

Wave Function Properties and Shifted Energy Levels of Bound States in a Plasma

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On the basis of earlier work we show a simple way to estimate the properties of bound states in a plasma. The Bethe-Salpeter equation is approximated by an effective Schrödinger equation. The energy eigenvalues are found via a variation procedure. The treatment is applied to helium-like bound states and excited hydrogen-like states. The effect of the new energy eigenvalues on the plasma composition is discussed for the symmetrical electron-positron plasma.

Key words: Effective Schrödinger equation, Variation principle, Ionization energies, Plasma composition.

1. Introduction

Due to new experimental possibilities, Coulomb plasmas under extreme density and temperature conditions are of growing interest. For a consistent understanding of the pressure ionization it is necessary to take the spatial properties of bound states and the respective shift in the energy levels into account. It is one of the oldest problems of plasma physics to divide the actual many particle wave function into a bound and a free part. In our model the bound electrons are influenced by the surrounding plasma. With the length scaling obtained from the variation we have made the first step to find a density and temperature dependent radius for the bound state which may enter the thermodynamical calculation. In the preceding papers [1, 2] for hydrogen-like ions an effective Bohr radius was obtained by an analytical approximation based on a perturbation calculation. In the present paper we employ instead a simple variation theory and extend the range of application to helium-like bound states. Thus the main difference from [1, 2] is that the plasma influences the wave function consistently with the energy eigenvalues. The applied variation can be understood either formally as a standard procedure to evaluate any Schrödinger equation or as adjusting an electron density to a given environment. The latter interpretation yields the link to the Density Functional Theory (DFT) [5, 6] in which the bound state is regarded as a microscopic inhomogeneity and the

electron distribution as the quantity over which the energy has to be minimized.

2. The Theoretical Approach

In [3, 4] the basic plasma equation, the Bethe-Salpeter-Equation, (BSE) was established in the form of a two particle wave equation. In analogy to [3, 4] we formally write the more general equation

$$\begin{aligned} & \left\{ \sum_i \varepsilon_i(p_i) - E \right\} \Psi(p_1, \dots, p_N E) \\ & + \sum_{i < j} \sum_q V_{ij}(q_{ij}) \Psi(p_1, \dots, p_i - q_{ij}, \dots, p_j + q_{ij} E) \\ & = \sum_{i < j} \sum_{q_{ij}} H_{ij}^{pl}(p_i p_j; p_i - q_{ij}, p_j + q_{ij}; \omega) \\ & \cdot \Psi(\dots p_i - q_{ij}, \dots, p_j + q_{ij} E). \end{aligned} \quad (1)$$

It has to be mentioned that in this formulation N is not the total particle number. Equation (1) is written in the chemical picture, i.e. it describes the behaviour of N particles imbedded in a plasma whose influence is contained in the operator H^{pl} . Thus for $H^{pl} = 0$ the N particle Schrödinger equation arises. As outlined in [4] the plasma Hamiltonian may be split up into

$$H_{ij}^{pl} = \Delta_{ij} + \Delta V_{ij}^{eff}, \quad (2)$$

where between Δ and ΔV a consistency rule has to be obeyed [4]. The formulation (2) implies that the plasma effects can be understood as replacing the actual Coulomb-Potential by an effective one and the particle energies by shifted ones (i.e. including the self

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energy). This idea shall be the basis of the present paper, where the self energies are taken into account on a thermodynamic level (nonideal contributions to the thermodynamical potentials) whereas the effective potential establishes in lowest order an effective Schrödinger equation. For a first crude evaluation of the theory we shall restrict ourselves to the simplest case which consists in understanding the plasma as statistically screening the interactions. Then the key quantity is the inverse Debye radius κ :

$$\kappa^2 = 4\pi\beta e^2(n_e + \langle z^2 \rangle n_+).$$

Here $\beta = 1/(kT)$, n_e^* is the density of the free electrons and n_+ the overall ionic density

$$n_+ = \sum_{k=1}^Z k n_k$$

with Z the nuclear charge and $\langle f(z) \rangle$ denoting a charge average of a function $f(z)$:

$$\langle f(z) \rangle = \frac{1}{n_+} \sum_{k=1}^Z f(k) n_k.$$

If we thus replace the bare Coulomb potential by the screened one

$$\frac{1}{r} \rightarrow \frac{1}{r} \exp\{-\kappa r\},$$

we take the plasma effects into account. For hydrogen-like bound states one obtains immediately a Schrödinger equation for the relative motion. For more complex bound states the separation of the electron wave function,

$$\Psi(r_1, \dots, r_N) = \prod_{i=1}^N \Psi_0(r_i), \quad (3)$$

holds not generally, and thus any Schrödinger equation means an approximation. The Schrödinger equation which one obtains as the result of the Kohn-Sham treatment [5, 6] of the DFT yields not the true eigenvalues and eigenfunctions either, as has been pointed out in the refined applications of the DFT for plasmas [7–9]. We believe that the above separation is applicable for helium-like ions in the ground state. In contrast to the hydrogen-like case, where screening only means to weaken the binding of the electron to the nucleus, in the helium-like case we have the additional effect of screening the repulsion of the two bound electrons. This new effect is opposite to the first.

3. Application to Hydrogenlike Bound States

3.1. The Ground State

The treatment of the Schrödinger equation with the screened Coulomb potential has already been carried out by Krieger [10] for the ground state. We shall benefit from his result that a more-parameter variation can be reduced to a one-parameter procedure. With the test function

$$\Psi_0(r) = (\alpha^3 \pi)^{-1/2} \exp\{-r/\alpha\},$$

where $\alpha = a_0/Z = a_0^Z$ is the variation parameter and $a_0 = \hbar^2/m_e^2$ the Bohr radius, the expectation value of the ground state energy of a hydrogen-like ion with nuclear charge Ze is

$$\langle H_{\text{hydrogen-like}} \rangle = \frac{\hbar^2}{2m\alpha^2} - \frac{4Ze^2}{\alpha(2+\kappa\alpha)^2}. \quad (4)$$

The ground state is found via $\langle H \rangle'(\alpha) = 0$, which yields the equation for α :

$$a_0^Z = \alpha \frac{4}{(2+\kappa\alpha)^2} \left(1 + \frac{2\kappa\alpha}{2+\kappa\alpha} \right). \quad (5)$$

Equation (5) is written in an iterable implicate form which makes clear the transition $\alpha \rightarrow a_0^Z$ for vanishing plasma effects. The solution of (5) requires knowledge of the plasma composition, i.e. (5) has to be imbedded in thermodynamical calculations, either the minimization of the Helmholtz Free Energy or the solution of the Mass Action Law. But assuming a fully ionized plasma one has an upper limit for α :

$$n_e^* + \langle z^2 \rangle n_+ \rightarrow (Z^2 + Z) n_N, \quad n_N = \sum_{k=0}^Z n_k,$$

$$\kappa_{\max}^2 = 4\pi\beta e^2(Z^2 + Z) n_N,$$

Studying (5) with κ_{\max} yields a rough estimate for the heavy particle density for which the Mott transition occurs, i.e. the density for which in (4) holds

$$\langle H \rangle \geq 0 \quad \text{for all } \alpha \text{ (see Figure 1).}$$

Mott [11] obtained the critical values $\alpha = 2a_0^Z$ and $(\kappa\alpha) = 2$. Rogers et al. [12] evaluated the equation numerically and found the critical value $(\kappa a_0^Z) \cong 1.19$. The energy eigenvalues we obtain agree completely with those of Rogers up to relatively high screening parameters. Even the last value before the Mott transition deviates by less than 10%. Other variational and numerical treatments of the problem can be found in the literature [13, 14]. In contrast to them we main-

tain the simple α -scaling for the reasons explained above.

If we expand the expression (4) with respect to $(\kappa\alpha)$ and set in zeroth order $\alpha = a_0^Z$, we may extract the unperturbed term and arrive at

$$\langle H \rangle(a_0^Z) \cong -Z^2 \text{ Ryd} + Z e^2 \kappa - \frac{3}{4} Z e^2 \kappa^2 a_0^Z.$$

If we compare this result with the expressions for the shift in [1, 2] we find coincidence for the linear term. The deviation in the quadratic term contains the qualitatively new effect of the shift in the kinetic energy. Expanding the r.h.s. of (5) in the same sense, one sees that the linear terms in $\kappa\alpha$ cancel. The first order correction to a_0^Z thus is

$$\alpha \cong a_0^Z / [1 - \frac{1}{2} (\kappa a_0^Z)^2].$$

This estimate obviously holds only for small κa_0^Z . One may summarize that the results of [1, 2] coincide with the present one for the low density case. For the high density limit, in [1, 2] the shift is calculated with the assumption of perfect screening. This is contradictory since a perfectly screened nuclear charge should not be able to bind an electron. We believe the present formulation to be nearer to the actual physical situation since the Mott transition in (4) can thus be read as the point where the kinetic energy overtakes the potential energy.

3.2. Excited States

If the Ritz variation procedure is applied to an excited state, exact quantum mechanics requires orthogonality of the test function to the eigenfunctions

$$\begin{aligned} \langle H \rangle / Z^2 \text{ Ry} = & c_0^2 \left[\left(\frac{a_0^Z}{\alpha_0} \right)^2 - 8 \frac{a_0^Z}{\alpha_0} \frac{1}{(2 + \kappa \alpha_0)^2} \right] + \frac{c_1^2}{4} \left[\left(\frac{a_0^Z}{\alpha_1} \right)^2 - \frac{2 a_0^Z}{\alpha_1} \frac{1 + 2(\kappa \alpha_1)^2}{(1 + \kappa \alpha_1)^4} \right] \\ & + 16 \sqrt{2} c_0 c_1 (\alpha_0 \alpha_1)^{1/2} \left[\frac{a_0^Z (4 \alpha_1 - \alpha_0)}{(2 \alpha_1 + \alpha_0)^4} - a_0^Z \frac{2 \alpha_1 - \alpha_0 + 2 \kappa \alpha_0 \alpha_1}{(2 \alpha_1 + \alpha_0 + 2 \kappa \alpha_0 \alpha_1)^3} \right]; \quad \langle H \rangle'(\alpha_1) = 0 \end{aligned}$$

then yields the implicate equation for α_1 :

$$a_0^Z = \alpha_1 \left\{ \frac{1 + 5 \kappa \alpha_1 - 2 (\kappa \alpha_1)^2 + 6 (\kappa \alpha_1)^3}{(1 + \kappa \alpha_1)^5} + 2 \alpha_1^2 \left[\frac{A A'}{1 - A^2} K_1 + 16 \sqrt{2} \frac{A' (1 + A^2)}{1 - A^2} (\alpha_0 \alpha_1)^{1/2} K_2 + 8 \sqrt{2} A (\alpha_0 / \alpha_1)^{1/2} K_4 \right] \right\} \quad (7)$$

with

$$A = 32 \sqrt{2} (\alpha_0 \alpha_1)^{3/2} \frac{(\alpha_1 - \alpha_0)}{(2 \alpha_1 + \alpha_0)^4}, \quad A' = 16 \sqrt{2} \alpha_0 (\alpha_0 \alpha_1)^{1/2} \frac{-3 \alpha_0^2 + 15 \alpha_0 \alpha_1 - 6 \alpha_1^2}{(2 \alpha_1 + \alpha_0)^5},$$

$$K_1 = -\frac{16}{\alpha_0 (2 + \kappa \alpha_0)^2} + \frac{2 a_0^Z}{\alpha_0^2} - \frac{1 + 2(\kappa \alpha_1)^2}{\alpha_1 (1 + \kappa \alpha_1)^4} + \frac{a_0^Z}{2 \alpha_1^2}, \quad K_2 = \frac{2 \alpha_1 - \alpha_0 + 2 \kappa \alpha_0 \alpha_1}{(2 \alpha_1 + \alpha_0 + 2 \kappa \alpha_0 \alpha_1)^3} - \frac{a_0^Z (4 \alpha_1 - \alpha_0)}{(2 \alpha_1 + \alpha_0)^4},$$

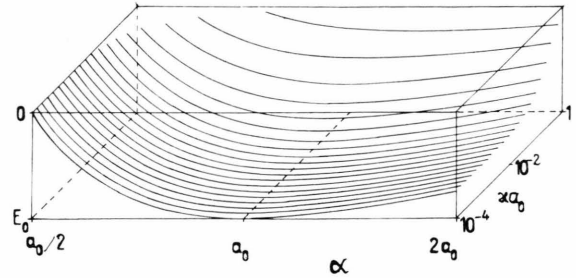


Fig. 1. $\langle H \rangle(\alpha)$ according to (4) vs. logarithmic scales of α and the nonideality parameter κa_0 for hydrogen.

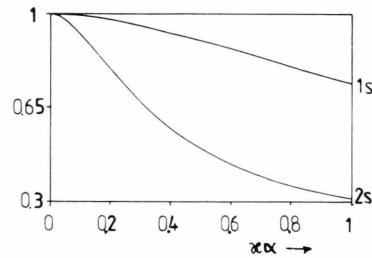


Fig. 2. The coefficients α_0 and α_1 in the implicate equations (5) and (7) for the 1s and 2s state versus the nonideality parameter $(\kappa \alpha_i)$.

belonging to the spectrum below. Thus we have the following test function:

$$\bar{\psi}_1 = c_0 \psi_0(r; \alpha_0) + c_1 \psi_1(r; \alpha_1),$$

with

$$\psi_1(r) = \frac{1}{2} (2 \alpha_1^3 \pi)^{-1/2} \left(1 - \frac{r}{2 \alpha_1} \right) \exp \left\{ -\frac{r}{2 \alpha_1} \right\}.$$

Here again $\alpha_1 = a_0/Z$ is the varied radius. We now evaluate the corresponding eigenvalue of H and minimize this with respect to α_1 :

and

$$K_4 = \frac{-\alpha_0^2 + 16\alpha_0\alpha_1 - 12\alpha_1^2 - 8\alpha_0\alpha_1(3\alpha_1 - 2\alpha_0) - 6(\alpha_0\alpha_1)^2}{(2\alpha_1 + \alpha_0 + 2\alpha_0\alpha_1)^4} + a_0^Z \frac{\alpha_0^2 - 26\alpha_0\alpha_1 + 40\alpha_1^2}{(2\alpha_1 + \alpha_0)^5}.$$

Due to the fifth power in the denominator the expansion for small ($\alpha\alpha$) gives again cancellation for the linear term, and for the ideal plasma the correct hydrogen parameter a_0^Z arises. In Fig. 2 the r.h.s. coefficients α_0 of (5) and α_1 of (6) with $c_0=0$ are plotted vs. $\alpha\alpha$ and show that the first excited state has a much faster increasing "radius" than the ground state. In the following we shall try a general estimate for higher order excitations. Though we will restrict ourselves to the unorthogonalized s-states the results should be a good estimate at least for weak screening. Dependences on the spherical harmonics should not change the α -behaviour because of the spherical symmetry of the Kepler Problem. The general s-state wave function is

$$\psi_s(r) = \alpha^{-3/2} c_s P_s(r) \exp\left(-\frac{r}{s\alpha}\right),$$

where the polynomial $P_s(r)$ is the Laguerre polynomial of s-th order. Then we have the expectation value of the Hamiltonian:

$$\begin{aligned} -\frac{\langle H \rangle}{2\pi Z e^2 c_s^2} &= \alpha^{-3} \left[a_0^Z \int_0^\infty dr \exp\left(-\frac{2r}{s\alpha}\right) P_s \left[r^2 P_s'' + 2r \left(1 - \frac{r}{s\alpha}\right) P_s' + \frac{r}{s\alpha} \left(\frac{r}{s\alpha} - 2\right) P_s \right] \right. \\ &\quad \left. + 2 \int_0^\infty dr r P_s^2(r) \exp\left\{-r \frac{2+s\alpha}{s\alpha}\right\} \right], \end{aligned} \quad (8)$$

where the first term is the kinetic energy expectation value $\langle T \rangle$ and the second that of the potential energy $\langle V \rangle$. Because of the structure

$$P_s(r) = \sum_{m=0}^s b_m \alpha^{-m} r^m$$

the first term may be expressed as

$$\begin{aligned} -\frac{\langle T \rangle}{2\pi Z e^2 c_s^2} &= \alpha^{-3} a_0^Z \int_0^\infty dr \exp\left(-\frac{2r}{s\alpha}\right) \sum_{m=0}^{2s+2} d_m \left(\frac{r}{\alpha}\right)^m \\ &= \alpha^{-3} a_0^Z \sum_{m=0}^{2s+2} d_m \alpha^{-m} m! \left(\frac{s\alpha}{2}\right)^{m+1} \\ &= -\alpha^{-2} t(s) a_0^Z. \end{aligned} \quad (9)$$

Analogously one finds

$$-\frac{\langle V \rangle}{2\pi Z e^2 c_s^2} = 2\alpha^{-1} \sum_{m=2}^{2s} f_m \left(\frac{s}{2+s\alpha}\right)^m. \quad (10)$$

The variational equation

$$\langle H' \rangle(\alpha) = 0$$

then yields

$$a_0^Z = \alpha t^{-1}(s) \sum_{m=2}^{2s} f_m \left(\frac{s}{2+s\alpha}\right)^m \left(1 + \frac{ms\alpha}{2+s\alpha}\right). \quad (11)$$

Further information we get from the request that for vanishing α the solution has to be $\alpha = a_0^Z$. This gives

$$\sum_{m=2}^{2s} f_m (s/2)^m = t(s). \quad (12)$$

To extract this term from (11) we expand the power series on the r.h.s. of (11) with respect to $\alpha\alpha$ and arrive at

$$a_0^Z = \alpha \left[1 - (s\alpha)^2 t^{-1}(s) \sum_{m=0}^{2s} f_m (s/2)^m \frac{m(m+1)}{4} \right] \quad (13)$$

and finally at

$$a_0^Z = \alpha(1 - (s\alpha)^2 g_s), \quad (14)$$

where for the constant g_s upper and lower bounds can be given. This equation proves that the "radii" of all excited states of the hydrogen spectrum increase with the density of the surrounding plasma. Another dependence is the increase with the square of the principle quantum number of the respective state. Thus we may expect that in nonideal plasmas the spectrum rapidly shrinks to some states at the energetic bottom. The shown behaviour of hydrogen-like bound states in a nonideal plasma leads to the assumption that the density ionization (the Mott-transition) has to be thought of as a delocalization process. With the flat-

tening of the bound electron probability distribution around the nucleus the link of the parameter α with a classical radius becomes more and more senseless.

4. Application to Helium-like Bound States

As already mentioned above, we will assume that the two electron wave function separates (see (3)):

$$\psi_0(r_1, r_2) = \frac{1}{\pi \alpha^3} \exp \left\{ -\frac{r_1 + r_2}{\alpha} \right\}.$$

Here again $\alpha = a_0^2/Z$ the variation parameter. In contrast to the hydrogen-like case the expectation value of the Hamiltonian contains an inneratomic electron repulsion term:

$$\langle H \rangle = \langle T \rangle + \langle V_{ez} \rangle + \langle V_{ee} \rangle.$$

For $\langle T \rangle$ and the electron-nucleus interaction the results are known from the computation above:

$$\langle T \rangle = \frac{\hbar^2}{m \alpha^2}, \quad \langle V_{ez} \rangle = -\frac{8 Z e^2}{\alpha (2 + \alpha)^2}.$$

The electron-electron interaction term is given by

$$\langle V_{ee} \rangle = \frac{8 e^2}{\alpha^6} I, \quad I = \int_0^\infty \int_0^\infty \int_{-1}^1 dr_1 dr_2 dz r_1^2 r_2^2 \frac{\exp \left\{ -\frac{2}{\alpha} (r_1 + r_2) - \alpha (r_1^2 + r_2^2 - 2 r_1 r_2 z)^{1/2} \right\}}{(r_1^2 + r_2^2 - 2 r_1 r_2 z)^{1/2}}.$$

After some calculation one arrives at

$$\langle V_{ee} \rangle = \frac{e^2}{2 \alpha (2 - \alpha)^2 (2 + \alpha)^4} (80 - 48 \alpha - 8 (\alpha)^2 + 4 (\alpha)^3 + (\alpha)^4). \quad (15)$$

It should be noted that for $(\alpha) \rightarrow 0$ the value

$$\langle V_{ee} \rangle = \frac{5}{8} \frac{e^2}{\alpha}$$

arises. This is in accordance with the known result of the Ritz procedure for the Helium atom (see for instance [15]). The defining relation for α

$$\langle H \rangle'(\alpha) = 0$$

has now the form

$$4 a_0 = \alpha \left[\frac{16 Z}{(2 + \alpha)^2} \left(1 + \frac{2 \alpha}{2 + \alpha} \right) - \frac{[4 + 4 \alpha - 7 (\alpha)^2] [80 - 48 \alpha - 8 (\alpha)^2 + 4 (\alpha)^3 + (\alpha)^4]}{(2 - \alpha)^3 (2 + \alpha)^5} - \alpha \frac{48 + 16 \alpha - 12 (\alpha)^2 - 4 (\alpha)^3}{(2 - \alpha)^2 (2 + \alpha)^4} \right]. \quad (16)$$

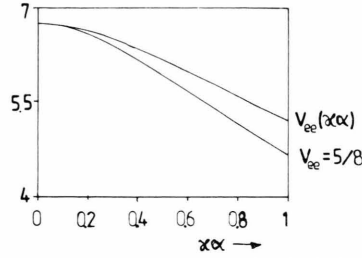


Fig. 3. The bracket expression in (16) for fully screened electron repulsion in comparison with the value for the decoupled atom vs. the nonideality parameter (α) .

The first term on the r.h.s. refers to the screened nucleus-electron interaction and is of the same structure as in the above discussed hydrogen-like theory. The second and third terms are of opposite sign and refer to the electron-electron interaction. In Fig. 3 the expression in the brackets is plotted as a function of $x = \alpha$. For comparison the same is plotted for the decoupled value $\langle V_{ee} \rangle = 5/8$. This illustrates the expected effect that the additional inneratomic electron effect hinders the increase of the "radius" parameter α though it is not capable to change the sign. It would

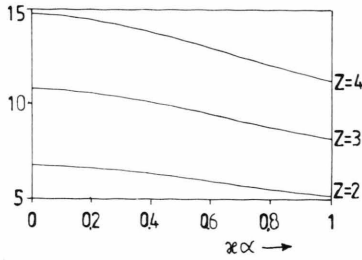


Fig. 4. The bracket expression in (16) for helium-like bound states with nuclear charges $Z=2, 3$ and 4 , respectively.

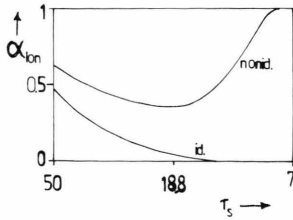


Fig. 5. The degree of ionization for the symmetrical electron-positron plasma (see (19)) for $\tau=0.1$. For comparison the ideal solution ($E_0 = -1 \text{ Ry}^*$) for the Saha-Equation is plotted.

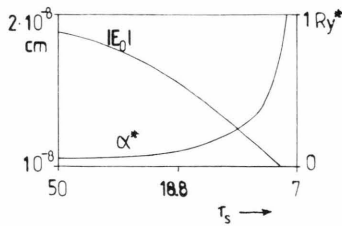


Fig. 6. The variation parameter α^* and the binding energy E_0 corresponding to the calculation of Figure 5. The Mott transition corresponds to a strongly increasing "radius" which is a hint for a delocalization process.

be a desirable theoretical result to show the general behaviour of a many-electron atom within this variational ansatz. In Fig. 4 the bracket expression is plotted for helium-like bound states with nuclear charges 2, 3, and 4, respectively. Since a thermodynamic calculation for a helium plasma can not yet be performed consistently we choose a simpler plasma to illustrate the thermodynamical consequences in the following paragraph.

5. Application to the Composition of the Symmetrical Plasma

For the bound states in symmetrical plasmas the hydrogen theory can be applied with a simple scaling.

The simplest possible case is the electron-positron plasma in vacuum. The thermodynamics of this plasma may be well approximated with the Coulomb interaction as the only source of nonideality [16]. Then we have the scaling laws

$$m^* = m_e/2, \quad a_0^* = 2a_0, \quad \text{Ry}^* = \text{Ry}/2$$

and get for the ground state

$$\langle H \rangle(x^*)/\text{Ry}^* = \left(\frac{a_0^*}{x^*} \right)^2 - \frac{a_0^*}{x^*} \frac{8}{(2 + x^*)^2}. \quad (17)$$

In an analogous manner one may exploit all results from paragraph 3. To estimate the plasma properties we regard the simplest kind of a Saha-equation. This is an equation for the degree of ionization $\alpha_{\text{ion}} = n_e^*/n_e^{\text{total}}$:

$$\frac{1 - \alpha_{\text{ion}}}{\alpha_{\text{ion}}^2} = n_e A_{\text{ep}}^3 \sum_s s^2 w_s \exp \{ -\beta \langle H \rangle^{(s)}(x_s) \}. \quad (18)$$

Here the electron-proton de-Broglie wavelength is

$$\Lambda_{\text{ep}} = 2^{3/2} \Lambda_e,$$

and the w_s 's contain the Planck-Brillouin-Larkin convention for the sum of states

$$w_s = 1 - \exp(\beta E_s^{(0)}) + \beta E_s^{(0)} \exp(\beta E_s^{(0)}),$$

where the unperturbed energy values have to be used. With the dimensionless parameters for density and temperature

$$r_s = \left(\frac{3}{4\pi n_e^*} \right)^{1/3} / a_0, \quad \tau = \frac{k_B T}{\text{Ry}}$$

we finally find

$$\frac{1 - \alpha_{\text{ion}}}{\alpha_{\text{ion}}} = 12 \sqrt{2\pi} r_s^{-3} \tau^{-3/2} \sum_s s^2 w_s \exp \left\{ -\frac{h_s}{\tau} \right\}, \quad (19)$$

where $h_s = \langle H \rangle^{(s)}(x_s)/\text{Ry}$. In this equation nonideality enters only via the h_s . This is in contrast to [16] where a similar equation has been formulated with the help of nonideal contributions to the chemical potentials. In Fig. 5 an example has been calculated which shows that already this very simple model yields all properties of a nonideal Coulomb plasma including the density ionization. In Fig. 6 over the same density scale the corresponding values for the binding energy E_0 and the respective values for α^* are plotted. Though the electron-positron plasma may be regarded as a study case far from reality, this model might easily be applied to "almost" symmetrical plasmas as excitation plasmas in semiconductors [16]. The application to

the thermodynamics of atomic plasmas is much more difficult since one has to deal with the different contributions to the Free Energy. The border of application for our simple model is given by the request that α has to be a small parameter. Approximating α by a_0^Z we may derive

$$n_c^* \ll \frac{1}{8\pi} \frac{\tau}{(a_0^Z)^3}. \quad (20)$$

If one is interested in the population of the excited states, (18) may easily be split up into a set of equations

$$n_s = n_c^{*2} A_{cp} w_s \exp \{ -\beta \langle H \rangle^{(s)}(\alpha_s) \}, \quad (21)$$

where s is the index of the excited state, the sum over which yields the overall bound states density

$$\sum_{s=0}^{\infty} n_s = n_{\text{bound}}.$$

The relative population may then be found by

$$n_s = n_{\text{bound}} \frac{w_s s^2 \exp \{ -\beta \langle H \rangle^{(s)} \}}{\sum_j w_j j^2 \exp \{ -\beta \langle H \rangle^{(j)} \}}. \quad (22)$$

Remembering now the result (14) one sees that the population distribution strongly deviates from the

Boltzmann distribution. Equations (21) and (22) are applicable to hydrogen plasmas as well.

7. Discussion

The presented model is on the one hand side a quantum statistically poor one since it does not contain the nowadays available refined corrections for Coulomb interaction. On the other hand it takes into account the change of the kinetic and potential part of the energy eigenvalues $\langle T \rangle$ and $\langle V \rangle$ consistently, which is beyond the reach for perturbation theories. In the application to a very simple case, the symmetrical electron-positron plasma we have shown that the model is sufficient to describe the so called density ionization. As a consequence for atomic plasmas the physical understanding of the Mott-transition has to be that of a delocalization process. This makes it more difficult to maintain the modelling of plasmas with different contributions to the Free Energy. This problem must be solved with better approximations for the effective potential. Another possibility to improve the model is to employ an inhomogeneous theory (DFT) which allows for a better treatment of the microscopic structure.

- [1] W. Ebeling and K. Kilimann, Z. Naturforsch. **44a**, 519 (1989).
- [2] K. Kilimann and W. Ebeling, Z. Naturforsch. **45a**, 613 (1990).
- [3] R. Zimmermann, K. Kilimann, W. D. Kraeft, D. Kremp, and G. Röpke, phys. stat. sol. (b) **90**, 175 (1978).
- [4] W. D. Kraeft et al., Quantum Statistics of Charged Particle Systems, Akademie-Verlag, Berlin 1986; Plenum Press, New York 1986.
- [5] E. Hohenberg and W. Kohn, Phys. Rev. **136B**, 864 (1964).
- [6] W. Kohn and L. Sham, Phys. Rev. **140A**, 1133 (1965).
- [7] F. Perrot, Strongly Coupled Plasma Physics (F. Rogers and H. DeWitt, eds.), Plenum Press, New York 1987.
- [8] C. Dharmawardana, ibid.
- [9] D. Ofer, E. Nardi, and Y. Rosenfeld, in press.
- [10] J. B. Krieger, Phys. Rev. **178**, 1337 (1969).
- [11] N. F. Mott, Phil. Mag. **6**, 287 (1961).
- [12] F. J. Rogers, H. C. Graboske, and D. J. Harwood, Phys. Rev. **A1**, 1577 (1970).
- [13] C. S. Lam and Y. P. Varshni, Phys. Rev. **A4**, 1875 (1971).
- [14] K. M. Roussel and O'Connell, Phys. Rev. **A9**, 52 (1974).
- [15] A. S. Davydow, Quantenmechanik, Deutscher Verlag der Wissenschaften, Berlin 1972.
- [16] W. Ebeling and H. Lehmann, Ann. Phys. **45**, 529 (1988).