op}(\mathbf{R},\mathbf{R}')F(\mathbf{R}') = 0, \tag{41}$$

where the optical potential $V_{op}(\mathbf{R},\mathbf{R}')$ is given by

$$V_{op}(\mathbf{R},\mathbf{R}') = \sum_m \sum_n \frac{\phi_m(\mathbf{R})\phi_m^\dagger(\mathbf{R}')}{E - e_m - \frac{\kappa_n^2}{2\mu_f} - \epsilon_{ps}(1s)} \tilde{V}_{\kappa_n a}(\mathbf{R})\tilde{V}_{a\kappa_n}(\mathbf{R}') + \delta^3(\mathbf{R}-\mathbf{R}')\sum_n \frac{|\tilde{V}_{a\kappa_n}(\mathbf{R})|^2}{\Delta\epsilon(\mathbf{R})_{\kappa_n}}. \tag{42}$$

In the continuum limit, we get

$$V_{op}(\mathbf{R},\mathbf{R}') = \sum_m \int_0^\infty d\epsilon \frac{\phi_m(\mathbf{R})\phi_m^\dagger(\mathbf{R}')}{E - e_m - \epsilon - \epsilon_{ps}(1s)} \tilde{U}_\epsilon(\mathbf{R})\tilde{U}_\epsilon^*(\mathbf{R}') + \delta^3(\mathbf{R}-\mathbf{R}')\int_0^\infty d\epsilon \frac{|\tilde{U}_\epsilon(\mathbf{R})|^2}{\Delta\epsilon(\mathbf{R})}, \tag{43}$$

where $\epsilon = k^2/2\mu_f$ is the kinetic energy of the positronium fragment,

$$\tilde{U}_\epsilon(\mathbf{R}) \equiv \langle\epsilon|\tilde{V}_f|a\rangle = \langle\epsilon|V_f|a\rangle/\sqrt{\Omega(\mathbf{R})},$$

$$\langle\epsilon|V_f|a\rangle \equiv \sqrt{\frac{\mu_f}{2k\pi^2}}\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \frac{\sin(kR_c)}{R_c}\varphi_{1s}(\boldsymbol{\xi})V_f\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{R}),$$

$$\Omega(\mathbf{R}) \equiv \det S = 1 - \int_0^\infty d\epsilon |\langle\epsilon|a\rangle|^2 = 1 - \int_0^\infty d\epsilon \frac{|\langle\epsilon|V_f|a\rangle|^2}{|\Delta\epsilon(\mathbf{R})|^2}, \tag{44}$$

R_c and $\boldsymbol{\xi}$ are defined in Eq. (22). $\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{R}) = \langle\mathbf{X}|a\rangle$ is the adiabatic eigenstate and $|\epsilon\rangle$ is the *s*-wave positronium wave function that is energy normalized $[\langle\epsilon|\epsilon'\rangle = \delta(\epsilon-\epsilon') = \delta(k^2/2\mu_f - k'^2/2\mu_f)]$. The states $|\epsilon\rangle$ obey the closure relation,

$$\sum_\epsilon \langle\mathbf{x}_1\mathbf{x}_2|\epsilon\rangle\langle\epsilon|\mathbf{x}_1'\mathbf{x}_2'\rangle = \frac{1}{4\pi}\frac{\delta(R_c - R_c')}{R_c R_c'}\varphi_{1s}(\boldsymbol{\xi})\varphi_{1s}(\boldsymbol{\xi}'). \tag{45}$$

It is instructive to examine the second term in Eq. (25), $\Psi_{frag} \equiv \Sigma_n f_{\kappa_n}(\mathbf{R})|\kappa_n\rangle$, so that its asymptotic form is explicit. Using Eqs. (25) and (31), and invoking the continuum limit, we get

$$\Psi_{frag} = -\sum_m \int \frac{d^3\mathbf{R}'}{4\pi}\int d^3x_1' \int d^3x_2' \phi_m(\mathbf{R})\phi_m^\dagger(\mathbf{R}') \times F(\mathbf{R}')\frac{V_f}{\sqrt{\Omega}}\varphi_{1s}(\boldsymbol{\xi})\varphi_{1s}(\boldsymbol{\xi}')\Psi(\mathbf{x}_1',\mathbf{x}_2',\mathbf{R}')G_{k_m}(R_c,R_c'), \tag{46}$$

where

$$G_{k_m}(R_c,R_c') \equiv \frac{4\mu_f}{\pi}\int_0^\infty dk \frac{\sin(kR_c)\sin(kR_c')}{R_c'R_c(k^2-k_m^2)}, \qquad k_m^2 \equiv 2\mu_f(E - e_m - \epsilon_{ps}(1s)). \tag{47}$$

The manner in which we integrate around the poles of the Green's function $G_{k_m}(R_c,R_c')$ determines the asymptotic boundary condition. We adopt the Feshbach prescription [11] $1/(k^2-k_m^2) \to 1/[(k^2-k_m^2) - i\eta]$, where η is a positive infinitesimal, and get

$$G_{k_m}(R_c,R_c') = \frac{2\mu_f}{k_m R_c R_c'}\exp(ik_m R_{c>})\sin(k_m R_{c<}), \tag{48}$$

where $R_{c<}$, $R_{c>}$ is the lesser, greater of R_c, R_c', respectively, and $k_m > 0$. Inserting the retarded Green's function into Eq. (46) we obtain for the fragment wave function

$$\Psi_{frag} \sim -\sum_m \sqrt{\frac{\mu_f}{2k_m}}\frac{\exp(ik_m R_c)}{R_c}\varphi_{1s}(\boldsymbol{\xi})\phi_m(\mathbf{R})T(k_m), \qquad T(k_m) \equiv \int d^3\mathbf{R}\phi_m(\mathbf{R})F(\mathbf{R})\langle\Psi_a|\tilde{V}_f|\epsilon(k_m)\rangle, \tag{49}$$

where we have taken the limit $R_c \to \infty$, used definition (44), and defined $|\epsilon(k_m)\rangle \equiv |\epsilon = k^2/2\mu_f\rangle$.

Equation (49) has the desired asymptotic limit for the fragment wave function, an outgoing *s* wave describing a positronium atom-protonium system. Using Eq. (49), we obtain an expression for the differential cross section for the rearrangement process (1),

$$d\sigma = \frac{(2\pi)^3}{2k_i^2}\sum_m |T(k_m)|^2 d\Omega, \tag{50}$$

where k_i is the wave number of the incident wave $F_{inc}(\mathbf{R}) = \sqrt{k_i\mu_i/(2\pi)^3}\exp(ik_i z)$ in the elastic channel, Ω is the solid angle, with respect to the quantization axis $\mathbf{z}$, in which the positronium-protonium fragment is found. Expression (50) predicts fragmentation cross sections for the case where the positronium atom is found in the ground 1*s* state. A generalization is given later in the paper. If we further assume that $T(k_m)$ is isotropic, we obtain for the total fragmentation cross section,

$$\sigma_{frag} = \frac{(2\pi)^4}{k_i^2}\sum_m |T(k_m)|^2. \tag{51}$$

In the discussion that follows we enforce the Feshbach prescription by the application of the following identity:

$$\frac{1}{(k^2-k_m^2) - i\eta} = \frac{P}{(k-k_m)(k+k_m)} + \pi i\delta(k^2-k_m^2), \tag{52}$$

when evaluating the energy integral in the expression for the optical potential (43).

Using relation (52) in expression (43) we obtain two distinct contributions to the optical potential,

$$V_{op}(\mathbf{R},\mathbf{R}') = V_{op}^{I}(\mathbf{R},\mathbf{R}') + V_{op}^{R}(\mathbf{R},\mathbf{R}'), \tag{53}$$

where

$$V_{op}^{I}(\mathbf{R},\mathbf{R}') = -\pi i \sum_{m} \phi_m(\mathbf{R})\phi_m^{\dagger}(\mathbf{R}')\tilde{U}_{\epsilon(k_m)}(\mathbf{R})\tilde{U}^{*}_{\epsilon(k_m)}(\mathbf{R}'), \tag{54}$$

$$\epsilon(k_m) \equiv E - e_m - \epsilon_{ps}(1s),$$

and

$$V_{op}^{R}(\mathbf{R},\mathbf{R}') = \sum_{m} \int_0^{\infty} d\epsilon \phi_m(\mathbf{R})\phi_m^{\dagger}(\mathbf{R}')\tilde{U}_{\epsilon}(\mathbf{R})\tilde{U}^{*}_{\epsilon}(\mathbf{R}') \times \left[\mathrm{P}\frac{1}{E - e_m - \epsilon - \epsilon_{ps}(1s)} + \mathrm{P}\frac{1}{\epsilon + \epsilon_{ps}(1s) + V_{p\bar{p}}(\mathbf{R}) - e(R)} \right], \tag{55}$$

symbol P standing for the principal value of the integral. In deriving Eq. (55) we made use of the closure property of the states $\phi_m(\mathbf{R})$ and definition (36). $V^{I}(\mathbf{R},\mathbf{R}')$ is an absorptive potential and it accounts for the loss of flux, in the elastic channel, due to the fragmentation of the $\mathrm{H}(1s)+\overline{\mathrm{H}}(1s)$ into $p\bar{p}+e^{-}e^{+}$. The potential $V_{op}^{R}(\mathbf{R},\mathbf{R}')$ is a correction to the Born-Oppenheimer energy $e(R)$.

IV. DISTORTED-WAVE APPROXIMATION

We seek solutions to the Schrödinger equation,

$$-\frac{\nabla^2}{2\mu_i}F(\mathbf{R}) + e(R)F(\mathbf{R}) - EF(\mathbf{R}) + \int d^3\mathbf{R}' V_{op}(\mathbf{R},\mathbf{R}')F(\mathbf{R}') = 0, \tag{56}$$

where the optical potential $V_{op}(\mathbf{R},\mathbf{R}')$ is given in Eq. (53). The real part, $V_{op}^{R}(\mathbf{R},\mathbf{R}')$, of the optical potential represents a nonadiabatic correction to the BO ground-state potential $e(R)$, and the imaginary part, $V_{op}^{I}(\mathbf{R},\mathbf{R}')$, determines the rate for the reaction, $\mathrm{H}(1s)+\overline{\mathrm{H}}(1s)\rightarrow p\bar{p}+e^{+}e^{-}$. Because the optical potential is complex, so is the s-wave scattering phase shift. In the discussion below we show that a distorted wave treatment of Eq. (56) leads to an expression for the imaginary part of the $\mathrm{H}(1s)+\overline{\mathrm{H}}(1s)$ scattering length that is in harmony with that obtained using a post-prior description [8].

We restrict our discussion to the energy regime where s-wave scattering dominates and where the phase shift is given by the effective range expansion

$$k\cot\delta = -\frac{1}{a} + \frac{1}{2}r_0 k^2, \tag{57}$$

where δ is the s-wave phase shift, a the scattering length, r_0 the effective range, and $k=\sqrt{2\mu_i E}$ the wave number corresponding to the motion, during the initial approach, of the $\mathrm{H}+\overline{\mathrm{H}}$ system.

In the limit where s-wave scattering dominates we obtain, from Eq. (56), the radial equation for the s-wave amplitude,

$$-\frac{1}{2\mu_i}\frac{d^2F(R)}{dR^2} + e(R)F(R) - EF(R) + \int_0^{\infty} dR' R' R V_{op}(R,R')F(R') = 0, \tag{58}$$

where

$$V_{op}(R,R') \equiv \int d\Omega \int d\Omega' Y_{00}(\Omega)V_{op}(\mathbf{R},\mathbf{R}')Y_{00}(\Omega') = \sum_{m}\int_0^{\infty} d\epsilon \phi_m(R)\phi_m^{\dagger}(R')\tilde{U}_{\epsilon}(R)\tilde{U}^{*}_{\epsilon}(R') \times \left[\frac{1}{E - e_m - \epsilon - \epsilon_{ps}(1s) + i\eta} + \mathrm{P}\frac{1}{\epsilon + \epsilon_{ps}(1s) + V_{p\bar{p}}(R) - e(R)} \right] \tag{59}$$

and the sum m is restricted to $l=0$ protonium states. In definition (59), $\phi_m(R)$ are $l=0$ radial functions and in deriving this expression, we used Eqs. (54) and (55) and invoked the approximation $\tilde{U}_{\epsilon}(\mathbf{R})\rightarrow\langle\tilde{U}_{\epsilon}(\mathbf{R})\rangle=\tilde{U}_{\epsilon}(R)$ where the brackets imply averaging over all angles of the internuclear vector $\mathbf{R}$.

We rewrite Eq. (58) in integral form,

$$F(R) = f(kR) + 2\mu_i\int_0^{\infty} dR' R' g(R_<,R_>) \times \int_0^{\infty} dR'' R'' V_{op}(R',R'')F(R''), \tag{60}$$

where the Green's function $g(R_<,R_>)$ is given by

$$g(R_<,R_>) = -kf(kR_<)h(kR_>) \tag{61}$$

and $\{f(kR),h(kR)\}=u$ are independent solutions of the homogeneous equation

$$\frac{d^2u(R)}{dR^2} - 2\mu_i e(R)u(R) + k^2u(R) = 0 \tag{62}$$

that satisfy the boundary conditions

$$f(kR) \rightarrow \frac{\sin(kR+\delta_0)}{k}, \qquad h(kR) \rightarrow \frac{\cos(kR+\delta_0)}{k} \tag{63}$$

as $R\rightarrow\infty$. The phase shift δ_0 is a consequence of elastic scattering by the BO potential $e(R)$, and we refer to it as the BO phase shift. In the asymptotic limit $R\rightarrow\infty$, Eq. (60) becomes

$$F(R) = f(kR) - 2\mu_i kh(kR)\int_0^\infty dR' R' f(kR') \times \int_0^\infty dR'' R'' V_{op}(R',R'')F(R'') = \frac{\sin(kR+\delta_0)}{k} + \frac{\cos(kR+\delta_0)}{k}\tan\,\delta, \tag{64}$$

$$\tan\,\delta = -2\mu_i k\int_0^\infty dR'\; R' f(kR')\int_0^\infty dR''\; R'' V_{op} f(R',R'')F(R''). \tag{65}$$

Equation (65) is an integral equation for the phase shift $\delta = \delta_T - \delta_0$, the difference of the total phase shift δ_T and the BO phase shift δ_0. We now invoke the distorted-wave approximation, in which the radial function $F(R)$ in the integral in Eq. (65) is replaced by $f(kR)$. Applying it we obtain an expression for the imaginary part of the phase shift β,

$$\beta \equiv \mathrm{Im}(\delta) = 2\mu_i k\pi\sum_m \left| \int_0^\infty dRRf(kR)\phi_m(R)\tilde{U}_{\epsilon(k_m)}(R) \right|^2, \tag{66}$$

where we ignored the real part of optical potential and set $\tan\,\delta \approx \delta$.

Because $F(R)$ is normalized to unit incident flux, we can use the expression [20]

$$\sigma_{abs} = \frac{4\pi}{k^2}\beta = \frac{4\pi^2}{k}2\mu_i\sum_m \left| \int_0^\infty dRRf(kR)\phi_m(R)\tilde{U}_{\epsilon(k_m)}(R) \right|^2 \tag{67}$$

that relates the absorption cross section, due to an absorptive complex optical potential, to the imaginary part of the phase shift. Because the imaginary part of the optical potential describes the fragmentation reaction $\mathrm{H}(1s)+\overline{\mathrm{H}}(1s)\rightarrow p\overline{p}+e^+e^-$, we equate σ_{abs} with the fragmentation cross section σ_{frag}. Using Eqs. (67) and (44) we get

$$\sigma_{frag} = \frac{(2\pi)^4}{k^2}\sum_m \left| \int d^3\mathbf{R}F_0(\mathbf{R})\phi_m(\mathbf{R})\langle a|\tilde{V}_f|\epsilon(k_m)\rangle \right|^2, \tag{68}$$

where $F_0(\mathbf{R})$ is a solution to the homogeneous Schrödinger equation

$$-\frac{1}{2\mu_i}\nabla^2 F_0(\mathbf{R}) + e(R)F_0(\mathbf{R}) = \frac{k^2}{2\mu_i}F_0(\mathbf{R}) \tag{69}$$

that satisfies the asymptotic boundary condition,

$$F_0(\mathbf{R}) \sim \sqrt{\frac{k\mu_i}{(2\pi)^3}}\left\{ \exp(ikz) + f(\theta\phi)\frac{\exp(ikR)}{R} \right\} \tag{70}$$

and where $f(\theta\phi)$ is the BO elastic scattering amplitude.

Expression (68) is in harmony with the derivation for the fragmentation cross section given in Eq. (51). However, in that expression $F(\mathbf{R})$ is a solution to the fully coupled equation (41). If we replace $F(\mathbf{R})$ by $F_0(\mathbf{R})$ in Eq. (51), we obtain the result given above.

An expression similar to Eq. (68) was derived in a previous treatment [7,8,21] of the collision process. The major difference between the two approaches, for the expression of the fragmentation cross sections, involves the higher-order effect of the projection operator P. Here, the coupling elements involve the use of a renormalized interaction $\tilde{V}_f \equiv V_f/\sqrt{\Omega}$, where Ω is defined in Eq. (44). In the former treatment matrix elements are calculated using interaction V_f. The effect of the real part of the optical potential on the scattering length will be discussed elsewhere.

V. CALCULATIONS

A. Fragmentation cross section

The construction of the optical potential requires a calculation of the rearrangement coupling coefficients $\tilde{U}_\epsilon(R)$ defined in Eq. (44). They are overlap integrals of the Born-Oppenheimer wave function for the ground state of the H -H system with the free positronium states $|\epsilon\rangle$ and the interaction $\tilde{V}_f$.

The BO wave functions take the form

$$\Psi(\mathbf{r}_e,\mathbf{r}_{\bar{e}},R) = \sum_i c_i \exp[-\alpha(\lambda_1+\lambda_2) - \beta(\mu_1-\mu_2)] \times \lambda_1^{p_i}\lambda_2^{s_i}\mu_1^{q_i}\mu_2^{t_i}r_{12}^{m_i}, \tag{71}$$

where λ_i, μ_i are the prolate spheroidal coordinates

$$\lambda_i \equiv \frac{(r_{ia}+r_{ib})}{R}, \qquad \mu_i \equiv \frac{(r_{ia}-r_{ib})}{R}, \tag{72}$$

and r_{1a}, r_{1b} are the distances of the electron from the proton center and antiproton center, respectively, and r_{2a}, r_{2b} are the corresponding distances for the positron. The proton is centered at $-R/2$ and the antiproton at $R/2$ along the z axis. The parameters $\alpha, \beta, c_i, p_i, s_i, t_i, q_i, m_i$ are variational parameters chosen to minimize the BO eigenvalue. A full discussion concerning the details of this wave function is presented in Ref. [8]. Using the optimized Born-Oppenheimer wave functions, we calculated the integrals defined in Eq. (44) $\tilde{U}_\epsilon(R) = U_\epsilon(R)/\sqrt{\Omega}; U_\epsilon(R) \equiv \langle\epsilon|V_f|a\rangle$. Since the integrals involve wave functions for different lepton arrangements, numerical evaluation was necessary. We employed Monte Carlo integration and found that acceptable convergence is achieved by sampling about 10^8 points in a six-dimensional cavity of radius $R \approx 12a_0$, for the interbaryon separations considered. The results for the coupling parameter $U_\epsilon(R)$ are shown, as a function of positronium momentum k in Figs. 1(a) and 1(b). The graphs correspond to the coupling functions for various proton-antiproton separations that are identified in the figure.

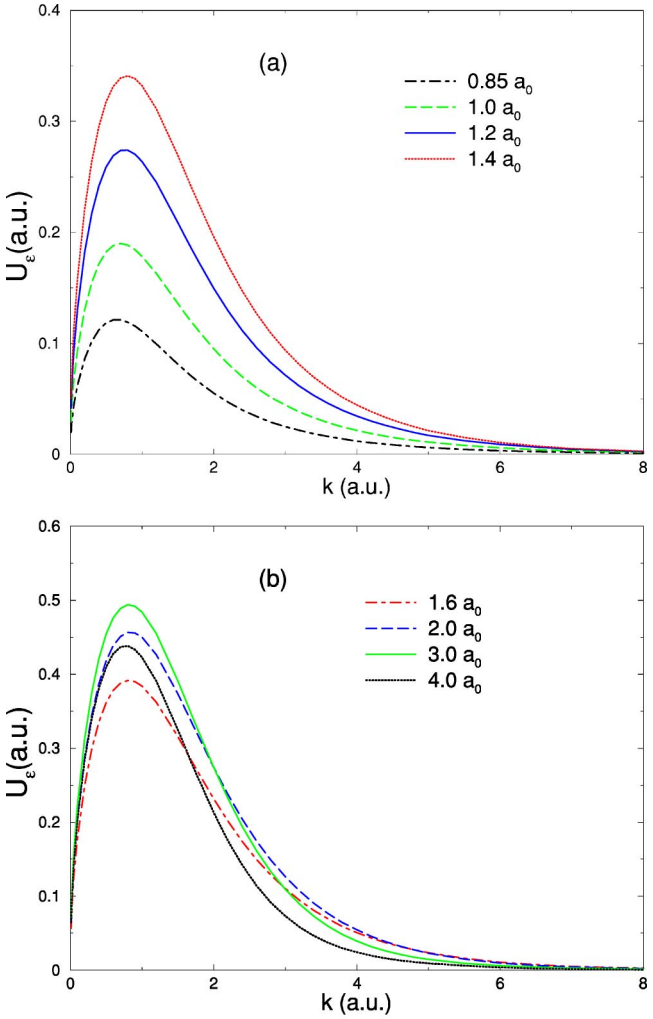

FIG. 1. (a) Coupling coefficients $U_\epsilon(R)$ as a function of the protonium-positronium relative momentum k, where $\epsilon=k^2/2\mu_f$, for the values $R=0.85a_0, 1.00a_0, 1.2a_0, 1.4a_0$. (b) Coupling coefficients for the values $R=1.6a_0, 2.0a_0, 3.0a_0, 4.0a_0$.

We imposed a self-consistency test to gauge the integrity of the wave functions used in the calculations for the coupling parameter $\tilde{U}_\epsilon$. According to Eq. (38) the identity $\Delta\epsilon(R)_{\kappa_n}\langle a|\kappa_n\rangle=-\langle a|V_f|\kappa_n\rangle$ must hold if the BO state $|a\rangle$ and the cavity normalized state $|\epsilon(\kappa_n)\rangle$ are good eigenstates of their respective Hamiltonians. The identity must also hold if we replace the cavity normalized functions with continuum normalized states, i.e., $|\kappa_n\rangle\rightarrow|\epsilon\rangle$. In Fig. 2. we compare the values of the integrals $\langle a|V_f|\epsilon\rangle$ (open circles) with the ones given by $\Delta\epsilon(R)_k\langle a|\epsilon\rangle$ (open squares). We find that, and show in Fig. 2, there is good to excellent agreement for the values obtained using the different methods.

With the coupling parameters $\tilde{U}_\epsilon$ we can calculate both the real and imaginary components of the optical potential. In Fig. 3 we plot the dependence of the coupling $U_\epsilon(R)$ matrix on the BO distance R for $\epsilon=k_f^2/2\mu_f=0.0469$, the energy of the fragment where the protonium is found in the $n=24$ state and positronium in its ground state. In that figure we also plot the renormalized coupling $\tilde{U}$ obtained by dividing

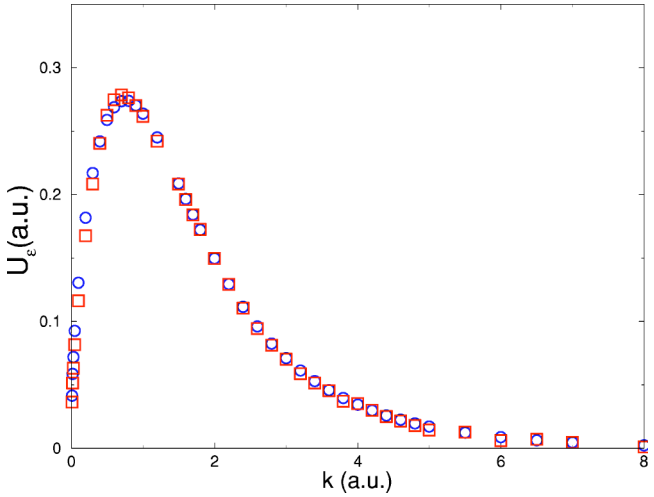

FIG. 2. Matrix elements $\langle\epsilon|V_f|a\rangle$ (open squares), and $\Delta\epsilon(R)_k\langle a|\epsilon\rangle$ (open circles), as a function of the relative momentum k. The proton-antiproton separation has the value $R=1.2a_0$.

the former by the quantity $\Omega^{1/2}(R)$ and whose values are plotted in Table I. We note that as R decreases so does Ω. The question arises, what is the value for $\Omega(R)$ at $R=R_{critical}$, the BO distance at which the leptons are no longer bound to the nuclear centers [23]? This question is addressed in Appendix A where we conclude that $\tilde{U}_\epsilon\rightarrow 0$ as $R\rightarrow R_{critical}$ from above. Likewise, we show that Ω becomes small but must remain finite in this limit. In Fig. 3 this behavior is illustrated by the dashed lines, which are extrapolations of the calculated data (our minimum value for $R=0.85a_0$) to $R=R_{critical}$, which we take to have the value $R_{critical}=0.74a_0$ [24]. For $R<R_{critical}$ we set $\tilde{U}_\epsilon=0$ (see Appendix A).

The results of our calculation for the fragmentation cross sections are tabulated in Table II. We compare the results obtained in the distorted-wave approximation with those ob-

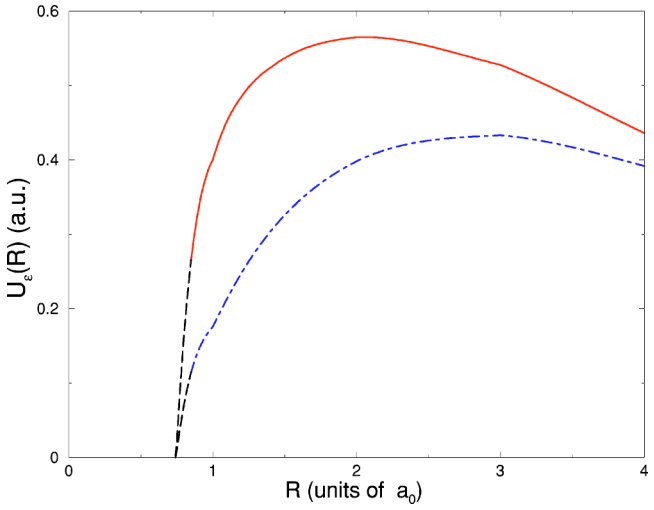

FIG. 3. Coupling elements $U_\epsilon(R)$ (dot-dashed line) and renormalized coupling $\tilde{U}_\epsilon(R)$ (solid line), as a function of internuclear distance for positronium fragment energy $\epsilon=0.0469$. Dashed line is an extrapolation.

TABLE I. Calculated values for renormalization parameter Ω_a defined in Eq. (44). The second column lists Ω obtained by direct evaluation of the matrix elements $|\langle\epsilon|a\rangle|$. Data listed in the third column are obtained by calculation of $|\langle a|V_f|\epsilon\rangle|$ and the use of identity (37).

R	Ω	Ω
4	0.807	0.807
3	0.674	0.674
2	0.497	0.496
1.6	0.398	0.397
1.4	0.336	0.334
1.2	0.262	0.257
1.0	0.193	0.185
0.85	0.186	

tained using full solutions to the Schrödinger equation including the imaginary component of the optical potential. Using the unrenormalized coupling V_f, we find good agreement in the predictions of both approaches. However, with the renormalized interaction $\tilde{V}_f$ we find that the distorted-wave approximation considerably overestimates the fragmentation cross sections. The cross sections corresponding to the $n=24,23$ protonium fragments, and obtained using $\tilde{V}_f$, are in good agreement with the results recently obtained by Armour and Chamberlain [22] using a Kohn variational theory. However, we also find significant fragmentation into the $n=22,21$ states whereas Armour and Chamberlain find a very small contribution into these states.

We also find a significant effect on the calculated value for the elastic scattering length. This is illustrated in Fig. 4 where we plot the real part of the wave function using both the BO approximation and that obtained including the imaginary part of the optical potential. We find that the scattering length for the latter case has a value $5.6a_0$, compared with $8.1a_0$ [8] obtained in the BO approximation.

TABLE II. Cross sections for fragmentation into protonium states, of principal quantum number n, and positronium in its ground state. The cross sections are expressed as $C/\sqrt{\epsilon}$, where ϵ is the collision energy and C is a constant listed in the columns.

	Distorted wave		Optical potential			
n	V_f	$\tilde{V}_f$	V_f	$\tilde{V}_f$	Ref. [8]	Ref. [22]
24	0.15	0.38	0.13	0.32	0.09	0.21
23	0.24	1.40	0.21	0.48		0.45
22	0.002	0.02	0.01	0.14		0.01
21	0.02	0.13	0.025	0.10		
20	0.001	0.004	0.001	0.04		
19	0.003	0.017	0.004	0.03		
18	0.0	0.002	0.0	0.003		
Total	0.39	1.95	0.38	1.1	0.09	0.67

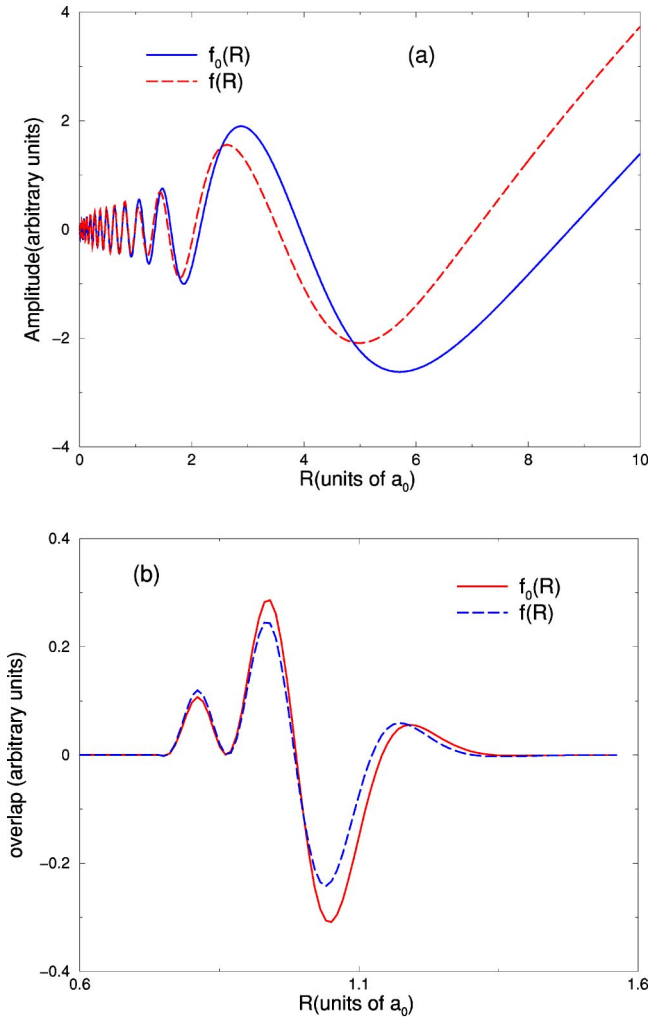

FIG. 4. (a) Solid line is the amplitude for the elastic scattering radial wave function, $f_0(R)$, in the Born-Oppenheimer approximation. It is characterized by the scattering length $a=8.10a_0$. The dashed line represents the real part of the radial wave function, $f(R)$, obtained by including the imaginary part of the optical potential to the BO potential. (b) Dependence of the radial integrand on the choice for the real part of the radial wave function.

B. Lifetimes of quasi bound $H\bar{H}$ levels

The time-dependent Schrödinger equation for the H-$\bar{H}$ system is

$$-\frac{1}{2\mu_i}\nabla^2\psi(\mathbf{R},t)+e(R)\psi(\mathbf{R},t)+\int d^3\mathbf{R}'V_{op}(\mathbf{R},\mathbf{R}')\psi(\mathbf{R}',t)=i\frac{\partial\psi(\mathbf{R},t)}{\partial t}, \tag{73}$$

where $V_{op}(\mathbf{R},\mathbf{R}')$ is given in Eq. (53). The proton-antiproton annihilation in-flight rate is largely determined by the value of the proton-antiproton wave function at their point of coalescence [8], and so we can ignore this process for states in which the relative angular momentum, for the atom-antiatom pair $j>0$. We also ignore the effects of lepton annihilation

TABLE III. Fragmentation lifetimes for selected quasibound states of $H\bar{H}$. ν is the radial quantum number, where $\nu-1$ is the number of nodes in the radial wave function, and j is the orbital angular momentum, $E_{\nu j}$ is the dissociation energy. $-E_n$ is the bound protonium energy with principal quantum number n, ϵ is the fragment energy, and τ, in units of seconds, is the partial lifetime for state $H\bar{H}(\nu j)$.

ν	j	$E_{\nu j}$	n	E_n	ϵ	τ
27	1	1.239×10^{-5}	24	0.7969	0.0469	5.7×10^{-13}
27	1	1.239×10^{-5}	23	0.8676	0.1177	2.9×10^{-13}
27	1	1.239×10^{-5}	22	0.9484	0.1984	3.4×10^{-11}
27	1	1.239×10^{-5}	21	1.0409	0.2909	2.5×10^{-12}
26	1	5.561×10^{-4}	24	0.7969	0.0464	1.6×10^{-13}
26	1	5.561×10^{-4}	23	0.8676	0.1172	7.5×10^{-14}
26	1	5.561×10^{-4}	22	0.9484	0.1979	8.2×10^{-12}
26	1	5.561×10^{-4}	21	1.0409	0.2903	6.6×10^{-13}
25	1	5.709×10^{-3}	24	0.7969	0.0412	1.9×10^{-14}
25	1	5.709×10^{-3}	23	0.8676	0.1120	5.1×10^{-15}
25	1	5.709×10^{-3}	22	0.9484	0.1927	2.8×10^{-13}
25	1	5.709×10^{-3}	21	1.0409	0.2852	4.9×10^{-14}
25	2	3.833×10^{-4}	24	0.7969	0.0466	1.6×10^{-13}
25	2	3.833×10^{-4}	23	0.8676	0.1174	9.8×10^{-14}
25	2	3.833×10^{-4}	22	0.9484	0.1980	2.6×10^{-11}
25	2	3.833×10^{-4}	21	1.0409	0.2905	8.2×10^{-13}
24	2	5.285×10^{-3}	24	0.7969	0.0417	1.3×10^{-14}
24	2	5.285×10^{-3}	23	0.8676	0.1125	5.0×10^{-15}
24	2	5.285×10^{-3}	22	0.9484	0.1931	5.2×10^{-13}
24	2	5.285×10^{-3}	21	1.0409	0.2856	4.6×10^{-14}
23	3	4.650×10^{-3}	24	0.7969	0.0423	8.8×10^{-15}
23	3	4.650×10^{-3}	23	0.8676	0.1131	5.0×10^{-15}
23	3	4.650×10^{-3}	22	0.9484	0.1938	2.6×10^{-12}
23	3	4.650×10^{-3}	21	1.0409	0.2863	4.3×10^{-14}

in-flight [10]. From Eq. (73) we obtain the conservation equation,

$$i\frac{\partial P(t)}{\partial t} = 2\int d^3\mathbf{R}' \int d^3\mathbf{R}\psi^*(\mathbf{R},t)V_{op}^I(\mathbf{R},\mathbf{R}')\psi(\mathbf{R}',t),$$
$$P(t) \equiv \int d^3\mathbf{R}\psi^*(\mathbf{R},t)\psi(\mathbf{R},t). \tag{74}$$

We assume that the probability $P(t)$ for the system to be found in state $\psi(\mathbf{R},t)$ at time t has the form $P(t)=P_0\exp(-\Gamma t)$. Because $V_{op}^I(\mathbf{R},\mathbf{R}')$ is of finite range, we assume that $\psi(\mathbf{R},t)=\exp(-iEt)\exp(-\Gamma/2t)\psi(\mathbf{R})$, where $\psi(\mathbf{R})$ is normalized to unity, and it follows

$$\Gamma = 2\pi\sum_m \left|\int_0^\infty \phi_m(R)\tilde{U}_{\epsilon(k_m)}(R)\psi(R)dR\right|^2, \tag{75}$$

where we used Eq. (54). $\phi_m(R)$ is the radial protonium wave function with principal quantum number m, and we made the isotropic approximation Eq. (59). We make the additional approximation that the radial wave function $\psi(R)$ is a bound-state solution to the equation

$$-\frac{1}{2\mu_i}\frac{d^2\psi(R)}{dR^2} + \frac{j(j+1)}{2\mu_i R^2}\psi(R) + e(R)\psi(R) - E\psi(R) = 0, \tag{76}$$

where E is its energy eigenvalue. We label these states and energies by the radial quantum number ν and angular-momentum quantum number j. We define a lifetime, which according to Eq. (75) is given by

$$\tau_n \equiv \frac{1}{\Gamma_n},$$
$$\Gamma_n = 2\pi\left|\int_0^\infty \phi_n(R)\tilde{U}_{\epsilon(k_n)}(R)\psi_{\nu j}(R)dR\right|^2, \tag{77}$$

for a quasibound state with quantum number νj to fragment into a $p\bar{p}(nj)$ and $e^+e^-(1s)$ pair.

In Table III, we tabulate the partial lifetimes for selected high-lying, $j>0$, levels of the $H\bar{H}$ system. We find that fragmentation is most probable into the $n=24,23$ protonium states. A more accurate calculation, including the real part of the optical potential, is the focus of current efforts.

In this discussion we restricted the fragmentation channels to positronium atoms in their ground 1*s* state which is justified by the observation [8] that in the limit of ultracold collisions it is the dominant fragmentation channel. If we relax the constraints imposed in the discussion of the previous sections, expression (54) and Eq. (55) are generalized to

$$V_{op}^{I}(\mathbf{R},\mathbf{R}') = -\pi i \sum_{m}\sum_{nl} \phi_m(\mathbf{R})\phi_m^{\dagger}(\mathbf{R}') \times \tilde{U}_{\epsilon(\mathbf{k}_m),nl}(\mathbf{R})\tilde{U}^{*}_{\epsilon(\mathbf{k}_m),nl}(\mathbf{R}'),$$

$$\epsilon(k_m) \equiv E - e_m - \epsilon_{ps}(nl), \tag{78}$$

$$V_{op}^{R}(\mathbf{R},\mathbf{R}') = \sum_{m}\sum_{nl}\int_0^{\infty} d\epsilon \phi_m(\mathbf{R})\phi_m^{\dagger}(\mathbf{R}') \times \tilde{U}_{\epsilon(\mathbf{k}),nl}(\mathbf{R})\tilde{U}^{*}_{\epsilon(\mathbf{k}),nl}(\mathbf{R}')\left[\mathrm{P}\frac{1}{E - e_m - \epsilon - \epsilon_{ps}(nl)} + \mathrm{P}\frac{1}{\epsilon + \epsilon_{ps}(nl) + V_{p\bar{p}}(\mathbf{R}) - e(R)}\right], \tag{79}$$

where *nl* are the principal and angular momentum, quantum numbers of the positronium atom, $\tilde{U}_{\epsilon(\mathbf{k}),nl}(\mathbf{R}) \equiv \langle \epsilon(\mathbf{k})nl|\tilde{V}_f|a\rangle$, and where the *s*-wave positronium continuum function is replaced by $|\epsilon(\mathbf{k})\rangle \equiv \sqrt{k\mu_f/2\pi^3}\exp[i\mathbf{k}\cdot(\mathbf{x}_1+\mathbf{x}_2)/2]$. We will apply Eqs. (78) and (79) in future studies to find the probability for rearrangement that involves excited states of the positronium fragment. As pointed out in Sec. III, care must be exercised so that the basis set is not overcomplete.

VI. SUMMARY AND DISCUSSION

Equation (56) states the central result of this paper and describes an effective Schrödinger equation that provides a description of hydrogen-atom–antihydrogen-atom interactions at very low collision energies. The Born-Oppenheimer potential $e(R)$ gives the leading-order interaction between the H and $\bar{\mathrm{H}}$ atoms, but even at ultracold collision energies the H-$\bar{\mathrm{H}}$ system is degenerate and embedded in a continuum of states involving $p\bar{p}$ and e^+e^- fragments. In addition to elastic scattering of the atoms, there exists the possibility of fragmentation into protonium and positronium. The single channel BO picture does not accommodate that possibility and a multichannel description is necessary. In Eq. (56) multichannel effects are incorporated by the introduction of the nonlocal optical potential V_{op}. Its imaginary component describes the breakup of the atom-antiatom pair into protonium and positronium fragments.

We showed, using a distorted-wave treatment of the optical potential, how to recover the post-prior theory employed in our previous calculations. We showed that the optical potential includes a renormalized interaction strength that governs the fragmentation process. We calculated the cross sections for fragmentation using the imaginary part of the optical potential and compared the results with those obtained in a distorted-wave treatment. For the renormalized interaction, we find that the distorted-wave approximation overestimates the fragmentation cross sections. We also find a significant higher-order effect induced by the imaginary component of the optical potential. Its inclusion in the Schrödinger equation leads to a scattering length having the value $a = 5.6a_0$, a 35% decrease in value from that obtained in the Born-Oppenheimer approximation [8]. The partial cross sections for fragmentation into the $n = 24, 23$ protonium states are in good agreement with recent values obtained using a Kohn variational approach [22], however, we also find significant fragmentation into the $n = 22, 21$ states. Our total fragmentation cross section is $1.1/\sqrt{\epsilon}$, where ϵ is the collision energy. We used the imaginary part of the optical potential to estimate the lifetimes for quasibound states of this complex to fragment into protonium-positronium pairs. The theory presented here provides a framework for additional and more accurate calculations that include the real part of the optical potential.

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APPENDIX A

In order to study the nature of the positronium-nuclei interaction at values for $R < R_{critical}$, we represent V_f by a multipole series whose leading term is

$$V_f \approx \frac{\boldsymbol{\xi}\cdot\boldsymbol{R}}{|R_c|^3} - \frac{3(\boldsymbol{\xi}\cdot\boldsymbol{R}_c)(\boldsymbol{R}\cdot\boldsymbol{R}_c)}{|R_c|^5}, \tag{A1}$$

where $\boldsymbol{\xi}$, $\boldsymbol{R}_c$ are the positronium coordinates defined in Eq. (22). In deriving Eq. (A1) we have assumed that $|\boldsymbol{\xi}| \ll |\boldsymbol{R}_c|$ and $|\boldsymbol{R}_c| \gg |\boldsymbol{R}|$. Equation (A1) represents the interaction between two electric dipoles and it is an appropriate description for the asymptotic interaction between the positronium atom and nuclei at BO separations $R < R_{critical}$. Since the positronium atom in its ground state does not have a permanent dipole moment V_f contributes only in second order. Consider the leptonic Hamiltonian

$$H_{lepton} = \frac{\boldsymbol{p}_c^2}{2\mu_f} + \frac{\boldsymbol{p}_{ps}^2}{m} - \frac{1}{|\boldsymbol{\xi}|} + V_f, \tag{A2}$$

which, when taken to second order, leads to the effective positronium-protonium interaction

$$V_{ef} = \frac{-C_6(\boldsymbol{R},\boldsymbol{R}_c)}{R_c^6},$$

$$C_6(\boldsymbol{R},\boldsymbol{R}_c) = \sum_n [\boldsymbol{d}_n \cdot \boldsymbol{R} - 3(\boldsymbol{d}_n \cdot \hat{\boldsymbol{R}}_c)(\boldsymbol{R} \cdot \hat{\boldsymbol{R}}_c)]^2, \quad \text{(A3)}$$

$$\boldsymbol{d}_n \equiv \langle \phi_{1s}|\boldsymbol{\xi}|\phi_n\rangle/(|E_{1s} - E_n|),$$

where ϕ_n is an unperturbed positronium state with energy eigenvalue E_n.

We can always express the Born-Oppenheimer wave function in the form

$$\Psi(\boldsymbol{R},\boldsymbol{\xi},\boldsymbol{R}_c) = \sum_n F_n(\boldsymbol{R}_c)\phi_n(\boldsymbol{\xi}), \quad \text{(A4)}$$

where $F_n(\boldsymbol{R}_c)$ is a positronium atom amplitude, it is understood that F_n is parametrized by the BO separation vector $\boldsymbol{R}$ and n is an index representing both discrete and continuous components. Using Eq. (A4), the partial wave expansion,

$$F_n(\boldsymbol{R}_c) = \sum_{lm} \frac{F_n^{lm}(R_c)}{R_c} Y_{lm}(\hat{\Omega}_c), \quad \text{(A5)}$$

we obtain for the expression defined in Eq. (44),

$$\Omega = \left(1 - \int_0^\infty dR_c |F_{n=1}^{l=0}(R_c)|^2\right)^{1/2}. \quad \text{(A6)}$$

In the region $R > R_{critical}$ Ψ is normalizable and

$$\sum_n \sum_{lm} \int_0^\infty dR_c |F_n^{lm}(R_c)|^2 = 1. \quad \text{(A7)}$$

Therefore Ω is either positive definite or vanishes. In the region $R < R_{critical}$ we enforce the condition $\langle\Psi|\Psi\rangle = 1$ by employing box normalization as in Sec. III for the fragment functions. In that case the normalization factor for amplitude $F_n(R)$ is proportional to $1/\sqrt{V}$, where V is the cavity volume. However, Ω remains independent of cavity volume. According to Eq. (A7) equality $\Omega = 0$ can only be satisfied if $F_n^{lm} = 0$ for all $n > 1$. Because V_f mixes the positronium ground state with states of $n > 1$ at all R (with the exception of the origin $R = 0$), we argue that $0 > \Omega \leqslant 1$ for all R. This inequality was satisfied in our numerical calculations.

We now study the behavior of the matrix element $\langle \epsilon_k|V_f|\Psi\rangle$ defined in Eq. (44). If we represent the BO state Ψ by expansion (A4) we obtain an effective radial equation for the s-wave amplitude $f(R_c) \equiv F_{n=1}^{l=0}(R_c)$, in the region where $R_c \gg R$,

$$-\frac{1}{2\mu_f}\frac{d^2 f(R_c)}{dR_c^2} - \frac{C_6(R)}{R_c^6} f(R_c) = \epsilon f(R_c), \quad \text{(A8)}$$

where

$$C_6(R) \equiv \langle C_6(\boldsymbol{R},\hat{\boldsymbol{R}}_c)\rangle \quad \text{(A9)}$$

is a spherical average over all angles of the positronium coordinate $\boldsymbol{R}_c$ defined with respect to a coordinate system in which the BO vector $\boldsymbol{R}$ is directed along the z axis. Though this s-wave average vanishes for the dipole-dipole interaction given by Eq. (A1), it can be shown that the average of $C_6(\boldsymbol{R},\boldsymbol{R}_c)$ does not vanish and that it is positive definite.

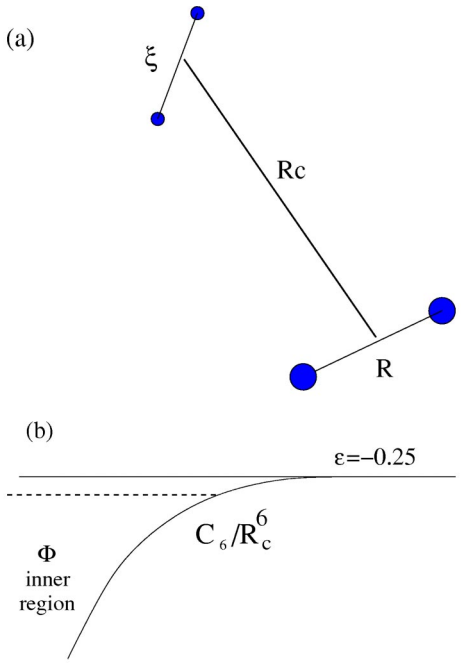

FIG. 5. (a) Graphical representation of coordinates defined in Appendix A. (b) Effective long-range component of the protonium-positronium interaction. Φ represents the contribution to the action from the region where $R_c < |\boldsymbol{R}|$.

We study bound-state solutions to Eq. (A8) whose energy eigenvalues ϵ are near, but below, the first excitation threshold energy of -0.25. Figure 5(b) illustrates the asymptotic potential included in Eq. (A8) and the bound-state energy eigenvalue ϵ is shown by the dashed line in that figure. For a given BO separation $R > R_{critical}$, the value for ϵ is primarily determined by the inner range potential, not included in Eq. (A8) but represented by the quantity Φ, the contribution to the total action from the potential in the inner region. If, at this R, ϵ is slightly below the threshold shown in Fig. 5(b), small, continuous, shifts of R toward $R_{critical}$ continuously shift ϵ toward the ionization limit. The outer classical turning point is determined by the value of the long range potential given in Eq. (A9) and the value for ϵ. As $\epsilon \to -0.25$ from below and for large R_c, the wave function $f(R_c)$ assumes the form

$$f(R_c) \approx C R_c \exp[-\sqrt{2\mu_f \Delta\epsilon} R_c], \quad \text{(A10)}$$

where $C \approx (2\mu_f \Delta\epsilon)^{3/4}$ is a normalization constant and $\Delta\epsilon \equiv |\epsilon| - 0.25$ is the binding energy. Using expressions (A10) and (A4) we evaluate the coupling matrix element $\langle \epsilon(k)|\Psi\rangle$ defined in Sec. III,

$$\begin{aligned}\langle \epsilon(k)|\Psi\rangle &= \int d^3\boldsymbol{R}_c \sqrt{\frac{\mu_f}{2\pi^2 k}} \frac{\sin(kR_c)}{R_c} F_{1s}(\mathbf{R}_c) \\ &= \sqrt{\frac{2\mu_f}{\pi k}} \int_0^\infty dR_c \sin(kR_c) f(R_c) \\ &= 2\sqrt{\frac{\mu_f k}{\pi}} \frac{(2\mu_f \Delta\epsilon)^{5/4}}{(k^2 + 2\mu_f \Delta\epsilon)^2}, \end{aligned} \quad \text{(A11)}$$

where k is the wave number associated with the fragment kinetic energy. According to relation (A11), the coupling matrix element tends to zero as $\Delta\epsilon\to 0$. By the same token, $\langle\epsilon(k)|V_f|\Psi\rangle\to 0$ as $\Delta\epsilon\to 0$ where we have used relation (38) and the fact that the energy defect does not vanish for fragments of finite kinetic energy. In the region $R<R_{critical}$ the overlap integral $\langle\epsilon(k)|\Psi\rangle$ does not necessarily vanish. In our formulation, $|\Psi\rangle$ is cavity (box) normalized (in the same way the functions $|\kappa_n\rangle$ are normalized) in this region. Thus, for $R<R_{critical}$, $|\Psi\rangle=1/\sqrt{V}|\Psi'\rangle$ where $|\Psi'\rangle$ is a continuum function with respect to coordinate R_c. However, $\langle\epsilon(k)|V_f|\Psi'\rangle$ remains finite since V_f has the asymptotic form (A3). Thus in the limit $V\to\infty$ the optical potential coupling elements, defined in Eq. (39), $\sqrt{\det S}\tilde{V}_{a\kappa_n}=\langle\Psi|V_f|\kappa_n\rangle\to 1/V\langle\Psi'|V_f|\epsilon(k)\rangle$ since both $|\Psi\rangle$ and $|\kappa_n\rangle$ are cavity normalized. Proceeding as in Eqs. (42) and (43), we find that the optical potential vanishes in the $V\to\infty$ limit. We stress that for $R>R_{critical}$ the matrix element $\langle\Psi|V_f|\kappa_n\rangle\to 1/\sqrt{V}\langle\Psi|V_f|\epsilon(k)\rangle$ and leads to the nontrivial continuum limit Eq. (53). A simple model is introduced in Appendix B, which provides more physical insight into the mechanism by which the optical potential vanishes as a bound state merges into a continuum state.

According to Eq. (A11) the coupling matrix element $\langle\epsilon(k)|\Psi\rangle$ has a maximum peak at fragment energy

$$E_{max}=\frac{k_{max}^2}{2\mu_f}=\frac{\Delta\epsilon}{7}. \tag{A12}$$

In our calculations we have seen that the peaks in the coupling matrix elements shift to lower fragment energies as we approach $R_{critical}$, behavior that is consistent with the prediction of Eq. (A11). At $R=1a_0$ the binding energy of the positronium has a value [24] 0.0244, and according to Eq. (A12) a peak in the coupling matrix element, corresponding to this binding energy, would occur at $E_{max}=0.0035$. In our calculations, we observe a maximum at $E_{max}=0.01$ (see Fig. 1) within the same order of magnitude as the value predicted by Eq. (A12).

APPENDIX B

We express the equation

$$(H-E)|\Psi\rangle=0 \tag{B1}$$

in the form [11]

$$\begin{aligned} PHP|\Psi_P\rangle+PHQ|\Psi_Q\rangle&=E|\Psi_P\rangle,\\ QHQ|\Psi_Q\rangle+QHP|\Psi_P\rangle&=E|\Psi_Q\rangle \end{aligned} \tag{B2}$$

where the projection operators obey the relations $P+Q=1$, $P^2=P$, $Q^2=Q$, $QP=0$, and $\Psi_P\equiv P|\Psi\rangle$, $\Psi_Q\equiv Q|\Psi\rangle$. It follows that [11]

$$\left(PHP+PHQ\frac{1}{H-E}QHP\right)|\Psi_P\rangle=E|\Psi_P\rangle. \tag{B3}$$

If $H=H_0+V$ so that $[P,H_0]=[Q,H_0]=0$ we further simplify

$$\left(PH_0P+PVP+PVQ\frac{1}{H-E}QVP\right)|\Psi_P\rangle=E|\Psi_P\rangle, \tag{B4}$$

where $1/(H-E)\equiv(H-E)^{-1}$.

We consider a particle in one dimension subjected to periodic boundary conditions at $x=\pm L/2$. We define periodic basis functions $|\kappa_n\rangle$ so that

$$\begin{aligned} \langle x|\kappa_n\rangle&\equiv u_n(x)=\frac{\exp(i\kappa_n x)}{\sqrt{L}},\\ \kappa_n&=\frac{2n\pi}{L},\quad n=0,\pm 1,\pm 2,... \end{aligned} \tag{B5}$$

and $\langle\kappa_n|\kappa_m\rangle=\delta_{nm}$. They are eigenstates of H_0,

$$H_0|\kappa_n\rangle=\frac{\kappa^2}{2}|\kappa_n\rangle \tag{B6}$$

and are complete so that

$$\sum_n|\kappa_n\rangle\langle\kappa_n|=1 \tag{B7}$$

in the domain $-L/2\leqslant x\leqslant L/2$. Let $P=|\kappa_n\rangle\langle\kappa_n|$, then $Q=\Sigma_{m\neq n}|\kappa_m\rangle\langle\kappa_m|$. V is an arbitrary short-range potential and

$$\langle\kappa_n|V|\kappa_m\rangle=\frac{v_{nm}}{L}, \tag{B8}$$

where v_{nm} is independent of the boundary dimension L. For example, if $V(x)=g\delta(x)$ then $v_{nm}=g$. The optical potential

$$U\equiv PVQ\frac{1}{H-E}QVP \tag{B9}$$

can be expressed as the sum

$$PVQ\frac{1}{H_0-E}QVP-PVQ\frac{1}{H_0-E}V\frac{1}{H_0-E}QVP+\cdots \tag{B10}$$

or

$$\begin{aligned} &|n\rangle\langle n|\left(\frac{1}{L^2}\sum_{m\neq n}\frac{v_{nm}v_{mn}}{(\kappa_m^2/2-E)}\right)-|n\rangle\langle n|\\ &\times\left(\frac{1}{L^3}\sum_{m\neq n}\sum_{q\neq n}\frac{v_{nm}v_{mq}v_{qn}}{(\kappa_m^2/2-E)(\kappa_q^2/2-E)}\right)+\cdots, \end{aligned}$$

where we have used Eq. (B8). We take the continuum limit $\Sigma_m\to L\int d\kappa$ as $L\to\infty$ and obtain

$$U\to\frac{|n\rangle\langle n|}{L}\tilde{U}_{nn}, \tag{B11}$$

where

$$\tilde{U}_{nn} \equiv \int d\kappa \frac{v_{nk}v_{kn}}{(\kappa^2/2 - E)} - \int d\kappa \int d\kappa' \frac{v_{n\kappa}v_{\kappa\kappa'}v_{\kappa' n}}{(\kappa^2/2 - E)(\kappa'^2/2 - E)} + \cdots \tag{B12}$$

is independent of the boundary dimension L. Defining the amplitude $\Psi_P(x) \equiv \langle x|P|\Psi\rangle = \langle x|\Psi_P\rangle$ using

$$\langle x|PVP|\Psi\rangle = \frac{v_{nn}}{L}\Psi_P(x), \tag{B13}$$

$$\langle x|PH_0P|\Psi\rangle = \frac{\kappa_n^2}{2}\Psi_P(x) = -\frac{1}{2}\frac{d^2\Psi_P(x)}{dx^2}.$$

We obtain the continuum limit of Eq. (B3),

$$-\frac{1}{2}\frac{d^2\Psi_P(x)}{dx^2} + \frac{1}{L}\left[v_{nn} + \tilde{U}_{nn}\right]\Psi_P(x) = E\Psi_P(x). \tag{B14}$$

The optical potential vanishes in this limit and Eq. (B14) for $\Psi_P(x)$ is that of a free particle. The above exercise could have been avoided if we recognized that for a solution to Eq. (B1) $\Psi(x) = \langle x|\Psi\rangle$, the projected function

$$\Psi_P(x) = u_n(x)\langle n|\Psi\rangle \tag{B15}$$

is a free particle solution in the limit $L \to \infty$. The optical potential must vanish, in this limit, in order for the equations to be consistent. We recognize that if P projects onto a true bound state $\phi(x)$, so that $\mathrm{Lim}_{L\to\infty}\int_{-L/2}^{L/2} dx\phi^*(x)V(x)\phi(x)$ is independent of L, the optical potential is also independent of L, and leads to a nontrivial interaction in the $L \to \infty$ limit.

We introduced this simple model in order to illustrate a mechanism that is at work, and discussed in Appendix A, in our general treatment of the H-$\bar{\mathrm{H}}$ optical potential. In that discussion, we projected onto true bound BO wave function at $R > R_{critical}$. This led to an optical potential that describes the interaction of the bound state with the continuum. However, for $R < R_{critical}$, the BO wave function merges into the continuum and the optical potential vanishes, in the infinite box limit, via a mechanism that is analogous to that seen in the simple model discussed above.

In order to treat the continuum-continuum interaction at $R < R_{critical}$ we need to relax and extend the assumptions employed in the present approach. The off-diagonal $\langle \kappa_m|V_f|\kappa_n\rangle$ terms in Eq. (29), treated here as a higher-order contribution to the optical potential, need to be included in a multichannel continuum treatment. One possibility is to exploit an R-matrix approach in this region. This is beyond the scope of the present discussion and will be the subject of future investigations.

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