Solution of the effective wave equation by perturbation theory in a dense hydrogen plasma

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The density dependence of two-particle states is an essential feature of nonideal plasmas and has to be taken into account for the investigation of the ionization equilibrium and the ionization and recombination processes in such plasmas. In this paper, we provide a rather simple method to calculate two-particle bound states in a dense hydrogen plasma and show that this problem can be dealt with in first order perturbation theory.

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I. INTRODUCTION AND THEORETICAL BACKGROUND

Strongly coupled plasmas are interesting many particle systems both from the theoretical and from the experimental points of view. Certain astrophysical objects such as the giant planets and the sun are dense strongly coupled plasmas. In laboratories, dense plasmas are investigated in heavy ion experiments in connection with inertially confined fusion. For references see, e.g., [1–6] and papers quoted therein.

Dense nonideal plasmas show a number of features which are essentially connected with the coupling of the particles. Here we mention the dynamical screening, the dynamical self energy, and the formation of bound states. The last is of special importance for the understanding of partially ionized plasmas. As we will show in detail, the energy levels of two-particle bound states and the continuum edge become density dependent, so that there is a crossover and thus a vanishing of localized states which is referred to as the Mott effect. Moreover, the effect of the surroundings leads to a damping and thus to a finite lifetime of bound states.

In this way, the optical, thermodynamic, and transport properties of partially ionized plasmas are changed drastically as compared with those of fully ionized plasmas on one hand and those of neutral gases on the other and may show, e.g., new types of phase transitions [7,8].

In the past, much work has been done in order to study the problem of two-particle states in different approximations, especially to deal with the numerical difficulties of a fully dynamical description. In 1970, Rogers *et al.* [9] published a solution of the Schrödinger equation, including many particle effects via the Debye potential. A Bethe-Salpeter equation with a dynamically screened Coulomb potential as an effective potential was given in 1977 using a Green's function technique [10] [see Eq. (1.4) below]. For the solution a pole approximation for the screening function was used in [10]. For electron-hole plasmas a consequent inclusion of many particle effects was done in [11–13], and the derivation of optical properties is described in [14,15]. In [16], a coupled nonlinear system of equations for Green's functions was solved numerically in order to determine two-particle properties. Recently, in [17] calculations were carried out with the full RPA (random phase approximation) dielectric function. It has been shown that the screening has to be taken into account dynamically and that the static description is valid only in the low density limit. Because of the complexity of such calculations, we investigate the question whether the procedure may be adequately replaced by a more simple (perturbative) one.

The appropriate starting point is the quantum statistical Green's function technique [18]. In this framework, one describes the properties of bound particles by the two-particle Green's function G_{ab}. We write the so called Bethe-Salpeter equation in the particle-particle channel [18,19]

$$G_{ab}(121'2') = G^0_{ab}(121'2') \pm i\hbar\int d3d4d\bar{3}d\bar{4}\, G_a(13) \times G_b(24)K_{ab}(34\bar{3}\,\bar{4})G_{ab}(\bar{3}\,\bar{4}1'2') \ , \quad (1.1)$$

where K_{ab} is the effective two-particle potential, which still contains all interactions of two particles. Here, e.g., $\bar{3} = (r_{\bar{3}}t_{\bar{3}})$, etc. In the screened potential approximation, K_{ab} is taken to be the screened two-particle potential

$$i\hbar K_{ab}(34\bar{3}\,\bar{4}) \approx i\hbar V^s_{ab}(34)\delta(3\bar{3})\delta(4\bar{4}). \quad (1.2)$$

This approximation means the restriction to dynamically screened two-particle interactions only. For the single-particle Green's function, we use a Dyson equation with self energy in the Montroll-Ward approximation [18]

$$G_a(11') = G^0_a(11') + \int d\bar{1}d2G^0_a(1\bar{1})\Sigma_a(\bar{1}2)G_a(21'),$$
$$\Sigma_a(\bar{1}2) = \Sigma^{\mathrm{HF}}_a(\bar{1}2) + \Sigma^{\mathrm{MW}}_a(\bar{1}2). \quad (1.3)$$

If we consider the relative motion with respect to the center of mass, the latter being at rest, and restrict ourselves to the region of nondegeneracy and therefore to the first order in density concerning the distribution functions, we get the following effective wave equation in momentum Matsubara representation [18]:

$$\left(\frac{\vec{p}^2}{2m_{ab}}-\hbar z\right)\psi_{ab}(\vec{p},z)+\int\frac{d\vec{q}}{(2\pi\hbar)^3}V_{ab}(q)\psi_{ab}(\vec{p}+\vec{q},z) = -\int\frac{d\vec{q}}{(2\pi\hbar)^3}\{V_{ab}(q)[-f_a(\vec{p})-f_b(\vec{p})]\psi_{ab}(\vec{p}+\vec{q},z)$$
$$-V_{ab}(q)[f_a(\vec{p}+\vec{q})+f_b(\vec{p}-\vec{q})]\psi_{ab}(\vec{p},z)\}$$
$$+\int\frac{d\vec{q}}{(2\pi\hbar)^3}\Delta V_{ab}^{\text{eff}}(\vec{q},\vec{p},z)\,[\psi_{ab}(\vec{p}+\vec{q},z)-\psi_{ab}(\vec{p},z)] \tag{1.4}$$

with

$$\Delta V_{ab}^{\text{eff}}(\vec{q},\vec{p},z) = V_{ab}(q)\int_{-\infty}^{+\infty}\frac{d(\hbar\omega)}{2\pi}\text{Im}\,\epsilon^{-1}(\vec{q},\omega+i\epsilon)$$
$$\times\left\{\frac{n_B(\hbar\omega)+1}{\hbar z-\hbar\omega-E_a(\vec{p})-E_b(-\vec{p}-\vec{q})}\right.$$
$$\left.+\frac{n_B(\hbar\omega)+1}{\hbar z-\hbar\omega-E_a(\vec{p}+\vec{q})-E_b(-\vec{p})}\right\}. \tag{1.5}$$

The one-particle Green's functions are taken with dynamical self energies. Here we have included in the first line of the right-hand side of Eq. (1.4) the phase space occupation effect (Pauli blocking) (i), in the second the exchange self energy (ii), and in the third line the dynamically screened effective potential correction (iii) and the dynamical self energy correction (iv). One can see that a compensation occurs between (i) and (ii) on one hand and (iii) and (iv) on the other in the limit $q \longrightarrow 0$. But this compensation acts only for bound states, where the wave function is sharply localized in coordinate space and not for scattering states, and so a Mott transition can take place. This results in a lowering of the effective ionization energy and thus influences such properties like the ionization cross section and recombination rates. For the continuum one has to take into account the self energies only:

$$E_{\text{cont}} = \Sigma_a^{\text{HF}}(p=0)+\Sigma_b^{\text{HF}}(p=0)+\Sigma^{\text{MW}}(p=0,E_{\text{cont}}) \tag{1.6}$$

with

$$\Sigma^{\text{MW}}(p=0,E_{\text{cont}}) = \int\frac{d\vec{q}}{(2\pi\hbar)^3}\,\Delta V_{ab}^{\text{eff}}(\vec{q},p=0,E_{\text{cont}}). \tag{1.7}$$

II. NUMERICAL SOLUTION

We assume that the solution of Eq. (1.4) is close to that of the Debye problem and that the perturbation is relatively small. This perturbation becomes larger in the region of the Mott transition, as one can see also from the results. We carry out first order perturbation theory

$$H_{ab} = H_{ab}^{\text{Debye}} + H_{ab}^{\text{plasma}}, \tag{2.1a}$$
$$E' = \frac{{}^D\langle\psi(\vec{p})|H_{ab}^{\text{plasma}}(\vec{p})|\psi(\vec{p})\rangle^D}{{}^D\langle\psi(\vec{p})|\psi(\vec{p})\rangle^D}, \tag{2.1b}$$
$$E = E^{\text{Debye}} + E'. \tag{2.1c}$$

In order to have the unperturbed problem on the left-hand side of the following equation (2.2) we add the Debye potential V^D on both sides, so that the perturbative plasma operator H_{ab}^{plasma} is represented by the right-hand side

$$\left(\frac{\vec{p}^2}{2m_{ab}}-\hbar z\right)\psi_{ab}^D(\vec{p},z)+\int\frac{d\vec{q}}{(2\pi\hbar)^3}V_{ab}^D(q)\psi_{ab}^D(\vec{p}+\vec{q},z)$$
$$=\int\frac{d\vec{q}}{(2\pi\hbar)^3}[V_{ab}^D(q)-V_{ab}(q)]\psi_{ab}^D(\vec{p}+\vec{q},z)$$
$$-\int\frac{d\vec{q}}{(2\pi\hbar)^3}V_{ab}(q)\,\{[-f_a(\vec{p})-f_b(-\vec{p})]\psi_{ab}^D(\vec{p}+\vec{q},z)-[f_a(\vec{p}+\vec{q})+f_b(\vec{p}-\vec{q})]\psi_{ab}^D(\vec{p},z)\}$$
$$+\int\frac{d\vec{q}}{(2\pi\hbar)^3}\Delta V_{ab}^{\text{eff}}(\vec{q},\vec{p},z)\,[\psi_{ab}^D(\vec{p}+\vec{q},z)-\psi_{ab}^D(\vec{p},z)]\,. \tag{2.2}$$

The Debye wave functions are determined by a simple Numerov algorithm and transformed into momentum space. In Fig. 1 one can see a delocalization tendency of the wave functions in position space, which means that bound states and scattering states become more similiar with increasing density. Using Legendre polynomials and orthogonality relations we can manage the angle dependence.

A. Static case

In the static case we replace the effective potential by the Debye potential, and for the self energy we simply take the Debye shift (this scheme corresponds to the Ecker-Weizel potential)

$$\Delta V_{ab}^{\text{eff}} = V_{ab}^D - V_{ab}, \qquad \Delta\Sigma_{ab}^{\text{eff}} = -\kappa e^2\,. \tag{2.3}$$

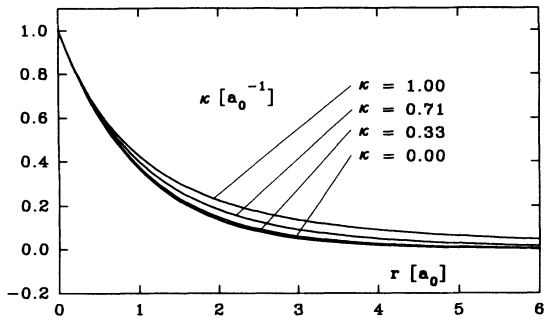

FIG. 1. Debye wave functions in position space. a_0 is the Bohr radius and $\kappa = \left(\sum_a \frac{n_a e^2}{\epsilon_0 k_B T}\right)^{1/2}$; one can see the delocalization with increasing density.

So we have

$$\left(\frac{\vec{p}^2}{2m_{ab}} - \kappa e^2 + \Sigma_a^{\rm HF} + \Sigma_b^{\rm HF}\right)\psi_{nlm}^D(\vec{p})$$

$$+[1 - f_a(\vec{p}) - f_b(\vec{p})]\int \frac{d\vec{q}}{(2\pi\hbar)^3} V_{ab}(\vec{q})\psi_{nlm}^D(\vec{p}+\vec{q})$$

$$+\int \frac{d\vec{q}}{(2\pi\hbar)^3}[V_{ab}^D(\vec{q}) - V_{ab}(\vec{q})]\psi_{nlm}^D(\vec{p}+\vec{q}) = E\psi_{nlm}^D(\vec{p}). \tag{2.4}$$

There are no numerical problems, and the results are the same as in [17,20].

B. Dynamical case

In order to find a better description of the screening we use the dynamical one. The behavior of the (dynamical) dielectric function, which we take in RPA, follows from

$$\epsilon^{\rm RPA}(\vec{q}, \omega + i\varepsilon)$$

$$= 1 + \sum_a \int \frac{d\vec{k}}{(2\pi\hbar)^3} V_{aa}(q) \frac{f_a(\vec{k}) - f_a(\vec{q}+\vec{k})}{E_a(\vec{k}) - E_a(\vec{q}+\vec{k}) + \hbar(\omega + i\varepsilon)}. \tag{2.5}$$

Using Heaviside units

$$\frac{e^2}{2} = 2m_e = \hbar = 4\pi\epsilon_o = 1, \tag{2.6}$$

and the parameters and dimensionless quantities

$$K = \sqrt{\frac{\hbar\omega_{pl}^e}{k_B T}}, \quad \delta_a = \frac{m_a}{m_e}, \quad \omega_e^{pl} = \sqrt{\frac{4\pi n_e e^2}{m_e}},$$
$$X^2 = \frac{\hbar^2 q^2}{2m_e}\frac{1}{\hbar\omega_{pl}^e}, \quad Y = \frac{\hbar\omega}{\hbar\omega_{pl}^e}, \quad X_0^2 = \frac{\hbar^2 p^2}{2m_e}\frac{1}{\hbar\omega_{pl}^e}, \tag{2.7}$$

we find in the nondegenerate case [18]

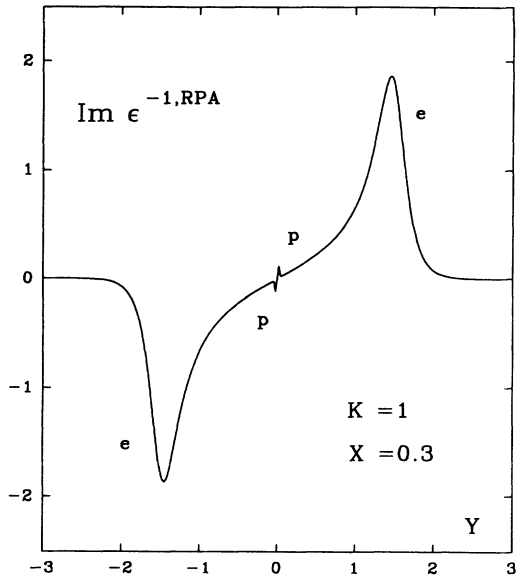

FIG. 2. $\mathrm{Im}\epsilon^{-1,\mathrm{RPA}}$. The peaks due to the electrons (e) are more pronounced than those due to the ions (p).

$$\mathrm{Re}\,\epsilon^{\rm RPA}(X,Y) = 1 + \frac{K^2}{4X^2}\sum_a \sum_{j=0}^{1}(-1)^j \left(\delta_a \frac{Y}{X^2} + (-1)^j\right) \times {}_1F_1\left[1, \frac{3}{2}; -\frac{1}{4\delta_a}\left(\delta_a \frac{Y}{X^2} + (-1)^j\right) \times K^2X^2\right],$$

$$\mathrm{Im}\,\epsilon^{\rm RPA}(X,Y) = \frac{\sqrt{\pi}}{4}\frac{K}{X^3}\sum_a \sum_{j=0}^{1} \delta_a^{1/2}(-1)^j e^{-\frac{1}{4\delta_a}A^2K^2X^2},$$

$$A = A(X,Y) = \delta_a \frac{Y}{X^2} + (-1)^j. \tag{2.8}$$

In Fig. 2 one can see that $\mathrm{Im}\epsilon^{-1,\mathrm{RPA}}$ becomes very sharply peaked for small momenta as a function of the frequency Y. This is the plasmon peak. The other singularity near the kinetic energies in the denominator of Eq. (1.5) has to be dealt with in the sense of the principal value.

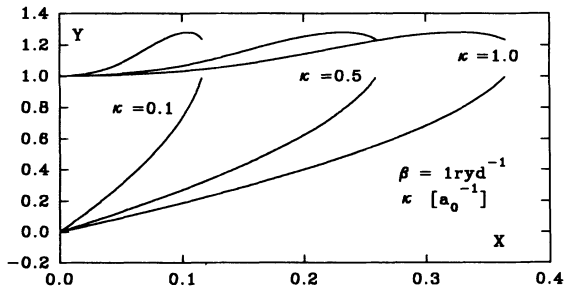

FIG. 3. Dispersion relation $\mathrm{Re}\epsilon^{\rm RPA}(X,Y) = 0$ for different densities. κ as in Fig. 1.

TABLE I. $1s$ two-particle bound state energies. Comparison of the results from [17] and this paper in different approximations. In the perturbative plasma operator H_{ab}^{plasma} (dynamical calculation). In the energy denominators of Eq. (1.5) $\hbar z$ is taken to be (1) E^{Coulomb} and (2) $E^{\text{Debye}} - \kappa e^2$. The continuum is taken from [17], $k_BT = 1$ Ry $= 13.6$ eV, $m_{ep} = 0.9995 m_e$.

κ_D	Debye	n_e (cm^{-3})	[17]	(1)	(2)	E_{cont}
1×10^{-6}	-0.9995	1.343×10^{11}	-0.9995	-0.9995	-0.9995	-2×10^{-6}
0.001	-0.9995	1.343×10^{17}	-0.9995	-0.9995	-0.9995	-0.0632
0.010	-0.9996	1.343×10^{19}	-0.9996	-0.9995	-0.9995	-0.1994
0.200	-1.0001	5.370×10^{19}	-0.9997	-0.9999	-0.9999	-0.2814
0.025	-1.0004	8.391×10^{19}	-0.9998	-1.0001	-1.0001	-0.3166
0.050	-1.0031	3.356×10^{20}	-1.0021	-1.0017	-1.0016	-0.4424
0.100	-1.0137	1.343×10^{21}	-1.0095	-1.0088	-1.0086	-0.6208
0.200	-1.0532	5.370×10^{21}	-1.0376	-1.0345	-1.0334	-0.8685
0.250	-1.0815	8.391×10^{21}	-1.0582	-1.0535	-1.0506	-0.9711
0.300	-1.1129	1.208×10^{22}	-1.0841	-1.0804	-1.0778	-1.0571

To manage the peaks in $\text{Im}\epsilon^{-1,\text{RPA}}$ near the plasmon frequency, we use a sum rule

$$\int_{-\infty}^{+\infty} dY\, Y \frac{\text{Im}\,\epsilon(X,Y)}{|\epsilon(X,Y)|^2} = -\pi. \tag{2.9}$$

The plasmon peaks are determined approximately by $\text{Re}\epsilon^{\text{RPA}}(X,Y) = 0$ (see Fig. 3).

As in [21,22] we rearrange the integrand in such a way that there is a zero contribution at the peak position. This is indicated for the electrons in $\text{Im}\epsilon^{-1}(X,Y)$ and one energy denominator in Eq. (1.5) only, namely,

$$\begin{aligned}\int_{-\infty}^{+\infty} \frac{1}{Y-Y_1^0} B(X,Y)\,dY &= \int_0^{+\infty} \left\{ \frac{1}{Y-Y_1^0} - \frac{Y}{Y_{\text{pl}}} \frac{n_B(Y_{\text{pl}})}{n_B(Y)(Y_{\text{pl}}-Y_1^0)} \right\} B(X,Y)\,dY \\ &+ \int_{-\infty}^{0} \left\{ \frac{1}{Y-Y_1^0} - \frac{Y}{Y_{\text{pl}}} \frac{n_B(-Y_{\text{pl}})}{n_B(Y)(Y_{\text{pl}}+Y_1^0)} \right\} B(X,Y)\,dY \\ &- \frac{\pi}{2} \left\{ \frac{n_B(Y_{\text{pl}})}{Y_{\text{pl}}(Y_{\text{pl}}-Y_1^0)} + \frac{n_B(-Y_{\text{pl}})}{Y_{\text{pl}}(Y_{\text{pl}}+Y_1^0)} \right\},\end{aligned} \tag{2.10}$$

with $B(X,Y) = \frac{\text{Im}\,\epsilon(X,Y)\, n_B(Y)}{|\epsilon(X,Y)|^2}$. Here $\pm Y_{\text{pl}}$ are the extrema of $\text{Im}\epsilon^{-1,\text{RPA}}$ located near the solution of the dispersion relation $\text{Re}\epsilon(X, \pm Y_{\text{pl}}) = 0$, and Y_1^0 stands for $E_a(X,X_0) + E_b(X,X_0) - \frac{\hbar z}{\omega_{\text{pl}}}$. Using this scheme one has to be aware of another singularity that occurs in the case $Y_{\text{pl}} \to Y_1^0$ in the subsequent angle or momentum integration, respectively. We used a principal value like integration method and got satisfying results.

Regarding Fig. 2 one may wonder why we take the ions in the dielectric function into the same account as the electrons although the peaks in $\text{Im}\epsilon^{-1,\text{RPA}}$ due to the ions are very small and could be neglected as compared to the electrons. But the ions change the behavior of such quantities like the self energy in a drastic way (see, e.g., [22]). To understand this one has to look at the combination of $\text{Im}\epsilon^{-1}$ with the other terms like the Bose function. One can see that for $Y \to 0$ ($\omega \to 0$) (see also Fig. 4)

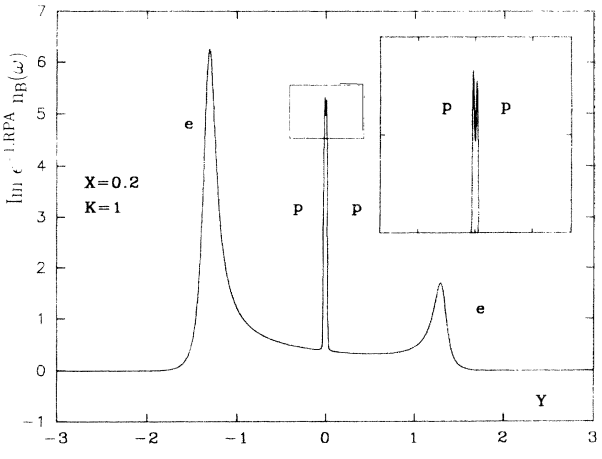

FIG. 4. $\text{Im}\epsilon^{-1,\text{RPA}} n_B(\omega)$. Now the peaks due to the ions (p) are not negligible.

$$\lim_{Y\to 0} \mathrm{Im}\epsilon(X,Y) n_B(Y) \sim \left(\frac{m_p}{m_e}\right)^{1/2}. \qquad (2.11)$$

And so in a hydrogenlike plasma with its big mass difference, we perhaps overestimate the contribution of the ions in the RPA and have to look for better approximations, while for electron-hole plasmas with equal masses of the components, the RPA works rather well [11,12].

III. RESULTS

We did our calculations for the real part of the two-particle state energies in the temperature range from 0.85 to 13.6 eV, which means for temperatures from 9.86×10^3 to 1.575×10^5 K and for densities up to the Mott transition depending on temperature. For temperatures $\leq 1.97 \times 10^4$ K and high densities one reaches the region of degeneracy where our approximations are no longer valid.

The numerical results show especially the compensation effect as stated in Sec. I. So the bound state levels are only weakly density dependent. This is not the case for plasmas with multiply charged ions, where there is a level shift proportional to $n^{1/2}$ [23].

Despite the fact that the plasma Hamiltonian H_{ab}^{plasma} is not small near the Mott transition and the basic assumption for perturbation theory becomes questionable, the general agreement with exact solutions of Eq. (1.4) in [17] is rather good.

The aim of this paper was to show that, in the temperature and density region of interest, perturbation theory gives reasonably good results. This may be concluded from the comparision with exact numerical solutions, which are much more time consuming. Moreover, one can see from Table I that the simple Ecker-Weizel level (Debye Hamiltonian) is sufficient to a good approximation. The latter case can be dealt with numerically even more simply than the perturbative scheme on a dynamical level.

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