Low-energy capture of antiprotons by helium ions

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Low-energy antiproton capture, \( \bar{p} + \text{He}^+ \rightarrow \bar{p}\text{He}^{2+} + e \), is investigated using a wave-packet-propagation full-quantum-mechanical method or a quantum-classical hybrid (i.e., semiclassical) approximation. If the adiabatic picture (i.e., Born-Oppenheimer separation) is a good approximation, the antiproton capture, which is a typical nonadiabatic process, can rarely occur. It is found that the probability of the nonadiabatic transition is small (at most \( \sim 0.1 \)). However, even in the zero energy limit \( E \rightarrow 0 \), the antiproton capture always occurs for the total angular momenta \( J \leq 40 \). Correspondingly, the cross section for the antiproton capture diverges as \( E \rightarrow 0 \). This happens due to the peculiarity that the Coulomb force range is longer than the centrifugal one. The importance of a Rydberg series of resonances in the capture process is emphasized. On the low-energy dynamical feature, some interesting similarities to the \( e + \text{ion} \) system are also found.

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I. INTRODUCTION

Recently, much progress has been made in the theoretical study of low-energy collisions of antiprotons \( (\bar{p}) \) with atoms or molecules. Performing a full quantum-mechanical (QM) calculation has become possible especially for \( \bar{p} + \text{H} \) collisions \([1–3]\). As usually done in the study of heavy particle collisions, we look at the \( \bar{p} + \text{H} \) system by using the adiabatic picture (Born-Oppenheimer separation). Owing to the negative charge of \( \bar{p} \), the lowest adiabatic potential curve crosses with its ionized (\( \bar{p} + p \)) one at the so-called Fermi-Teller critical distance \( (R_{\text{FT}}=0.639 \text{ a.u.)}) \) \([4]\). Evidently, the adiabatic approximation is unacceptable in the vicinity of \( R_{\text{FT}} \). The presence of the critical distance brings about the situation that the ionization occurs very easily (its probability is indeed close to unity) whenever \( \bar{p} \) could sufficiently approach \( \text{H} \) \([2, 3]\). Accordingly, the cross section for the \( \bar{p} \) capture \( \bar{p} + \text{H} \rightarrow \bar{p}p + e \) becomes extremely large as the energy decreases. Such a behavior is expected to be commonly observed for most of the neutral targets.

To see how the situation changes for the \( \bar{p} \) collisions with ion targets, the present study investigates the \( \bar{p} \) capture by \( \text{He}^+ \) in the \( 1s \) state at energies below the first excitation threshold (=40.82 eV), i.e.,

\[ \bar{p} + \text{He}^+ \rightarrow \bar{p}\text{He}^{2+} + e. \]

In the adiabatic approximation, the electron can be bound for all the distances between \( \bar{p} \) and \( \text{He}^+ \) (no critical distance like \( R_{\text{FT}} \) exists). In previous studies \([5–7]\), the adiabatic approximation was found to be very useful for the description of the metastable states of antiprotonic helium atoms \( \bar{p}\text{He}^+ \). If the adiabatic condition were well satisfied also in the \( \bar{p} + \text{He}^+ \) collisions as frequently happened in slow atomic collisions, the nonadiabatic process \([1]\) would be negligible. However, even if the incident energy is very small, as \( \bar{p} \) approaches \( \text{He}^+ \) the Coulomb attraction yields a large gain of the relative kinetic energy, which may be sufficient to induce a nonadiabatic transition. Using the fermion-molecular-dynamics (FMD) method, Cohen \([8]\) obtained the result that the capture cross section became much larger for \( \bar{p} + \text{He}^+ \) than for \( \bar{p} + \text{H} \) at very low energies. This may suggest the significance of the nonadiabatic effect in the low energy \( \bar{p} + \text{He}^+ \) collisions. At the present time, only a few studies have been made for the ion targets at low energies \([8–11]\). It is an important subject to clarify to what extent the adiabatic approximation is applicable to the \( \bar{p} + \text{ion} \) collisions.

In the present study, we consider the QM method based on the wave-packet-propagation technique, which is the same as applied to the \( \bar{p} + \text{H} \) system \([2, 3]\). However, the stronger Coulomb attraction causes the QM calculation to be much more laborious for \( \bar{p} + \text{He}^+ \) than for \( \bar{p} + \text{H} \). We also consider a quantum-classical (QC) hybrid (i.e., semiclassical) method, which was found to be very useful for the \( \bar{p} \) capture in \( \bar{p} + \text{H} \) \([12, 13]\). The QM and QC calculations are both carried out to be complementary.

II. OVERVIEW OF THE COLLISION SYSTEM

First, we overview the \( \bar{p} + \text{He}^+ \) system using the adiabatic picture. The adiabatic wave function \( \chi_{\alpha\lambda} \) of this system for a fixed distance \( R \) between \( \bar{p} \) and \( \text{He}^+ \) satisfies the Schrödinger equation

\[ \tilde{H}_{\text{AD}} \chi_{\alpha\lambda}(r, \theta; R) = E_{\alpha\lambda}(R) \chi_{\alpha\lambda}(r, \theta; R), \]

with

\[ \tilde{H}_{\text{AD}} = -\frac{1}{2m_r} \frac{\partial^2}{\partial r^2} + \frac{1}{2m_e} \frac{\partial^2}{\partial \varphi^2} + U(R, r, \theta), \]

where \( r \) is the distance between \( e \) and \( \text{He}^{2+} \), \( \theta \) the angle between \( \textbf{R} \) and \( \textbf{r} \), \( m_r \) the reduced mass of the \( e + \text{He}^{2+} \) system, \( \varphi \) the electronic angular momentum operators, and \( U \) the sum of all the Coulomb interactions. The subscript \( \lambda = l \) is the magnetic quantum number along the \( \textbf{R} \) axis, and \( \alpha = 1, 2, \ldots \) identify the adiabatic states having the same \( \lambda \). Here and in the following, atomic units are used unless otherwise stated explicitly.

Figure 1 summarizes the adiabatic potentials \( E_{\alpha\lambda}(R) \) as a function of \( R \). The electronic excited levels form an infinite Rydberg series converging to the ionization limit for each
fixed $R$. For the collision process (1), we introduce the total energy $E_{\text{tot}}$ defined by

$$E_{\text{tot}} = E + E_{1\sigma}(R = \infty),$$

where $E$ is the center-of-mass relative collision energy, and $E_{1\sigma}(R = \infty) = -2$ a.u. In the present study, the excitation channels $(\alpha, \lambda) \neq 1\sigma$ are all closed in the separation limit. However, all the potential curves go down far below $E_{1\sigma}(R = \infty)$ u.a as $R$ becomes small. Therefore, no matter how the collision energy is small (i.e., $E \to 0$), the nonadiabatic transition becomes possible at small distances. From the figure, the range that any nonadiabatic transition as well as ionization can occur is estimated to be $R_c \sim 1$ a.u. at $E \sim 0$. [The potential $-2/R$ is equal to $E_{1\sigma}(R = \infty)$ at $R=1$ a.u.] This situation implies that the $\bar{\rho} + \text{He}^+$ collision system reveals a Rydberg series of Feshbach-type resonances, i.e.,

$$\bar{\rho} + \text{He}^+ \leftrightarrow (\bar{\rho}\text{He}^+)^* \to \bar{\rho}\text{He}^{2+} + e.$$  

Although the three-body break-up ionization is a closed channel, the ionization can take place by leading to the formation of the $\bar{\rho}\text{He}^{2+}$ atoms. The Coulomb attraction ($-1/R$) between $\bar{\rho}$ and $\text{He}^+$ in each electronic excited state can support bound states in another Rydberg series. Therefore, at energies just below the ionization threshold of $\text{He}^+$, the collision process would have a feature of quite complicated energy dependence due to the double Rydberg series of resonances.

At low collision energies, the angular momentum plays a very important role in the relative ($R$) motion. Figure 2 shows the effective potential

$$V_{\text{eff}}^{\alpha\lambda}(R) = \frac{L(L+1)}{2m_R R^2} + E_{\alpha\lambda}(R),$$

where $m_R$ is the reduced mass of the $\bar{\rho} + \text{He}^+$ system and $L$ the relative angular momentum quantum number. When $L < L_c = 38$, the lowest energy $E_{\text{ion}}^{\alpha\lambda} = -2m_R/(L+1)^2$ of atomic states of $\bar{\rho}\text{He}^{2+}$, given by the effective potential $L(L+1)/(2m_R R^2) - 2/R$, is below $E_{1\sigma}(R = \infty)$. In this case, the ionization is certainly possible at any energy. When $L \geq L_c$, the fact that $E_{\text{ion}}^{L} > E_{1\sigma}(R = \infty)$ implies that the ionization seldom occurs at $E \sim 0$. Strictly speaking, the ionization can still occur in this case by the nonadiabatic coupling with the ionized states having $L < L_c$ ($L$ is not a good quantum number). However, the transition following the large change $|\Delta L|$ is negligible [5–7,14]. In any way, we can anticipate that in the zero energy limit, a wide range of the angular momenta up to $L \sim L_c$ has non-negligible contribution to the ionization. This peculiarity occurs because the Coulomb potential range ($\sim R^{-1}$) is longer than the centrifugal one ($\sim R^{-2}$). A very similar situation arises in $e^+\text{ion}$ scattering.

### III. COLLISION THEORY

#### A. Full quantum-mechanical theory

The time-dependent Schrödinger equation of the $\bar{\rho} + \text{He}^+$ collision is given by [2]

$$i\hbar \frac{\partial}{\partial t} \Psi^{JM}(\mathbf{r}, t) = \hat{H} \Psi^{JM}(\mathbf{r}, t),$$

where $J$ is the total angular momentum quantum number, $M$ its magnetic component in the space-fixed (SF) frame, and $p = \pm$ the total parity. The total Hamiltonian $\hat{H}$ is given by

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**FIG. 1.** Adiabatic potential $E_{\alpha\lambda}(R)$ of the $\bar{\rho} + \text{He}^+$ system.

**FIG. 2.** Effective potential $V_{\text{eff}}^{\alpha\lambda}(R)$ of the $\bar{\rho} + \text{He}^+$ system for $L=20$ and 40.
\[ \hat{H} = -\frac{1}{2m_rR} \frac{\partial^2}{\partial r^2} R + \frac{\mathbf{L}^2}{2m_rR^2} - \frac{1}{2m_r} \frac{\partial^2}{\partial \varpi^2} + \frac{\mathbf{L}^2}{2m_r} + U(R, r, \theta), \]

where \( \mathbf{L} \) is the angular momentum operator of the relative motion. We employ a body-fixed (BF) frame in which the \( z \) axis is chosen along \( \mathbf{R} \). Hence, \( \mathbf{L}^2 \) is replaced by \((\mathbf{\hat{J}} - \mathbf{\hat{I}})^2\), with \( \mathbf{\hat{J}} \) being the total angular momentum operator. The total wave function \( \Psi^{JM}(p) \) can be expanded in the form

\[ \Psi^{JM}(p)(\mathbf{R}, r, t) = (\mathbf{R}r)^{-1} \sum_{\lambda} \tilde{D}^{JM}_{M\lambda}(\mathbf{\hat{R}}) \psi^{JM}(p)(\mathbf{R}, r, \theta, t), \]  

where

\[ \tilde{D}^{JM}_{M\lambda}(\mathbf{\hat{R}}) = \left[ \frac{2J + 1}{16 \pi^2 (1 + \delta_{J,0})} \right]^{1/2} \times \left[ D^J_{M\lambda}(\mathbf{\hat{R}}) + p(-1)^{J+\lambda} D^{J}_{M-\lambda}(\mathbf{\hat{R}}) \right], \]

and the initial condition can be given by

\[ \psi^{JM}(p)(\mathbf{R}, r, \theta, t = 0) = \chi_{1, \sigma}(r, \theta, R) \xi_0, \]

where \( \chi_{1, \sigma} \) is the ground-state \((1, \sigma)\) adiabatic function defined by (2), and \( \xi \) the Gaussian wave packet representing the incoming radial \((R)\) motion.

**B. Quantum-classical hybrid approximation**

We also consider the QC approximation, in which the relative radial distance \( R \) is given as a time dependent parameter, and the other degrees of freedom are described by quantum mechanics. In this case, the time-dependent Schrödinger equation becomes [15]

\[ i \frac{\partial}{\partial t} \Psi^{JM}_{QC}(p)(\mathbf{R}, r, t) = \hat{H}_{QC} \Psi^{JM}_{QC}(p)(\mathbf{R}, r, t), \]

where

\[ \hat{H}_{QC} = (\mathbf{\hat{J}} - \mathbf{\hat{I}})^2 + \frac{1}{2m_r} \frac{\partial^2}{\partial \varpi^2} + \frac{\mathbf{L}^2}{2m_r} + U(R, r, \theta), \]

and

\[ \Psi^{JM}_{QC}(p)(\mathbf{R}, r, t) = r^{-J} \sum_{\lambda} \tilde{D}^{JM}_{M\lambda}(\mathbf{\hat{R}}) \psi^{JM}(p)(r, \theta, t). \]

In the QC approximation, \( R(t) \) is considered to be a classical trajectory representing the relative radial motion. Unfortunately, we have no way of giving such a classical trajectory without any ambiguity. Previous studies [3,12,13] suggest that one of the best choices is to use the adiabatic potential \( E_{\text{eff}}(R) \): Namely, the time dependence of \( R \) is determined from

\[ E_{\text{eff}} = \frac{m_r}{2} \left( \frac{dR}{dt} \right)^2 + V_{\text{eff}}(R). \]

In \( V_{\text{eff}}(R) \), \( L \) is replaced by \( J \) because the electronic angular momentum is much smaller than \( L \) in most cases.

The initial condition is given by

\[ \psi^{JM}_{QC}(p)(r, \theta, t = 0) = \chi_{1, \sigma}(r, \theta; R_0) \delta_{t,0}, \]

where \( R_0 = R(t=0) \).

**C. Numerical solution**

The wave packet propagation was calculated on a grid of points in the \((R, r, \theta)\) space for \( \psi^{JM}_{QC}(p)(R, r, \theta, t) \) and on a grid of points in the \((r, \theta)\) space for \( \psi^{JM}_{QC}(p)(r, \theta, t) \) by using a discrete-variable-representation (DVR) technique [16,17]. The grid points are taken to be the zero points of orthogonal polynomials. We used the \( N_r \) zero points of the Chebyshev polynomial [18] for \( R \), the \( N_\varpi \) zero points of the generalized Laguerre polynomial [18] for \( r \), and the \( N_{\theta} \) zero points of the Legendre [18] or Gegenbauer polynomial [18] for \( \theta \). As in the pre-H system [2,3], the inclusion of the \(|\lambda|=0 \) and 1 states is sufficient. A fourth-order Runge-Kutta formula was applied for the time evolution.

**IV. PRELIMINARY INQUIRY USING QUANTUM-CLASSICAL HYBRID METHOD**

For the QC calculation, we chose a sufficiently large number of grid points, i.e., \((N_r, N_\varpi, N_{\theta})=(40,5,5)\). We checked the accuracy of this choice by carrying out some calculations for the larger number set \((N_r, N_\varpi, N_{\theta})=(50,6,6)\), and a relative error of the transition probability was estimated to be mostly less than 1%.

We introduce the probability that the system is in the adiabatic state \((\alpha, \lambda)\) at each time \( t_i \), i.e.,

\[ P^{J}_{QC}(\alpha; t_i) = \left| \langle \chi_{\alpha}(r; R) | \psi^{JM}_{QC}(p)(r, t_i) \rangle \right|^2, \]

where \( R = R(t_i) \), and the subscript \( r \) means the integration over \( r \). In the QC calculation, we cannot directly describe the pHe\(^+\) formation as long as the \( R \) motion is given by the potential scattering (15). However, as in previous studies [12,13], we can assume that the probability of pHe\(^+\) formation is equal to the probability of the ionization obtainable from the QC calculation. Accordingly, we define the direct capture probability by

\[ P^{J}_{QC, \text{dir}}(t_i) = 1 - \sum_{\alpha \lambda} P^{J}_{QC}(\alpha; t = t_i), \]

where the final time \( t_i \) is given by \( R(t_i) = R_0 \), and the summation is taken over all the adiabatic bound states. Although the excitation channels are all closed in the separation limit, the QC method provides non-negligible probabilities for the excitations. This may seem to happen due to the defect of the QC method. However, as demonstrated in section V, the finite excitation probability has a physical significance. Here, the capture probability (18) is defined as the one coming from the direct ionization.

First, we show the \( R_0 \) dependence of the direct capture probability \( P^{J}_{QC, \text{dir}}(t_i) \) in Fig. 3. As noted in Sec. II, the range of the interaction that can induce ionization is \( \sim 1 \) a.u. Correspondingly, the probability is almost independent of \( R_0 \) for \( R_0 \approx 1 \) a.u. This is a great advantage in our performing the
QM calculation because we can set the center of the initial wave packet at a relatively small distance, and can make the total propagation time shorter and the number of grid points smaller.

Next, we plot the direct capture probability \( P_{QC,\text{dir}}(t_i) \) as a function of the collision energy \( E \) in Fig. 4. It is very interesting that the probability is almost independent of \( E \) over a wide range. This is easily understood from the fact that the effective local kinetic energy at small \( R \) can be much larger than the incident collision energy owing to the strong Coulomb attraction (Fig. 2). The same feature has been found in the \( e+\text{ion} \) system, and serves as the basis of the quantum defect theory (QDT) [19,20]. An important point is that we need no repetition of the calculation at different energies in the low energy region. As \( J \) increases, a shallower effective potential well causes the \( E \) dependence to be more significant. However, as seen in Fig. 4, the probability itself becomes negligibly small.

V. FULL QUANTUM-MECHANICAL CALCULATION

A. Numerical parameters

Unfortunately, it is quite difficult to carry out the QM calculation for the number of grid points \( N_R \). In the QM calculation, we chose the smaller number set \( N_R = 30, 5 \). To check the validity of this choice, we calculated the direct capture probabilities for \( N_R = 40, 5 \) and \( 30, 5 \) by using the QC method, and show the results of the opacity \( (2J+1)P_{QC,\text{dir}}(t_i) \) in Fig. 5. On the whole, the agreement between the two results is sufficient for the present purpose. The agreement becomes better for the calculation of the cross section, which is 1.69 a.u. for \( N_R = 30, 2 \) and 1.70 a.u. for \( 40, 5 \).

The motion of the wave packet along \( R \) is confined in the box of \( 0 \leq R \leq 3.5 \) a.u. As \( J \) decreases, the deeper well of the effective potential requires a larger number of gird points \( N_R \). We chose \( N_R = 105 \) for \( J \geq 30 \), \( N_R = 175 \) for \( J = 29 \sim 23 \), \( N_R = 262 \) for \( J = 22 \sim 18 \), \( N_R = 437 \) for \( J = 13 \), and \( N_R = 700 \) for \( J = 8 \). The largest error of the transition probabilities is estimated to be \( \sim 3.5\% \). We could not obtain a sufficiently converged result by \( N_R = 875 \) for \( J = 5 \). To avoid an artificial reflection by the outer boundary, we applied the absorbing optical potential to the outgoing wave at \( R > 2.3 \) a.u. The Laguerre grid can cover a large distance \( r \) (\( r \approx 110 \) a.u. for \( N_r = 30 \)) so that no optical potential was introduced for the propagation along \( r \). However, if a much longer time evolution were considered, a larger \( N_r \) would be needed (otherwise the optical potential should be applied at large \( r \)).
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B. Initial wave packet

We prepared the initial Gaussian wave packet \( \zeta(R) \) in which the center was \( R_c = 2 \) a.u. and the collision energy corresponding to the central momentum was \( E_c = 0.5 \) eV, as shown in Fig. 6. Because \( \zeta(R) \) has a finite value in the range of \( 1 \leq R \leq 3 \) a.u., the \( R \) dependence of \( \chi(r, \theta; R) \) must be explicitly taken into account in (11). In the QM calculations of \( \bar{p} + \text{H} \) [2,3], the transition probability for each collision energy was extracted by the Fourier transformation from \( t \) to \( E \) of the scattered wave. The present wave packet has a very broad energy distribution up to \( E \approx 6 \) eV. In such a case, however, it becomes quite difficult to extract each energy component in a numerically accurate manner. A sharp energy distribution needs the wave packet broadly spreading in the \( R \) space. For this reason, the calculation of wave packet propagation becomes more troublesome as the energy decreases. Without extracting each energy component, we must characterize the dynamical process by using the probabilities averaged over a wide energy range \( 0 \leq E \leq 6 \) eV. However, as was seen in the QC calculation, the transition probability is almost independent of \( E \) in this energy range.

Therefore, no worry is needed for the information loss suffered from the energy average, and the present energy averaged probability is still useful for the understanding of the dynamical process.

C. Time evolution of the wave packet

The time evolution of the wave packet for \( J = 25 \) is visualized in Fig. 7 by the contour plot of \( \Sigma_p R^2 r^2 |\psi(\hat{p}p)(R, r, t)|^2 d\mathbf{r} \) at the different times \( t = 4.5, 49.5, 74.5 \), and 119.5 a.u. The panel (a) shows the incoming wave before the collision. At \( t = 49.5 \) a.u., the wave packet is reflected by the centrifugal potential. After that \( (t \approx 74.5 \) a.u.), the prompt electron emission, occurring locally at \( R \approx 0.8 \) a.u., means that the \( \bar{p}\text{He}^{2+} \) atoms are formed with the average radius of \( \approx 0.8 \) a.u. We can call this process direct capture of \( \bar{p} \). Examination of the wave packet propagation shows that the direct capture process completes up to the time \( t \approx 80 \) a.u. In the panel (d), the wave packet corresponding to the direct capture is out of scope. The majority of the wave packet goes back along \( R \) (outgoing wave), and fades away at \( R \approx 2.5 \) a.u. by the action of the optical potential. An interesting thing is that some portion of the wave packet remains localized at \( R < 1 \) a.u. and \( 2 \leq r \leq 8 \) a.u. for a long time after the direct capture completed. This portion indicates a compound of the three particles \( e, \bar{p}, \text{and He}^{2+} \). Because the average distance between \( e \) and \( \text{He}^{2+} \) is very large (\( \approx 5 \) a.u.), we can see that this compound is in electronic excited states. It is evident that the compound is formed as a Feshbach-type resonance state \( (\bar{p}\text{He}^+) \) (i.e., resonance capture).

VI. CAPTURE PROBABILITIES

Also in the QM calculation, corresponding to (17) defined in the QC method, the probability that the system is in the adiabatic state \( (a, \lambda) \) at each time \( t \) can be given by

![Figure 6](image6.png)

![Figure 7](image7.png)

FIG. 6. Properties of the initial Gaussian wave packet \( \zeta(R) \) in the QM calculation: (a) The radial distance distribution \( |\zeta(R)|^2 \); (b) the kinetic energy distribution.

FIG. 7. Time evolution of the wave packet projected on the \( Rr \) plane in the QM calculation for \( J = 25 \), \( R_c = 2 \) a.u. and \( E_c = 0.5 \) eV. The four panels show (a) the incoming phase; (b) the reflection by the centrifugal potential; (c) the electron emission and \( \bar{p}\text{He}^{2+} \) formation; (d) the feature after the direct collision.
becomes independent of $t$ when $t > 80$ a.u. This time independent part is considered to represent the total amount of the localized compound portion seen in Fig. 7(d). Thus, the sum $P_{\text{res}}^J(t_0)$ with $t_0 > 80$ a.u. has a physical significance, and can be interpreted as the total net of the resonance capture probabilities.

It should be noted that the particle absorption due to the optical potential takes place only for the open channel $(\alpha, \lambda) = 1 \sigma$. Therefore, corresponding to (18) defined in the QC method, the time-dependent direct capture probability in the QM calculation can be given by

$$P_{\text{dir}}^J(t) = P_{\text{tot}}^J(t) - \sum_{\alpha \lambda} P^J(\alpha \lambda ; t),$$

with

$$P^J(\alpha \lambda ; t) = \int |\langle \chi_{\alpha \lambda}(r;R) \eta^{R}(R,r,t) \rangle_{\tau} |^2 R^2 dR.$$  (19)

Figure 8 shows the time evolution of $P^J(\alpha \lambda ; t)$ for $(\alpha, \lambda) \neq 1 \sigma$. Although the excited channels are all closed in the separation limit, these probabilities remain finite even after the direct capture completed (i.e., at $t \approx 80$ a.u.). This implies that $P^J(\alpha \lambda ; t)$ for $(\alpha, \lambda) \neq 1 \sigma$ is related to the probability of the capture into the resonance compound. Unfortunately, these probabilities have obvious time variation all the time, and hence the adiabatic approximation is not suitable for the description of each resonance state [21]. However, we can find that the total sum of $P^J(\alpha \lambda ; t)$ over $(\alpha, \lambda) \neq 1 \sigma$,

$$P_{\text{res}}^J(t) = \sum_{(\alpha, \lambda) \neq 1 \sigma} P^J(\alpha \lambda ; t),$$

becomes independent of $t$ when $t > 80$ a.u. This time independent part is considered to represent the total amount of the localized compound portion seen in Fig. 7(d). Thus, the sum $P_{\text{res}}^J(t_0)$ with $t_0 > 80$ a.u. has a physical significance, and can be interpreted as the total net of the resonance capture probabilities.

We can find in Fig. 9 that the QC direct capture probability $P_{\text{dir}}^J(t)$ calculated for $E = E_c = 0.5$ eV and $R_0 = R_c = 2$ a.u. becomes very close to the QM direct capture probability $P_{\text{dir}}^J(t)$ when $t > 70$ a.u. Although $P_{\text{dir}}^J(t)$ is the energy averaged probability, this comparison has significance because $P_{\text{dir}}^J$ is almost independent of $E$ (Fig. 4). We further consider the QC version of $P_{\text{res}}^J(t)$, i.e.,

$$P_{\text{res}}^J(t) = \sum_{(\alpha, \lambda) \neq 1 \sigma} P_{\text{QC}}^J(\alpha \lambda ; t).$$

Also for this probability, the $E$ dependence is very loose over a wide range (Fig. 10). We can find again in Fig. 9 that the QC probability $P_{\text{res}}^J(t)$ for $E = E_c$ and $R_0 = R_c$ is very close to the QM resonance capture probability $P_{\text{res}}^J(t)$ when $t > 80$ a.u. It should be noted that $P_{\text{res}}^J(t)$ is identically the total excitation probability. Thus, it is evident that the total excitation probability obtained in the QM calculation can be regarded as the net amount of the resonance capture probability.

In the $\tilde{p}+{\text{He}}^+$ system, an infinite series of resonances should produce a rich structure in the transition probabilities plotted as a function of $E$, although $P_{\text{dir}}^J(t)$ and $P_{\text{res}}^J(t)$ have very weak $E$ dependence. In this respect, the $e+{\text{ion}}$ scattering, likewise revealing a prominent Rydberg series of
resonances, is of some help. In the e+ ion scattering, an important physical quantity, obtained by the average over resonances (known as the Gailitis average), can characterize the resonances, and is usually found to be weakly dependent on the energy [20,22]. We can naturally consider that the present QM probabilities $P_{\text{dir}}^J(t_0)$ and $P_{\text{res}}^J(t_0)$ are the resonance averaged ones similar to those defined in the e+ ion study. Although of course the QC method cannot describe the details of the resonance phenomena, it is found to be still very useful for the calculation of the probabilities averaged over resonances.

Because the resonance state has a finite lifetime, the localized compound wave packet [Fig. 7(d)] will decay as time goes on. Figure 11 shows the time evolution of the probabilities $P_{\text{dir}}^J(t_0)$, $P_{\text{res}}^J(t_0)$, $P_{\text{sum}}^J(t_0)=P_{\text{dir}}^J(t_0)+P_{\text{res}}^J(t_0)$, and $P_{\text{tot}}^J(t_0)$ up to the longer time $t=300$ a.u. (although a larger number of $N_0$ might have been needed for such long time propagation). At $t \approx 120$ a.u., we can see that $P_{\text{res}}^J(t)$ decreases gradually. This represents the decay of resonance states. For the time $t > 150$ a.u., the decay channel is considered to be mainly $\bar{p}$He$^{2+}+e$ because the sum $P_{\text{sum}}^J(t)$ becomes independent of $t$. The fact that $P_{\text{sum}}^J(t)$ rather decreases just before $t \approx 150$ a.u. may suggest that also the decay channel $\bar{p}+\text{He}^+$ is important in this short time duration. (The outgoing wave corresponding to this decay channel is absorbed by the optical potential.) It should be mentioned, however, that these interpretations remain speculation. A more quantitative analysis and an extremely-long-time propagation are needed for the examination of resonance decay channels.

In the resonance state, the compound $\bar{p}$He$^+$ reveals vibrational motion along $R$. The resonance decay cannot take place at any time of the vibrational motion because the occurrence of electron emission is always localized at $R \sim 0.8$ a.u. As a result, the resonance process has a time period of no electron emission (i.e., plateau), which corresponds to the time independent part of $P_{\text{res}}^J(t)$ observed at $t \sim 95$ a.u. We expect that the plateau appears in a periodic manner. This may be the reason that $P_{\text{res}}^J(t)$ seems to be flat again at $t \sim 150$ a.u. in Fig. 11. As the time goes on, the plateau would be more obscure because the accuracy of the present calculation would be inadequate. In any way, as long as $80 \leq t \leq 110$ a.u., we can have a clear initial plateau each for $P_{\text{dir}}^J(t)$ and $P_{\text{res}}^J(t)$. Furthermore, as a matter of course, the QC probabilities $P_{\text{dir}}^J(t_0)$ and $P_{\text{res}}^J(t_0)$ become inevitably $t$ independent $[\rightarrow P_{\text{dir}}^J(t)$ and $P_{\text{res}}^J(t)]$ in the limit as $t \rightarrow \infty$. As a result, we can define the net amounts of the direct and resonance capture probabilities without ambiguity. We set $t_0=100$ a.u. for the calculation of $P_{\text{dir}}^J(t_0)$ and $P_{\text{res}}^J(t_0)$.

VII. CAPTURE CROSS SECTIONS

Figure 12 shows the $J$ dependence of the probabilities, $P_{\text{dir}}^J(t_0)$ and $P_{\text{res}}^J(t_0)$ in the QM calculation at $E_c=0.5$ eV, and $P_{\text{dir}}^J(t_0)$ and $P_{\text{res}}^J(t_0)$ in the QC calculation at $E=0.5$ eV. The QC probability differs from the QM one by only $\leq 0.004$ for $J>10$. At very low $J$, as might be expected, the agreement would be worse. However, the contribution of the low $J$ to the cross section is relatively less important (e.g., Fig. 5).

The resonance capture probability is much larger than the direct capture probability except at very low $J$. Cohen found in the FMD calculation that a relatively significant number of $\bar{p}$ were temporarily trapped as compounds [8]. Its implication was unclear because the FMD method was based on the classical trajectory calculation. The present study evidently shows that the resonances are prominent in the capture process. Nevertheless, the total nonadiabatic transition probabilities $P_{\text{sum}}^J(t_0)$ are at most $\sim 0.1$ except for $J \sim 0$. Although
the resonance phenomena is very interesting, the nonadiabatic process itself is less important in the present system. Therefore, we can conclude that the adiabatic approximation is appropriate in a large sense for the $\bar{p}+$He$^+$ collisions, as well as for the metastable states of antiprotonic helium $\bar{p}$He$^+$ [5–7].

In both the QM and QC methods, if $P^J$ is the probability of some transition for $J$, the corresponding cross section $\sigma$ is calculated by

$$\sigma = \frac{\pi}{2m_R}E\Omega,$$

where $\Omega=\Sigma J(2J+1)P^J$ is the opacity sum. Table I shows the opacity sums $\Omega_{\text{QC,dire}}=\Sigma J(2J+1)P^J_{\text{QC,dire}}(t_f)$ and $\Omega_{\text{QC, res}}=\Sigma J(2J+1)P^J_{\text{QC, res}}(t_f)$ obtained in the QC calculation at $E=0.5$, $2.5$, $5.0$, and $10.0$ eV. The opacity sums are mostly independent of $E$ for these energies. Therefore, the cross sections $\sigma_{\text{dire}}$ and $\sigma_{\text{res}}$ are found to be simply proportional to $E^{-1}$ in a very good approximation over a wide energy range. The $E^{-1}$ dependence, which is exact in the limit as $E\rightarrow 0$, is evidently due to the Coulomb peculiarity. In the study of e+ion scattering, the opacity sum $\Omega$ is often called collision strength, which reveals loose energy dependence if averaged over resonances [20,22].

![Graph showing the J dependence of the probabilities P^J_{\text{dire}}(t_f) and P^J_{\text{res}}(t_f) in the QM calculation at E=0.5 eV, and P^J_{\text{QC,dire}}(t_f) and P^J_{\text{QC, res}}(t_f) in the QC calculation [(N_r,N_f)=(40,5)] at E=0.5 eV.](image)

**FIG. 12.** J dependence of the probabilities $P^J_{\text{dire}}(t_f)$ and $P^J_{\text{res}}(t_f)$ in the QM calculation at $E=0.5$ eV, and $P^J_{\text{QC,dire}}(t_f)$ and $P^J_{\text{QC, res}}(t_f)$ in the QC calculation [(N_r,N_f)=(40,5)] at $E=0.5$ eV.

We can fit the direct and resonance capture cross sections in the form

$$\sigma_{\text{a.u.}} = \frac{C}{E},$$

(25)

The fitting parameter $C$ was determined from the QM ($E_c=0.5$ eV) and QC ($E_c=0.5$ eV) cross sections, and is shown in Table II. For the QM result, the cross section was calculated by assuming that $P^J=P^{08}$ for $J<8$. The error due to this substitution would not be so significant.

The direct and resonance capture cross sections calculated by the QC method and the fitting form (25) are drawn in Fig. 13. We can see that the cross sections are nicely approximated by the simple form (25) except at high energies. Also shown are the capture cross sections calculated by Cohen [8] using the FMD method. Although his results are for the radioactive isotope $^8$He$^+$, the isotope effect was found to be negligibly small for the capture. We see that the FMD method gives the cross sections too large compared with the present results except at high energies, and in addition the FMD results do not lie on a single curve $C/E$ even at very low energies. The classical treatment sometimes fails for the process having a small transition probability. In the $\bar{p}+H$ collision, the capture probabilities were close to unity in the

**TABLE II.** Fitting parameter $C$ in $\sigma_{\text{a.u.}}=C/E$ [eV].

<table>
<thead>
<tr>
<th></th>
<th>Direct</th>
<th>Resonance</th>
</tr>
</thead>
<tbody>
<tr>
<td>QM</td>
<td>0.844</td>
<td>1.896</td>
</tr>
<tr>
<td>QC</td>
<td>0.852</td>
<td>1.848</td>
</tr>
</tbody>
</table>

![Graph showing the cross section (a.u.) vs. E (eV) for QM and QC results.](image)

**FIG. 13.** Direct and resonance capture cross sections obtained by the QC calculation (closed circles) and the equation $C/E$ fitted to the QC result at $E=0.5$ eV (solid lines). The capture cross sections obtained by the FMD calculation of Cohen [8] and the curve $C/E$ fitted to the FMD result at $E=0.271$ eV (dashed line) are also shown.
important range of total angular momenta, and accordingly the FMD or classical trajectory Monte Carlo (CTMC) results would not have been so different from the QM results [2].

VIII. DISCUSSION AND FURTHER REMARKS

The adiabatic approximation has proved basically tolerable for the understanding of the main characteristic of the low energy \( \bar{p} + \text{He}^+ \) collision process. This conclusion was obtained for the \( \bar{p} + \text{H}_2^+ \) system [9]. Probably, the adiabatic approximation is better for \( \bar{p} + \text{H}_2^+ \) than for \( \bar{p} + \text{He}^+ \) because the electron can escape from \( \bar{p} \) by the H atom formation in \( \bar{p} + \text{H}_2^+ \). Under the adiabatic approximation, the rearrangement process \( \bar{p} + \text{H}_2^+ \rightarrow \bar{p}\text{H} + \text{H} \) could be treated in the same way as the conventional chemical reaction problems [10]. In this way, the adiabatic approximation is expected to work as a useful tool generally for the study of the \( \bar{p} + \text{ion} \) system. It should be remembered however that the nonadiabatic coupling is by no means negligible in the \( \bar{p} + \text{ion} \) system, and can generate an interesting dynamical process even at extremely low energies.

Here, we consider the iso electronic sequence of the present system, i.e., \( \bar{p} + \Lambda \rightleftharpoons Z \rightleftharpoons \Lambda + \text{e} \rightleftharpoons \text{e} \rightleftharpoons \Lambda \rightleftharpoons Z \rightleftharpoons \text{e} \rightleftharpoons \Lambda \rightleftharpoons \text{e} \rightleftharpoons \Lambda \rightleftharpoons Z \rightarrow \infty \). As shown in the appendix, the relative importance of the \( e \bar{p} \) interaction is measured by the factor \( Z^{-1} \). Using perturbation theory, we can see that the electronic excitation probability is proportional to \( Z^{-2} \) [23]. Therefore, as \( Z \) increases, the nonadiabatic transition is expected to occur less frequently. However, even if the nonadiabatic transition probabilities were very small, the capture cross section would diverge as \( E^{-1} \) in the limit as \( E \rightarrow 0 \) just due to the Coulomb peculiarity.

The fact that the Coulomb force dominates the dynamical process and further the non-adiabatic transition probability is small causes the resonance effect to be relatively significant in the capture process. The present QM and also QC methods were successful in indicating the importance of the resonances. It is further interesting to see the resonance profile and to know the branching ratio of the decay channels. However, the time-dependent wave-packet method would not be suitable for this purpose. Rather, a time-independent method might be more efficient. Considering the similarity to the \( e \bar{p} \) system and the nearly energy independence of the transition probabilities, we can expect that the \( R \) matrix method [24] is useful for the detailed study of the present resonance process. This study is now in progress.

From the reduction rate of \( P_{\text{res}}(t) \) plotted as a function of \( t \), we may calculate the decay rate \( \Gamma \) of the resonance state. Although this is a very crude estimate, we have \( \Gamma \approx 1 \times 10^6 \text{ sec}^{-1} \) for \( J = 25 \) from Fig. 11. When the energy is negative \( E = E_{\text{el}} < 0 \) (i.e., \( E_{\text{el}} < -2 \text{ a.u.} \)), the effective potential \( V_{\text{eff}}(R) \) can support bound states of \( \bar{p} + \text{He}^+ \), identified by the vibrational \( (v) \) and angular momentum \( (L) \) quantum numbers (cf., Fig. 2). Actually, these bound states are unstable against electron emission. We can roughly estimate the decay rate \( \Gamma_{\text{el}} \) of such unstable states by using the present results. Let \( \tau_{\text{el}} \) be the period of the \( \bar{p} - \text{He}^+ \) vibrational motion. If \( v \gg 1 \), noticing the energy independence of the ionization probability we may have \( \Gamma_{\text{el}} = I_{\text{dir}} \frac{1}{\tau_{\text{el}}} \approx 4P_{\text{dir}}(v + L + 1)^3 \times 10^{12} \text{ sec}^{-1} \), in which the pure Coulomb interaction has been assumed for the evaluation of \( \tau_{\text{el}} \). For instance, \( \Gamma_{\text{el}} \approx 4 \times 10^{11} \text{ sec}^{-1} \) for the state \( (v,L) = (70,30) \). If the energy \( E_{\text{ion}} \) of \( \bar{p} \text{He}^+ \) is above \( E_{\text{el}} \), the angular momentum change \( |\Delta L| \approx 1 \) is required for electron emission [5,6]. Such states have very long lifetimes [14], and as a consequence could be rather directly observed in experimental studies [7].

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APPENDIX: TIME-DEPENDENT SCHRODINGER EQUATION IN THE LIMIT OF INFINITE NUCLEAR CHARGE

We introduce the following scaled quantities:

\[ t' = Z^2 t, \]
\[ R' = ZR, \]
\[ r' = Zr, \]
\[ \bar{H}' = Z^2 \bar{H}. \]

The last implies that the energy is scaled as \( E' = E/Z^2 \). For heavy ions, we have practically \( m_e = 1 \) and \( m_p = m_\bar{p} \), where \( m_\bar{p} \) is the \( \bar{p} \) mass. Then, the time-dependent Schrödinger equation for \( \bar{p} + \Lambda \rightleftharpoons Z \rightleftharpoons \Lambda \rightleftharpoons Z \rightarrow \infty \) becomes

\[ i \frac{\partial}{\partial t'} \Psi_{\text{JM}(p)}(R',r',t') = \bar{H}' \Psi_{\text{JM}(p)}(R',r',t'), \]

with

\[ \bar{H}' = \bar{H}_p' + \bar{H}_e' + \frac{1}{Z^2 |R' - r'|}, \]

where

\[ \bar{H}_p' = -\frac{1}{2m_\bar{p}} \frac{\partial^2}{\partial R'^2} R' + \frac{\bar{L}^2}{2m_\bar{p} R'^2} - \frac{1}{R'} \]

is the same as the Hamiltonian for the \( \bar{p} + p \) system without a mass factor, and

\[ \bar{H}_e' = -\frac{1}{2r'} \frac{\partial^2}{\partial r'^2} r' + \frac{\bar{L}^2}{2r'^2} - \frac{1}{r'}, \]

is exactly the same as the Hamiltonian for the \( e + p \) system. In (A5), only the interaction between \( e \) and \( \bar{p} \) explicitly depends on \( Z \), and is proportional to \( Z^{-1} \).