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Metastable compound states of an antiproton and a hydrogen atom

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The stability of antiproton-hydrogen compound states ($\bar{p}$H) is investigated theoretically. The $\bar{p}$H compound state has decay channels of atomic electron detachment ($\rightarrow e^- + \bar{p}p$) and hadronic pair ($\bar{p}$-$p$) annihilation, and hence it cannot be permanently stable even if the dissociation channel ($\rightarrow \bar{p} + \mathrm{H}$) is energetically closed. In this paper, information on the metastable $\bar{p}$H states at energies below the dissociation limit is obtained by analyzing low-energy resonances in $e^- + \bar{p}p$ scattering. The scattering calculation is carried out by using an R-matrix method, which also allows for the annihilation channel simultaneously. The metastable states are found to be identified as vibrational levels supported by a Born-Oppenheimer (BO) potential. The energy-level widths attributed to the electron detachment and the annihilation are also calculated using a model based on the BO picture.

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I. INTRODUCTION

Recently, large progress has been made in experimental studies to produce and trap antihydrogen atoms ($\bar{\mathrm{H}}$) at very low ($\sim$10 K) temperatures [1–6]. In such studies, of serious concern to the experimentalists are processes leading to unfavorable trap loss of $\bar{\mathrm{H}}$, and particular attention is paid to $\bar{\mathrm{H}} + \mathrm{H}$ collisions. At very low energies, besides merely the elastic one, the $\bar{\mathrm{H}} + \mathrm{H}$ system has reactive channels of matter-antimatter annihilation due to hadronic interaction and of atomic rearrangement producing a positronium (e^+e^-) and a protonium ($\bar{p}p$). Meanwhile, the $\bar{\mathrm{H}} + \mathrm{H}$ system has deeper scientific significance since it is one of the simplest and most fundamental matter-antimatter combinations. So far, a lot of theoretical studies have been done on this matter-antimatter collision system in atomic physics [7–18]. In most of these studies, the Born-Oppenheimer (BO) approximation is a starting point for treating the atomic four-body dynamics in $\bar{\mathrm{H}} + \mathrm{H}$, and first-order perturbation theory is applied to the rearrangement reaction. Hereafter, let us call this type of approach the BO model. As for more sophisticated studies, Armour and Chamberlain [14] performed a nonperturbative quantum-mechanical (QM) calculation by using a Kohn variational method, and Zygelman *et al.* [17] introduced an optical potential approach.

Taking note of the fact that the BO potential of $\bar{\mathrm{H}} + \mathrm{H}$ reveals an attractive nature at least at large separations [7,8], one might expect that this system could have vibrationally bound states as if it were a molecule. Zygelman *et al.* [9] suggested the possibility of forming the $\bar{\mathrm{H}}$H molecule by radiative association in $\bar{\mathrm{H}} + \mathrm{H}$ collisions. However, there is a basic difficulty with this idea because the heavy particles ($\bar{p}$ and p) are unable to bind the light particles (e^+ and e^-) at $\bar{p}$-p distances R less than the critical value $R_0 = 0.744$ a.u., even within the BO approximation [8,13,16]. For this reason, any compound state of $\bar{\mathrm{H}}$H has a non-negligible decay channel of a breakup into $\bar{p}p + e^+e^-$ and is eventually unstable (or perhaps metastable). Considering that the vibrational wave function can have high amplitudes at $R > R_0$ for a high vibrational state, it is expected that the $\bar{\mathrm{H}}$H compound state having an energy close to the dissociation limit ($\rightarrow \bar{\mathrm{H}} + \mathrm{H}$) can become metastable. The energy widths of such vibrational levels attributed to the breakup and annihilation reactions were calculated using the BO picture and a distorted-wave (DW) method in several theoretical studies [19–21]. However, Strasburger [16] found that the correction to the BO approximation would diverge when $R \rightarrow R_0$ in the $\bar{\mathrm{H}} + \mathrm{H}$ system. It is not certain that the BO model is satisfactory for understanding the physical properties of the $\bar{\mathrm{H}}$H compound state.

The present study investigates the $\bar{p} + \mathrm{H}$ system at energies E below the dissociation limit D. A noteworthy fact is that the BO property of $\bar{p} + \mathrm{H}$ is very similar to that of $\bar{\mathrm{H}} + \mathrm{H}$. Also in the $\bar{p} + \mathrm{H}$ system, there exists the so-called Fermi-Teller critical value $R_{\mathrm{FT}} = 0.639$ a.u. [22]; at distances $R \leqslant R_{\mathrm{FT}}$, the electronic bound state is absent. Therefore, the $\bar{p}$H molecule is unstable as well as $\bar{\mathrm{H}}$H and has a decay channel of electron detachment ($\rightarrow \bar{p}p + e^-$). In the case of $\bar{p} + \mathrm{H}$, since the long-range polarization force $\propto -R^{-4}$ works at large R, the vibrational wave function can have high amplitudes even at $R \sim 100$ a.u. $\gg R_{\mathrm{FT}}$ if the vibrational energy is close to the dissociation limit (see later). Thus, one may be able to expect that high vibrational states of $\bar{p}$H are more stable than those of $\bar{\mathrm{H}}$H. It is hence very interesting to investigate the physical properties of the $\bar{p}$H compound state.

From the viewpoint of electron scattering, the $\bar{p}$H compound should be described as a metastable state in a resonance phenomenon,

$$e^- + \bar{p}p(N,L) \rightleftarrows \bar{p}\mathrm{H}, \tag{1}$$

where (N,L) are the principal and angular-momentum quantum numbers of the hydrogenic $\bar{p}p$ atom. Recently, accurate QM calculations were carried out for the collision process $\bar{p} + \mathrm{H} \rightarrow \bar{p}p + e^-$ using time-dependent approaches [23,24] and an R-matrix approach [25]. These approaches can also be used for the study of the electron resonance scattering of Eq. (1). It should be mentioned here that a QM calculation would become extremely unrealistic if the resonance process were described by a brute-force method of simple close-coupling expansion with respect to the (N,L) states: $\bar{p}p$ states with $N \sim 250$ are required for describing the resonance wave

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function, which extends up to $\bar{p}$-p distances of $R \sim 100$ a.u., while open channels are $N \leqslant 30$ at energies $E < D$. Such resonance channels can be effectively handled by using the R-matrix method. The $\bar{p}$H compound state also has another decay channel attributed to pair annihilation of $\bar{p}$ and p:

$$\bar{p}\text{H} \to e^- + \bar{p}\text{-}p \text{ annihilation}. \tag{2}$$

In the R-matrix calculation of $\bar{p} + \text{H}$ collisions [25], both the atomic rearrangement and the hadronic annihilation channels were coherently taken into account, and the annihilation was found to be important mostly for the total angular momentum $J = 0$. Also, for investigating the annihilation effect on the $\bar{p}$H compound state, the R-matrix method is expected to be useful.

The present study focuses on the energy region of $E < D$. In the case of $E > D$, one may expect that a quasibound state is formed in $\bar{p} + \text{H}$ collisions at energies below the centrifugal barrier height (i.e., a *tunneling* resonance). This quasibound state would also be regarded as a $\bar{p}$H compound. However, only minor peaks due to *overbarrier* resonance were actually observed in $\bar{p} + \text{H}$ collisions [25]. Using the WKB (Wentzel-Kramers-Brillouin) and uniform approximations, it is shown that this system cannot satisfy the condition of tunneling resonance because of its high reactivity [26]. It is unlikely that an important quasibound state exists at energies $E > D$ in this system.

In this paper, first, Sec. II presents the BO model (i.e., a molecular treatment) for the $\bar{p}$H compound state. The electron detachment and the annihilation are described using a local optical potential model (having an imaginary part of the interaction). In Sec. III, the R-matrix method is introduced for describing the $\bar{p}$H compound state as the resonance $e^- + \bar{p}p$ scattering. In Sec. IV, the results of the $\bar{p}$H properties calculated by the molecular and the R-matrix treatments are compared, and the applicability of the BO model is examined.

II. MOLECULAR TREATMENT OF METASTABLE COMPOUND STATES

Let $\mathbf{R}$ and $\mathbf{r}$ be the position vectors of $\bar{p}$ and e^-, respectively, measured from p. In the BO approximation, the total wave function of the $\bar{p} + \text{H}$ system is given in the form

$$\Psi_{\text{BO}}^{JM}(\mathbf{R},\mathbf{r}) = \chi(R;\mathbf{r})Y_{JM}(\hat{\mathbf{R}})F_v^J(R), \tag{3}$$

where $\chi(R;\mathbf{r})$ is the ground-state (1σ) electronic wave function providing the adiabatic electron energy $\epsilon_{\text{BO}}(R)$ [27,28], and $Y_{JM}(\hat{\mathbf{R}})$ is the spherical harmonics, with (J,M) being the total angular momentum quantum numbers. The BO potential governing the relative motion in $\bar{p} + \text{H}$ is given by

$$V_{\text{BO}}(R) = \begin{cases} -\frac{1}{R} - \epsilon_{\text{H}} & \text{for} \quad R < R_{\text{FT}}, \\ \epsilon_{\text{BO}}(R) - \frac{1}{R} - \epsilon_{\text{H}} & \text{for} \quad R \geqslant R_{\text{FT}}, \end{cases} \tag{4}$$

where ϵ_{H} is the ground-state energy of the H atom, and $V_{\text{BO}}(R) \to D = 0$ as $R \to \infty$ (D being the dissociation limit of $\bar{p}$H). The electronic bound state is absent at $R < R_{\text{FT}}$, and in the present study the BO potential is defined by assuming $\epsilon_{\text{BO}}(R) = 0$ at $R < R_{\text{FT}}$. The values of $\epsilon_{\text{BO}}(R)$ in the vicinity of $R = R_{\text{FT}}$ were calculated by Turner *et al.* [28]. Their result shows that $\epsilon_{\text{BO}}(R)$ seems to take a stationary value at $R = R_{\text{FT}}$.

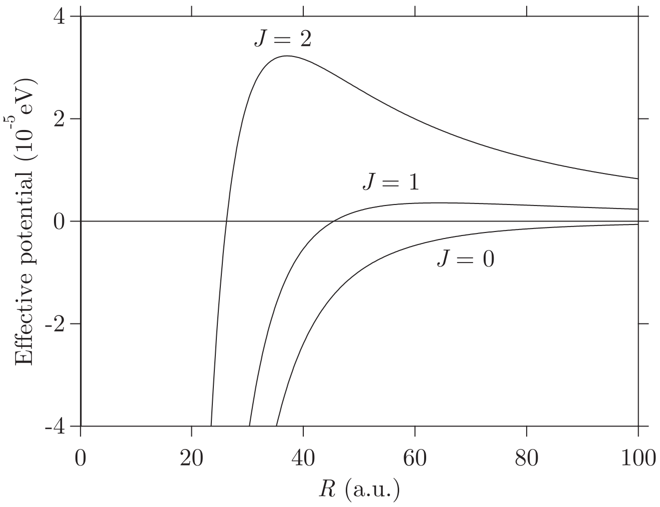

FIG. 1. Effective potential $V_{\text{eff}}(R)$ of $\bar{p} + \text{H}$ for $J = 0$, 1, and 2.

Therefore, the definition of Eq. (4) provides a smooth function around $R = R_{\text{FT}}$.

The radial function $F_v^J(R)$ is given by solving

$$\left[-\frac{1}{2mR^2}\frac{d}{dR}R^2\frac{d}{dR} + V_{\text{eff}}(R)\right]F_v^J(R) = EF_v^J(R), \tag{5}$$

where the effective potential $V_{\text{eff}}(R)$ is

$$V_{\text{eff}}(R) = \frac{J(J+1)}{2mR^2} + V_{\text{BO}}(R), \tag{6}$$

and m is the reduced mass of the system. Here and in the following, a.u. is used unless otherwise stated. If the energy is $E < D$, the $\bar{p}$H molecule is in a vibrational bound state identified by $v = 0, 1, \ldots$, and the vibrational energy is discrete, i.e., $E = E_{Jv}$.

The behavior of the effective potential $V_{\text{eff}}(R)$ at large distances R is shown in Fig. 1 for low angular momenta $J = 0$, 1, and 2. The effective potential supports a finite number of the vibrational states. Table I summarizes the highest vibrational quantum number v_{max}, the highest vibrational energy $E_{J,v_{\text{max}}}$, and the classical outer turning point R_{TP} of the vibrational motion with $v = v_{\text{max}}$. For low J, the $v = v_{\text{max}}$ turning point

TABLE I. Energies E_{Jv} and classical outer turning points R_{TP} of the $\bar{p}$H vibrational motion supported by the BO potential for the highest state $v = v_{\text{max}}$ of $J = 0$–10.

J	v_{max}	$E_{J,v_{\text{max}}}$ (eV)	R_{TP} (a.u.)
0	39	-4.816×10^{-5}	33.58
1	38	-3.112×10^{-6}	41.79
2	36	-8.039×10^{-4}	15.04
3	34	-6.050×10^{-3}	9.36
4	33	-3.769×10^{-3}	9.74
5	32	-1.202×10^{-3}	10.38
6	30	-1.181×10^{-2}	7.12
7	29	-5.479×10^{-3}	7.40
8	27	-2.982×10^{-2}	5.55
9	26	-1.752×10^{-2}	5.68
10	25	-4.462×10^{-3}	5.86

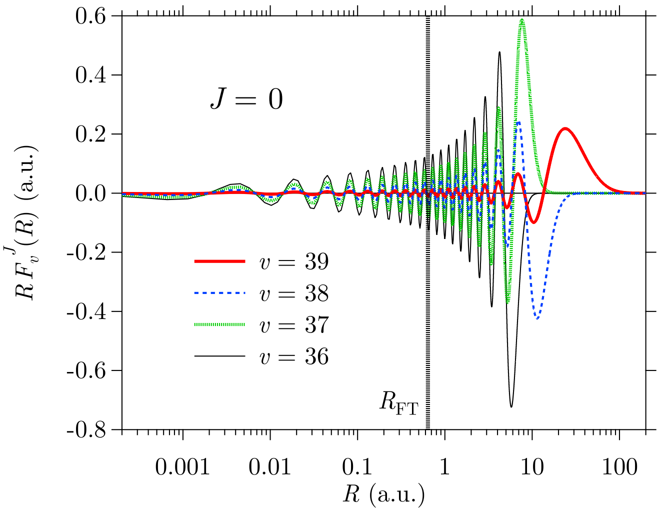

FIG. 2. (Color online) $J = 0$ vibrational wave functions $F_v^J(R) \times R$ obtained using the BO potential for $v = 39$–36. The vertical line indicates the Fermi-Teller critical distance $R = R_{\rm FT}$.

$R_{\rm TP}$ is > 10 a.u., and this fact actually confirms that the vibrational motion extends to very long distances of $R \gg R_{\rm FT}$. In the case of $J = 0$, the vibrational wave functions in the form of $R \times F_v^J(R)$ are drawn as a function of R in Fig. 2 for the vibrational states $v = 39$–36. A notable feature in the figure is that the wave function can have much higher amplitudes at distances $R \gg R_{\rm FT}$ than at $R \lesssim R_{\rm FT}$ (and furthermore, that it has finite amplitudes even up to $R \sim 100$ a.u. for $v = v_{\rm max}$). Thus, one can certainly expect the possible existence of a metastable compound state for low J and high v.

From the results of an accurate QM calculation, the present author empirically derived an imaginary part of the potential, which accounts for the decay by the electron detachment, in the form [29]

$$i\,V^{\rm I}_{\rm det}(R) = -i\,\frac{2.2}{87.5+R}\exp[-3.13(R-0.394)^4]. \tag{7}$$

This potential has the range of $R \lesssim R_{\rm det} \simeq 1.5$ a.u. Using Eq. (7) and the BO potential as the real part, the probability of electron detachment in $\bar{p} + {\rm H}$ collisions can be calculated satisfactorily [29]. This optical potential is expected to be useful also for the present purpose. With the use of Eq. (7), the energy level width $\Gamma^{\rm det}_{Jv}$ of the $\bar{p}$H molecule due to the electron detachment can be simply given by first-order perturbation theory, i.e.,

$$-\frac{i}{2}\Gamma^{\rm det}_{Jv} = \langle F_v^J | V^{\rm I}_{\rm det} | F_v^J \rangle. \tag{8}$$

The $\bar{p}$H molecule also has the decay channel of annihilation, Eq. (2). The imaginary part of the interaction accounting for the annihilation decay may be assumed to be a δ-function form [10], i.e.,

$$i\,V^{\rm I}_{\rm ann}(R) = -i\,\frac{A}{R^2}\delta(R), \tag{9}$$

where A is constant. This potential can be used to calculate the level width of the $\bar{p}p$ atom. For $\bar{p}p$ in the $1s$ state, first-order perturbation theory provides

$$-\frac{i}{2}\Gamma^{\rm ann}_{1s}(\bar{p}p) = \langle G^{\bar{p}p}_{1s} | V^{\rm I}_{\rm ann} | G^{\bar{p}p}_{1s} \rangle = -i\,A\,\big|G^{\bar{p}p}_{1s}(0)\big|^2, \tag{10}$$

where $G^{\bar{p}p}_{1s}(R)$ is the radial Coulomb function of $\bar{p}p(1s)$. From this result, one has

$$A = \frac{\Gamma^{\rm ann}_{1s}(\bar{p}p)}{8m^3}. \tag{11}$$

Then, using the recommended value $\Gamma^{\rm ann}_{1s}(\bar{p}p) = 1060$ eV given in Ref. [30], one can obtain $A = 6.29 \times 10^{-9}$ a.u. The δ-function assumption of Eq. (9) was found to be reasonable for the annihilation in $\bar{\rm H} + {\rm H}$ [15]. In the same way, the annihilation width of the $\bar{p}$H molecule is given by

$$-\frac{i}{2}\Gamma^{\rm ann}_{Jv} = \langle F_v^J | V^{\rm I}_{\rm ann} | F_v^J \rangle = -i\,A\,\big|F_v^J(0)\big|^2\delta_{J0}. \tag{12}$$

As long as the δ-function form is assumed, Eq. (12) yields no annihilation width except for $J = 0$.

III. SCATTERING CALCULATION USING THE *R*-MATRIX METHOD

Let us consider e^- scattering from $\bar{p}p(N,L)$ in the (N,L) state. The time-independent Schrödinger equation is

$$\mathsf{H}\Psi^{JM}(\mathbf{R},\mathbf{r}) = E_{\rm tot}\Psi^{JM}(\mathbf{R},\mathbf{r}), \tag{13}$$

with H being the Hamiltonian of the Coulomb three-body (e^--p-$\bar{p}$) system and $E_{\rm tot}$ being the total energy given by

$$E_{\rm tot} = \epsilon + E_N = \epsilon_{\rm H} + E, \tag{14}$$

where ϵ is the electron kinetic energy, and E_N is the $\bar{p}p$ energy. The last term in Eq. (14) is expressed in the $\bar{p} + {\rm H}$ channel related to the resonance state (cf. Sec. II). In the present study, Eq. (13) is solved using an R-matrix technique [31], in which the configuration space can be conveniently partitioned into several domains [25,32,33]. Let us introduce the boundary lines $R = B$, $r = b$, and $r = r_{\rm dip}$. The values of B and b are chosen such that the scattering wave function $\Psi^{JM}(\mathbf{R},\mathbf{r})$ has negligible amplitudes in the domain of $R \gtrsim B$ and $r \gtrsim b$. Specifically, $B = 2.7$ a.u. and $b = 8$ a.u. are appropriate in Ref. [25] and also in the present study. The significance of $r = r_{\rm dip}$ is discussed later.

In the inner domain ($R \leqslant B$ and $r \leqslant b$), the scattering wave function Ψ^{JM} can be expanded in terms of the R-matrix eigenfunctions, which are normalized to unity with respect to the integration over the inner domain. For the details of the calculation, see Ref. [25]. For low angular momenta $J \sim 0$, the annihilation is important, and its effect can be taken into account by imposing a boundary condition of a complex-valued R matrix at a very small distance ($R \sim 10^{-4}$ a.u.) [25], in the same way as developed for the $\bar{\rm H} + {\rm H}$ system by Jonsell *et al.* [15]. The R-matrix calculation in the inner domain is the most time-consuming part. The R-matrix data obtained in Ref. [25] can also be used for the present case.

The outer $R \gtrsim B$ (and $r < b$) domain is associated with the $\bar{p} + {\rm H}$ channel. Although this channel is closed at energies $E < D = 0$, the scattering wave function can have finite amplitudes at $R \gg B$ as easily imagined from the discussion in the previous section. The presence of this closed channel is closely related to the formation of a $\bar{p}$H resonance state in the $e^- + \bar{p}p$ scattering. Therefore, the contribution of the $\bar{p} + \mathrm{H}$ channel must be carefully handled in the $R > B$ domain. At sufficiently large R, the scattering wave function can be given in the BO separation form of Eq. (3), i.e.,

$$\Psi^{JM}(\mathbf{R},\mathbf{r}) = \chi(R;\mathbf{r})Y_{JM}(\hat{\mathbf{R}})F^J(R), \tag{15}$$

where the radial solution $F^J(R)$ satisfies the same equation as Eq. (5). At $R = B$, the scattering wave function obtained by the R-matrix calculation in the inner domain is matched to Eq. (15). In the case of $E < D$, the radial solution has a tail,

$$F^J(R) \underset{R\to\infty}{\sim} R^{-1}\exp(-\sqrt{2m|E|}R). \tag{16}$$

In the present calculation, $F^J(R)$ was assumed to have a starting value given by Eq. (16) at a sufficiently large distance (e.g., $R = 350$ a.u. for $J = 0$), and was inward solved down to $R = B$.

At $r = b$ (and $R < B$), the scattering wave function can be appropriately matched to the close-coupling expansion form using the basis set associated with the $e^- + \bar{p}p$ channel: i.e.,

$$\Psi^{JM}(\mathbf{R},\mathbf{r}) = \sum_{NLl}\mathcal{Y}^{JM}_{Ll}(\hat{\mathbf{R}},\hat{\mathbf{r}})G^{\bar{p}p}_{NL}(R)f^J_{NLl}(r), \tag{17}$$

with $G^{\bar{p}p}_{NL}(R)$ being the radial Coulomb function of $\bar{p}p(N,L)$, and

$$\mathcal{Y}^{JM}_{Ll}(\hat{\mathbf{r}},\hat{\mathbf{R}}) = \sum_{m_l}(L,M-m_l,lm_l|JM)Y_{LM-m_l}(\hat{\mathbf{R}})Y_{lm_l}(\hat{\mathbf{r}}), \tag{18}$$

where $(L,M-m_l,lm_l|JM)$ is the Clebsch-Gordan coefficients, and l is the electronic angular momentum quantum number. For the purpose of calculating the decay width of the $\bar{p}$H compound state, the annihilation effect can be disregarded in the outer $r > b$ domain. This domain corresponds to the $e^- + \bar{p}p$ channel, which is a breakup decay channel of the $\bar{p}$H compound state. Therefore, the annihilation occurring in the $r > b$ domain is the annihilation of $\bar{p}p$ after the breakup of $\bar{p}$H, but not the direct annihilation from $\bar{p}$H. Thus, the annihilation process at $r > b$ is a matter of no importance in the study of the $\bar{p}$H compound state. In the present scattering calculation including the annihilation effect, the resonance width corresponds to the one due to the processes of both electron detachment and direct annihilation from $\bar{p}$H.

In the $e^- + \bar{p}p$ scattering, the sum of the centrifugal potential $\mathbf{l}^2/(2r^2)$ and the interaction becomes, as $r \to \infty$,

$$\frac{\mathbf{l}^2}{2r^2} - \frac{1}{r} + \frac{1}{|\mathbf{r}-\mathbf{R}|} - \frac{1}{R} \longrightarrow \frac{\mathbf{l}^2 + 2\mathbf{R}\cdot\hat{\mathbf{r}}}{2r^2} - \frac{1}{R}. \tag{19}$$

Since the $\bar{p}p(N,L)$ energies are degenerate with respect to L, the presence of the dipole interaction $\mathbf{R}\cdot\hat{\mathbf{r}}/r^2$ provides strong coupling among L and l even at very large distances r. This can cause a significant effect on elastic scattering and, especially, on the resonance position. In such a case, it is more convenient to introduce a new channel α, which is defined by the diagonalization of the operator $\mathbf{l}^2 + 2\mathbf{R}\cdot\hat{\mathbf{r}}$ within the same N [34,35]:

$$(\mathbf{l}^2 + 2\mathbf{R}\cdot\hat{\mathbf{r}})\phi^{JMN}_\alpha(\mathbf{R},\hat{\mathbf{r}}) = \Lambda^{JN}_\alpha\phi^{JMN}_\alpha(\mathbf{R},\hat{\mathbf{r}}), \tag{20}$$

where Λ^{JN}_α is the eigenvalue with $\alpha = 1,2,\ldots$, and the eigenfunction is expanded as

$$\phi^{JMN}_\alpha(\mathbf{R},\hat{\mathbf{r}}) = \sum_{Ll}U^{JMN}_{\alpha,Ll}\mathcal{Y}^{JM}_{Ll}(\hat{\mathbf{R}},\hat{\mathbf{r}})G^{\bar{p}p}_{NL}(R). \tag{21}$$

At sufficiently large $r \geqslant r_{\mathrm{dip}} \gg b$, where Eq. (19) is valid, the scattering wave function can be expressed as

$$\Psi^{JM}(\mathbf{R},\mathbf{r}) = \sum_{N\alpha}\phi^{JMN}_\alpha(\mathbf{R},\hat{\mathbf{r}})g^J_{N\alpha}(r), \tag{22}$$

where the radial function $g^J_{N\alpha}(r)$ satisfies

$$\left[-\frac{1}{2r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\Lambda^{JN}_\alpha}{2r^2}\right]g^J_{N\alpha}(r) = \epsilon g^J_{N\alpha}(r). \tag{23}$$

Then, expressing $g^J_{N\alpha}(r)$ in terms of the incoming and outgoing solutions of Eq. (23), one can define the scattering S matrix $\mathbb{S}$, which has the elements $S^J_{N\alpha,N'\alpha'}$.

The information on the dynamics in a domain can be fully expressed in terms of an R matrix given on the boundary of the domain [31], and one can propagate the R matrix from a domain to an adjacent or broader domain by imposing the continuity condition of the scattering wave function on the boundary [32,33]. For example, by matching $\Psi^{JM}(\mathbf{R},\mathbf{r})$ obtained in the inner domain ($R \leqslant B$ and $r \leqslant b$) to the form of Eq. (17) at $r = b$, the R matrix can be propagated from $r = b$ outward to $r = r_{\mathrm{dip}}$ [25]. At $r = r_{\mathrm{dip}}$, the propagated R matrix in the (N,L,l) representation is transformed into the eventual one in the (N,α) representation by the unitary matrix having the elements $U^{JMN}_{\alpha,Ll}$. In the present calculation, $r_{\mathrm{dip}} = 20$ a.u. was chosen. The suitability of this value was confirmed by carrying out a calculation for $r_{\mathrm{dip}} = 100$ a.u., which yielded <0.5% differences in the resonance position and width. The derivation of the S matrix from the eventual R matrix, including the effect of the closed channel, is summarized by Berrington *et al.* [36].

For the analysis of resonances, Smith [37] introduced the time-delay matrix $\mathbb{Q}$, which is defined in terms of $\mathbb{S}$ by

$$\mathbb{Q} = i\mathbb{S}\frac{d\mathbb{S}^\dagger}{dE} = -i\frac{d\mathbb{S}}{dE}\mathbb{S}^\dagger. \tag{24}$$

Igarashi and Shimamura [38] showed that the trace of $\mathbb{Q}$ satisfies the relation to the eigenphase sum δ [39],

$$\mathrm{Tr}\mathbb{Q} = 2\frac{d\delta}{dE}, \tag{25}$$

and is directly expressible, around a resonance energy ($E \sim E_0$), as

$$\mathrm{Tr}\mathbb{Q} = \frac{\Gamma}{(E-E_0)^2 + (\Gamma/2)^2} + 2\frac{d\delta_{\mathrm{BG}}}{dE}, \tag{26}$$

where $2d\delta_{\mathrm{BG}}/dE$ is the background contribution. The expression of Eq. (26) is appropriate for determining the resonance energy E_0 and the width Γ by the scattering calculation. For the calculation of E_0 and Γ, the second term in (26) was further fitted to

$$2\frac{d\delta_{\mathrm{BG}}}{dE} = C_0 + C_1E + C_2E^2, \tag{27}$$

where C_0, C_1, and C_2 are constant. For $J = 0$ and 1, the scattering calculation was carried out for the two cases

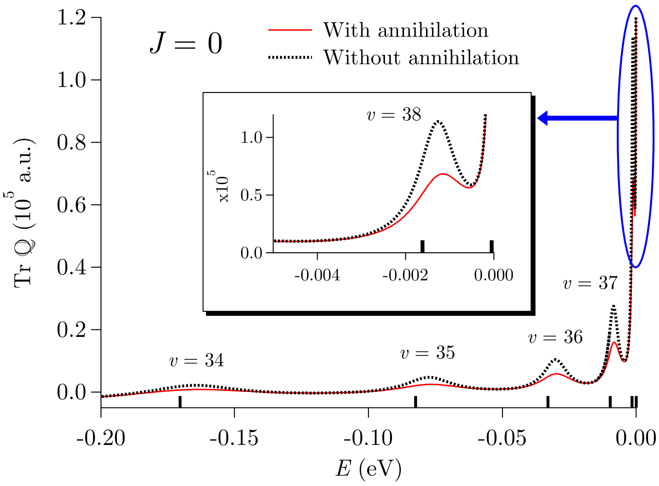

FIG. 3. (Color online) Traces of the time-delay matrix Trℚ in the R-matrix calculation of $e^- + \bar{p}p$ for $J = 0$ with and without annihilation as a function of the energy E of $\bar{p} + \mathrm{H}$. For each resonance peak, the corresponding vibrational quantum number v of $\bar{p}$H is assigned. Vertical bars indicate the vibrational energies in the molecular treatment.

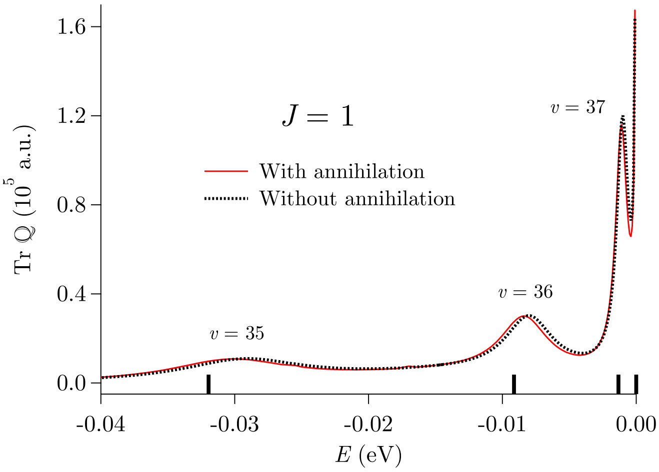

FIG. 4. (Color online) Traces of the time-delay matrix Trℚ in the R-matrix calculation for $J = 1$ with and without annihilation as a function of the energy E. For each resonance peak, the corresponding vibrational quantum number v is assigned. Vertical bars indicate the vibrational energies in the molecular treatment.

including and neglecting the annihilation effect. For $J = 2$, the annihilation effect was neglected in the calculation.

IV. RESULTS AND DISCUSSION

Figure 3 shows the trace of the time-delay matrix, Trℚ, for $J = 0$ obtained by the R-matrix calculations of $e^- + \bar{p}p$ with and without the inclusion of annihilation effects. The results are plotted against the relative energy E of $\bar{p} + \mathrm{H}$ in the range of $-0.2 \leqslant E < 0.0$ eV below the dissociation limit $D = 0$. Several clear peaks recognized in the trace Trℚ are evidently due to resonances, which correspond to the formation of metastable $\bar{p}$H compound states. The resonance lying just under the dissociation limit is the most prominent, and the resonance profile becomes vaguer as the energy decreases. The peak position differs only slightly between the two calculations with and without the inclusion of annihilation effects; However, the peak height is significantly lowered by including the annihilation effect. The traces Trℚ for $J = 1$ obtained by the calculations with and without the inclusion of annihilation are shown in Fig. 4 at energies $E = -0.04 \sim 0.0$ eV. In contrast to the trace for $J = 0$, the annihilation decay is found to always produce very little effect for $J = 1$. As J increases, the probability of finding the $\bar{p}$-p distance within the range of hadronic interaction (i.e., $R < 5 \times 10^{-5}$ a.u.) drops steeply. It can be concluded that the annihilation channel is practically negligible for $J \geqslant 1$. The trace (without annihilation) for $J = 2$ in the neighborhood of the dissociation limit ($E = -0.015$ to 0.0 eV) is displayed in Fig. 5. At energies just below the dissociation limit, the appearance feature for $J = 2$ becomes somewhat different from that for $J = 0$ and 1 (see later).

The resonance energies and widths are obtained by fitting the trace Trℚ to the form of Eq. (26) with Eq. (27). The resonance energies in the R-matrix calculation neglecting the annihilation effect are shown in Table II for $J = 0$, 1, and 2 and are compared with the vibrational energies of $\bar{p}$H obtained using the BO potential. Because the difference in the resonance energy between the R-matrix calculations with and without the inclusion of annihilation effects is <5%, the resonance energies are not shown for the R-matrix calculation with annihilation. As also shown in Figs. 3, 4, and 5, the peak in Trℚ corresponds nicely with a molecular vibrational level supported by the BO potential, though there is the exception that the R-matrix calculation shows no peak-like structure corresponding to $v = v_{\mathrm{max}}$ for $J = 0$ and 1. The reason for the latter fact would be that the vibrational energies of these molecular states are too close to the dissociation limit. Apart from these $v = v_{\mathrm{max}}$ states, it is expected that the BO picture can be used for analyzing the resonance in $e^- + \bar{p}p$ scattering.

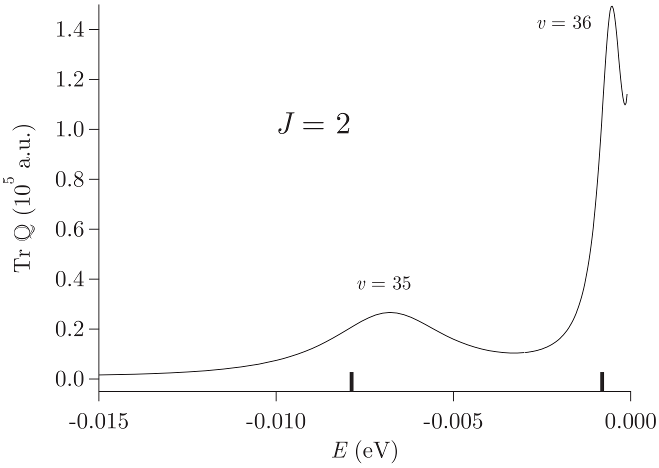

FIG. 5. Traces of the time-delay matrix Trℚ in the R-matrix calculation for $J = 2$ without annihilation as a function of the energy E. For each resonance peak, the corresponding vibrational quantum number v is assigned. Vertical bars indicate the vibrational energies in the molecular treatment.

TABLE II. Vibrational energies E_{Jv} in the molecular treatment of $\bar{p}$H (BO) and resonance energies in the R-matrix calculation of $e^- + \bar{p}p$ without annihilation (RM) for $J = 0$, 1, and 2.

	E_{Jv} (eV)		
	$J = 0$	$J = 1$	$J = 2$
$v = 39$			
BO	-4.816×10^{-5}	–	–
RM	–	–	–
$v = 38$			
BO	-1.616×10^{-3}	-3.112×10^{-6}	–
RM	-1.276×10^{-3}	–	–
$v = 37$			
BO	-9.778×10^{-3}	-1.331×10^{-3}	–
RM	-8.558×10^{-3}	-1.030×10^{-3}	–
$v = 36$			
BO	-3.302×10^{-2}	-9.133×10^{-3}	-8.039×10^{-4}
RM	-3.023×10^{-2}	-8.037×10^{-3}	-5.493×10^{-4}
$v = 35$			
BO	-8.232×10^{-2}	-3.195×10^{-2}	-7.871×10^{-3}
RM	-7.753×10^{-2}	-2.937×10^{-2}	-6.819×10^{-3}
$v = 34$			
BO	-1.703×10^{-1}	-8.081×10^{-2}	-2.982×10^{-2}
RM	-1.652×10^{-1}	-7.610×10^{-2}	-2.719×10^{-2}

The R-matrix results of the resonance width for $e^- + \bar{p}p$ are listed in Table III. The annihilation effect was neglected in these R-matrix calculations, and hence the resonance width can be directly compared with the detachment width $\Gamma^{\mathrm{det}}_{Jv}$ obtained by the BO model of Eq. (8). One can see that the agreement between the two methods is surprisingly good. In the present system, the imaginary part of the optical potential, Eq. (7), produces actually a very strong interaction causing electron detachment [29]. As shown in Fig. 2, however, the vibrational wave functions for very high v states have very low amplitudes in the interaction region ($R \lesssim R_{\mathrm{det}}$). For this reason, first-order treatment of Eq. (8) would be satisfactory. In contrast to the present case, the BO model is not as good for the calculations of the rearrangement cross section in $\bar{\mathrm{H}} + \mathrm{H}$ [14,17]. In the BO model for $\bar{\mathrm{H}} + \mathrm{H}$, the rearrangement reaction was calculated using the DW method [10,15,17,21]. Unlike this approach, the present BO model employs the empirically determined imaginary potential and might be able to effectively include higher-order contribution in terms of the DW method. Furthermore, it should be pointed out that the range R_{det} of the imaginary potential is much shorter than that of the perturbation assumed in the DW method.

TABLE III. Electron detachment widths $\Gamma^{\mathrm{det}}_{Jv}$ in the BO model (BO) and resonance widths in the R-matrix calculation without annihilation (RM) for $J = 0$, 1, and 2.

	$\Gamma^{\mathrm{det}}_{Jv}$ (eV)		
	$J = 0$	$J = 1$	$J = 2$
$v = 39$			
BO	8.86×10^{-5}	–	–
RM	–	–	–
$v = 38$			
BO	1.18×10^{-3}	3.46×10^{-5}	–
RM	1.05×10^{-3}	–	–
$v = 37$			
BO	4.47×10^{-3}	1.08×10^{-3}	–
RM	4.20×10^{-3}	1.03×10^{-3}	–
$v = 36$			
BO	1.09×10^{-2}	4.35×10^{-3}	8.84×10^{-4}
RM	1.06×10^{-2}	4.36×10^{-3}	8.23×10^{-4}
$v = 35$			
BO	2.13×10^{-2}	1.08×10^{-2}	4.11×10^{-3}
RM	2.11×10^{-2}	1.12×10^{-2}	4.11×10^{-3}
$v = 34$			
BO	3.59×10^{-2}	2.12×10^{-2}	1.06×10^{-2}
RM	3.50×10^{-2}	2.27×10^{-2}	1.10×10^{-2}

TABLE IV. Energy widths $\Gamma^{\mathrm{ann}}_{Jv}$ and $\Gamma^{\mathrm{tot}}_{Jv} = \Gamma^{\mathrm{det}}_{Jv} + \Gamma^{\mathrm{ann}}_{Jv}$ in the BO model (BO) and resonance widths in the R-matrix calculation with annihilation (RM) for $J = 0$.

	$J = 0$	
	$\Gamma^{\mathrm{ann}}_{Jv}$ (eV)	$\Gamma^{\mathrm{tot}}_{Jv}$ (eV)
$v = 39$		
BO	1.18×10^{-5}	1.00×10^{-4}
RM		–
$v = 38$		
BO	1.57×10^{-4}	1.34×10^{-3}
RM		1.62×10^{-3}
$v = 37$		
BO	5.96×10^{-4}	5.07×10^{-3}
RM		6.37×10^{-3}
$v = 36$		
BO	1.46×10^{-3}	1.24×10^{-2}
RM		1.61×10^{-2}
$v = 35$		
BO	2.83×10^{-3}	2.41×10^{-2}
RM		3.20×10^{-2}
$v = 34$		
BO	4.77×10^{-3}	4.07×10^{-2}
RM		5.11×10^{-2}

In the case of $J = 0$ and 1, Tables II and III show that the width $\Gamma^{\mathrm{det}}_{Jv}$ for $v = v_{\mathrm{max}}$ is evidently larger than the dissociation energy $|E_{J,v=v_{\mathrm{max}}}|$ in the BO model. This is consistent with the fact that the resonances identified as $(J,v_{\mathrm{max}}) = (0,39)$ and (1,38) are missing in the $e^- + \bar{p}p$ scattering (cf. Figs. 3 and 4). In the case of $J = 2$, the BO model provides $\Gamma^{\mathrm{det}}_{Jv} \sim |E_{Jv}|$ for $v = v_{\mathrm{max}}$, and it is understandable that the resonance peak corresponding to $v = v_{\mathrm{max}}$ is marginally observable as shown in Fig. 5. Since the detachment width increases with decreasing v, the $\bar{p}$H compound state is more stable against electron detachment for higher v, as expected.

If the angular momentum is $J = 0$, the $\bar{p}$H compound state can be significantly influenced by the annihilation decay. Table IV shows the annihilation width $\Gamma^{\mathrm{ann}}_{J=0,v}$ and the total width $\Gamma^{\mathrm{tot}}_{J=0,v} = \Gamma^{\mathrm{det}}_{J=0,v} + \Gamma^{\mathrm{ann}}_{J=0,v}$ obtained using the present BO model. The ratio $\Gamma^{\mathrm{ann}}_{J=0,v}/\Gamma^{\mathrm{tot}}_{J=0,v} \sim 0.1$ suggests that the annihilation effect is not as striking in the BO model. The resonance width in the R-matrix calculation including the annihilation process is also listed in Table IV. This resonance width is reflected by both the detachment decay and the annihilation decay, and it can be compared with $\Gamma^{\rm tot}_{J=0,v}$ in the BO model. Unlike in the detachment width listed in Table III, there is a clear difference of about 20% in the total width between the BO model and the R-matrix calculation. It turns out that the annihilation effect is more considerable in the R-matrix calculation. In the calculation of the annihilation width, sufficient accuracy is required for the wave function at $R \simeq 0$, as understood through Eq. (12). Probably, the accurate wave function at $R \sim 0$ could not be obtained by merely solving the simple equation of Eq. (5). A previous study on $\bar{p} + {\rm H}$ collisions [25] shows that the BO model is applicable to the calculation of the annihilation probability only if the collision energy is extremely low, $E \lesssim 10^{-7}$ eV. In view of this fact, the BO model may become good by some chance if $|E| \lesssim 10^{-7}$ eV also for the calculation of $\Gamma^{\rm ann}_{J=0,v}$.

The present study indicates that the resonances in the scattering are nicely identified as the formation of molecular vibration. However, since the condition $\Gamma^{\rm det}_{Jv} \ll |E_{Jv} - E_{Jv\pm1}|$ is not satisfied, one cannot conclude that the $\bar{p}$H compound is a long-lived molecule which can vibrate many times during its lifetime. In the study of electron scattering from molecules, such short-lived resonances were observed experimentally (e.g., low-energy metastable $\rm H_2^-$ [40] and $\rm N_2^-$ [41] states) and are described reasonably by the so-called boomerang model [42–44]. The present $\bar{p}$H compound state has a resonance property very similar to that of $\rm H_2^-$ and $\rm N_2^-$.

V. CONCLUSION

In the scattering calculation using the R-matrix method, the lifetimes τ_{Jv} $(=1/\Gamma^{\rm tot}_{Jv}$ or $1/\Gamma^{\rm det}_{Jv})$ of the resonance compound $\bar{p}$H formed at energies not far below the dissociation limit are $\tau_{Jv} = 4.07 \times 10^{-13}$ s for the $(J,v) = (0{,}38)$ state, $\tau_{Jv} = 6.40 \times 10^{-13}$ s for the (1,37) state, and $\tau_{Jv} = 7.99 \times 10^{-13}$ s for the (2,36) state. The annihilation width is ~50% of the detachment width for the angular momentum state $J = 0$ and negligible for $J \geqslant 1$. The BO model, in which decay processes are described by the optical potentials, is very useful for estimating the electron detachment width but not good for the annihilation width. Although the metastable $\bar{p}$H compound can be related to the vibrational bound motion (v) supported by the BO potential, it cannot be regarded as a long-lived molecule. With decreasing v, the compound state becomes more unstable. Some metastable compound states to be formed at an energy just below the dissociation limit are missing because the dissociation energy is smaller than the decay width.

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