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Ionic transitions and oscillator strengths in Debye plasma – a case study

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Abstract. Stability and energy of the excited states of the C^{4+} ion in plasmas are investigated theoretically using the Debye model. The transition energies of $\Delta n = 0$ and $\Delta n \neq 0$ transitions are seen to follow completely opposite trends of variation with the plasma screening strength. The dependence of absorption oscillator strength values on the screening strength is also discussed.

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1 Introduction

Theoretical investigation of atomic phenomena occuring in hot and dense plasmas has emerged as a highly active area of research in recent years. One- and two-electron properties of ions in vacuum are modified considerably in plasma environments due to short-range order and static and dynamic screening effects introduced by surrounding plasma charges consisting of ions and fast electrons. Of all the models now available to approximate the effect of static plasma screening on atomic processes, the analytic exponential Yukawa-type potential *i.e.* the Debye model is the most well-known. This model has been the subject of several investigations in the past in relation to the energy levels of single-electron systems [1,2] or, in considering collisional excitations of ions in plasma environments [3]. Of late, the detachment criterion for the two-electron hydrogen negative ion in this potential has been predicted accurately in a variational calculation [4].

The aim of the present communication is to report the results of our investigation of the plasma effects on some transition properties of the stripped positive ions which are commonly seen in high-temperature laboratory or astrophysical plasmas besides the neutral species. Such studies are almost non-existent in the literature, although atomic data are abundant for highly stripped ions *in vacuo*. We have considered the C^{4+} ion as a representative case because such a two-electron ion is the simplest prototype of the complicated many-electron systems where the degree of stripping is maximal, yet the nuclear charge Z is not too high to render the plasma effects on the optical electron of the ion inconspicuous. The screened coulomb potential model of plasma screening is retained in this study because of its immediate appeal to the plasma parameters *i.e.* the temperature and density in terms of a single screening constant. More specifically, we are interested in the ionic properties like the transition energy and the transition strength together with their systematics of variation in plasma environments that are relevant for diagnostic purposes. A few dipole-allowed as well as dipole-forbidden transitions of the ion are discussed in this paper. The method of our calculation is briefly outlined in the next section and the results are presented in Section 3.

2 Method

The non-relativistic Hamiltonian of the two-electron ion with the analytic exponential model for plasma screening takes the form (atomic units are used throughout in this article):

$$H_0 = -\frac{1}{2}\sum_{j=1}^{2}\nabla_j^2 - \sum_{j=1}^{2}\frac{Z}{r_j}\exp\left(-\frac{r_j}{D}\right) + \frac{1}{r_{12}} \qquad (1)$$

where, Z denotes the nuclear charge and D is the familiar Debye screening constant. For a highly-stripped ion the electron-nuclear attraction being more important than the interelectronic repulsion, the former is kept screened while the latter is assumed to remain a pure coulomb potential.

The excitation spectrum of the plasma-embedded system is now studied following a time-dependent perturbation-variation procedure which (i) considers the linear response of the system to an external harmonic multipolar perturbation, spin-free for the present study:

$$H'(\mathbf{r},t) = \lambda\sum_{j=1}^{2} r_j^l Y_{l0}(\theta_j,\phi_j)\exp(-i\omega t) + \text{complex conjugate} \qquad (2)$$

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and (ii) seeks and analyses the poles of the following time-dependent, normalised and cycle-averaged Dirac-Frenkel variational functional [5–7] of the perturbed function Φ of the system in plasma environment through standard optimisation procedure:

$$J[\Phi] = \frac{1}{T}\int_0^T \mathrm{d}t \frac{\langle\Phi|H_0 + H' - i(\partial/\partial t)|\Phi\rangle}{\langle\Phi|\Phi\rangle} \qquad (3)$$

where l, ω and T are the multipolarity, angular frequency and time-period of perturbation H' respectively. The methodology is similar to that elaborated in a recent article [8] although in a somewhat different context (dealing with ionic response in crystalline environments), and will not be repeated here. In the following section the results of our calculation are described at some length.

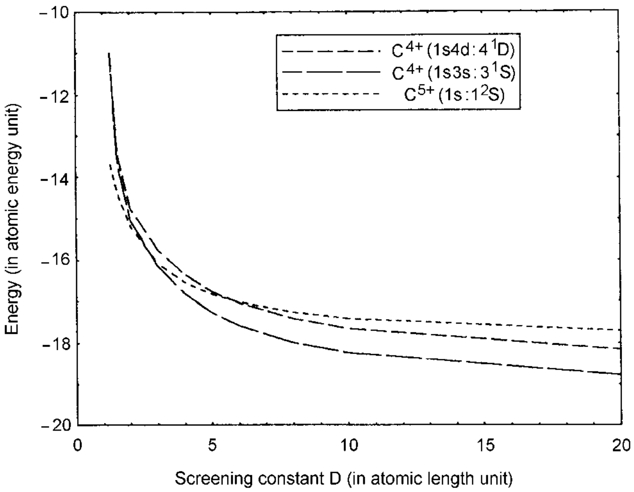


Fig. 1. Dependence of energy of the states of carbon ions on the plasma screening constant.

3 Results

In this paper we have considered the ground state $1s^2 : {}^1S$ and the following singlet terms arising out of the singly-excited configurations:

$$1sns: {}^1S(n = 2\text{–}5),\ 1snp: {}^1P(n = 2\text{–}5)$$
$$\text{and } 1snd : {}^1D(n = 3\text{–}5) \qquad (4)$$

of the C^{4+} ion in a variety of Debye Plasma. The screening constant D is a function of both the electron density n_0 and temperature T of the plasma. So, a particular value of D relates to a set of plasma parameters, and by varying its magnitude a variety of plasma conditions may be simulated. Starting from the free-ion limit *i.e.* "zero" screening characterised by $D = \infty$ (or alternatively, $1/D = 0$) strong plasma conditions can be achieved gradually by reducing the Debye Constant in successive steps.

In presence of plasma screening the system should become less bound, so it is reasonable to expect "continuum lowering" which is clearly demonstrated in Table 1 in the progressively reduced magnitude of the complete or double ionisation potential (given as the negative energy of the ground configuration $1s^2 : {}^1S$ in the Table) of the C^{4+} ion with increased plasma strength. Similar trend holds for the orbital ionisation continuum also (*i.e.* the $-\varepsilon[1s]$ values), which are not shown in the Table. On the other hand, the negative energy of any excited configuration of C^{4+} is a monotonically decreasing function of the growing plasma strength too, but with one important distinction: It is seen that there is a limiting plasma strength that the positive ion in the excited state can survive, *i.e.* beyond which it becomes unstable. To examine this point we have necessarily computed the dependence of the ionisation potential of the further-singly- ionised system, the H-like C^{5+} ion, and have noticed that at around $D = 1.15$, the most strongly bound of all the configurations ($1s2s : {}^1S$) considered here for C^{4+} becomes unstable as its energy exceeds that of C^{5+}. Relatively loosely bound higher excited configurations can survive only weaker plasma conditions as evident from Table 1 from the shift of the critical magnitude of D towards smaller screening strengths with increasing orbital quantum number of the "active" electron. This indicates that for a positive ion embedded in a Debye plasma, corresponding to a definite value of the screening constant only a finite number of discrete bound states is available as opposed to the free-ion case with infinite number of bound states below the continuum in a purely coulomb potential. Some of the results of Table 1 are displayed graphically in Figure 1. The crossing points of the C^{4+} excited state energy curves against the C^{5+} ground state curve determine the critical values of plasma screening for the survival of the excited states of the former ion (in this and all the subsequent figures the screening magnitude increases towards the origin).

Next are studied the energy differences between the ground - excited and excited - excited configurations of C^{4+} under various plasma conditions. Not all of these transitions are optically allowed in an isolated ion, yet forbidden line formations are common in plasmas due to the temporary breaking of the spherical symmetry and are in fact a valuable tool for plasma modeling and diagnostics. As to the behaviour of the transition energy of the plasma-embedded ion as a function of the screening strength it is noticed that all the transitions in such an ion can be classified in two groups. From what we have presented in Figures 2a,b as the representative cases it can be seen that, for transitions maintaining no change in the principal quantum number of the active electron, *i.e.* for $\Delta n = 0$ transitions the transition energy increases with larger plasma screening strength. Conversely, for the $\Delta n \neq 0$ transitions involving a change in the principal quantum number the transition energy decreases with stronger screening. These trends are equally valid for transitions connecting states of the same (Δn always non-zero) or different (Δn can be zero or non-zero both) orbital symmetries. In this context it is worthwhile to point out that a reversal in the relative magnitude of the $1s^2 \rightarrow 1snp$ and the corresponding $1s^2 \rightarrow 1snd$ ($n = 3\text{–}5$) energy is observed when the free ion gradually passes into plasma environments with stronger screening-the former transition energy is larger

Table 1. Stability of the excited states of the C^{4+} ion under various plasma screening conditions.

	−Energy												
State	$D=\infty$	$D=20$	$D=10$	$D=8$	$D=6$	$D=5$	$D=4$	$D=3$	$D=2$	$D=1.5$	$D=1.25$	$D=1.15$	$D=1.05$
							(C^{5+})						
1s : ^{2}S	18.0000	17.7019	17.4074	17.2616	17.0205	16.8293	16.5456	16.0804	15.1776	14.3102	13.6406	13.2995	12.9005
							(C^{4+})						
1s^2 : 1^{1}S	32.3612	31.7652	31.1770	30.8858	30.4048	30.0237	29.4584	28.5324	26.7395	25.0223	23.7006	23.0287	22.2444
1s2s : 2^{1}S	21.1592	20.5697	20.0002	19.7227	19.2707	18.9180	18.4037	17.5840	16.0744	14.7266	13.7575	13.2896[a]	
1s3s : 3^{1}S	19.3609	18.7818	18.2411	17.9840	17.5740	17.2615	16.8176	16.1394	15.0311[a]				
1s4s : 4^{1}S	18.7374	18.1721	17.6677	17.4355	17.0754	16.8101[a]							
1s5s : 5^{1}S	18.4504	17.9018	17.4387	17.2342[a]									
1s2p : 2^{1}P	21.0284	20.4378	19.8653	19.5856	19.1289	18.7718	18.2497	17.4144	15.8693	14.4872	13.5038[a]		
1s3p : 3^{1}P	19.3229	18.7429	18.1999	17.9413	17.5283	17.2132	16.7656	16.0829	15.0239[a]				
1s4p : 4^{1}P	18.7215	18.1555	17.6496	17.4166	17.0556	16.7901[a]							
1s5p : 5^{1}P	18.4423	17.8932	17.4295	17.2252[a]									
1s3d : 3^{1}D	19.3327	18.7498	18.1991	17.9352	17.5117	17.1871	16.7237	16.0151[a]					
1s4d : 4^{1}D	18.7253	18.1566	17.6441	17.4070	17.0388	16.7683[a]							
1s5d : 5^{1}D	18.4442	17.8926	17.4238	17.2169[a]									

[a] correspond to unstable states under specific plasma screening.

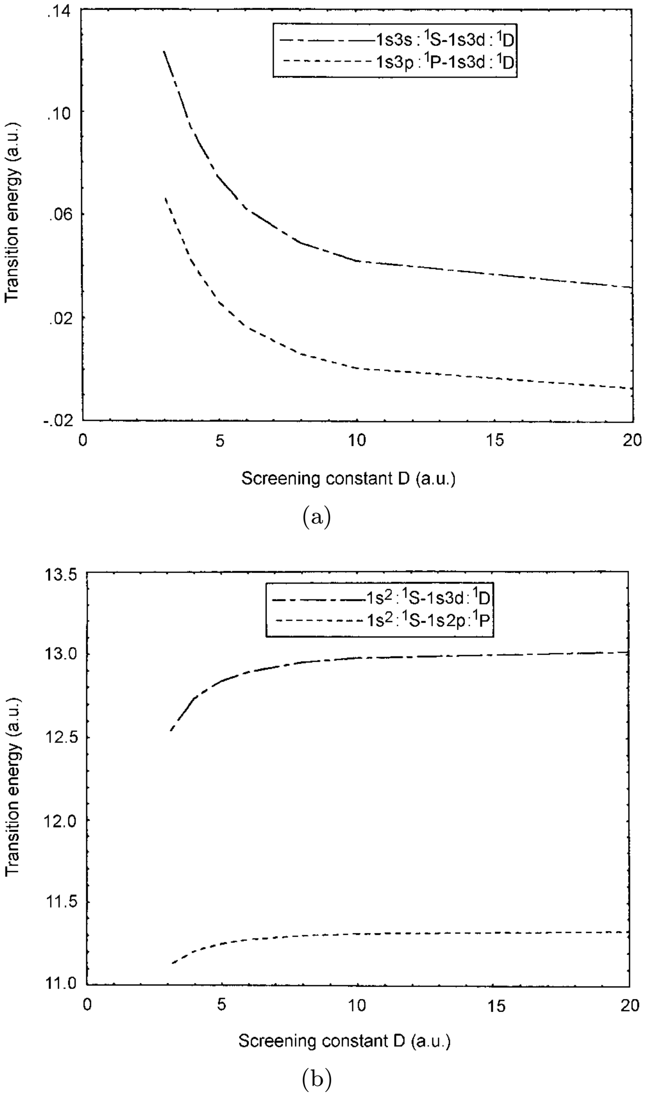
Table 2. Variation of the dipole (f_d) and the quadrupole (f_q) absorption oscillator strength values for different transitions of the C^{4+} ion with Debye screening constant D.

	Transitions						
1s^2 : ^{1}S →	1s2p : ^{1}P	1s3p : ^{1}P	1s4p : ^{1}P	1s5p : ^{1}P	1s3d : ^{1}D	1s4d : ^{1}D	1s5d : ^{1}D
	f_d				f_q		
$D=\infty$	0.6435	0.1411	0.0539	0.0264	1.765(−5)[a]	9.029(−6)	4.937(−6)
=20	0.6418	0.1396	0.0520	0.0242	1.731(−5)	8.598(−6)	4.440(−6)
=10	0.6372	0.1352	0.0470	0.0187	1.636(−5)	7.482(−6)	3.227(−6)
=8	0.6338	0.1322	0.0435	0.0147[b]	1.571(−5)	6.733(−6)	2.412(−6)[b]
=6	0.6266	0.1258	0.0363		1.438(−5)	5.242(−6)	
=5	0.6196	0.1196	0.0291[b]		1.313(−5)	3.821(−6)[b]	
=4	0.6069	0.1085			1.099(−5)		
=3	0.5822	0.0842			6.879(−6)[b]		
=2	0.5080	0.00023[b]					
=1.5	0.4063						
=1.25	0.2821[b]						

[a] $M(N) \equiv M \times 10^N$.
[b] denote that the upper level is unstable.

than the latter until a typical screening strength is reached to reverse the trend, which itself shifts towards the weaker screening side with larger n. The same is also manifested from the relative positions of all the 1snp and 1snd pairs of states in Table 1. The screening-dependence of the transition energies can easily be calculated from the data given in Table 1 and no separate tabulation is made for it.

In the last part of this work we have studied the modification brought about in the transition strengths as the free ion gradually faces stringent plasma conditions. We have considered the dipole absorption oscillator strength f_d for the transitions 1s^2 → 1snp ($n = 2$–5) and the quadrupole absorption oscillator strength f_q for the transitions 1s^2 → 1snd ($n = 3$–5) for different screening constants. The result is summarised in Table 2. The data exhibits a gradual reduction in these values with increased screening magnitude. The lower-lying states are seen to remain less affected at smaller screening strengths as it should be from physical considerations because the screening effect influences the outer orbital more than the inner one. The variations of f_d and f_q with the screening constant D are smooth and are depicted in Figures 3a,b respectively.

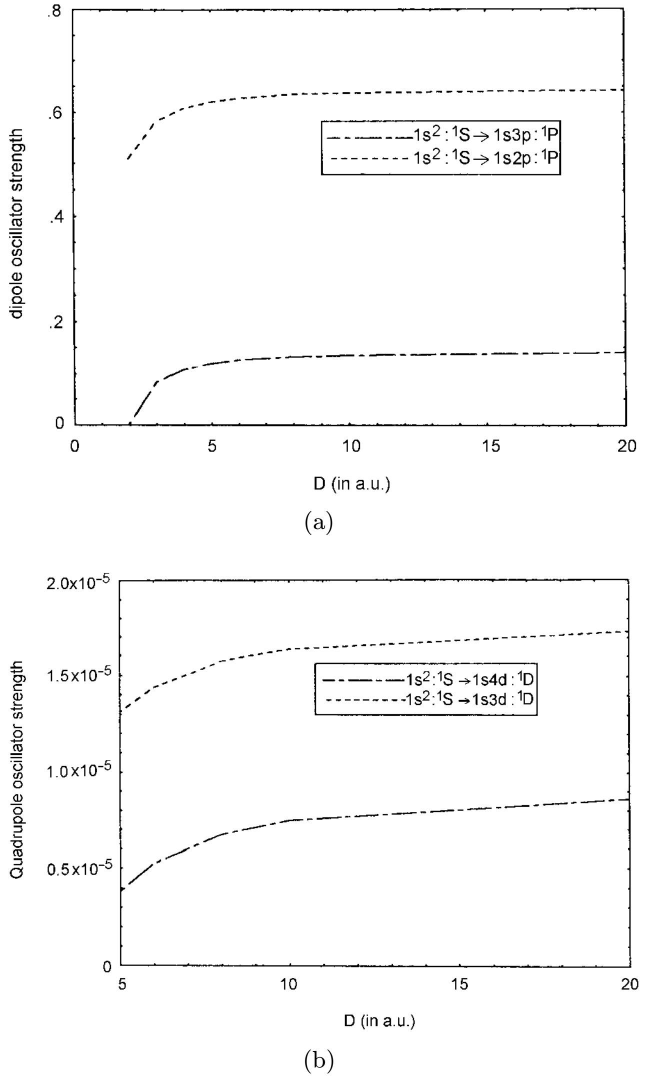


(a)

(b)

Fig. 2. a) Transition energy *versus* screening constant for some $\Delta n = 0$ transitions in C^{4+} ion. b) Transition energy *versus* screening constant for some $\Delta n \neq 0$ transitions in C^{4+} ion.

To conclude, the Debye model has been utilised in the present calculation to investigate the effect of plasma screening on the survival of the excited states, and the behaviour of the transition energy as well as some allowed and forbidden transition strengths for the typical C^{4+} ion under a wide range of plasma conditions represented by the varying screening constant D. The information obtained from this study seems to be consistent and interesting, and it has to be further enriched from the analysis of the free - bound transitions as well as the spin-forbidden and intercombination transitions among the other types of bound-bound transitions in order to link up the data with plasma diagnostics. This is currently in progress and the results will be reported in due course.



(a)

(b)

Fig. 3. a) Variation of the dipole absorption oscillator strength (f_d) with plasma screening constant (D) for a few allowed transitions in C^{4+} ion. b) Variation of the quadrupole absorption oscillator strength (f_q) with plasma screening constant (D) for a few electric quadrupole transitions in C^{4+} ion.

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