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Near-threshold positron impact ionization of hydrogen

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Abstract

The hyperspherical hidden crossing method (HHCM) is used to investigate positron impact ionization of hydrogen near threshold. An important feature of this method is that it can provide valuable insight into scattering processes. In the calculation of positron–hydrogen ionization, the adiabatic Hamiltonian is expanded about the Wannier saddle point; anharmonic corrections are treated perturbatively. The S-wave results are consistent with the Wannier threshold law and with the extended threshold law that was previously derived using the HHCM. We have extended the previous HHCM calculation to higher angular momenta L and have calculated the absolute ionization cross-section for $L = 0$, 1 and 2. The HHCM calculation confirms that the S-wave ionization cross-section is small and provides the reason why it is small. The HHCM ionization cross-section (summed over the lowest partial waves) is compared with a convergent close-coupling calculation, a 33-state close-coupling calculation and experimental data.

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1. Introduction

The process of positron impact ionization of hydrogen near threshold is a particularly sensitive test of three-particle correlations. The cross-section for positron–hydrogen ionization has been measured in the energy range 15–700 eV [1]. Measurements close to threshold have been made for positron impact ionization of helium and molecular hydrogen [2,3].

Using a classical treatment, Wannier obtained a threshold law for the cross-section $\sigma(E)$ for electron impact ionization of neutral atoms:

$$\sigma(E) \propto E^{\zeta}, \tag{1}$$

where E is the excess energy and the exponent is 1.127 [4]. Klar extended Wannier's theory to positron impact ionization and showed that $\zeta = 2.65011$ [5]. The near threshold measurements of positron impact ionization [2] are in accord with the Wannier threshold law [5] in that the cross-section could be fitted to a power law, but the value of the exponent is smaller than predicted.

The near-threshold measurements for helium [2] have been interpreted by two different calculations. The first of these calculations was an extension of the Wannier threshold law to higher energies [6,7]. This extension was achieved by expanding the adiabatic Hamiltonian about the saddle point and using the hyperspherical hidden crossing method (HHCM) [8] to take into account perturbatively the correction terms. The calculation was limited to the S-wave, and the cross-section computed was relative. The second calculation was quantal-semiclassical [9] and stressed the importance of higher partial waves for interpreting the data.

The HHCM is ideally suited for treating the near-threshold region of positron–hydrogen ionization.

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Previously, the HHCM successfully described near-threshold electron impact ionization of hydrogen [8,10]. In addition, the method provided an explanation for the very small S-wave cross-section for ground-state positronium formation in positron–hydrogen collisions [11]. An important feature of the HHCM is that it does not suffer from overcompleteness, which can be a problem with standard close-coupling (CC) calculations that expand the wave function about both the target and positronium states. In addition, the HHCM does not yield ill-conditioned numerical equations, which is a problem with a full convergent close-coupling (CCC) calculation in the near-threshold region [12].

In this paper, we extend the earlier HHCM analysis of near-threshold positron–hydrogen ionization [6,7] to higher partial waves and to the calculation of the absolute ionization cross-section for total angular momentum $L = 0$, 1 and 2. In Section 2, we present the application of the HHCM to near-threshold positron–hydrogen ionization. In Section 3, we present our results and compare them with an S-wave model CCC calculation [12], a full CCC calculation [12], a 33-state CC calculation [13] and experimental data [1]. We give concluding remarks in Section 4. Atomic units are used throughout this paper.

2. Application of the HHCM to near-threshold positron–hydrogen ionization

2.1. Expansion of the eigenvalue $2R^2\varepsilon'(R)$

The HHCM [8] for positron–hydrogen collisions is formulated by using hyperspherical coordinates, which are the hyperradius $R = \sqrt{r_+^2 + r_-^2}$ and the two hyperangles $\alpha = \tan^{-1}(r_-/r_+)$ and $\theta = \cos^{-1}(\hat{\mathbf{r}}_+ \cdot \hat{\mathbf{r}}_-)$, where $\mathbf{r}_+$ and $\mathbf{r}_-$ are the position vectors of the positron and electron, respectively, relative to the proton [14]. The Schrödinger wave function ψ depends on R, α, θ and the three Euler angles $(\omega_1, \omega_2, \omega_3)$ which specify the orientation of the body fixed frame. The reduced wave function is defined as

$$\Psi(R,\Omega) = R^{5/2} \sin\alpha \cos\alpha \, \psi(R,\Omega), \tag{2}$$

where Ω represents the two hyperangles and the three Euler angles. The Schrödinger equation is expressed as

$$\left[-\frac{\partial^2}{\partial R^2} + \frac{\Lambda^2 + 2RC(\alpha,\theta)}{R^2} - 2E\right]\Psi(R,\Omega) = 0, \tag{3}$$

where Λ^2 is the grand angular momentum operator [14] and

$$C(\alpha,\theta) = \frac{1}{\cos\alpha} - \frac{1}{\sin\alpha} - \frac{1}{(1-\sin 2\alpha\cos\theta)^{1/2}} \tag{4}$$

is the reduced potential. The adiabatic Hamiltonian is $\frac{1}{2}[\Lambda^2 + 2RC(\alpha,\theta)]$. The adiabatic basis functions $\varphi_\mu(R;\Omega)$ are found by holding R fixed and solving

$$[\Lambda^2 + 2RC(\alpha,\theta)]\varphi_\mu(R;\Omega) = 2R^2\varepsilon_\mu(R)\varphi_\mu(R;\Omega). \tag{5}$$

The reduced potential $C(\alpha,\theta)$ has a saddle point at $(\alpha_0,\theta_0) = (0.4347, 0)$, corresponding to the collinear configuration of the proton, electron and positron in which the ratio of the lengths is $r_-/r_+ = 0.4643$. For ionization, the wave function is localized around the saddle point as $R \to \infty$.

We first obtain the expansion of the eigenvalue $2R^2\varepsilon(R)$ about the saddle point for $L = 0$. In this case since the grand angular momentum operator depends only on α and θ, Eq. (5) can be written as

$$\left[-\frac{\partial^2}{\partial\alpha^2} - \frac{1}{\sin^2\alpha\cos^2\alpha}\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}\right) + 2RC(\alpha,\theta)\right] \varphi_\mu(R;\alpha,\theta) = 2R^2\varepsilon'_\mu(R)\varphi_\mu(R;\alpha,\theta), \tag{6}$$

where

$$\varepsilon'_\mu(R) = \varepsilon_\mu(R) + \frac{1}{8R^2}. \tag{7}$$

We define coordinates $x = \alpha - \alpha_0$ and $y = \theta - \theta_0$ and expand the Hamiltonian about the point $(x,y) = (0,0)$:

$$\begin{aligned}&\left[-\frac{\partial^2}{\partial x^2} - \{B_0 - B_1 x + B_2 x^2 + \cdots\}\right. \\ &\times\left(\frac{\partial^2}{\partial y^2} + \left\{\frac{1}{y} - \frac{1}{3}y + \cdots\right\}\frac{\partial}{\partial y}\right) + 2R\{-C_{00} - C_{20}x^2 + C_{02}y^2 \\ &\left.+ C_{12}xy^2 - C_{30}x^3 + C_{22}x^2y^2 - C_{40}x^4 - C_{04}y^4 + \cdots\}\right] \\ &\times \varphi(R;x,y) = 2R^2\varepsilon'(R)\varphi(R;x,y),\end{aligned} \tag{8}$$

where the expansion coefficients B_j and C_{jk}, are defined by

$$B_j = \left|\frac{1}{j!}\left[\frac{d^j}{dx^j}\frac{1}{\sin^2(x+\alpha_0)\cos^2(x+\alpha_0)}\right]_{x=0}\right| \qquad j = 0,1,2, \tag{9}$$

and

$$C_{jk} = \left|\frac{1}{j!k!}\left[\frac{\partial^{j+k}}{\partial x^j \partial y^k}C(x+\alpha_0,y)\right]_{x=0,y=0}\right| \qquad j,k = 0,\cdots,4, \tag{10}$$

respectively.

Retaining only the lowest order terms gives a partial differential equation that is separable in x and y:

$$[p_x^2 - 2RC_{20}x^2 + B_0 p_y^2 + 2RC_{02}y^2 - 2RC_{00}]\varphi(R;x,y) = 2R^2\varepsilon'(R)\varphi(R;x,y), \tag{11}$$

where

$$p_x^2 = -\frac{\partial^2}{\partial x^2} \tag{12}$$

and

$$p_y^2 = -\left(\frac{\partial^2}{\partial y^2} + \frac{1}{y}\frac{\partial}{\partial y}\right). \tag{13}$$