

Mass polarization effect on the resonant energies of \bar{p} -He⁺ ions and the protonium formation in low-energy antiproton–hydrogen-atom collisions

X. M. Tong^{1,2,*} and N. Toshima¹

¹*Institute of Materials Science, Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan*

²*Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577, Japan*

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We present a time-dependent method to investigate the mass polarization effect on the resonant energies of \bar{p} -He⁺ and the state-specified protonium formation in low-energy antiproton–hydrogen-atom collisions in Jacobi coordinates. Comparing with our previous calculations in the V-shaped coordinates by neglecting the mass polarization, we confirm that the mass polarization effect on the protonium formation is negligibly small. We also calculated the resonant energies of \bar{p} -He⁺ in the V coordinates and Jacobi coordinates. The differences of the resonant energies between the two calculations are less than 4 meV. This also confirms that the mass polarization effect is negligibly small even in the resonant region.

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I. INTRODUCTION

The first production of cold antihydrogen atoms [1] and the recent success of trapped antihydrogen [2] in experiments have stimulated further theoretical studies on antimatter physics. Even for the capture of antiprotons by hydrogen atoms, a simple Coulomb three-body system, the exact quantum solutions do not exist due to the huge mass difference between an antiproton and electron. Cohen [3] calculated the state-specified protonium-formation cross sections by the classical trajectory Monte Carlo method, not a quantum simulation. Esry and Sadeghpour [4] showed that hundreds or even thousands of adiabatic potentials have to be taken into account for a real antiproton and hydrogen atom system and they had to solve the scattering equations by reducing the antiproton mass artificially. Using the diabatization technique, Hesse *et al.* [5] have extended the calculation of the protonium-formation cross sections for scaled proton and antiproton masses of $100m_e$, which is much lighter than the real antiproton mass, $1836m_e$ with m_e the mass of an electron. So far, the best available quantum calculations of the state-specified protonium formation are obtained by using a time-dependent method [6,7] in the V coordinates as shown in Fig. 1(b), in which the mass polarization (MP) ($-\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{R}}/m_z$) [8] is neglected, where m_z is the mass of nucleus Z. The justification of the V coordinates is based on that the MP does not contribute to the initial state (a hydrogen atom and a free antiproton) or the final states (a protonium and a free electron). It only affects the dynamics when the three particles are close to each other and the effect should be small.

Recently, Sakimoto [9] has investigated the capture of antiproton by a He⁺ ion using the R-matrix method [10]. He found that the MP shifts the resonant energies significantly and the capture cross sections obtained in the two coordinates differ by orders in the resonant region. Since the MP effect should be smaller in the capture process of antiproton by He⁺ than by hydrogen atoms due to the mass difference between

a proton and α particle, he wonders if the V coordinates are applicable to the protonium-formation calculations.

To check the validity of the V coordinates and MP effect on the protonium formation and the resonant energies of \bar{p} -He⁺, we extended our time-dependent method in the V coordinates to the Jacobi coordinates [Jacobi set 2 as shown in Fig. 1(c)], the same coordinates as used by Sakimoto [9]. Comparing the resonant energies obtained in the V coordinates and Jacobi coordinates, we find that the MP effect shifts the resonant energies by less than 4 meV, much smaller than the values reported by Sakimoto [9]. Furthermore, we calculate the state-specified protonium-formation cross sections in the Jacobi coordinates and show that the results are in good agreement with the ones obtained in the V coordinates. Since the computational resource needed for the Jacobi coordinates is more than hundred times larger than that needed for the V coordinates, the V-coordinate method is very useful for the protonium-formation study and the issue raised by Sakimoto [9], the invalidity of the V-coordinate method, is questionable.

II. THEORETICAL METHODS

In Jacobi set 2 as shown in Fig. 1(c), the Hamiltonian of a Coulomb three-body system composed of an electron, an antiproton, and a nucleus with charge Z is written as (atomic units $\hbar = m_e = e = 1$ are used throughout the paper unless stated otherwise)

$$H = -\frac{\nabla_{\mathbf{r}}^2}{2\mu_e} - \frac{\nabla_{\mathbf{R}}^2}{2\mu_p} - \frac{Z}{R} - \frac{Z}{|\mathbf{r} + b_0\mathbf{R}|} + \frac{1}{|\mathbf{r} - b_1\mathbf{R}|}, \quad (1)$$

where

$$\mu_e = \frac{m_e(m_z + m_{\bar{p}})}{m_e + m_z + m_{\bar{p}}}, \quad \mu_p = \frac{m_z m_{\bar{p}}}{m_z + m_{\bar{p}}},$$

$$b_0 = \frac{m_{\bar{p}}}{m_{\bar{p}} + m_z}, \quad b_1 = \frac{m_z}{m_{\bar{p}} + m_z}.$$

Here $m_{\bar{p}}$ is the mass of antiproton, and \mathbf{R}, \mathbf{r} are the position vectors of the antiproton with respect to the nucleus and the electron to the center of mass of the antiproton and nucleus, respectively. For a Coulomb three-body system, the total

*tong@ims.tsukuba.ac.jp

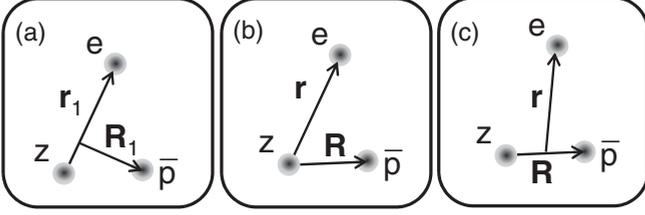


FIG. 1. Schematics of the coordinate systems for an antiproton and a hydrogen-like atomic ion: (a) Jacobi set 1 which describes the initial state naturally; (b) \mathbf{V} coordinate; and (c) Jacobi set 2 which describes the capture states naturally.

angular momentum and the parity are good quantum numbers, thus the wave function for a given total angular momentum (J) and its projection onto the z direction (M_J) can be expressed as

$$\Psi_{JM_J}(\mathbf{r}, \mathbf{R}) = \sum_{L,l} F_{JM_J}^{L,l}(r, R) \Omega_{JM_J}^{L,l} \quad (2)$$

with

$$\Omega_{JM_J}^{L,l} = \sum_{m,M} \langle LM \, lm | JM_J \rangle Y_{LM}(\hat{\mathbf{R}}) Y_{lm}(\hat{\mathbf{r}}),$$

where L , l and M , m are the angular momenta and their projections onto the z direction for the relative motions of \mathbf{R} and \mathbf{r} .

A. Resonant energy

For $Z > 1$, the antiproton can be captured via resonant states. The resonant energies of the Coulomb three-body system can be calculated by an autocorrelation function [11,12] defined as

$$C(t) = \langle \Psi(\mathbf{r}, \mathbf{R}) | e^{-iHt} | \Psi(\mathbf{r}, \mathbf{R}) \rangle. \quad (3)$$

For any given wave function $\Psi(\mathbf{r}, \mathbf{R})$, it can be expanded as

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum C_i \Psi_i^r(\mathbf{r}, \mathbf{R}) + \int C(\epsilon) \Psi_\epsilon(\mathbf{r}, \mathbf{R}) d\epsilon,$$

where $\Psi_i^r(\mathbf{r}, \mathbf{R})$ is a bound or resonant state wave function, and $\Psi_\epsilon(\mathbf{r}, \mathbf{R})$ is a continuum wave function of the total Hamiltonian in Eq. (1), and C_i and $C(\epsilon)$ are the corresponding coefficients. Mathematically, the defined autocorrelation function can be written as

$$C(t) = \sum_i |C_i|^2 e^{-i\epsilon_i^r t} + \int |C(\epsilon)|^2 e^{-i\epsilon t} d\epsilon, \quad (4)$$

where $\{\epsilon_i^r\}$ are the complex resonant energies. The time-dependent wave function $|\Psi(t)\rangle = e^{-iHt} |\Psi(\mathbf{r}, \mathbf{R})\rangle$ is obtained by solving the following time-dependent Schrödinger equation

$$i \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle \quad (5)$$

numerically [13] with the initial condition $|\Psi(0)\rangle = |\Psi(\mathbf{r}, \mathbf{R})\rangle$. Then we can obtain the autocorrelation function as $C(t) = \langle \Psi(0) | \Psi(t) \rangle$. Since we introduce an optical absorber [14] in the outer region, only the resonant states contribute to the autocorrelation function after a long time propagation. The

peak positions of the Fourier transformation

$$C(\omega) = \int C(t) e^{i\omega t} dt \quad (6)$$

provide the resonant energies.

B. Protonium formation

Instead of obtaining the scattering wave function by solving the time-integral equation in the \mathbf{V} coordinates, we obtain it in the Jacobi coordinates [set 2 as shown in Fig. 1(c)]. The numerical procedure is similar to our previous work [15] so that we only present how to prepare the initial wave function, which is different from the one used in the \mathbf{V} coordinates. Here we choose $Z = 1$ and $m_z = m_p = m_{\bar{p}}$ with m_p the mass of proton. The initial wave function is expressed as

$$\Psi_0(\mathbf{r}_1, \mathbf{R}_1) = \psi_{1s}(\mathbf{r}_1) e^{i\mathbf{k}_0 \cdot \mathbf{R}_1}$$

in Jacobi set 1 as shown in Fig. 1(a), where \mathbf{k}_0 is the momentum of the antiproton in the center of mass frame. Since the Jacobian of the mapping $(\mathbf{r}_1, \mathbf{R}_1) \rightarrow (\mathbf{r}, \mathbf{R})$

$$J = \left| \frac{\partial(\mathbf{r}_1, \mathbf{R}_1)}{\partial(\mathbf{r}, \mathbf{R})} \right| = 1, \quad (7)$$

the initial wave function in Jacobi set 2 is written as

$$\begin{aligned} \Psi_0(\mathbf{r}, \mathbf{R}) &= \psi_{1s}(\mathbf{r} + b_0 \mathbf{R}) e^{i\mathbf{k}_0 \cdot [(1-a_0 b_0) \mathbf{R} - a_0 \mathbf{r}]} \\ &= \sum_{JM_J} \sum_{L,l} F_J^{L,l}(r, R) \Omega_{JM_J}^{L,l} \end{aligned}$$

for a given JM_J , where $a_0 = m_e/(m_e + m_p)$. Note that in the \mathbf{V} coordinates or Jacobi set 1, only the electron s -partial wave is involved. In Jacobi set 2 we need a lot of partial waves to describe the initial electron wave function since the origin of vector \mathbf{r} is shifted from the proton to the middle point of the proton and antiproton. The scattering wave function is obtained from the time-integral equation as [6]

$$\Psi_f^+(0) = -i \int_{-\infty}^0 e^{iH\tau} e^{\eta\tau} e^{-iE_0\tau} V_{\text{res}} \Psi_0 d\tau + \Psi_0, \quad (8)$$

with

$$V_{\text{res}} = -\frac{1}{R} + \frac{1}{|\mathbf{r} - b_1 \mathbf{R}|},$$

which represents the interaction between the antiproton and hydrogen atom. η is an infinitesimal introduced to adiabatically switch on the interaction. In the simulation we replaced $e^{\eta\tau}$ by $e^{-\eta^2\tau^2}$ to accelerate the evolution [15]. Once we have the scattering wave function, we can obtain the state-specified protonium-formation cross section as

$$\sigma_{NL}^l(J) = \frac{4\mu_e \mu_p k_{NL}}{k_0} |\langle \Psi_f^{L,l} | V_f | \Psi_f^+(0) \rangle|^2, \quad (9)$$

with

$$V_f = -\frac{1}{|\mathbf{r} + b_0 \mathbf{R}|} + \frac{1}{|\mathbf{r} - b_1 \mathbf{R}|},$$

which represents the electron protonium interaction, and

$$\Psi_f^{L,l} = j_l(k_{NL} r) \psi_{NL}(R) \Omega_{JM_J}^{L,l},$$

which represents the final state wave function for the protonium with principle quantum number N and angular momentum L and the ejected electron with angular momentum l and momentum k_{NL} . We also calculated the cross sections by monitoring the outgoing electron current as described in Ref. [15] to check the convergence.

III. RESULTS AND DISCUSSION

Since Sakimoto [9] found that the MP is important in the formation of \bar{p} -He⁺ for both the resonant energies and the formation cross sections, we will check the resonant energies. We calculate the autocorrelation function $C(t)$ in Eq. (3) using the generalized pseudospectral method and the split-operator method in the energy representation [13]. To compare with Sakimoto's results, we also ignored the fine and hyperfine structures, which are very small for an antiprotonic helium [16]. We show the resonant energies for $J = 32$ in the same energy regime in Fig. 2. In the simulation we recast the Hamiltonian of \bar{p} -He⁺ as (we choose $Z = 2$ and $m_z = 4m_p$)

$$H = H_r + H_R + V,$$

with

$$\begin{aligned} H_r &= -\frac{1}{2\mu_e} \nabla_r^2 - \frac{1}{r}, \\ H_R &= -\frac{1}{2\mu_p} \nabla_R^2 - \frac{2}{R}, \\ V &= \frac{1}{r} - \frac{2}{|\mathbf{r} + b_0 \mathbf{R}|} + \frac{1}{|\mathbf{r} - b_1 \mathbf{R}|}. \end{aligned}$$

Here V stands for the residual correlation between the electron and \bar{p} -He⁺⁺ core apart from the Coulomb interaction ($-1/r$). When the antiproton is deeply bound by the α particle and the electron is in a highly excited state, the resonant energy can be simply expressed in a good approximation as

$$E_r = 2.0 - \frac{2\mu_p}{N^2} - \frac{\mu_e}{2n^2} \quad (10)$$

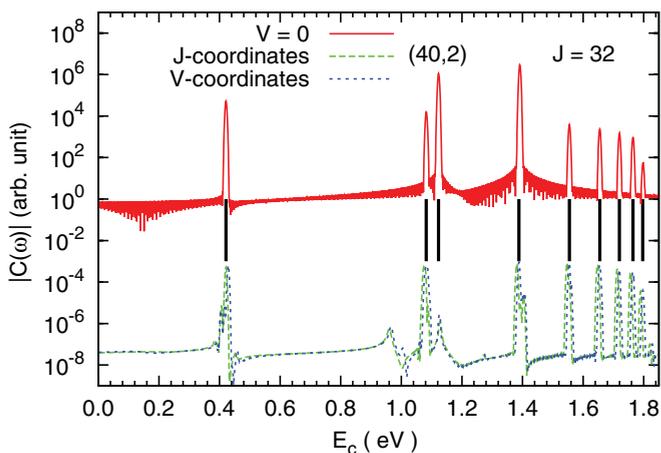


FIG. 2. (Color online) Resonant energies of \bar{p} -He⁺ calculated in the Jacobi coordinates (dashed curve) and in the V coordinates without the mass polarization term (dotted curve). The vertical lines show the predicted values by Eq. (10) and the solid curve shows the resonant energy without the residual correlation between the antiproton and electron.

since V approaches zero. Here $N(n)$ is the principle quantum number of \bar{p} -He⁺⁺ (hydrogen-like atom). Hereafter we choose the ground state energy of He⁺ as zero. To check the validity of the numerical method, we switch off the residual correlation V and obtain the resonant energies as shown in the upper curve in Fig. 2. The peak positions of the curve are in good agreement with the prediction from Eq. (10), the vertical lines in the middle of the figure. The width of the peaks is attributed to the finite time propagation. The peaks in the figure represent $N = 39, 3 \leq n \leq 10$. $N = 40$ and $n = 2$ state is also located in this energy regime as indicated in the figure. Then we switch on the residual correlation V and calculate the spectra in the Jacobi coordinates (dashed curve) and the V coordinates (dotted curve). The two calculations are in good agreement as shown in Fig. 2. Analyzing the numerical value in detail, we find that the MP shifts the resonant energies by less than 4 meV, which is negligibly small. To avoid missing any resonant states, we choose different initial wave functions (in case that it is orthogonal with a resonant state) and propagation time (in case that we miss short-lifetime states). The results in Fig. 2 are obtained by choosing

$$\Psi(\mathbf{r}, \mathbf{R}) = (1 + r/10)e^{-r/2-R} \sum_{L,l} \Omega_{JM}^{L,l}, \quad (11)$$

which covers all the resonant states in this energy range. The results showed in Fig. 2 are obtained by time propagation of one million time steps with $\Delta t = 0.2$ a.u. We also varied the number of grids in space to check the convergence.

Based on the perturbation theory, we can estimate that the upper limit of the MP ($-\nabla_r \cdot \nabla_R / m_z$) is smaller than 40 meV if we replace ∇_R (∇_r) by $2\mu_p/N$ ($1/n$) with $N = 39, n = 3$. Note that this is an upper limit and the real shift due to the MP is much smaller since this term vanishes for a single configuration as

$$\langle \Omega_{JM}^{L,l} | \nabla_R \cdot \nabla_r | \Omega_{JM}^{L,l} \rangle = 0.$$

We did not find the large energy shifts (larger than this upper limit) reported by Sakimoto [9].

As shown in Fig. 2, we see that the residual correlation V does not modify the resonant energies significantly. Since an antiproton is very heavy, its wave function mainly locates near $N^2/(Z\mu_p) \approx 0.5$ a.u. for $N = 40$. The electron wave function locates in the range around $n^2 \approx 4$ for $n = 2$. For other higher n , the electron is well separated from \bar{p} -He⁺⁺ so that the residual correlation should be even smaller. Therefore, the largest split should be around $N = 40, n = 2$ peak which is consistent with our calculations. From all the discussion and our calculations, we may conclude that the MP does not affect the resonant energies significantly.

In principle, if we replace the plane wave by a Coulomb wave, we can also study the formation cross section of \bar{p} -He⁺⁺ in the collision of antiprotons with He⁺ ions. However, it requires huge computational work and it is not our goal to study this process but to investigate the MP effect on the resonant energies.

Sakimoto [9] stated that the V coordinates could be more problematic in the protonium-formation process since the antiproton and proton masses are equal. We have to investigate the MP effect on the protonium formation. We calculate the state-specified protonium-formation cross sections in the

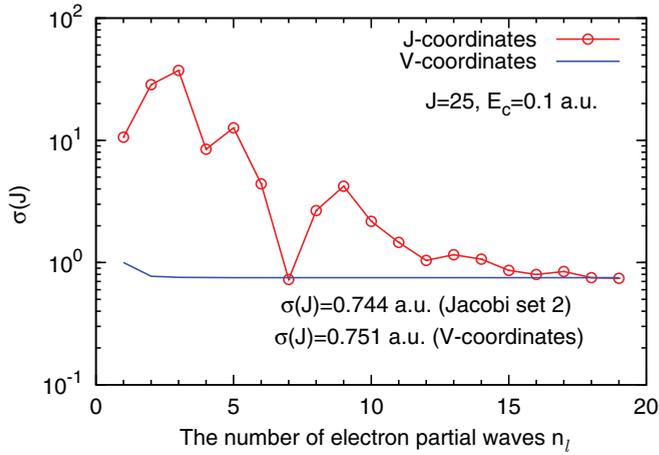


FIG. 3. (Color online) Partial protonium-formation cross sections obtained in the Jacobi coordinates (solid curve with open circles) and V coordinates (solid curve) as a function of the number of electron partial waves.

Jacobi coordinates. Figure 3 shows the partial cross section defined as

$$\sigma(J) = \sum_{N,L,l} \sigma_{NL}^l(J)$$

for a given $J = 25$ at $E_c = 0.1$ a.u., the incident energy in the center of mass frame, as a function of the number of electron partial waves (n_l) involved in the calculation. The number of channels (L, l) involved in the simulation is proportional to n_l^2 and the computational time goes up to n_l^4 . In the figure we see that the cross section converges very fast in the V coordinates below $n_l = 3$. On the other hand, the cross section converges slowly in the Jacobi coordinates. The converged results of the two coordinate sets are very close to each other and this means that the MP does not affect the partial protonium-formation cross sections much. The numerical values show that the difference is less than 1%.

Since the number of electron partial waves needed in the two coordinate systems differs almost by an order of magnitude, we need to check how the MP affects the individual formation cross sections. Figure 4 shows the formation cross sections, defined by

$$\sigma_N(J) = \sum_{L,l} \sigma_{NL}^l(J),$$

as a function of the principle quantum number N of the protonium. We see that the two calculations are in reasonable agreement over a broad range which covers more than six orders. Since the plot is in a logarithm scale, in which we cannot see the difference distinctly, we compared the numerical values directly. The differences between the two calculations are less than 10%. As the formation cross sections become larger, the differences get smaller. The differences may also come from the numerical inaccuracy in the Jacobi coordinates as we will discuss later. Nevertheless, we can safely say that the MP effect on the state-specified protonium-formation cross sections is less than 10%.

In Fig. 3 we have seen that the partial cross sections are larger than the converged one if we do not include enough

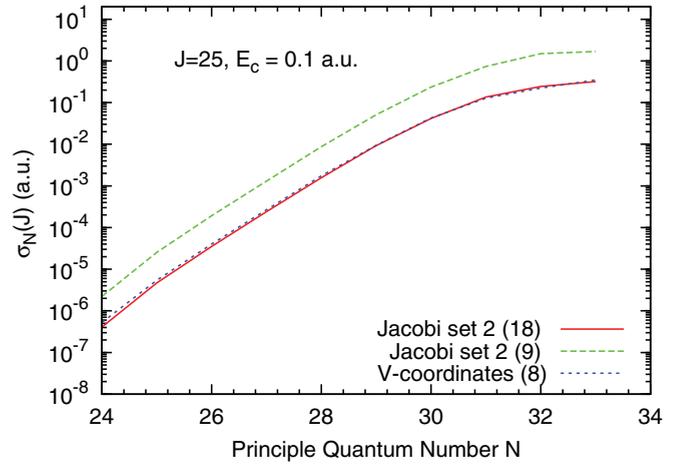


FIG. 4. (Color online) Principle quantum number dependent protonium-formation cross sections calculated in the Jacobi coordinates (solid curve) and V coordinates (dotted curve). Unconverged results (dashed curve) are also plotted. The number in parentheses is the number of electron partial waves n_l used in the calculation.

electron partial waves. Initially, the electron is located around the proton and its wave function is analytically known if we choose the proton as the origin of the electron coordinates. In Jacobi set 2 we choose the middle point of the proton and antiproton as the origin of the electron coordinates, and the initial electron wave function can be written as

$$\psi_{1s}(\mathbf{r} + b_0\mathbf{R}) = \sum_{l=0}^{L_{\max}} F_l(r, R) P_l(\cos \theta), \quad (12)$$

where θ is the angle between \mathbf{r} and \mathbf{R} . Define

$$S(R) = \sum_{l=0}^{L_{\max}} \frac{2}{2l+1} \int_0^\infty F_l^2(r, R) r^2 dr, \quad (13)$$

then we can study how many partial waves are needed to describe the initial electron wave function at a given R . We plot $S(R)$ in Fig. 5. For a large R we need many partial waves to describe the initial electron wave function. If the number of the partial waves is not large enough, the electron is “distributed” to a place far away from the proton and becomes loosely bound.

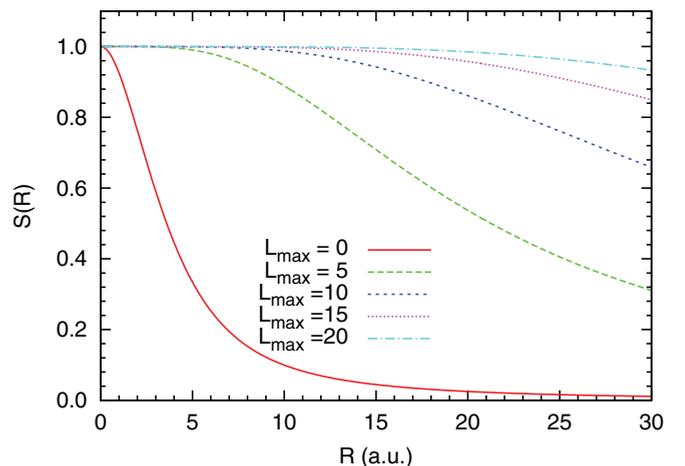


FIG. 5. (Color online) $S(R)$ for different L_{\max} .

For example, if we only take s wave into account, the electron is symmetrically distributed around the middle point of the proton and antiproton, not around the proton. The loosely bound electron is easily knocked out when the antiproton approaches the proton. This increases the formation cross sections unphysically. When R is large, we need both a lot of partial waves and many grid points in r to accurately describe the initial wave function. All these make the calculations in the Jacobi coordinates very difficult. Insufficient space grid points will also result in numerical inaccuracy.

Interestingly, although the partial cross sections are overestimated by almost 8 times for $n_l = 9$, the relative dependence on N does not differ much as shown in Fig. 4. This also infers that the MP effect is not important for the state-specified protonium formation, or at least not important for the relative formation cross sections. Although in Jacobi set 2 we need a large n_l to get a convergent result, the ejected electron is mainly distributed at low angular momentum states. This is in agreement with the results of the V coordinates.

We have presented two examples, the resonant energies of \bar{p} -He⁺ and the protonium-formation cross sections of \bar{p} +H, and have shown that the MP is not important, or more specifically, its contribution to dynamical processes is less than a few percent. Now we estimate the MP effect on the capture processes of antiproton in a general way without numerical calculations. In the V coordinates one can also perform high precision calculations by including the mass polarization term $-\nabla_{\mathbf{R}} \cdot \nabla_{\mathbf{r}}/m_z$ properly [17]. The MP term, unlike the Coulomb interaction which affects either the initial state or final states or both, does not affect the initial and final states if one particle is far away from the other two. The

MP contribution reaches its maximum when the electron and antiproton are located close to each other. For He atoms, it is well known that the MP modifies the ground state energy about 0.6 meV [18]. If we scale the MP contribution by $\sqrt{\mu_p}$ since the momentum of the antiproton is $\sqrt{\mu_p}$ times larger than that of the electron for a given energy, the MP term is about 20 meV, which is less than 1% of the Coulomb interaction. Thus the maximum contribution of the MP to the state-specified protonium-formation cross section is a few percent regardless of the incident energy and the total angular momentum.

To summarize, we have studied the resonant energies of \bar{p} -He⁺ and the protonium-formation cross sections in antiproton-hydrogen-atom collisions in the Jacobi coordinates and the V coordinates. Although the computational effort needed for the Jacobi coordinates is much larger than that for the V coordinates, the calculated results, both of the resonant energies of \bar{p} -He⁺ and of the state-specified protonium-formation cross sections, are in good agreements for the two coordinate sets. Thus, it is proved that the V coordinates are very useful for the Coulomb three-body system involving an antiproton and a hydrogen-like ion, and that the MP has a small contribution to both the energy structures and the capture cross sections for such a system. The large MP effects reported by Sakimoto [9] are questionable and need to be reinvestigated.

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- [1] M. Amoretti *et al.*, *Nature (London)* **419**, 456 (2002).
 - [2] G. B. Andresen *et al.*, *Nature (London)* **468**, 673 (2011).
 - [3] J. S. Cohen, *Phys. Rev. A* **36**, 2024 (1987).
 - [4] B. D. Esry and H. R. Sadeghpour, *Phys. Rev. A* **67**, 012704 (2003).
 - [5] M. Hesse, A. T. Le, and C. D. Lin, *Phys. Rev. A* **69**, 052712 (2004).
 - [6] X. M. Tong, K. Hino, and N. Toshima, *Phys. Rev. Lett.* **97**, 243202 (2006).
 - [7] X. M. Tong, K. Hino, and N. Toshima, *Phys. Rev. Lett.* **101**, 163201 (2008).
 - [8] F. Weinhold, *J. Phys. Chem.* **86**, 1111 (1982).
 - [9] K. Sakimoto, *Phys. Rev. A* **82**, 012501 (2010).
 - [10] K. Sakimoto, *Phys. Rev. A* **80**, 012517 (2009).
 - [11] X. M. Tong and Shih-I. Chu, *Phys. Rev. A* **61**, 031401(R) (2000).
 - [12] Shih-I. Chu and X. M. Tong, *Chem. Phys. Lett.* **294**, 31 (1998).
 - [13] X. M. Tong and S. I. Chu, *Chem. Phys.* **217**, 119 (1997).
 - [14] J. Perie and G. Jolicard, *J. Phys. B* **26**, 4491 (1993).
 - [15] X. M. Tong, T. Shirahama, K. Hino, and N. Toshima, *Phys. Rev. A* **75**, 052711 (2007).
 - [16] D. Bakalov and V. I. Korobov, *Phys. Rev. A* **57**, 1662 (1998).
 - [17] V. I. Korobov, *Phys. Rev. A* **67**, 062501 (2003).
 - [18] B. H. Bransden and C. J. Joachain, *Physics of Atoms and Molecules* (Prentice Hall, Englewood Cliffs, NJ, 2003).