Threshold law for ionization of atomic hydrogen by positron impact

N. C. Sil* and K. Roy
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India

(Received 12 February 1996)

The cross section σ for the positron-impact ionization of the hydrogen atom near threshold has been evaluated analytically with the final-state wave function involving three Coulomb functions. Contrary to the earlier result that σ vanishes exponentially, we find the threshold law as $\sigma \sim E^{3/2}$. [S1050-2947(96)08007-9]

PACS number(s): 34.80.Dp, 32.80.Fb

In a quantum-mechanical calculation the energy dependence of the cross section σ for the positron-impact ionization of hydrogen atoms near threshold is determined to a large extent, only by the form of the final-state wave function used to calculate the transition matrix element. With one attractive Coulomb function corresponding to full screening of the target nuclear charge, one gets identical results for electron and positron impact in which σ varies as $E^{3/2}$. For positron-impact ionization with two Coulomb functions, one attractive and the other repulsive, Geltman [1] gets a very unphysical result; the cross section is almost insignificant over a considerable portion of the energy interval near the threshold due to the normalization constant vanishing exponentially. The phase condition [2] of the final-state wave function in the asymptotic region, where both the positron and the electron are far from the nucleus as well as from each other, is satisfied in neither of these two cases of full screening and no screening. On the basis of Coulomb dipole theory, Temkin [3] obtained a modulated linear law for threshold ionization cross section by positron impact.

In recent years a final-state wave function with three Coulomb functions that is asymptotically correct has been extensively used to calculate electron- and positron-impact ionization of atoms [4,5], and the results thus obtained are in good agreement with the experimental data at intermediate and high energies. Here, one of these three Coulomb functions is always repulsive and therefore according to Brauner *et al.* [6] the use of the three Coulomb function final state for the calculation of the ionization cross section near threshold would lead to unphysical results due to the exponential vanishing of the normalization constant.

In the present work we present the detailed evaluation of the matrix element for positron-impact ionization of atomic hydrogen near threshold with the above three Coulomb final-state wave functions to show how the exponentially vanishing normalization factor due to the repulsive positron-proton interaction is appropriately compensated for and a physical threshold law, $\sigma \sim E^{3/2}$ is obtained. For electron-impact ionization near threshold the Wannier model [7] based on the classical theory, which gives a threshold law $\sigma \sim E^{1.127}$ for atomic hydrogen is, in general, considered to be more or less satisfactory. A quantum-mechanical extension of this model was attempted by Peterkop [8], Rau [9], and others. Klar [10] has extended the Wannier model to positron-impact ionization and obtained analytically a threshold law $\sigma \sim E^{2.65}$ for the hydrogen atom. Modification of the Wannier threshold law for small but finite energy excess above the threshold has been considered by Kazansky, Ostrovsky, and Sergeeva [11]. For positron impact the Wannier threshold law is rather controversial. Dimitrijević and Grujić [12] have obtained a threshold law $\sigma \sim E^{1.64}$ for positron-impact ionization of the hydrogen atom by their classical trajectory study. The classical trajectory Monte Carlo calculations of Wetmore and Olson [13], on the other hand, agree with the power law $\sigma \sim E^{3.01}$.

The total cross section in atomic units for positron impact ionization of the hydrogen atom may be written as

$$\sigma = (1/k) \int \int |M|^2 d\vec{k}_1 d\vec{k}_2 \delta(E - k_1^2/2 - k_2^2/2), \qquad (1)$$

where M, the matrix element at threshold, is given by

$$M = (4\pi^3 k_1 k_2 k_{12})^{-1/2} \exp(-\pi\alpha_1) I, \qquad (2)$$

with

$$I = \int \exp(i\vec{k}_0 \cdot \vec{r}_1 - \lambda r_2)(1/r_1 - 1/r_{12}) \exp(-i\vec{k}_1 \cdot \vec{r}_1 - i\vec{k}_2 \cdot \vec{r}_2)\, {}_1F_1(-i\alpha_1; 1; i(k_1 r_1 + \vec{k}_1 \cdot \vec{r}_1))$$
$$\times {}_1F_1(i\alpha_2; 1; i(k_2 r_2 + \vec{k}_2 \cdot \vec{r}_2))\, {}_1F_1(i\alpha_3; 1; i(q r_{12} + \vec{q} \cdot \vec{r}_{12})) d\vec{r}_1 d\vec{r}_2, \qquad (3)$$

*Electronic address: tpkr@iacs.ernet.in

$\vec{r}_1$ ($\vec{r}_2$) and $\vec{k}_1$ ($\vec{k}_2$) are, respectively, the position vector and momentum of the positron (electron), $\vec{k}_0$ is the incident momentum, $k_0=1$ at threshold; $\lambda=1$, $\alpha_1=1/k_1$, $\alpha_2=1/k_2$, $\alpha_3=1/k_{12}$, $\vec{q}=(\vec{k}_1-\vec{k}_2)/2$. Making use of the contour integral representation [14]

$$_1F_1(i\alpha;1;z)=(1/2\pi i)\int \exp(zt)p(\alpha,t)dt,$$

wherein

$$p(\alpha,t)=t^{-1+i\alpha}(t-1)^{-i\alpha},$$

and the Fourier transformation technique we can write

$$I=\lim_{\substack{\mu\to 0\\ \eta\to 0}}\left(-\frac{\delta}{\delta\lambda}\right)\left[\left(-\frac{\delta}{\delta\mu}\right)+\left(\frac{\delta}{\delta\eta}\right)\right] \times[1/(2\pi i)^3]\int\int\int dt_1dt_2dt_3p(-\alpha_1,t_1) \times p(\alpha_2,t_2)p(\alpha_3,t_3)J, \tag{4}$$

where

$$J=8\int d\vec{P}([(\vec{P}-\vec{q}t_3)^2+(\eta-iqt_3)^2]\{[\vec{P}+\vec{k}_0-\vec{k}_1(1-t_1)]^2 +(\mu-ik_1t_1)^2\}\{[\vec{P}+\vec{k}_2(1-t_2)]^2+(\lambda-ik_2t_2)^2\})^{-1}. \tag{5}$$

On carrying out the contour integrations with respect to t_1, t_2, t_3 and differentiating with respect to λ,μ,η we get

$$I=64\int d\vec{P}(P^2+i\vec{P}\cdot\hat{\vec{k}}_2+\vec{P}\cdot\vec{k}_2)[(\vec{P}+\vec{k}_2)^2+\lambda^2]^{-2+i\alpha_2}[P^2+(\lambda-ik_2)^2]^{-1-i\alpha_2}[(\vec{P}+\vec{k}_0-\vec{k}_1)^2]^{-1-i\alpha_1}[P]^{-1+i\alpha_3}(\alpha_1k_1) \times[(\vec{P}+\vec{k}_0)^2-k_1^2-i0_+]^{-1+i\alpha_1}[(\vec{P}-\vec{q})^2-q^2-i0_+]^{-i\alpha_3}+(\alpha_3q)[(\vec{P}+\vec{k}_0)^2-k_1^2-i0_+]^{i\alpha_1} \times[(\vec{P}-\vec{q})^2-q^2-i0_+]^{-1+i\alpha_3}. \tag{6}$$

Let us now put $\vec{p}=\vec{P}+\vec{k}_0-\vec{k}_1$, then

$$(\vec{P}+\vec{k}_0)^2-k_1^2-i0_+=p(p-X-i0_+),$$

where $X=-2\vec{k}_1\cdot\hat{\vec{p}}$.

In the very small region where $p<X$, on account of the negative imaginary infinitesimal phase $-i0_+$, we have

$$[(\vec{P}+\vec{k}_0)^2-k_1^2-i0_+]^{-n+i\alpha_1} =(-1)^n\exp(\pi\alpha_1)p^{-n+i\alpha_1}(X-p)^{-n+i\alpha_1}.$$

Evidently the contribution from this region only to the integral in Eq. (6) is significant since the effect of the vanishingly small normalization factor $\exp(-\pi\alpha_1)$ in Eq. (2) is compensated for. Over this very small region $P^2\approx k_0^2$ and $\vec{P}\cdot\hat{\vec{k}}_2\approx-\vec{k}_0\cdot\hat{\vec{k}}_2$, etc. Thus considering only the dominant contribution we get after integration over the azimuthal angle

$$I=(8\pi/k_1)(1-i\hat{\vec{k}}_0\cdot\hat{\vec{k}}_2)\exp(-1-iC+\pi\alpha_1) \times\int_{\varepsilon_2}^{2k_1}dp\,p^{-1-i\alpha_1}\int_{p+\varepsilon_1}^{2k_1}(X-p)^{-1+i\alpha_1}dX, \tag{7}$$

where $C=\hat{\vec{k}}_0\cdot\hat{\vec{k}}_2+\hat{\vec{k}}_0\cdot\hat{\vec{q}}$. We next perform the integration with respect to X. In view of the fact that

$$\lim_{\varepsilon_2\to 0_+}\int_{\varepsilon_2}^{2k_1}p^{-1-i\alpha_1}(2k_1-p)^{i\alpha_1}dp=B(-i\alpha_1,1+i\alpha_1),$$

which is proportional to $\exp(-\pi\alpha_1)$, we have

$$I=(8\pi/\alpha_1)(1-i\hat{\vec{k}}_0\cdot\hat{\vec{k}}_2)\exp(\pi\alpha_1) \times[(\varepsilon_1/2k_1)^{i\alpha_1}-(\varepsilon_1/\varepsilon_2)^{i\alpha_1}]. \tag{8}$$

The matrix element M is now obtained by the substitution of Eq. (8) into Eq. (2) and finally after carrying out the integrations in Eq. (1) we get

$$\sigma=3^{-1}\pi 2^{12}\exp(-2)(2^{1/2}-1)E^{3/2}. \tag{9}$$

The experimental value [15] of σ at $E=1.4$ eV, the lowest energy known to us, is 1.8×10^{-17} cm^2 (from graph), while our calculation gives 7.8×10^{-17} cm^2. No other theoretical value is available at such a low energy to our knowledge. It should be noted that the Wannier law does not give the absolute magnitude of the cross section, which is required for a quantitative comparison with experiment. Precise measurement of the ionization cross section very close to the threshold is urgently required for a comparison with the theoretical prediction.

[1] S. Geltman, J. Phys. B **16**, L525 (1983).
[2] M. R. H. Rudge and M. J. Seaton, Proc. R. Soc. London Ser. A **83**, 262 (1965).
[3] A. Temkin, Phys. Rev. Lett. **49**, 366 (1982).
[4] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[5] A. Bandyopadhyay, K. Roy, P. Mandal, and N. C. Sil, J. Phys. B **27**, 4337 (1994).
[6] M. Brauner, J. S. Briggs, H. Klar, J. T. Board, T. Rosel, K. Jung, and H. Ehrhardt, J. Phys. B **24**, 657 (1991).
[7] G. Wannier, Phys. Rev. **90**, 817 (1953).
[8] R. Peterkop, J. Phys. B **4**, 513 (1971).
[9] A. R. P. Rau, Phys. Rev. A **4**, 207 (1971).
[10] H. Klar, J. Phys. B **14**, 4165 (1981).
[11] A. K. Kazansky, V. N. Ostrovsky, and L. Yu. Sergeeva, Z. Phys. D **33**, 181 (1995).
[12] M. S. Dimitrijević and P. V. Grujić, J. Phys. B **16**, 297 (1983).
[13] A. E. Wetmore and R. E. Olson, Phys. Rev. A **34**, 2822 (1986).
[14] A. Nordsieck, Phys. Rev. **93**, 785 (1954).
[15] G. O. Jones, M. Charlton, J. Slevin, G. Laricchia, A. Kover, M. R. Poulsen, and S. N. Chormaic, J. Phys. B **26**, L483 (1993).