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Screening of ionic cores in partially ionized plasmas within linear response

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We employ a pseudopotential approach to investigate the screening of ionic cores in partially ionized plasmas. Here, the effect of the tightly bound electrons is condensed into an effective potential between the (free) valence electrons and the ionic cores. Even for weak electron-ion coupling, the corresponding screening clouds show strong modifications from the Debye result for elements heavier than helium. Modifications of the theoretically predicted x-ray scattering signal and implications on measurements are discussed.

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I. INTRODUCTION

Partial ionization, degeneracy, and strong ionic correlations are often used to characterize warm dense matter (WDM) [1–3]. These are systems that cover the intermediate states between solids and hot plasmas, and they retain properties common to both. WDM states are of great interest for planetary physics [4–6] and also share direct similarities with other astrophysical systems such as nuclear matter and quark-gluon plasmas [2,7,8]. Indeed, WDM exhibits strongly coupled ions and degenerate electrons and, therefore, constitutes a strongly coupled quantum system.

Expansion techniques as used in traditional plasma physics incorporate correlations in a perturbative way and are thus not applicable in WDM. On the other hand, direct quantum simulations are limited by the number of particles and the region in parameter space they can treat with reasonable numerical effort (see, e.g., Refs. [9,10]). In this respect, experimental verifications of theoretical predictions becomes crucial for the progress in this field.

In the past decade time-resolved x-ray probing has been demonstrated to yield the basic plasma properties of dense matter as well as its ionic structure [11–14]. This experimental technique is particularly suited for a direct comparison with theoretical models for dense plasma and WDM since the main observable is the dynamic electron structure factor. This quantity contains rich information and, for low-Z plasmas which allow to neglect bound-free transitions, it can be decomposed as [15,16]

$$S_{ee}^{tot}(k,\omega) = [f_I(k) + q(k)]^2 S_{ii}(k,\omega) + S_{ee}^0(k,\omega). \qquad (1)$$

The first term corresponds to the quasielastic (Rayleigh) scattering by electrons that follow the ion motion: $f_I(k)$ denotes the atomic/ionic form factor, i.e., the density of tightly bound electrons in Fourier space, and $q(k)$ is the corresponding density of the electrons in the screening cloud. The ion-ion structure factor $S_{ii}(k,\omega)$ contains the information on the spatial structure and dynamics of the ions. Its dynamic range is less than twice the ion plasma frequency. In the experiments performed so far, this value is much smaller than the bandwidth of the x-ray probe radiation. Accordingly, one is not able to resolve the dynamics of the Rayleigh feature and, thus, we can treat ionic correlations frequency-integrated, i.e., statically: $S_{ii}(k) = \int S_{ii}(k,\omega)d\omega$.

The second term in Eq. (1) describes the scattering by dynamically free electrons. In the case of collective scattering from Langmuir waves, $S_{ee}^0(k,\omega)$ gives rise to a plasmon peak in the scattering spectrum [12]. For noncollective scattering, it samples the electron momentum distribution [11].

Most of the theoretical work presented in the past years has concentrated on the development of advanced models for the dynamics of correlated and degenerate electrons [17,18] and on the structure of the strongly coupled ion fluid [3,19–22]. Recent investigations of the ionic form factor $f_I(k)$ obtained shapes that are very close to such of wave functions of isolated atoms/ions [23,24]. On the other hand, the screening function $q(k)$ has not been given any significant attention. It is the main goal of this paper to show that more accurate modeling of $q(k)$ is required to describe quasielastic scattering from partially ionized warm dense matter. The small k-behavior of the signal is here of particular interest as present models fail to describe the strength of the Rayleigh feature measured in this limit.

II. SCREENING FUNCTION FOR FULLY IONIZED SYSTEMS

In a very general sense, the screening function $q(k)$ is defined via the partial structure factors in electron-ion systems [25]

$$q(k) = \sqrt{Z}\frac{S_{ei}(k)}{S_{ii}(k)}, \qquad (2)$$

where the electron-ion structure factor $S_{ei}(k)$ contains only free electrons and Z is the average ion charge. Thus, calculating $q(k)$ would require the electron-ion structure of fully coupled systems.

However, many systems from plasmas to solids can be treated within linear response as higher orders in the interaction potential cancel to a large extent [26,27]. Neglecting these higher order correlations, the screening function is given by

$$q(k) = \chi_e(k)V_{ei}(k) \tag{3}$$

with the susceptibility of the free electrons $\chi_e(k)$ in the static, that is $\omega \to 0$, limit. Applying the random phase approximation (RPA), the latter can be expressed as

$$\chi_e^{\mathrm{RPA}}(k) = \chi_e^0/[1 - \chi_e^0 V_{ee}(k)] = \chi_e^0/\varepsilon_e^{\mathrm{RPA}}(k), \tag{4}$$

where $\chi_e^0 = \kappa_e^2/4\pi e^2$ is the density response function of a noninteracting gas which becomes $\chi^0 = n_e/k_B T_e$ in the nondegenerate limit. $\varepsilon_e^{\mathrm{RPA}}(k) = (k^2+\kappa_e^2)/k^2$ is the well-known dielectric function in RPA. Combining Eqs. (2) and (3), we obtain for the electron-ion structure factor

$$S_{ei}(k) = \sqrt{Z}\frac{\kappa_e^2}{k^2} S_{ii}(k) S_{ee}^0(k), \tag{5}$$

where $S_{ee}^0(k) = k^2/(k^2+\kappa_e^2)$ [28], and

$$q^{\mathrm{RPA}}(k) = Z\frac{\kappa_e^2}{k^2+\kappa_e^2}. \tag{6}$$

for the screening function within linear response in fully ionized plasmas interacting by Coulomb forces. Note that RPA is the lowest order approximation that ensures the correct long wavelength limit $\lim_{k\to 0} q(k) = Z$.

To account for partial degeneracy of the electron gas, the inverse screening length κ_e should be calculated by $\kappa_e^2 = (4e^2 m_e)/(\pi\hbar^3)\int f_e(p)dp$, where $f_e(p)$ is the Fermi distribution. Practically, it might be more attractive to use the Debye form with an effective temperature [29]. Here, we suggest the form

$$\kappa_e^2 = \frac{4\pi e^2 n_e}{k_B T_e^{\mathrm{eff}}} \quad \text{with} \quad T_e^{\mathrm{eff}} = (T_e^4 + T_F^4)^{1/4}, \tag{7}$$

which interpolates between the Debye and the Thomas-Fermi screening length and yields results with less than 2% error for all densities.

III. SCREENING FUNCTION FOR PARTIALLY IONIZED MATTER

In a partially ionized plasma, the interaction between the free electrons and the ions is also influenced by the bound states that are occupied. The main effect is that core and valence electrons must build an antisymmetric state. Thus, the core electrons effectively block a volume close to the nucleus. If the core electrons are not considered explicitly, their effect might be described by an effective electron-ion potential that is strongly modified near the nucleus while it approaches the bare Coulomb potential at large distances [30]. The most simple form for such a pseudopotential is the empty core potential [31]

$$V_{ei}^{\mathrm{ec}}(r) = \begin{cases} \dfrac{Ze^2}{r} & \text{for } r > r_{cut} \\ 0 & \text{otherwise} \end{cases}. \tag{8}$$

The core radius r_{cut} is treated here as a free parameter and can be fit to match experimental data on transport and optical properties of the medium under investigation. This very simple potential was nevertheless successfully employed in the description of the properties of electrons in solids and liquid metals [30,32].

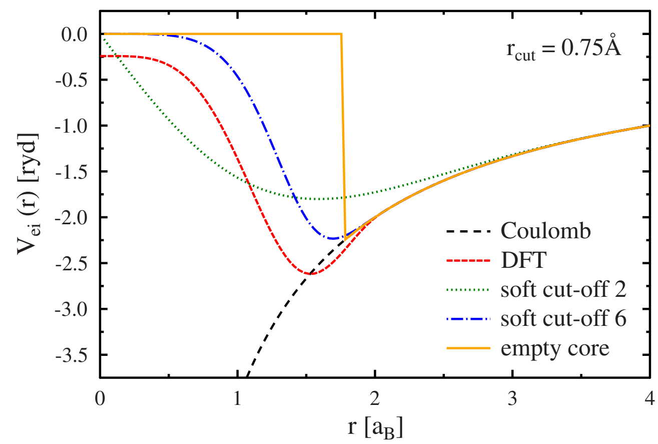

FIG. 1. (Color online) Effective electron-ion potentials that are considered in this paper. The soft core potential, defined by Eq. (10), is shown for exponents $\alpha=2$ and $\alpha=6$. The curve labeled DFT gives the norm-conserving potential for beryllium used in density functional calculation when the 1s electrons are frozen out.

Inserting the Fourier transform of the potential [Eq. (8)] into the expression (3), we obtain for the screening function

$$q(k) = Z\frac{\kappa_e^2}{k^2+\kappa_e^2}\cos(kr_{cut}). \tag{9}$$

Comparing Eqs. (6) and (9), we see that the main effect of the pseudopotential is a modulation of the screening function $q(k)$ with the possibility of negative values at intermediate wavelengths. Note that the density of the screening clouds in real space is positive definite, but not its Fourier components. Negative screening is a well-known effect in solid state physics [26,27]. This behavior arises from the fact that the bound electrons repel valence electrons near the nucleus and, thus, reducing the effect of screening at short distances; quasineutrality requires that screening is then compensated at large distances.

The empty core potential [Eq. (8)] is not the only possible choice to account for partial ionization. Indeed, the hard cut-off edge can constitute a problem as it triggers strong oscillations in Fourier space. Therefore, we also employ potentials with a soft empty core having the form

$$V_{ei}^{\mathrm{soft}}(r) = \frac{Ze^2}{r}\left[1 - \exp\left(-\frac{r^\alpha}{r_{cut}^\alpha}\right)\right]. \tag{10}$$

The parameter α controls the steepness of the core edge and, in combination with r_{cut}, the depth of the minimum: while the pseudopotential [Eq. (10)] is very soft for $\alpha=1$, it approaches the empty core potential [Eq. (8)] for $\alpha\to\infty$.

Figure 1 displays the different pseudopotentials and compares them with the bare Coulomb potential. We also show a potential that was created to describe the interaction of valence electrons with a beryllium nucleus that has the two 1s electrons attached. Similar norm-conserving pseudopotentials are very successfully used in density functional calcula-

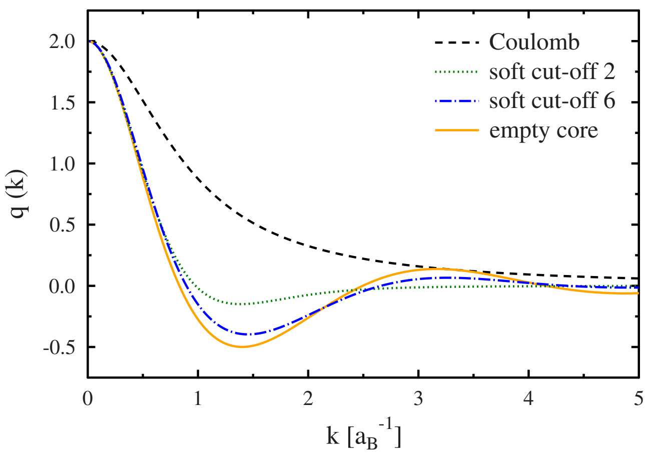

FIG. 2. (Color online) Screening function $q(k)$ obtained in linear response [Eq. (3)] applying different effective potentials. The plasma parameters were taken for beryllium at solid density ($\varrho = 1.848\ \mathrm{g/cm^{-3}}$) and $T=12$ eV. The ion charge state is $Z=2$. The free cutoff parameter in the pseudopotentials is set to be $r_{cut} = 1$ Å.

tions as they strongly reduce the computational effort. The potential shown here was taken from the VASP package [33,34]. Clearly, its form is best resembled by the soft cutoff potential [Eq. (10)] with an exponent of $\alpha=6$. Although these two potentials do not fully match, we can hope to catch the important physics qualitatively by the analytic potential.

The screening functions corresponding to the different pseudopotentials are plotted in Fig. 2 for isochorically heated beryllium as it was experimentally investigated in Refs. [11,12]. Compared to the calculations using Coulomb interactions (as it would be applicable in fully ionized plasmas), the screening function is significantly reduced for wavelengths $k < 3a_B^{-1}$ if we employ a pseudopotential. The extent of the reduction depends on both the functional form of the potential and the cutoff radius. The latter is demonstrated in Fig. 3 for the case of the soft core potential [Eq. (10)] with $\alpha=6$. In particular, we see that large cutoff radii are required to suppress screening at intermediate wavelengths. Unfortunately, data published for the cutoff radii show a considerable spread which is related to the different choice for the material property that was fit [35–37]. The values used for r_{cut} in Fig. 3 are within the published range.

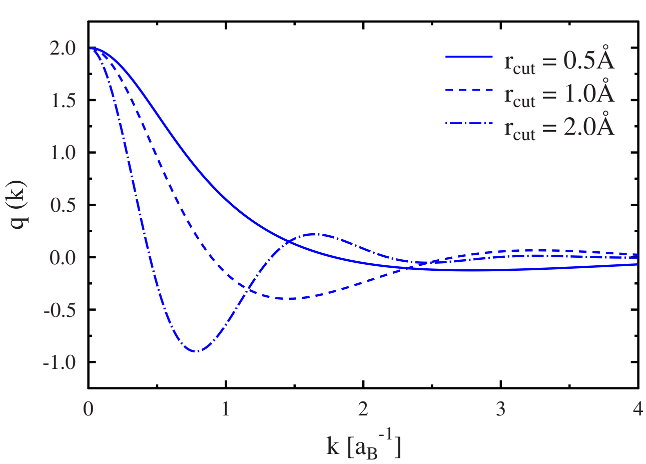

FIG. 3. (Color online) Influence of the cutoff radius r_{cut} on the screening function $q(k)$ using the soft cutoff potential [Eq. (10)] with $\alpha=6$. Plasma conditions as in Fig. 2.

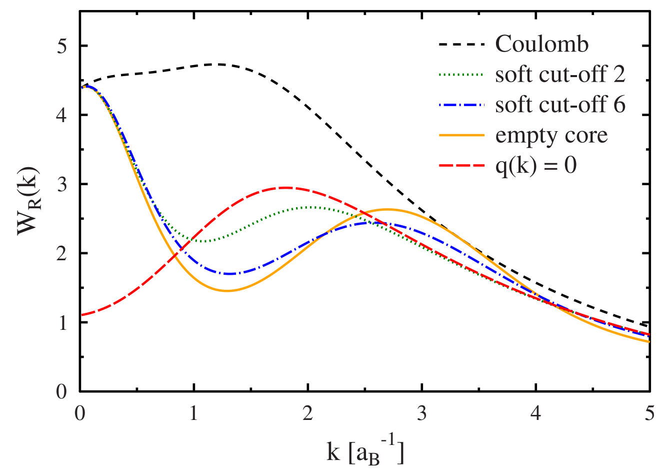

FIG. 4. (Color online) Weight of the Rayleigh peak in the scattering signal, that is $W_R(k) = |f_I(k) + q(k)|^2 S_{ii}(k)$ which is calculated for pseudopotentials and plasma conditions as in Fig. 2. For comparison, we also report $W_R(k)$ for the case where the screening function is set zero.

IV. IMPLICATIONS ON X-RAY SCATTERING EXPERIMENTS

The possibility of a significantly reduced (or even negative) screening function $q(k)$ has important implications on the interpretation of x-ray scattering signals. As discussed in the recent review [3], the intensity of the quasi-elastic Rayleigh peak in the collective regime, i.e., for small k, has been often found to be much lower than predicted by calculations using RPA and ion-ion structure factors obtained from screened interactions. As the weight of the Rayleigh feature can be summarized as

$$W_R(k) = |f_I(k) + q(k)|^2 S_{ii}(k), \tag{11}$$

the theoretical estimates of either the electron properties described by $f_I(k)$ and $q(k)$ or the ionic structure, i.e., $S_{ii}(k)$, must be revised.

HNC calculations based on a one-component plasma model using unscreened Coulomb interactions yield sufficiently low ion-ion structure factors [3]. However, these predictions are inconsistent as there should be $q(k)=0$ in this case. Moreover, this model was not confirmed by recent experimental findings [14] nor *ab initio* simulations [20,38].

On the other hand, a small or even negative screening function, that arises due to core electrons blocking the space around the nucleus, offers a viable and plausible interpretation of the small Rayleigh signals seen in the collective scattering regime. In Fig. 4, we plot the weight of the Rayleigh term $W_R(k)$ as calculated from different screening models. For the ionic form factor of the 1s electrons, we used hydrogenlike wave functions [40,39]. The ion-ion structure factor was calculated by the HNC method employing a linearly screened ion-ion potential which yields results similar to *ab initio* simulations [19,20]. Figure 4 shows that the intensity of the Rayleigh scattering is strongly reduced for $k < 3a_B^{-1}$ if pseudopotentials are applied. While $q(k)$ is reduced for small to intermediate k values, the long wavelength limit is still preserved, that is $\lim_{k\to 0} q(k)=Z$ and particle conservation is satisfied. Although this description needs improvements to allow for a quantitative comparison, the trend of the effect is in agreement with experimental findings.

V. CONCLUDING REMARKS

We have used a pseudopotential approach to investigate the effect of occupied core states on the interaction of free electrons with ions in partially ionized plasmas. Here, the effect of the tightly bound electrons is condensed into an effective potential between valence/free electrons and the ionic core. We have shown that even for weak electron-ion coupling, that allows a treatment within linear response, the corresponding form of the screening function $q(k)$ shows strong modifications from the Debye result for low-Z elements (using beryllium as an example). Such modifications manifest themselves as a reduction of the screening at intermediate wavelengths, with the possibility of negative screening. We suggest that this effect yield a major advantage toward a plausible interpretation of the reduced Rayleigh signals observed in recent x-ray scattering experiments. A quantitative comparison is however impossible here as we only applied model potentials. Future work will therefore concentrate to obtain more realistic electron-ion pseudopotentials that allow for a direct comparison with experiments and improve their interpretation.

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