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July 1974

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The Effects of Debye Screening on the Position of Spectral Lines*

C. Bruce Tarter

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I. INTRODUCTION

The purpose of this brief report is to write down for reference the shifts in spectral lines produced by the static screened Coulomb (Debye) potential.¹ The motivation for the work is described by Chapline,² who has proposed that line profiles be employed as diagnostics of density in early laser-fusion experiments. Although a theoretical understanding of the line shape as a function of density (and temperature) is the crucial element in such a diagnostic technique, an accurate knowledge of the position of the line center is also required. In addition, if the energy shift of the line center is comparable with the line broadening, then it will be difficult for an integral experiment to distinguish between these effects (and hence one should try to design experiments in which this is not the case). Finally, some experiments³ have indicated that mechanisms other than Debye shielding may be primarily responsible for line shifts at low density, so that the laser-fusion experiments may also serve as an experimental test of the Debye theory.

* This work performed under the auspices of the U. S. Atomic Energy Commission.

II. THEORY

In all of the calculations that follow we will assume that the atomic potential in a hydrogenic atom of charge Z is described by

$$V(r) = -\left(\frac{Ze^2}{r}\right) e^{-r/D} \quad (1)$$

where the Debye length is given by

$$D^{-2} = \frac{4\pi e^2 \rho}{\bar{A} H k T} \left[\frac{\bar{Z}^2}{Z^2} + \bar{Z} \frac{F_{-\frac{1}{2}}(\eta)}{2F_{\frac{1}{2}}(\eta)} \right] \quad (2)$$

where ρ is the density, T the temperature, $\bar{A}$ the mean molecular weight, H the hydrogen mass, and $\bar{Z}^2$ and $\bar{Z}$ are averages over the charges of the ions in the gas. $F_{-\frac{1}{2}}(\eta)$ and $F_{\frac{1}{2}}(\eta)$ are Fermi-Dirac functions of the degeneracy parameter η ; as $\eta \rightarrow -\infty$, one has $F_{-\frac{1}{2}}(\eta)/2F_{\frac{1}{2}}(\eta) \rightarrow 1$ for a nondegenerate gas. We can write equation (2) in more convenient units as

$$D/a_0 = 5.74 \left(\frac{T_k}{\rho} \right)^{\frac{1}{2}} h(\bar{Z}, \bar{A}) \quad (3)$$

where a_0 is the Bohr radius, T_k is the temperature in kilovolts, ρ is in gm/cc, and

$$h(\bar{Z}, \bar{A}) = \left\{ \bar{A} / \left[\bar{Z}^2 + \bar{Z} \frac{F_{-\frac{1}{2}}(\eta)}{2F_{\frac{1}{2}}(\eta)} \right] \right\}^{\frac{1}{2}} \quad (4)$$

Now, Rogers et al.¹ have shown that the transformations

$$\epsilon_{n\ell} = E_{n\ell}/Z^2 \quad (5a)$$

$$d = Z D/a_0 \quad (5b)$$

reduce the Schrödinger equation to a form which is independent of Z (except

through the dependence of D on Z). Consequently, a solution for $E_{nl}(d)$ leads simply to a solution for any hydrogenic atom of charge Z through equations (5a) and (5b). For relatively large screening lengths, $d/a_0 \gg 1$, we can write down an approximate expression for the energy of level n . We have,

$$E(r) = -\frac{Ze^2}{2r} \left(1 - \frac{2r}{D} + \frac{3}{2} \frac{r^2}{D^2} - \dots \right) \quad (6)$$

and for hydrogenic systems $\bar{r} \approx a_0 n^2/Z$ so that,

$$\epsilon_n = \frac{E_n}{Z^2} = -\frac{e^2}{2a_0} \left[\frac{1}{n^2} - \frac{2}{d} + \frac{3}{2} \frac{n^2}{d^2} - \dots \right] \quad (7)$$

Thus, the lowest order screening effect is to raise all levels n by an amount $2/d$, while the next order in powers of $1/d$ depresses them by an amount which increases with increasing quantum number n . Thus, the energy of any spectral line between levels n and upper level n' is given by

$$E_{nn'} \cong \left(\frac{Z^2 e^2}{2a_0} \right) \left[\left(\frac{1}{n^2} - \frac{1}{n'^2} \right) - \frac{3}{2d^2} (n'^2 - n^2) \right], \quad (8)$$

which corresponds to a decrease (red shift) in the line energy compared with its unscreened value.

Before considering specific applications two other points are worth noting. First, there is the well-known fact that level n only exists as a bound state for $d > 2n^2$, which obviously restricts the range of applicability of equation (8). Secondly, the oscillator strength $f_{nn'}$ will decrease with decreasing d ^{4,5} so that the intensity of a given line will be reduced as d decreases.

III. APPLICATIONS

Most of the proposed experimental situations involve the doping of a hydrogen pellet with a moderate Z impurity (or impurities), and using the

by a line of the impurity as the plasma diagnostic. Ignoring relativistic effects* the energy of that line is given by equation (8) as

$$E_{nn'} = \frac{Z^2 e^2}{2a_0} \left[\frac{3}{4} - \frac{9}{2d^2} \right] = \frac{3}{8} \frac{Z^2 e^2}{a_0} \left[1 - \frac{6}{d^2} \right] \quad (9)$$

Equation (9) is of course only valid for $d \gg 1$, and exact numerical solutions for arbitrary d have been obtained.¹ The results are plotted in Figure 1, where we also show the 1s-2p oscillator strength as a function of d .

Now consider a mixture of hydrogen and an impurity whose relative concentration is f ; and assume that the impurity is nearly fully ionized. The function h is then given by

$$h = \left\{ \frac{A_H (1-f) + f A_Z}{(1-f) + fZ^2 + [(1-f) + fZ] \frac{F_{-1/2}(\eta)}{2F_{1/2}(\eta)}} \right\}^{1/2} \quad (10)$$

In Table 1 we have tabulated h for various values of f and Z for an impurity embedded in a pure deuterium plasma (we have also assumed that the system is nondegenerate; it will turn out that for all systems of interest this affects the value of h by a completely negligible amount).

Table 1

$h(Z, f)$

Impurity	Z	f = 1.0	.1	.01	.001	0
Neon	10	.42	.54	.82	.98	1.0
Argon	18	.34	.40	.66	.93	1.0
Iron	26	.28	.32	.50	.87	1.0

* The relativistic correction to the line energy is $E_{rel} = E_{nr} \left[1 + \frac{(Z\alpha)^2}{3} \right]$ which ranges from .1% at $Z = 10$ to 1% for $Z = 26$.

To illustrate the possible effects of screening on the line positions in proposed experimental configurations, we have calculated the decrease in Ly α energy for deuterium plasmas doped with 1% neon and 1% argon, respectively. The results are shown in Table 2 for several densities and temperatures. We have also used the HANK code to compute the ionization equilibrium and degeneracy parameter for each ρ and T point. In all cases shown the degeneracy correction to the function h was insignificant, and except for the very lowest temperature the assumption of full ionization was satisfied quite well (at the lowest T point Z_{ionic} was typically $\sim Z_{\text{nuc}-1}$ to $Z_{\text{nuc}-2}$, which doesn't significantly alter the results).

Table 2

Shift of 2p-1s Line Due to Debye Screening*

a) Neon (1% in deuterium) - $E(2p-1s) = 1.02 \text{ keV}$

Redshift (eV)

$\rho \backslash T$	0.2	0.5	1.0	2.0
.03	<1	<1	<1	<1
.1	<1	<1	<1	<1
.3	1	<1	<1	<1
1	10	4	2	1
3	24	12	6	3
5	32	18	10	5

* In the tables ρ is in gm/cc and T in kilovolts.

b) Argon (1% in deuterium) - $E(2p-1s) = 3.34$ keV

Redshift (eV)

ρ / T	0.3	1.0	2.0	6.0
.03	<1	<1	<1	<1
.1	1	<1	<1	<1
.3	3	1	1	<1
1	10	3	2	1
3	23	9	4	2
5	45	25	8	3

IV. SUMMARY

This report has described the effects of Debye screening on the position of spectral lines, particularly the Ly α resonance line of hydrogen-like atoms. There are many theoretical approaches to the problem of continuum lowering in plasmas, the Debye theory being one of the simplest. Unfortunately, the spectral line shifts predicted by all such theories are first order rather than zero order quantities: most physical properties of interest, such as the equation of state and radiative opacity, are sensitive to the average magnitude of the continuum lowering but relatively insensitive to the differential effects on different quantum states. In addition the Debye picture certainly breaks down as $d \rightarrow 1$ and is probably obscured by other phenomena² for $d \gg 1$. However, if it is to have any validity it should produce at least semi-quantitative accuracy for intermediate values, say $10 \lesssim d \lesssim 100$, so that the predicted line shifts in this regime can initially be treated with some measure of confidence.

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