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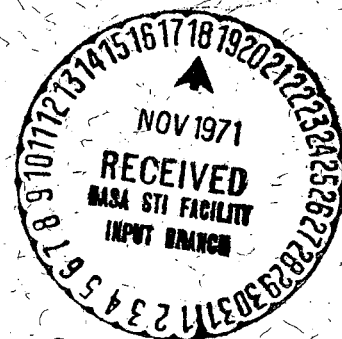
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COLLISIONAL EXCITATION OF THE HIGHLY EXCITED HYDROGEN ATOMS IN THE DIPOLE FORM OF THE SEMI CLASSICAL IMPACT PARAMETER AND BORN APPROXIMATIONS

KAZEM OMIDVAR

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COLLISIONAL EXCITATION OF THE HIGHLY
EXCITED HYDROGEN ATOMS IN THE
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Kazem Omidvar

Laboratory for Space Physics
NASA, Goddard Space Flight Center
Greenbelt, Maryland 20771

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ABSTRACT

Expressions for the excitation cross section of the highly excited states of the hydrogenlike atoms by fast charged particles have been derived in the dipole approximation of the semi classical impact parameter and the Born approximations, making use of a formula for the asymptotic expansion of the oscillator strength of the hydrogenlike atoms given by Menzel. When only the leading term in the asymptotic expansion is retained, the expression for the cross section becomes identical to the expression obtained by the method of the classical collision and correspondence principle given by Percival and Richards. Comparisons are made between the Bethe coefficients obtained here and the Bethe coefficients of the Born approximation for transitions where the Born calculation is available. Satisfactory agreement is obtained only for $n \rightarrow n + 1$ transitions, with n the principal quantum number of the excited state.

I. INTRODUCTION

A knowledge of accurate values for the excitation cross section of highly excited states of the hydrogenlike atoms by electron impact is necessary in order to understand the conditions under which the observed radio frequency transitions between the highly excited states of these atoms in the interstellar ionized region, or similar processes in the solar corona, take places. Using the classical collisions and the correspondence principle Percival and Richards (1970) give an expression for the excitation cross section valid for high impact energies. Similar expression is given by Presnyakov and Urnov (1970) making use of the impact parameter approximation and an atomic model based on an harmonic oscillator.

The work that is being reported here gives solution of the same problem in the dipole approximation of the semi classical impact parameter and Born approximations, making use of the asymptotic expansion of the hydrogenlike oscillator strength given by Menzel (1968, 1969). The results of the calculation are checked against the results of the Born approximation.

In collisional excitation the Born approximation becomes valid when the incident energy is some 50 times larger than the excitation energy. The Born

cross section then should not differ from the actual cross section by more than a few percent. In low impact energy excitation of highly excited states of atoms another consideration should be taken into account. Due to the closeness of their energy levels, many excitation channels are strongly coupled to each other, and validity of a two channel approximation such as the Born approximation becomes questionable (Seaton, private communication).

Nevertheless, here we assume the validity of the Born approximation at high impact energies, and compare the results of the dipole approximation, itself an approximation to the Born approximation, with the results of the full Born approximation. Instead of comparing the cross sectional values for the two approximations, it is more convenient and more useful to compare the corresponding Bethe coefficients which are independent of the mass, charge, and energy of the projectile. In Table I this comparison has been made.

We have also shown that when the leading term in the expansion of the oscillator strength is retained, the result of the impact parameter dipole approximation becomes identical to the result of the classical collision and correspondence principle method given by Percival and Richards.

II. FORMULATION AND RESULTS

Let n be the initial and n' the final principal quantum numbers of a hydrogen-like atom with atomic number Z in collision with a charged particle with charge $Z'e$, e being the absolute value of the electronic charge. According to the dipole form of the semi classical impact parameter method the excitation cross section

between these two levels is given by (Seaton, 1962)

$$\sigma(n \rightarrow n') = 2\pi \int_{b_{\min}}^{\infty} p(n \rightarrow n') b db \quad (1)$$

where b is the impact parameter and

$$p(n \rightarrow n') = \frac{(Z'e^2)^2}{3\hbar^2} |\langle n' | \underset{\sim}{r} | n \rangle|^2 \times \frac{4}{b^2} \frac{M}{m_e} \frac{Ry}{E} \frac{\hbar^2}{e^4} f\left(\frac{b\Delta E}{\hbar V}\right) \quad (2)$$

with $\underset{\sim}{r}$ the position vector of the bound electron, M , E , and V the reduced mass, the relative energy, and the relative velocity of the system, m_e the electronic mass, and ΔE the excitation energy. The function $f(x)$ is defined by

$$f(x) = x^2 [K_0^2(x) + K_1^2(x)] \quad (3)$$

where $K_0(x)$ and $K_1(x)$ are modified Bessel functions.

The matrix in (2) represents the expectation value of $\underset{\sim}{r}$ between sub-levels of n and n' , averaged with respect to the initial states and summed with respect to the final states, namely

$$|\langle n' | \underset{\sim}{r} | n \rangle|^2 = \frac{1}{n^2} \sum_{\ell m} \sum_{\ell' m'} |\langle n' \ell' m' | \underset{\sim}{r} | n \ell m \rangle|^2 \quad (4)$$

where $\ell \ell'$ and mm' are the azimuthal and magnetic quantum numbers.

Introducing s by $s = n' - n$ then for both n and n' large and s small the matrix in (4) is given by (Menzel 1968, 1969)

$$|\langle n' | \tilde{r} | n \rangle|^2 = \frac{3}{2} a^2 \left(1 + \frac{s}{n}\right) \times \frac{4}{3s^3} J_s(s) J'_s(s) g(s), \quad g(s) = 1 + \frac{1.5s}{n} + \frac{A(s)}{n^2} \quad (5)$$

where $a = n^2 a_0/Z$ is the atomic radius before excitation and a_0 the Bohr radius. $J_s(s)$ is the Bessel function of equal order and argument and $J'_s(s)$ is the first derivative with respect to the argument. $A(s)$ are constants of order of unity given by Menzel (1969). Substitution of (5) into (2) gives

$$p(n \rightarrow n') = Z'^2 \frac{M}{m_e} \left(1 + \frac{s}{n}\right) \frac{4}{3s^3} J_s(s) J'_s(s) g(s) \frac{2 Ry}{E} \frac{a^2}{b^2} f\left(\frac{b\Delta E}{\hbar V}\right) \quad (6)$$

To evaluate the cross section given by (1) we choose b_{\min} to be equal to a . A different choice for b_{\min} and of the same order of magnitude as a makes little difference in the high energy values of the cross section. Making use of a formula for an integral over the squared of the Bessel's functions (Morse and Feshbach, 1953) we obtain the following expression for the cross section

$$\frac{\sigma(n \rightarrow n')}{\pi a_0^2} = \frac{16 Z'^2 M Ry}{3Z^2 m_e E} n^4 \left(1 + \frac{s}{n}\right) \frac{J_s(s) J'_s(s)}{s^3} g(s) \left(\frac{a\Delta E}{\hbar V}\right) K_0\left(\frac{a\Delta E}{\hbar V}\right) K_1\left(\frac{a\Delta E}{\hbar V}\right) \quad (7)$$

By putting $g(s) = 1$ Equation (7) becomes identical to the expression for the cross section given by Percival and Richards (the right hand side of their expression should be multiplied by a factor of n^4). Since the impact parameter

method is valid when the incident momentum is much larger than the momentum of the orbiting electrons, and the dipole approximation is valid when the momentum transferred to the atom is small, we conclude that the results of Percival and Richards are also valid under the same conditions and provided $n \gg 1$.

Making use of the relation

$$\left(\frac{a \Delta E}{\hbar V}\right)^2 = \frac{M a^2 \Delta E^2}{4 m_e a_0^2 \text{Ry} E} \quad (8)$$

and the validity criteria for the impact parameter method and the dipole approximation it can be seen that $a \Delta E / (\hbar V) \ll 1$ always, except for the rare occasion that the incident velocity is much less than the orbital velocity. Then an expansion of the modified Bessel functions in (7) about the origin, as has been done by Percival and Richards, is permissible and will yield

$$\frac{\sigma(n \rightarrow n')}{\pi a_0^2} = \frac{8 Z'^2 M \text{Ry}}{3 Z^2 m_e E} n^4 \left(1 + \frac{s}{n}\right) \frac{J_s(s) J'_s(s)}{s^3} g(s) \ell_n \left(5.04 \frac{m_e a_0^2 \text{Ry} E}{M a^2 \Delta E^2}\right). \quad (9)$$

It should be emphasized that for the range of the incident energy that (7) is valid, (9) can be used instead (Percival and Richards have a factor of 4.5 instead of the factor of 5.04 in (9). The reason for this discrepancy is not understood).

To show more clearly the dependence of the cross section on the impact energy it is convenient to write (9) in the form

$$\frac{\sigma(n \rightarrow n')}{\pi a_0^2} = \frac{Z'^2 M Ry}{Z^2 m_e E} \left[A(n, n') \ell_n \left(\frac{m_e E}{M Z^2 Ry} \right) + B(n, n') \right] \quad (10a)$$

where $A(n, n')$ and $B(n, n')$ are pure numbers depending on n and n' only and are given by

$$A(n, n') = \frac{8}{3} n^4 \left(1 + \frac{s}{n} \right) s^{-3} J_s(s) J'_s(s) g(s),$$

$$B(n, n') = A(n, n') \ell_n [5.04 (1 - n^2/n'^2)^{-2}]. \quad (10b)$$

A numerical table for $M(s) = 4/3 s^{-2} J_s(s) J'_s(s)$ is given by Menzel (1969).

Similarly, the numerical values of $g(s)$ defined by (5) can be obtained using this reference.

To derive the dipole form of the Born approximation we start with the expression for the Born approximation given by

$$\sigma^B(n \rightarrow n') = \frac{8\pi}{E/Ry} \frac{M}{m_e} Z'^2 \int_{k_1 - k_2}^{k_1 + k_2} |\langle n' | e^{i\mathbf{q}' \cdot \mathbf{r}} | n \rangle|^2 \frac{dq}{q^3} \quad (11)$$

with k_1 the wave number of the relative motion before collision related to E by

$$k_1^2 = a_0^{-2} (M/m_e) (E/Ry), \quad (12)$$

and k_2 the wave number of the relative motion after collision related to k_1 by

$$k_1^2 - k_2^2 = a_0^{-2} (M/m_e) (\Delta E/Ry), \quad (13)$$

and \tilde{q} the momentum transfer between the particles. The matrix in (11) in analogy to (4) is defined by

$$|\langle n' | e^{i\tilde{q} \cdot \tilde{r}} | n \rangle|^2 = \frac{1}{n^2} \sum_{\ell m} \sum_{\ell' m'} |\langle n' \ell' m' | e^{i\tilde{q} \cdot \tilde{r}} | n \ell m \rangle|^2 \quad (14)$$

with $\ell m \ell' m'$ defined before.

When $a_0^2 k_1^2 \gg (M/m_e) (\Delta E/Ry)$ we have from (12), up to the first order terms,

$$k_1 - k_2 \cong [M/(2m_e a_0^2 k_1)] \Delta E/Ry, \quad k_1 + k_2 \cong 2k_1. \quad (15)$$

The radial part of the integral $\langle n' | \exp(i\tilde{q} \cdot \tilde{r}) | n \rangle$ decreases exponentially when $|\tilde{r}|$ becomes greater than the atomic radius $a = n^2 a_0/Z$. Following Bethe (1930) we expand $\exp(i\tilde{q} \cdot \tilde{r})$ under the integral sign and introduce a parameter q_0 such that

$$[M/(2m_e a_0^2 k_1)] \Delta E/Ry \ll q_0 \ll Z/(n^2 a_0), \quad (16)$$

then (11) can be written in the form

$$\sigma^B(n \rightarrow n') = \frac{8\pi}{E/Ry} \frac{M}{m_e} Z'^2 \left[\frac{1}{3} |\langle n' | \tilde{r} | n \rangle|^2 \ell n \frac{2m_e a_0^2 q_0 k_1 Ry}{M\Delta E} + \int_{q_0}^{2k_1} |\langle n' | e^{i\tilde{q} \cdot \tilde{r}} | n \rangle|^2 \frac{dq}{q^3} \right]. \quad (17)$$

In deriving (17) the range of integration in (11) has been divided into two parts; the first part running from $k_1 - k_2$ to q_0 , and the second from q_0 to $k_1 + k_2$. Due to (16), only the dipole term in the expansion of $\exp(i\mathbf{q} \cdot \mathbf{r})$ in the first integral has non-vanishing values. Integrating this term and using (15), we find the first term in the bracket of (17). The second integral cannot be integrated easily, but in any case the cross section is independent of q_0 . From inequality (16) it is evident that at high impact energies we can choose q_0 independent of the impact energy. With the help of (5) and (12) Equation (17) can then be written in the following form

$$\frac{\sigma^B(n \rightarrow n')}{\pi a_0^2} = \frac{Z'^2 M Ry}{Z^2 m_e E} \left[A^B(n, n') \ln \left(\frac{m_e E}{MZ^2 Ry} \right) + B^B(n, n') \right], \quad (18a)$$

$$A^B(n, n') \simeq \frac{8}{3} n^4 \left(1 + \frac{s}{n} \right) s^{-3} J_s(s) J'_s(s) g(s),$$

$$B^B(n, n') \simeq A^B(n, n') \ln \frac{4 a^2 q_0^2}{(1 - n^2/n'^2)^2} + \int_{q_0}^{2k_1} |\langle n' | e^{i\mathbf{q} \cdot \mathbf{r}} | n \rangle|^2 \frac{dq}{q^3}, \quad (18b)$$

n >> 1

Equations (17) and (18) have been derived within the validity of the Born approximation. It is seen that $A^B(n, n')$ is identical to $A(n, n')$ given by (10b). If we now make the approximation that $q_0 \cong 1/a$ instead of the second inequality in (16), that is q_0 is inversely proportional to the atomic radius, then (17) will be an approximation to the Born approximation in the sense that in its first term on the right hand side we have neglected contribution of all the multipoles higher than the dipole. From Equation (18) it can be seen that the choice

$q_0 \cong 1/a$ has no effect on the value of $A^B(n, n')$, but it lowers the value of $B^B(n, n')$ from its actual value. This is due to the neglect of the higher multipoles in the first term in the expression for $B^B(n, n')$. In Table I where we compare the Bethe coefficients derived here with the Bethe coefficients of the Born approximation we find this in fact to be the case.

For $q_0 = 1/a$ the value of the integral in the expression for $B^B(n, n')$ is small. This is due to the fact that when q becomes several times larger than the atomic radius, because of the factor $\exp(i \underline{q} \cdot \underline{r})$ the integrand of $\langle n' | \exp(i \underline{q} \cdot \underline{r}) | n \rangle$ will oscillate rapidly in its range, assuming positive and negative values, and the integral will be small. With $q_0 = 1/a$ and the neglect of the integral, $B^B(n, n')$ becomes the same as $B(n, n')$ given by (10b) except for an additional factor of 1.26 in the argument of the logarithm in (10b).

The Bethe coefficients in the Born approximation, $A^B(n, n')$ and $B^B(n, n')$, for $n = 1 - 9$ and many values of n' in the range 2 - 20 are given by Omidvar (1969). In Table I the ratios $A(n, n')/A^B(n, n')$ and $B(n, n')/B^B(n, n')$, where $A(n, n')$ and $B(n, n')$ are given by (10b), are given for a range of n from 5 to 9 and a range of s from 1 to 4. As is seen the A ratios range from 0.81 to 0.95. The reason that these ratios are different from unity is the use of the asymptotic expansion of the oscillator strength for calculation of $A(n, n')$ instead of the oscillator strength itself. The B ratios are, however, quite different from unity except for the $n \rightarrow n + 1$ transitions. The reason for the smallness of these ratios is the approximation $q_0 = 1/a$. Physically this approximation is equivalent

to an arbitrary cut off of the large momentum transfers to the atom, and a resulting smaller cross section.

We conclude that the dipole approximation of the semi classical impact parameter or Born approximation gives as expected the $A^B(n, n')$ coefficient correctly, but not the $B^B(n, n')$ coefficient. Contribution to the cross section coming from the $B^B(n, n')$ coefficient even at moderately high impact energies is appreciable. Then an adequate description of the cross section by the dipole approximation for moderately high impact energies, with a possible exception of $n \rightarrow n + 1$ transitions, can not be given. It has been shown that the method of classical collision with correspondence principle is equivalent to the dipole approximation.

REFERENCES

- Bethe, H. A., 1930, Ann. Phys. (Leipzig) 5, 325.
- Menzel, D. H., 1968, Nature, 218, 756.
- , 1969, Ap. J. 18, 221.
- Morse, P. M., and Feshbach, H., 1953, Methods of Theoretical Physics (New York: McGraw-Hill Co.Inc.) 2, 1322.
- Omidvar, K., 1969, Phys. Rev. 188, 140, Table IX.
- Percival, I. C., and Richards, D., 1970, J. Phys. B: Atom. Molec. Phys. 3, 315.
- Presnyakov, L. P., and Urnov, A. M., 1970, J. Phys. B: Atom. Molec. Phys. 3, 1267.
- Seaton, M. J., 1962, Proc. Phys. Soc. (London) 79, 1105.

Table I

Ratios of the Bethe Coefficients. For each n and $s = n' - n$ two numbers are specified. The top number is $A(n, n')/A^B(n, n')$ and the bottom number is $B(n, n')/B^B(n, n')$. $A(n, n')$ and $B(n, n')$ are the Bethe coefficients in the semi classical impact parameter, and $A^B(n, n')$ and $B^B(n, n')$ are the corresponding coefficients in the Born approximation.

$\begin{matrix} n \\ s \end{matrix}$	5	6	7	8	9
+1	0.9176	0.9292	0.9378	0.9451	0.9510
	0.8015	0.8015	0.8033	0.8069	0.8132
+2	0.8646	0.8800	0.8922	0.9026	
	0.4064	0.4111	0.4174	0.4250	
+3	0.8309	0.8460	0.8594	0.8713	
	0.2741	0.2739	0.2768	0.2913	
+4	0.8064	0.8200	0.8326		
	0.2117	0.2081	0.2079		