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A Study of Adiâbaticity in the Case of Target Degeneracy

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The validity of the adiabatic approximation in thecaseof the collision of a semi-classical charged projectile and a target atom in a degenerate state is examined. The target is Hydrogen atom in the first excited state, which allows calculations to be performed analytically, within the dipolar interaction and "no-quenching" assumptions. We confirm, in a precisely quantitative way, that the adiabatic approximation breaks down for impact parameters larger than the Weisskopf radius and we supply the exact wave functlon describing the collision.

A validade do tratamento adiabático da colisão de uma partícula carregada com um alvo em estado degenerado é examinada, dentro das aproximações de interação dipolar, de trajetória semi-clássica e de transições limitadas ao grupo de sub-níveis degenerados ("no-quenching"). O alvo é um átomo de Hidrogênio no primeiro estado excitado, para o qual os cálculos podem ser feitos analiticamente. Confirma-se de forma quantitativamente precisa que a aproximação adiabática deixa de valer quando o parâmetro de impacto se torna maior que o raio de Weisskopf e obtem-se a função de onda exata que descreve a colisão.

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1. INTRODUCTION

Textbooks mostly discuss the validity of the adiabatic approximation only in the non-degenerate case (see, for instance, Schiff[1]). The approximation is nonetheless used in cases of target degeneracy in some collision problems in order to simplify (cr even make possible) calculations: such is the case of some iine-broadening theories[2,3]. It is thus wcrth discussing its validity in the case of degeneracy as deeply as possible.

The adiabatic approximation depends essentially on the ratio of the time derivative of the transition matrix slement to the energy difference between states[1]: when this ratio is small, we can suppose that each possible initial state of the system simply undergoes a phase shift as time passes, the probability of "jumping" to another state being negiigible. In the case of a *degenerate* target state, the splitting in energy is induced by the collisional interaction *itself,* thus requiring a specific treatment. The problems connected with the breakdown of the approximation have been recently raised and discussed by Voslamber[4] but they were already dealt with since 1959 by Margenau and Lewis[5], among others.

In the case of a Hydrogen atom undergoing collision with a charged particle assumed to travel along a straight classical path, and within the electric dipolar interaction and no-quenching assumptions, calculation of probability amplitudes can be performed analytically, thus allowing a ráther clear insight of the problen. These calcuiations were first made hy Lisitsa and Sholin[6] and Pfennig[7], and were obtained independently by this author.

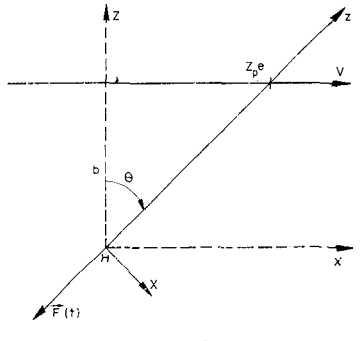

Fig.1

2. THEORY

We refer tu fig. 1 for the geometrical description of the collision between a fixed H atom in the state $n=2$ and a classical particle of charge $Z_p e$, impact parameter $\underline{b}$ and velocity V. Two coordinate systems are used: the fixed (X,Y,Z) system and the rotating $(x,y\equiv Y,z)$ systems. The angle θ describes the collision, as it takes values from $-\pi/2$ to $\pi/2$.

For each position of the pertuber we consider the Stark states $\psi_1 \equiv \psi_{211}(\vec{r})$, $\psi_2 \equiv \psi_{21-1}(\vec{r})$, $\psi_3 \equiv (\psi_{210}-\psi_{200})/\sqrt{2}$, $\psi_4 \equiv (\psi_{210}+\psi_{200})/\sqrt{2}$, where the $\psi_{n\ell m}$ are labeled in the usual way. In the fixed reference system (X,Y,Z) these wave functions are written $\phi_i = e^{-i\theta J_y}\psi_i$, $i = 1, 2, 3, 4$, and their energy-eigenvalues are $E_1 = E_2 = 0$ (taking the unperturbed energy as origin of the energies), $E_3 = -3e a_0 F$, $E_4 = 3e a_0 F$, where $F = Z_p e/4\pi\varepsilon_0 r^2$ is the interisity of the electric field created by the perturber of charge $Z_p e$. Writing the wave function of the atom as:

$$\psi(\vec{r},t) = \sum_{n=1}^{4} a_n(t)\ \phi_n(\vec{r})\ \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} E_n(\tau)d\tau\right\} \qquad (1)$$

the usual development[1] ieads to the set of coupled diiferentia! equations:

$$\begin{aligned}
-i\hbar\dot{a}_1 &= S_{11}a_1 + S_{12}a_2 + S_{13}F^*(t)a_3 + S_{14}F(t)a_4 \\
-i\hbar\dot{a}_2 &= S_{21}a_1 + S_{22}a_2 + S_{23}F^*(t)a_3 + S_{24}F(t)a_4 \\
-i\hbar\dot{a}_3 &= S_{31}F(t)a_1 + S_{32}F(t)a_2 + S_{33}a_3 + S_{34}\left[F(t)\right]^2 a_4 \\
-i\hbar\dot{a}_4 &= S_{41}F^*(t)a_1 + S_{42}F^*(t)a_2 + S_{43}\left[F^*(t)\right]^2 a_3 + S_{44}a_4
\end{aligned} \qquad (2)$$

where $S_{nm} = \dot{\theta} < \psi_n/J_y/\psi_m > \equiv \dot{\theta} J_{nm}$, with the property $S_{nm}=S^*_{mn}$, and

$$F(t) = \exp\left\{-\frac{i}{\hbar} 3ea_0 \int_{t_0}^{t} F(t')dt'\right\} = \exp\left\{-\frac{i}{\hbar}\frac{3e^2 a_0 Z_p}{4\pi\varepsilon_0 b V}\left[t_g^{-1}\frac{V}{b} - t_g^{-1}\frac{Vt_0}{b}\right]\right\} \qquad (3)$$

The J_{rm} matrix can be easily calculated, giving:

$$(J_{rm}) = \frac{i\hbar}{2}\begin{pmatrix} 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & 1 \\ 1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix} \tag{4}$$

Changing independent variables from t to θ and by choosing $t_0 = -\infty$, we obtain:

$$\begin{aligned} \frac{da_1}{d\theta} &= \frac{1}{2}\left[F^*(\theta)\,a_3 + F(\theta)\,a_4\right] \\ \frac{da_2}{d\theta} &= -\frac{1}{2}\left[F^*(\theta)\,a_3 + F(\theta)\,a_4\right] = -\frac{da_1}{d\theta} \\ \frac{da_3}{d\theta} &= -\frac{F(\theta)}{2}(a_1 - a_2) \\ \frac{da_4}{d\theta} &= -\frac{F^*(\theta)}{2}(a_1 - a_2) \end{aligned} \tag{5}$$

Here: $F(\theta) = \exp\{-iK(\theta + \pi/2)\}$. (5a)

$$K = \frac{3e^2 a_0 Z_p}{4\pi\varepsilon_0 b V} \tag{5b}$$

The system (5) reduces to the single equation:

$$\frac{d^2 a_1}{d\theta^2} = -(K^2 + 1)a_1 + \frac{c}{2} + \alpha K^2 \tag{6}$$

where c and α depend on the initial conditions through the relations:

$$c = a_2(-\pi/2) + a_1(-\pi/2) \quad \text{and} \quad \alpha = a_1(-\pi/2) - \frac{a_3(-\pi/2) - a_4(-\pi/2)}{2iK}$$

The solution of (6) is the well known expression

$$a_1(0) = E \cos\left(\sqrt{K^2+1}\,\theta + \phi_0\right) + \left(\frac{c}{2} + \alpha K^2\right)/(K^2+1) \quad . \tag{7}$$

where E and ϕ_0 also depend on initial conditions. As for the other probability amplitudes, we find:

$$a_2(\theta) = c - a_1(\theta) \tag{7b}$$

$$a_3(\theta) = F(\theta)\left[\frac{da_1}{d\theta} + iK(a_1 - \alpha)\right] \tag{7c}$$

$$a_4(\theta) = F(\theta)\left[\frac{da_1}{d\theta} - iK(a_1 - \alpha)\right] \tag{7d}$$

3. RESULTS

Choosing $a_i(-\pi/2) = \delta_{i,1}$, we put the H atom initially in state $|211>$. Equations (7a), (7b), (7c) and (7d) then give:

$$a_2(\theta) = (k^2+1)^{-1} \sin^2\left[\frac{\sqrt{K^2+1}\,(\theta + \pi/2)}{2}\right] \tag{8a}$$

$$a_1(\theta) = 1 - a_2(\theta) \tag{8b}$$

$$|a_3|^2 = |a_4|^2 = \frac{1}{2}\left(1 - |a_1|^2 - |a_2|^2\right) \tag{8c}$$

We choose V in the form of the thermal velocity of a proton $V = (3kT/M_P)^{1/2}$ (M_P is the mass of the proton), that is, $V = 1.574\times10^2\sqrt{T}$ ms^{-1}. As for b, we shall write $b = n_b\, b_0$ where n_b is an integer and b_0 is the atomic radius $4a_0 = 2{,}116 \times 10^{-10}$m. We take $Z_p = 1$.

Numerical results are given in figures 2 and 3, where $|a_1|^2$ and $|a_2|^2$ are respectively plotted.

The values of parameters are: for curves labeled (1), $T = 10^2$K, $n_b = 1$ (very close collision at low speed); for curves labeled (2), (3), (4) and (5), $4 = 10^4K$ and n_b respectively equal to 20, 50, 100 and 1000

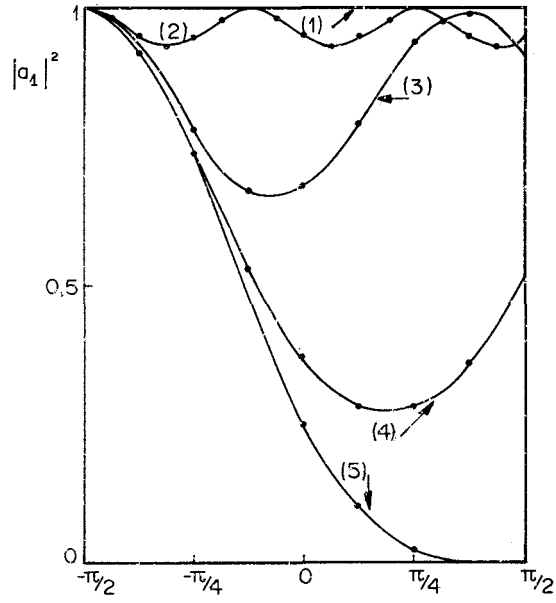

Fig.2 $|a_1|^2$ as a function of 6
For curve (1) $|a_1|^2$ = i.

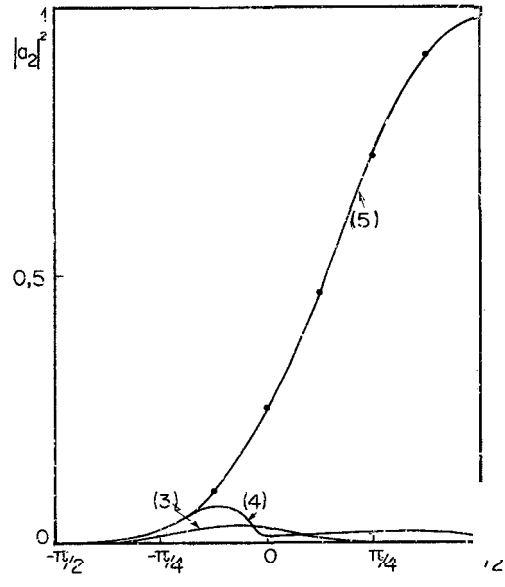

Fig.3 $|a_2|^2$ as a function of θ
Curves (1) and (2) practically coincide rith the θ axis.

(moderate speed and increasing impact parameter). The parameter K given by (5b), which is the relevant quantity, takes the values 1.043×10^3, 5.21, 2.09, 1.04 and 0.104 respectively for curves (1), (2), (3), (4) and (5).

It is worth remarking that a different choice of initial conditions such as $a_i(-\pi/2) = E_{i,3}$ would lead to the same results, through a re-labeling of the resulting curves.

4. ANALYSIS AND CONCLUSIONS

Only curves (1) and (2) can be considered adiabatic, that is, only for them is the initial population of levels conserved approximately throughout the collision process.

Curve (1) has little physical meaning: it corresponds to a slow very close collision, for which all our main assumptions (dipolar interaction, classical trajectory, no quenching) breakdown. Within a statistical treatment, such as a line broadening calculation, it might still be useful, provided a convenient correction is made in order to account for the effects just mentioned.

Curves (4) and (5) are at first sight difficult to understand: one might expect that, as it is usually the case, the perturbation would be more and more adiabatic as the perturber passes farther and farther from the target. Actually, as it was pointed out in the Introduction, in the degenerate case which is being dealt with the energy splitting, which is due to the perturbation itself, becames smaller that the variation of the transition matrix-element during the relevant interaction time. For further discussion of this point, see ref. 5. This fact explains the results expressed by curves (4) and (5).

Curve (2) supplies the criterium for adiabaticiy in our problem: it shows that for $K \gtrsim 5$, or equivalently $bV/Z_p \lesssim 7 \times 1$ —m²/s the adiabatic regime is valid.

This limiting value could have been obtained from the condition b << b_w, where $b_w = n^2\hbar^2 p/m_e V$ is the Weisskopf radius For the col-

lision with an ion of thermal velocity V (n is the principal quantum number and m_e the electron mass). This is the limiting impact parameter for strong collisions, and it could be presumed that such collisions cause a sufficiently large splitting to be adiabatic. Our calculation supplies a precise value for the limiting values of the parameters in this particular case.

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REFERENCES

1. L.I.Schiff, *Quantum Mechanics*, McGraw-Hill Book Company, Inc. (1955).
2. D.Voslamber and E.R.A. Segre, J.Quant.Spectrosc. Radiat. Transfer 25, 45 (1981).
3. A.J.Barnard, J.Cooper and E.W.Smith, J.Quant.Spectrosc.Radiat.Transfer *14*, 1025 (1974).
4. D.Voslamber, Ann. Phys. Fr. 5, 207 (1980).
5. H.Margenau and M.Lewis, Rev.Mod.Phys. *31*, 569 (1959).
6. V.S.Lisitsa and G.V.Sholin, Sov. Phys. JETP *34*, 484 (1972).
7. H.Pfennig, Z.Naturforsch *26a*, 1071 (1971).