

# Energy Gap and Line Shifts for H-Like Ions in Dense Plasmas

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Based on the results of a foregoing paper (Z. Naturforsch. **44a**, 519–523 (1989)) the density-dependence of the discrete energy states and the continuum level is calculated with better accuracy. A static approximation to the line shifts is derived and discussed.

## 1. Introduction

The recombination spectra of multiply charged ions yield rich information about the state of dense plasma and can therefore be used for the diagnostics of highly ionized dense plasmas. Prominent examples are arc plasmas and plasmas generated by high power devices.

Very important measurements of line profiles and of the full half-width were made recently in the Bochum group by Kunze and coworkers [1–5]. They used a gas-liner pinch as a plasma source and investigated hydrogen-like and lithium-like ions. Other important experimental and theoretical research of broadening and shift of emission lines in dense plasmas was performed by Vitel [6] and Ichimaru and coworkers [7].

But the recombination lines of multiply charged ions were found also in several astrophysical objects. The lines of O VIII e.g. appear in the spectra of certain hot Wolf-Rayet stars and in the nuclei of O VI planetary nebulae [8, 9]. Storey and Hummer [10] suppose that analogous lines of C VI and N VII will be found in the spectra of other highly ionized objects, such as old nova shells. They calculated the intensities of the recombination lines for the hydrogenic ions C VI, N VII, O VIII.

This work is dealing with an other aspect of the emission spectra. Here the line shift is studied as a function of density and temperature of the plasma.

The line shift is produced by the level shift of the ions. The latter, however, is a result of many-particle effects. Via these effects the plasma state enters the line shift and other spectroscopic characteristics.

The most consequent way to include many-body effects in the two-particle spectrum is the determination of the spectral density of the two-particle Green's function in the s-channel [11]. The singularities of the spectral density yield the spectral information about two-particle like quasi particles in the interacting many-particle system and about their damping. Because of interaction with surrounding particles they cannot be strictly stationary.

The method used here is based on the solution of the Bethe-Salpeter equation for the two-particle Green's function in the particle-particle channel (s-channel). The problem is reduced to the solution of an effective wave equation [11–14].

In a previous paper [15] we solved the wave equation for hydrogen-like ions by means of the perturbation method. In this work we want to extend the validity region of our results to higher densities. As in the previous paper [15] we shall consider a plasma of electrons with the total number density of electrons  $n_e$ , nuclei (charge:  $Z\epsilon$ ) with the number density  $n_n$ . All the other species with the charge  $z\epsilon$  and  $z \leq (Z-1)$  are assumed to be present only with very low densities  $n_z \ll n_e$ . Electrons carry the charge  $(-\epsilon)$ . From charge neutrality follows

$$n_e = Z n_n. \quad (1)$$

For the number densities of neutral atoms  $n_0$ , the singly charged ions  $n_1$ , doubly charged ions  $n_2$  etc. hold the balance equations

$$n_e = n_e^* + \sum_{z=0}^{Z-1} (Z-z) n_z, \quad (2)$$
$$n_n = \sum_{z=0}^Z n_z.$$

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Here  $n_e^*$  denotes the number density of free electrons. For a pair of one electron and a  $Z$ -fold charged nucleus we have to solve the effective wave equation.

## 2. The Effective Wave Equation

The bare interaction  $V_{en}$  between the electron and the  $Z$ -fold charged nucleus is

$$V_{en} = -Z\epsilon^2/r. \quad (3)$$

Let us mention that the consideration of more complex bound states, as e.g. lithium-like ions requires the use of more elaborated potentials like those proposed by Rogers et al. [16]. Using the bare potentials as input into a many-body theory one arrives at an equation for the screened potential [14]:

$$\bar{V}_{en} = V_{en} + V_{en} P_{nn} \bar{V}_{nn} + V_{ee} P_{ee} \bar{V}_{en}. \quad (4)$$

In the static Debye approximation one arrives at

$$\bar{V}_{en}(r) = -Z\epsilon^2 r^{-1} \exp(-\kappa r) \quad (5)$$

with

$$\kappa = r_D^{-1} = [4\pi\epsilon^2(n_e^* + Z^2 n_n)/k_B T]^{1/2}. \quad (6)$$

Assuming as in [15] a nondegenerate plasma the effective wave equation has the form

$$\begin{aligned} \{p_1^2/2m_e + p_2^2/2m_n + \Delta_{en}(p_1 p_2) - \tilde{E}^{(Z-1)}\} \psi(p_1 p_2) \\ + \sum_q \bar{V}_{en}(q) \psi(p_1 - q, p_2 + q) = 0. \end{aligned} \quad (7)$$

Through  $\Delta_{en}$  the self energies of electrons and nuclei enter the wave equation

$$\Delta_{en}(p_1 p_2) \approx \text{Re } \Sigma_e(p_1, p_1^2/2m_e) + \text{Re } \Sigma_n(p_2, p_2^2/2m_n). \quad (8)$$

Within the rigid shift approximation [17] this rather complicated expression is replaced by

$$\Delta_{en}(p_1 p_2) \approx \Delta_e + \Delta_n = \text{Re } \Sigma_e(0, 0) + \text{Re } \Sigma_n(0, 0). \quad (9)$$

As shown earlier (cf. [17]),  $\Delta_e$  and  $\Delta_n$  correspond to the exchange interaction parts of the chemical potential. In the Debye approximation [15] holds

$$\Delta_e \approx -\frac{1}{2}\epsilon^2 \kappa, \quad \Delta_n \approx -\frac{1}{2}Z^2 \epsilon^2 \kappa. \quad (10)$$

In our earlier paper [15] the eigen values were approximated by perturbation theory. At large  $\kappa a_B \gg 1$  this leads to an overestimation of the level shift by 100%.

On the other hand, numerical calculations showed, however, [18, 19] that at certain values ( $\kappa a_B^Z = X_{kl}$ ) the levels  $\tilde{E}_{kl}$  merge into the continuum.

For the ground state level, Rogers et al. [18] found, e.g.,

$$X_{1S} = (\kappa a_B^Z) \approx 1.19; \quad a_B^Z = \hbar^2/Z\epsilon^2 \mu_{en}. \quad (11)$$

At this point the system undergoes the Mott-transition. The last bound state disappears and the ionization energy vanishes. Following [15], we represent the energies as follows:

$$\tilde{E}_{kl}^{(Z-1)} = E_{kl}^{(Z-1)} + \Delta_e + \Delta_n + \Delta_{kl}^{(Z-1)} \quad (12)$$

with

$$E_{kl}^{(Z-1)} = -Z\epsilon^2/2a_B^Z k^2.$$

In the frame work of the static perturbation-theory, the shift may be written as [15]

$$\Delta_{kl}^{(Z-1)} \approx Z\epsilon^2 \langle r^{-1} - r^{-1} \exp(-\kappa r) \rangle_{kl}. \quad (13)$$

By expanding the exponential function we get a Taylor series which was used in [15] for the construction of a Padé approximation. Unfortunately, we committed a mistake in the determination of the Padé coefficients so that the explicite form should have been

$$\begin{aligned} \Delta_{kl}^{(Z-1)} &= Z\epsilon^2 \kappa \frac{1 + a_{kl}^Z \kappa}{1 + b_{kl}^Z \kappa + c_{kl}^Z \kappa^2}, \\ a_{kl}^Z &= \{\frac{1}{4} \langle r \rangle_{kl}^2 - \frac{1}{6} \langle r^2 \rangle_{kl}\} \langle r^{-1} \rangle_{kl} D^{-1}, \\ D &= 1 - \frac{1}{2} \langle r \rangle_{kl} \langle r^{-1} \rangle_{kl}, \\ b_{kl}^Z &= \frac{1}{2} \langle r \rangle_{kl} + a_{kl}^Z, \\ c_{kl}^Z &= a_{kl}^Z / \langle r^{-1} \rangle_{kl}. \end{aligned} \quad (13a)$$

This result, however, overestimates the shift at high values  $\kappa a_B \gg 1$ , as we mentioned in the introduction.

Here, we shall use an other method which is based on a polynomial approximation. We represent the full level shift by the first three terms of the Taylor series. Finally we fit the coefficient of the  $\kappa^3$ -contribution in such a way that the effective ionization energy of the level

$$I_{kl}^{(Z-1)} = |E_{kl}^{(Z-1)}| - \Delta_{kl}^{(Z-1)} = 0 \quad (14)$$

disappears at ( $\kappa a_B^Z = X_{kl}$ ) in accordance with the numerical results [18, 19]. In this way, we find a polynomial of third order

$$\begin{aligned} \Delta_{kl}^{(Z-1)} &= Z\epsilon^2 \kappa \{1 - \frac{1}{2} \kappa \langle r \rangle_{kl} + \frac{1}{6} \kappa^2 \langle r^2 \rangle_{kl} \\ &\quad - \frac{1}{24} \kappa^3 \langle r^3 \rangle_{kl} + f_{kl}^{(Z-1)} (\kappa a_B^Z)^4\}, \end{aligned} \quad (15)$$

which is consistent with the first terms of the perturbation theory and with the numerical solutions as well. Introducing in (15) the expressions for the average

values of  $r$ ,  $r^2$  and  $r^3$  [20],

$$\langle r \rangle_{kl} = \frac{1}{2} [3k^2 - l(l+1)] a_B^Z = \langle \varrho \rangle_{kl} a_B^Z, \quad (16)$$

$$\langle r^2 \rangle_{kl} = \frac{1}{2} [5k^2 + 1 - 3l(l+1)] k^2 (a_B^Z)^2 = \langle \varrho^2 \rangle_{kl} (a_B^Z)^2,$$

$$\langle r^3 \rangle_{kl} = \frac{7}{4} k^2 a_B^Z \langle r^2 \rangle_{kl} - \frac{3}{16} k^2 (a_B^Z)^2 [(2l+1)^2 - 9] \langle r \rangle_{kl} \\ = \langle \varrho^3 \rangle_{kl} (a_B^Z)^3; \quad \varrho = r/a_B^Z$$

and using (12), (14), and (15), we come to the following expression for  $f_{kl}^{(Z-1)}$ :

$$f_{kl}^{(Z-1)} = - \left\{ 1 - \frac{1}{2} X_{kl} \langle \varrho \rangle_{kl} + \frac{1}{6} X_{kl}^2 \langle \varrho^2 \rangle_{kl} \right. \\ \left. - \frac{1}{24} X_{kl}^3 \langle \varrho^3 \rangle_{kl} - \frac{1}{2} k^{-2} X_{kl}^{-1} \right\} / X_{kl}^3 \quad (17a)$$

with expression for  $\langle \varrho \rangle_{kl}$ ,  $\langle \varrho^2 \rangle_{kl}$  and  $\langle \varrho^3 \rangle_{kl}$  which can be obtained from (16):

$$\langle \varrho \rangle_{kl} = \frac{1}{2} [3k^2 - l(l+1)], \\ \langle \varrho^2 \rangle_{kl} = \frac{1}{2} k^2 [5k^2 + 1 - 3l(l+1)], \quad (17b)$$

$$\langle \varrho^3 \rangle_{kl} = \frac{7}{4} k^2 \langle \varrho^2 \rangle_{kl} - \frac{3}{16} k^2 [(2l+1)^2 - 9] \langle \varrho \rangle_{kl}.$$

So the coefficient  $f_{kl}^{(Z-1)}$  in the polynomial is expressed in terms of the critical values  $X_{kl}$  where the level  $\{kl\}$  merges into the continuum and the quantum numbers  $k, l$ .

In this way we obtain for the level shift a function which depends only on  $X = \kappa a_B^Z$ . From (15) and (17) we have

$$\Delta_{kl}^{(Z-1)} = 2X |E_{kl}^{(Z-1)}| \\ \cdot \{1 - a_{kl}^{(Z-1)} X + b_{kl}^{(Z-1)} X^2 - c_{kl}^{(Z-1)} X^3 + f_{kl}^{(Z-1)} X^4\}$$

with

$$X \leq X_{kl}; \quad a_{kl}^{(Z-1)} = \frac{1}{2} \langle \varrho \rangle_{kl}, \\ b_{kl}^{(Z-1)} = \frac{1}{6} \langle \varrho^2 \rangle_{kl}; \quad c_{kl}^{(Z-1)} = \frac{1}{24} \langle \varrho^3 \rangle_{kl}. \quad (18)$$

We further assume that bound state levels stay pinned to the lowest continuum level, when they reach the continuum edge. In this moment these levels become very broad because of damping. Then it is further not reasonable to regard them as quasi stationary bound states [21].

### 3. Discussion of Line Shifts

The theory of the effective energy levels developed so far leads to the qualitative picture shown in Fig. 1 for the example of C VI bound states. Similar drawings may be obtained for all H-like bound states. The most essential result is that at fixed density the lowering of the levels decreases with increasing principal

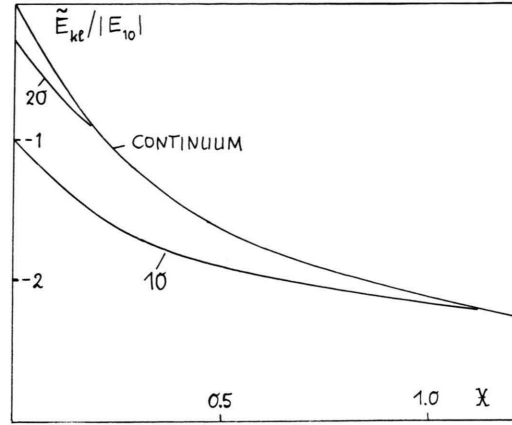


Fig. 1. The energy levels of C VI ions in dependence on the Mott-parameter  $X = a_B^Z / r_D$  ( $a_B^Z$  = Bohr radius,  $r_D$  = Debye radius).

quantum number. Further, at fixed principal quantum number the lowering is monotonously increased with the density up to certain density limit given by  $X_{kl}$  where the level merges into the continuum. An interesting result is, that in the line shifts calculated from (12)–(19) the self-energy contributions  $\Delta_e$  and  $\Delta_n$  cancel, which leads to line shifts

$$\Delta v(kl \rightarrow k'l') = h^{-1} \{ \Delta_{kl}^{(Z-1)} - \Delta_{k'l'}^{(Z-1)} \}. \quad (19)$$

Further, we see that  $\Delta v$  depends only on the dimensionless quantity

$$X = \kappa a_B^Z = a_B^Z / r_D, \quad r_D = \text{Debye radius.}$$

Inserting here the result (18) for  $\Delta_{kl}$ , the line shift agrees up to order  $X^2$  (coefficient  $a_{kl}^{(Z-1)}$ ) with the shifts determined by Pittman et al. [23]. Short range contributions to the interaction potential coming from occupied inner shells and leading e.g. to ion quadrupole effects in our case, however, are not taken into account.

At the critical values  $X = X_{kl}$  the lines merge, and therefore the shifts become constant (see Figure 2).

Here our approach differs from the confined ion model developed by Nguyen et al. [24]. They suppose generally that bound state energies merge into the continuum when the orbit radius  $r_{kl}$  comes into the order of the average particle distance  $R_0$ . Our result shows, however, that  $\Delta v$  depends only on the relation  $X$  between  $r_{kl}$  and the Debye radius  $r_D$ . At low densities and high temperatures ( $r_D > R_0$ ), the critical value  $X_{1s} = 1.19$  (or  $r_D = 0.84 a_B^Z$ ) for the ground state in our approach is reached at lower densities than the

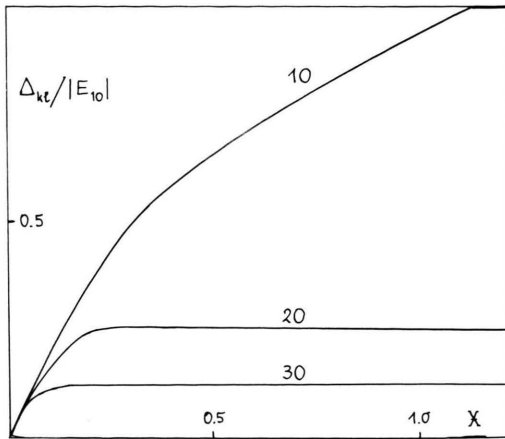


Fig. 2. The line shift as a function of the Mott-parameter and the quantum numbers.

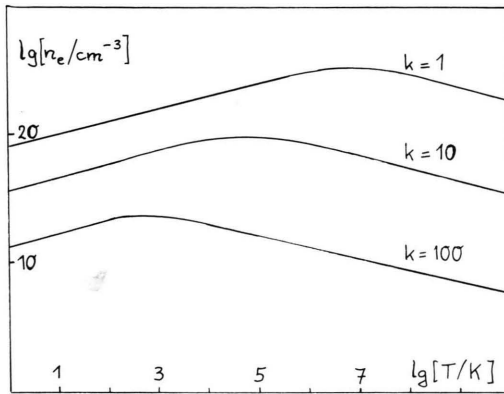


Fig. 3. Border lines in the density-temperature plane where the levels  $k l$  of C VI ions disappear. The l.h.s. of each border-line is determined by the Debye shift and the r.h.s. by the Pauli blocking effects.

confinement condition  $a_B^Z = R_0$  due to Nguen et al. So our level shifts at given densities are larger than those due to the confined ion model.

Let us discuss now the limits of the validity of this theory. The most serious limitation is due to the fact that we have neglected Pauli blocking effects. The essence of this is, that states occupied already by electrons cannot be occupied by other electrons. Among other effects, this leads to the relative “rigidness” of bound states. If a bound state (atom, ion etc.) is formed in a plasma, it needs some space which is not available to other electrons. Let us consider a simple estimate for these effects. A particle of radius  $R$  which is imbedded into a plasma shows (in the 2nd virial

coefficient approximation) the following shifts of the chemical potential:

$$\Delta\mu = \frac{1}{3} 4\pi k_B T R^3 (n_e^* + n_Z). \quad (20)$$

Following the general philosophy that shifts of energy levels correspond to shifts in the chemical potential [17], we may conclude that the finite volume required by a bound state  $k l$  leads to an energy level shift. With

$$R \sim a_B k^2$$

we get the estimate for the shift due to the Pauli blocking effects,

$$\Delta E_{kl}^{(Z-1)} \approx \frac{4\pi}{3} (a_B^Z k^2)^3 (n_e^* + n_Z). \quad (21)$$

In this way we have the following approximation for the level shift:

$$\Delta E_{kl}^{(Z-1)} \approx Z \varepsilon^2 \kappa + (4\pi k^6/3 Z^3) a_B^3 (1 + Z^{-1}) n_e^*. \quad (22)$$

Here we have used the Debye approximation for the contribution of screening and the 2nd virial approximation for the contribution of Pauli blocking (finite volume effects). We see in this way that the Coulombic approximation used in this paper is justified only if the inequality

$$\frac{4\pi}{3} k^6 (Z^{-3} + Z^{-4}) a_B^3 n_e^* \ll Z \varepsilon^2 \kappa \quad (23)$$

is fulfilled for all the existing energy levels. In general, this is not a severe restriction to the low levels but it might be relevant for high levels, so-called Rydberg states which require an enormous amount of space (Figure 2).

In this way we see that (23) provides upper limits for the temperature, density and the main quantum numbers which restrict the range of applicability of the theory presented here. Another restriction follows from the condition of degeneracy. Let us mention, however, that most “normal” plasmas do not violate the restrictions discussed here.

The estimate (21)–(22) is evidently in close relation to the formulae derived by Hummer, Mihalas, and Däppen [22] using quite other methods. This shows that the Pauli blocking effects discussed above bear physical reality. Let us underline, however, that a stronger theory of this effect, which seems to be important especially for the Rydberg states, does not yet exist. The way to a unique theory of the energy gap and line shifts requires more refined solutions of the Bethe-Salpeter equation [25].

- [1] U. Ackermann, K. H. Finken, and J. Musielok, *Phys. Rev. A* **31** (4), 2597 (1985).
- [2] F. Böttcher, J. Musielok, and H.-J. Kunze, *Phys. Rev.* **26** (5), 2265 (1987).
- [3] H.-J. Kunze, *Spectral Line Shapes*, Vol. 4 (R. J. Exton, ed.), A. Deepak Publishing, Hampton, Virginia, USA 1987.
- [4] F. Böttcher, P. Breger, J. D. Hey, and H.-J. Kunze, *Phys. Rev. A* (to be published).
- [5] A. Gawron, S. Maurmann, F. Böttcher, A. Meckler, and H.-J. Kunze, *Phys. Rev. A* (to be published).
- [6] Y. Vitel, *J. Phys. B, At. Mol. Phys.* **20**, 2327 (1987).
- [7] X. You and S. Ichimaru, *Phys. Rev. A* **34** (3), 2173 (1986).
- [8] M. J. Barlow, J. C. Blades, and D. G. Hummer, *Astrophys. J.* **241**, L 27 (1980).
- [9] R. H. Mendez and V. S. Niemala, *Wolf-Rayet Stars: Observations, Physics, Evolution*, p. 457 (C. W. H. de Loore and A. J. Willis, eds.), Reidel, Dordrecht, Holland 1982.
- [10] P. J. Storey and D. G. Hummer, *Mon. Nat. Roy. Astr. Soc.* **231**, 1139 (1988).
- [11] K. Kilimann, W. D. Kraeft, and D. Kremp, *Phys. Lett. A* **61**, 393 (1977).
- [12] R. Zimmermann, K. Kilimann, W. D. Kraeft, D. Kremp, and G. Röpke, *phys. stat. sol. (b)* **90**, 175 (1978).
- [13] K. Kilimann, D. Kremp, and G. Röpke, *Teoret. Matemat. Fizika* **55** (3), 448 (1983).
- [14] W. D. Kraeft, D. Kremp, W. Ebeling, and D. Röpke, *Quantum Statistics of Charged Particle Systems*, Akademie-Verlag 1986; Plenum Press, New York 1986.
- [15] W. Ebeling and K. Kilimann, *Z. Naturforsch.* **44a**, 519 (1989).
- [16] F. J. Rogers, B. G. Wilson, and C. A. Iglesias, *Phys. Rev. A* **38** (10), 5007 (1988).
- [17] R. Zimmermann, *Many-Particle Theory of Highly Excited Semiconductors*, Teubner-Texte zur Physik, Vol. 18, Leipzig 1988.
- [18] F. J. Rogers and H. C. Graboske, *Phys. Rev. A* **1**, 1577 (1970).
- [19] N. Bessis, G. Bessis, G. Corbel, and B. Dakhel, *J. Chem. Phys.* **63** (9), 3744 (1975).
- [20] A. Messiah, *Quantenmechanik I*, Appendix B 1.3, de Gruyter, Berlin 1976.
- [21] K. Kilimann, *Diss. B*, Rostock 1978.
- [22] D. G. Hummer and D. Mihalas, *Astrophys. J.* **331**, 794 (1988). – D. Mihalas, W. Däppen, and D. G. Hummer, *Astrophys. J.* **332**, 815 (1988). – W. Däppen, D. Mihalas, and D. G. Hummer, *Astrophys. J.* **332**, 261 (1988).
- [23] T. L. Pittman, P. Voigt, and D. E. Kelleher, *Phys. Rev. Lett.* **45**, 723 (1980).
- [24] H. Nguen, M. Koenig, D. Beuredjem, M. Caby, and G. Couland, *Phys. Rev. A* **33**, 1279 (1986).
- [25] G. Röpke and L. Hitschke, *Spectral Line Shapes* **5**, 49 (1989).