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Classical radiative electron capture by a proton

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Abstract. Partial radiative capture cross sections for very low energy (<100 eV) electrons and protons are calculated via the classical method of Fourier components. Comparisons of these cross sections are made with quantum mechanical calculations.

1. Introduction

The process of radiative electron capture by protons is important in interstellar H II regions. In these nebulae surrounding very hot stars ionised hydrogen atoms are continuously recombining. The temperatures of these clouds are of the order of 10 000 K and correspond to free-electron kinetic energies of about 1 eV.

A quantum mechanical study of this process was recently reported by Fazio and Copeland (1985). Among other results reported were partial cross sections for the capture of these very low energy electrons. For any specified state of principal quantum number n and for energies greater than 15 eV recombination into s states is preferred and cross sections decrease with increasing angular momentum. At energies below 15 eV, however, this 'normal' ordering changes. Recombination into s states is least preferred while states of higher angular momentum have greater cross sections. When plotted as a function of the kinetic energy of the incoming electron the cross section curves cross each other (see figure 1), and total reversal occurs at lower energies for higher n. This crossing behaviour was thought to be due to specific relationships between the bound-excited and free-state radial wavefunctions and substantiating evidence, in the form of matrix elements and transition strengths, was presented.

It is the purpose of this paper to examine the process of radiative electron capture—also known as radiative recombination—from a classical perspective in order to further substantiate the view that the curve crossings discussed above cannot be attributed to classical physics.

The classical electron capture problem is treated by the method of Fourier components. The initial state of the free electron is described by a Keplerian orbit and the Fourier transform of the acceleration gives the frequency of the emitted radiation. For a historical perspective the reader is referred to Kramers (1923) where the state of the free electron is described by a parabolic orbit ($\varepsilon = 1$), the shortest distance between the electron and the nucleus is required to be $\frac{1}{2}$ and the angular momentum mvb is set equal to m. Calculations for cross section are performed in two approximations—one for high energy and one for low.

In the treatment that follows the free electron is described by a hyperbolic orbit ($\varepsilon > 1$). This allows specification of the angular momentum, in addition to the energy

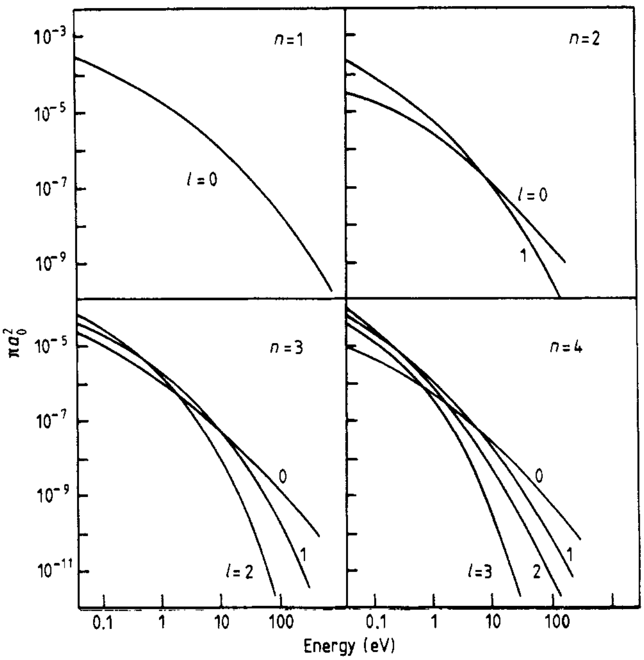

Figure 1. The quantum mechanical partial cross sections for radiative capture of an electron into all angular momentum states through $n = 4$.

of the incoming electron. No energy approximations are made and calculations of the Fourier components are done numerically.

2. Procedure

An electron incident on a proton describes an orbit that is the shape of a conic section. If the electron is not bound to the proton the orbit is in the shape of a parabola or hyperbola.

The formula relating eccentricity of the orbit (ε) to the energy and angular momentum of the system is

$$\varepsilon = [1 + (2EL^2/mK^2)]^{1/2} \tag{1}$$

where E is the total energy of the system (in this case the kinetic energy of the incoming electron), L is the angular momentum (mvb), m is the reduced mass of the system and K is the square of e.

The angle θ locates the electron from the positive x axis and the position of the electron is given by

$$\bar{r} = L^2\hat{r}/mK(1 + \varepsilon \cos\theta). \tag{2}$$

When $\theta = 0$ the electron is at the point of closest approach and when the angle $\theta = \theta_0 = \cos^{-1}(-1/\varepsilon)$ the electron is infinitely far away (see figure 2). From the law of conservation of angular momentum:

$$L = mr^2\, \mathrm{d}\theta/\mathrm{d}t$$

where time t can be expressed as a function of the angular position θ. After a change

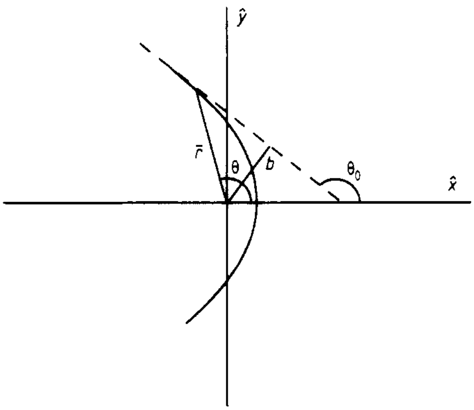

Figure 2. A hyperbolic orbit is presented. The electron is located by r and θ. The angle θ_0 locates the electron when it is infinitely far away and at the angle $\theta=0$ the electron is at the point of closest approach. The angular momentum of the incoming electron is mvb where b is the impact parameter.

of variables where $\tan(\theta/2)$ is set equal to x,

$$t=\frac{a_0L^3}{\alpha c\hbar^3(\varepsilon^2-1)^{3/2}}\left(\frac{2\varepsilon x_0x}{x_0^2-x^2}+\ln\left|\frac{x-x_0}{x+x_0}\right|\right).$$

Time t is zero at $\theta=0$. Therefore, at $t=-\infty$ the electron is located by the angle $\theta_0=\cos^{-1}(-1/\varepsilon)$ or by $x_0=\tan(\theta/2)$ and at $t=\infty$ by $-x_0$. The value of x_0 can be related to the eccentricity of the orbit: $x_0=((\varepsilon+1)/(\varepsilon-1))^{1/2}$.

The acceleration of the electron,

$$\bar{a}=e^2\hat{r}/mr^2$$

can be resolved into components parallel and perpendicular to the x axis: $a_{\parallel}=a\cos\theta$ and $a_{\perp}=a\sin\theta$. By writing the sine and cosine terms as functions of the variable x the components of acceleration can be written as

$$a_{\parallel}=a(1-x^2)/(1+x^2) \qquad a_{\perp}=2ax/(1+x^2)$$

where

$$a=e^2/mr^2=e^6(1+\varepsilon\cos\theta)^2/L^4$$
$$=\frac{\hbar^4(\alpha c)^2(\varepsilon-1)^2(x_0^2-x^2)}{a_0L^4(1+x^2)^2}.$$

The Fourier sine and cosine transforms can now be written:

$$\phi(\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}a_{\perp}\sin(\omega t)\,\mathrm{d}t=\frac{4\hbar^2c}{L^2}\int_{-x_0}^{x_0}\frac{\mathrm{d}x\,x\sin(\omega t)}{(1+x^2)^2}$$

and

$$\psi(\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}a_{\parallel}\cos(\omega t)\,\mathrm{d}t=\frac{2\hbar^2c}{L^2}\int_{-x_0}^{x_0}\frac{\mathrm{d}x\,(1-x^2)\cos(\omega t)}{(1+x^2)^2}.$$

It can be seen that as $x\to x_0$ ($\theta\to\theta_0$) the arguments of the sine and cosine functions grow rapidly, yielding negligible contributions to the integral near x_0. Hyperbolic and elliptical orbits of the same angular momenta (see equations (1) and (2)) are strikingly similar when $\theta < \theta_0$, especially when comparing more eccentric elliptical orbits ($\varepsilon \to 1$) with low energy hyperbolic orbits ($\varepsilon \to 1$). Thus, in the low energy region this classical approximation should yield fairly accurate results.

The cross section formula for the radiative capture of an electron into a bound state described by principal quantum number n and angular momentum quantum number l, in terms of these Fourier components, can now be derived. It is assumed that an electron will be captured into a state with principal quantum number n if its energy puts it in the range of $-Ry/(n+\frac{1}{2})^2$ and $-Ry/(n-\frac{1}{2})^2$. Electromagnetic energy with a frequency interval $d\omega$ will then be emitted. From the energy radiated per unit time (Jackson 1975, p 659)

$$dR/dt = 2e^2\bar{a}\cdot\bar{a}/3c^3$$

it can be written that

$$R = \frac{2e^2}{3c^3}\int (a_{\parallel}^2 + a_{\perp}^2)\,dt$$

or in terms of the Fourier components as

$$R = \frac{2e^2}{3c^3}\int [\phi(\omega)^2 + \psi(\omega)^2]\,d\omega.$$

From this formula the relative amount of radiated energy which lies between ω and $\omega + d\omega$ can be identified as

$$P(\omega) = \tfrac{1}{3}[\phi(\omega)^2 + \psi(\omega)^2].$$

The cross section for capture into a state of principal quantum number n is

$$\sigma_n = 2\pi\int_0^{\infty} q_n r\,dr$$

where the probability that a free electron of kinetic energy ke will be bound to the nth quantum state is q_n:

$$q_n = \frac{2^5\pi\alpha^4\hbar c P(\omega) n^3}{a_0 L^2(n^2 ke + Ry)(4n^2-1)^2}.$$

The frequency of the emitted radiation is related to the bound state and the free-electron energy by

$$\omega = \frac{1}{\hbar}\left(ke + \frac{Ry}{n^2}\right).$$

This cross section formula is for capture into a state described by the principal quantum number n and the integration limits include all possible angular momenta of the incoming electron. With the assumption that electrons having angular momentum $L = [l(l+1)]^{1/2}\hbar$ are captured into states with angular momentum quantum number l if their initial values lie between $l-\frac{1}{2}$ and $l+\frac{1}{2}$ the partial cross section formula is written

$$\sigma_{nl} = \frac{2^5\pi^2\alpha^5\hbar^2c^2n^3}{ke(4n^2-1)^2(n^2ke+Ry)}\int_{l-\frac{1}{2}}^{l+\frac{1}{2}} \frac{P(n,l)\,dl}{l}.$$

$P(n, l)$ is almost constant over the range of integration and little accuracy is lost by treating it as such; therefore, it can be brought outside the integral and the partial

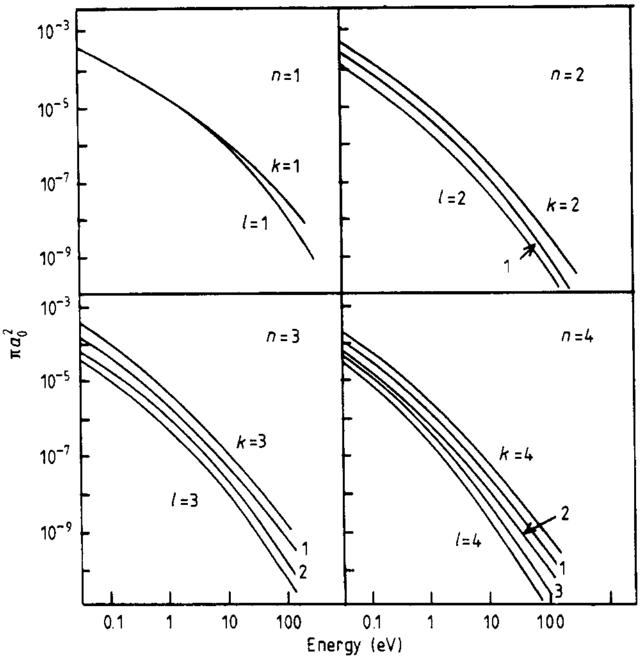

Figure 3. The classical cross sections for the capture of an electron into all angular momentum states through $n=4$. The curves $K=1$ through 4 are total cross sections for the special case of a parabola.

cross section formula (in units of πa_0^2) is

$$\sigma_{nl} = 2^5 \pi \alpha^5 \left(\frac{\hbar c}{a_0}\right)^2 \frac{n^3 P(n, l)}{ke(4n^2-1)^2(n^2 ke + Ry)} \ln \left|\frac{2l+1}{2l-1}\right|.$$

The partial cross sections for capture into all angular momentum states through $n=4$ are plotted in figure 3 along with the total cross sections for the special case of the parabolas that were calculated from Kramers' (1923) formulae.

3. Discussion

For very low kinetic energy electrons the total cross sections ($\Sigma_l \sigma_{nl} = \sigma_n$) calculated from this work agree with the total quantum mechanical cross sections and those calculated by Kramers (1923). At energies near 100 eV, however, the cross sections deviate by as much as 50% from the other two (which remain in agreement). This was not totally unexpected because electrons in hyperbolic orbits with large energies did not fall within the limits of the approximation.

The classical cross section curves for different angular momenta l of the same principal quantum state do not cross each other—or even hint at such behaviour. At all energies, capture into the lowest angular momentum state is most probable and the probability of capture decreases with increasing angular momentum and/or energy.

The best correlation between the quantum mechanical cross sections (see figure 1) and the classical cross sections (see figure 3) is for the ground state. For the excited states correspondence is good for higher angular momentum states but poor for the low. This deviation was expected since the crossing of the quantum mechanical curves was thought to be due to the wave relationship between the lower angular momentum bound-excited states and the free states with one angular momentum unit more. The quantum mechanical cross sections are large if the initial free state wavefunction and final bound state wavefunction have a large overlap. This is true, in general, at low energies. As the kinetic energy of the free electron increases the free state wavefunction contracts; positive and negative contributions to the radial integral cancel causing the matrix elements to decrease in value. Thus, the matrix elements have a maximum absolute value at zero energy of the free electron and decrease as energy increases. This general behaviour is modified by including information on angular momentum. Low angular momentum wavefunctions have values near the origin, while states of higher angular momentum are excluded further and further from the origin. Since the bound state wavefunctions are localised around the origin—especially zero angular momentum states—and the free state is not, low angular momentum bound states and free states with larger angular momentum values will produce smaller overlaps. The value of this overlap will decrease with decreasing energy because the amplitude of the free state wavefunction increases more rapidly with r for low energies than for high (Bethe and Salpeter 1977). Thus, the general behaviour of the cross section is modified, the most pronounced effect being on the cross sections for capture into zero angular momentum states. The result is that the curves for zero angular momentum cross under the other quantum mechanical curves and ultimately the cross section curves reverse order completely.

4. Conclusion

In this paper the classical partial cross section curves for the radiative capture of a low energy electron by a proton were calculated. The method of Fourier components was employed and integration was done numerically. The classical partial cross section curves do not cross and correlation between the quantum mechanical and the classical cross sections is poorest for low angular momentum recombinations. Since it is these very recombinations that are responsible for the crossing of the quantum mechanical curves the explanation seems to depend on the wave relationship between the free and the bound state. Therefore, it can be concluded that the reversal of the order of the radiative recombination cross sections presented by Fazio and Copeland (1985) is a result of the wave nature of the system and can be explained only in the realm of quantum mechanics.

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