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Static structure factor of electrons around a heavy positively charged impurity in a one-component quantum rare plasma

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Abstract. An expression for the static structure factor, $g^{+-}(r)$, of electrons at a distance r from an infinitely heavy positively charged particle in a one component quantum rare plasma has been obtained in linear response theory using an appropriate quantum dielectric function of the rare plasma. The expression is a complicated function of the electron plasma frequency, Debye screening length and r, but reduces to that of classical plasma when quantum corrections are neglected. For $r < r_s$ ($2r_s$ being the mean distance between two electrons), the temperature dependent $g^{+-}(r)$ has larger values in quantum case in comparison to that in classical situation and keeps increasing with decrease in r, more so at low temperatures when de-Broglie wavelength becomes larger and a considerable fraction of r_s.

Keywords. Static structure factor; charged impurity; one component quantum rare plasma.

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1. Introduction

An expression for the static structure factor of electrons around a massive positively charged particle, such as a proton or an heavy ion in a one component classical rare plasma which one encounters in semiconductors, ionosphere and intergalactic space to name a few examples, has been derived taking into account nonlinear effects [1]. The expression is dependent upon certain distance r_0, the distance of closest approach of electrons to the impurity, which is to be judiciously chosen. Since $r_0 \gg \lambda_{th}$ (thermal de Broglie wavelength of electrons), no quantum correction is needed. However, if the electrons build up close to the impurity, that is $r \sim \lambda_{th}$, is to be studied one would have to use an appropriate quantum dielectric function. In the present communication we report the results of such an investigation of static structure factor of electrons around a heavy positively charged impurity in one component quantum rare plasma in the linear response theory.

2. Mathematical formalism

The expression for the static structure factor is given as

$$g^{+-}(r) = 1 + \frac{1}{(2\pi)^3}\int v^{\pm}(\bar{q})\exp(-i\bar{q}\cdot\bar{r})\overline{\mathrm{d}q}. \tag{1}$$

When the density of positive charge introduced in the system is small then $v^{\pm}(q)$ [2] is given by

$$v^{\pm}(\bar{q}) = -\frac{Z}{n^{-}}\mathrm{Re}\left(\frac{1}{\varepsilon^{--}[\bar{q},(\hbar q^2/2m)]} - 1\right) + \frac{z}{n^{-}}\frac{2}{\pi}\int_0^{\infty}\mathrm{d}\omega\,\mathrm{Im}\left(\frac{1}{\varepsilon^{--}(\bar{q},\omega)}\right)P\left[\frac{\hbar q^2/2M}{\omega^2-(\hbar q^2/2M)^2}\right], \tag{2}$$

where $\varepsilon^{--}(q,\omega)$ is the dielectric function of the plasma, z is an integer, n^{-} is the number density of electrons of the system, $\omega, \bar{q}$ are the angular frequency and wave-vector respectively and M is the mass of positively charged impurity.

Since, we are considering $M = \infty$, $v^{\pm}(q)$ reduces to

$$v^{\pm}(\bar{q}) = -\frac{z}{n^{-}}\mathrm{Re}\left[\frac{1}{\varepsilon^{--}(\bar{q},0)} - 1\right]. \tag{3}$$

Using the quantum two particle distribution function in one component rare plasma assembly having Maxwellian momentum distribution funtion, the expression for quantum dielectric function at zero frequency [3, 4] is given as

$$\varepsilon_q(0) = 1 + \frac{1}{q^2 d^2}\left[\frac{z' + g(z')}{z'+1}\right], \tag{4}$$

$$z' = q\lambda_{\mathrm{th}}/2,$$

where

$$g(Z') = \exp(-z')^2\int_0^1 \exp(z'^2x^2)\mathrm{d}x, \tag{5}$$

and

$$d^2 = V^2/\omega_p^2(z'+1).$$

Substituting $\sqrt{\alpha}x = iu$ in (5) and integrating [5] we get

$$g(z') = \exp(-z')^2\left[1 - \frac{(\sqrt{\alpha}/i)^2}{3} + \frac{(\sqrt{\alpha}/i)^4}{10} - + \ldots\right] \tag{6}$$

which in the case of $z'^2 < 1$ reduces to

$$g(z') = 1 - \frac{2}{3}z'^2 - \frac{7}{30}z'^4 - \ldots \tag{7}$$

Using (7) in (4) we get

$$\varepsilon_q(0) = \left[1 + \frac{\omega_p^2}{q^2V^2} + \frac{1}{2\sqrt{2}}\frac{h\omega_p}{k_{\mathrm{B}}T}\frac{\omega_p}{qV} + \frac{1}{24}\left(\frac{h\omega_p}{k_{\mathrm{B}}T}\right)^2 + \ldots\right], \tag{8}$$

where h is Planck's constant; $\omega_p(=(4\pi n^{-}e^2/m)^{1/2})$ is the angular plasma frequency, e and m_e are the charge and mass of electrons respectively; $V(=(k_B T/m)^{1/2})$ is the thermal velocity of electron, k_{B} is the Boltzmann's constant and T is the temperature of the plasma.

When $h \to 0$ (8) reduces to the well-known classical expression for $\varepsilon_q(0)$ [1, 4–8],

$$\varepsilon_q(0) = 1 + \frac{\omega_p^2}{q^2V^2}. \tag{9}$$

Equation (8) represents the quantum mechanical dielectric function of the plasma in which contributions up to h^2 have been taken into account. One can go to higher order terms in h using further terms in (8).

It may be pointed out here, that these quantum corrections appear only because the rare plasma has become mildly degenerate so that consideration of Fermi-Dirac statistics which appear when the plasma becomes strongly degenerate, is not required. That is, one continues to use the Maxwellian distribution function with modified linear momenta only.

We can write down $\varepsilon_q(0)$ given by (8) in the following alternate form

$$\varepsilon_q(0) = D + \frac{c}{q} + \frac{a^2}{q^2}, \tag{10}$$

where

$$a^2 = \frac{\omega_p^2}{V^2} = \frac{1}{\lambda_D^2};\ \lambda_D \text{ is the Debye screening length,}$$

$$c = a^2 \lambda_{th}/2 = a\mu/2,\ \lambda_{th} = \frac{h}{(2mk_B T)^{1/2}},$$

$$D = 1 - \frac{1}{6}\mu^2 \text{ and } \mu = \lambda_{th}/\lambda_D.$$

Substituting (10) in (3) we get for

$$v^{\pm}(q) = \frac{z}{n^-}\left[\frac{a^2 + (\mu q/2)(a - \frac{1}{3}\mu q)}{a^2 + q^2 + (\mu q/2)(a - \frac{1}{3}\mu q)}\right]. \tag{11}$$

Using $v^{\pm}(q)$ given above in (1), performing θ and ϕ integrations and some mathematical manipulations we get an expression for the static structure factor as

$$g^{+-}(r) - 1 = \frac{z}{2\pi^2 r n^-}\left[a^2 \frac{d}{dr}\int_0^\infty \frac{(-\cos qr)dq}{a^2 + q^2 + (\mu q/2)(a - \frac{1}{3}\mu q)}\right.$$

$$+ \frac{a\mu}{2}\frac{d^2}{dr^2}\int_0^\infty \frac{(-\sin qr)dq}{a^2 + q^2 + (\mu q/2)(a - \frac{1}{3}\mu q)}$$

$$\left. - \frac{1}{6}\mu^2 \frac{d^3}{dr^3}\int_0^\infty \frac{\cos qr\, dq}{a^2 + q^2 + (\mu q/2)(a - \frac{1}{3}\mu q)}\right]. \tag{12}$$

After decomposing the various terms in partial fractions, integrations can be performed and finally taking the appropriate spatial derivatives of various terms one gets an expression for $g^{+-}(r)$ as

$$g^{+-}(r)-1=-\frac{z}{n^-}\frac{6-\mu^2}{3\pi^2 a\sqrt{3\cdot\bar{6}\mu^2-16}}\times$$
$$\left\{e^{ir\alpha}\left[a^2A+\frac{a\mu}{2}B+\frac{1}{6}\mu^2C\right]\right.$$
$$+e^{-ir\alpha}\left[a^2A^*+\frac{a\mu}{2}B^*+\frac{1}{6}\mu^2C^*\right]$$
$$+e^{ir\beta}\left[a^2E+\frac{a\mu}{2}F+\frac{1}{6}\mu^2G\right]$$
$$\left.+e^{-ir\beta}\left[a^2E^*+\frac{a\mu}{2}F^*+\frac{1}{6}\mu^2G^*\right]\right\} \tag{13}$$

where

$$A=\left[-\frac{1}{2r^2}-\frac{\alpha^2}{4}+(0{\cdot}423i-1{\cdot}57)\frac{\alpha}{2r}+\frac{ri\alpha^3}{24}+0{\cdot}0069r^2\alpha^4+\dots\right],$$

$$B=\left[-\frac{i}{2r^3}-\frac{\alpha}{r^2}+(0{\cdot}923i-1{\cdot}57)\frac{\alpha^2}{2r}-\frac{\alpha^3}{6}+\frac{r\alpha^4 i}{48}+\dots\right],$$

$$C=\left[-\frac{1}{r^4}+\frac{3\alpha i}{2r^3}+\frac{3\alpha^2}{2r^2}+(1{\cdot}57-i1{\cdot}256)\frac{\alpha^3}{2r}+\frac{0{\cdot}25}{2}\alpha^4+\dots\right],$$

$$E=\left[\frac{1}{2r^2}+\frac{\beta^2}{4}+\frac{\beta}{2r}(1{\cdot}57-0{\cdot}423i)-\frac{r\beta^3 i}{24}-0{\cdot}0069r^2\beta^4+\dots\right],$$

$$F=\left[\frac{i}{2r^3}+\frac{\beta}{r^2}+(1{\cdot}57-0{\cdot}923i)\frac{\beta^2}{2r}+\frac{1}{6}\beta^3-\frac{r\beta^4 i}{48}+\dots\right],$$

$$G=\left[\frac{1}{r^4}-\frac{3\beta i}{2r^3}-\frac{3\beta^2}{2r^2}+(-1{\cdot}57+1{\cdot}256i)\frac{\beta^3}{2r}-0{\cdot}125\beta^4+\dots\right],$$

$$A^*=[A]^*,\ B^*=[B]^*,\ C^*=[C]^*$$

$$E^*=[E]^*,\ F^*=[F]^*,\ G^*=[G]^*$$

with

$$\alpha=-\frac{a\mu}{4-0{\cdot}\bar{6}\mu^2}+\frac{a}{4-0{\cdot}\bar{6}\mu^2}(3{\cdot}\bar{6}\mu^2-16)^{1/2}$$

and

$$\beta=\frac{-a\mu}{4-0{\cdot}\bar{6}\mu^2}-\frac{a}{4-0{\cdot}\bar{6}\mu^2}(3{\cdot}\bar{6}\mu^2-16)^{1/2}.$$

3. Results and discussion

When $h=0$, $\mu=0$, the roots of the quadratic equations occurring in the denominators of (12) get simplified and the expression for $g^{+-}(r)$ reduces to the well-known classical expression of $g^{+-}(r)$ [1] i.e.

$$g^{+-}(r) = 1 + \frac{z}{n^-}\frac{a^2}{4\pi}\frac{e^{-ra}}{r}. \tag{14}$$

As is evident, the expression (13) for the distribution of electrons around a heavy positively charged impurity is quite complicated when one considers quantum corrections to the classical dielectric function up to h^2. When $h = 0$, it reduces to the simple classical expression given by (14). Equation (13) exhibits that the static structure factor in the present case is dependent, in a quite involved way, on the temperature, plasma frequency of the electrons and the distance r from the impurity. Equation (13) can be grouped into three types of terms: (i) independent of μ (ii) proportional to μ and (iii) dependent on μ^2. In each group there is a complicated dependence on r. However, one can observe that for a given temperature and electron density, as $r \to 0$, $g^{+-}(r)$ increases quite sharply.

We have also made computations on $g^{+-}(r)$ for a plasma having the electron density $n^- = 10^{15}\,\mathrm{cm}^{-3}$ and different temperatures 1200, 300, 60 and 30 K when $z = 1$, $n^-\lambda_{\mathrm{th}}^3 \ll 1$ in each of the cases, implying small degeneracy. The results of the calculation, omitting the terms of the form e^{ra} which lead to unphysical sharp build up of electrons for large r, have been shown in figure 1. Y-axis represents the ratio R, of $g^{+-}(r)_Q$ (the calculations using (13)) and $g^{+-}(r)_{\mathrm{cl}}$ (the calculations based on (14)) i.e. $R = g^{+-}(r)_Q/q^{+-}(r)_{\mathrm{cl}}$, while the X-axis represents r, the distance from the impurity in terms of r_s (r_s in this case $\sim 620\,\text{Å}$). As r is decreased and approaches zero, the ratio R, increases first slowly and then somewhat sharply for very small r. For r nearly equal to r_s, R is nearly equal to one for temperatures greater than 60 K implying thereby that no quantum corrections are needed for $r > r_s$. Further, the quantum corrections as one would expect become increasingly important for $r < r_s$ but the degree of their contribution is significantly dependent on the temperature. For example, as is clear from the figure for $r = 0{\cdot}25 r_s$, say, the value of R is equal to 1·25, 1·45 and 2·40 for $T = 1200$, 300 and 60 K respectively. This is what is expected because as we decrease temperature while λ_{th} increases, λ_D decreases resulting in somewhat large increase in μ. For r still smaller, the quantum correction for high temperatures becomes first comparable and then larger than the classical values implying thereby that when electrons are close to impurity, quantum nature of plasma plays a dominant role in the determination of their distribution around the impurity. In the figure we have also shown calculations for $T = 30$ K ($n^-\lambda_{\mathrm{th}}^3 \simeq 0{\cdot}014$). In this case the ratio R does not approach the value one even at $r = 2r_s$ as is shown in the inset (1a) of the figure.

If one neglects h^2 dependent terms and calculates the ratio, R, one finds that for $T = 1200$ K there is hardly any change in the ratio for all r from the one shown in figure 1. However, as the temperature is decreased, h^2 terms contribute. For example when $T = 60$ K, the ratio R with the neglect of h^2 terms, is shown in figure 1b by solid line and on comparison with figure 1, one finds that the contribution of h^2 is quite large for $r < 0{\cdot}3 r_s$. For $T = 30$ K, the contribution of h^2 is still more significant as can be seen by comparing the plots of R, as given in the inset (1b) with that given in the main figure. In the inset (1b), R does not take into account h^2 terms.

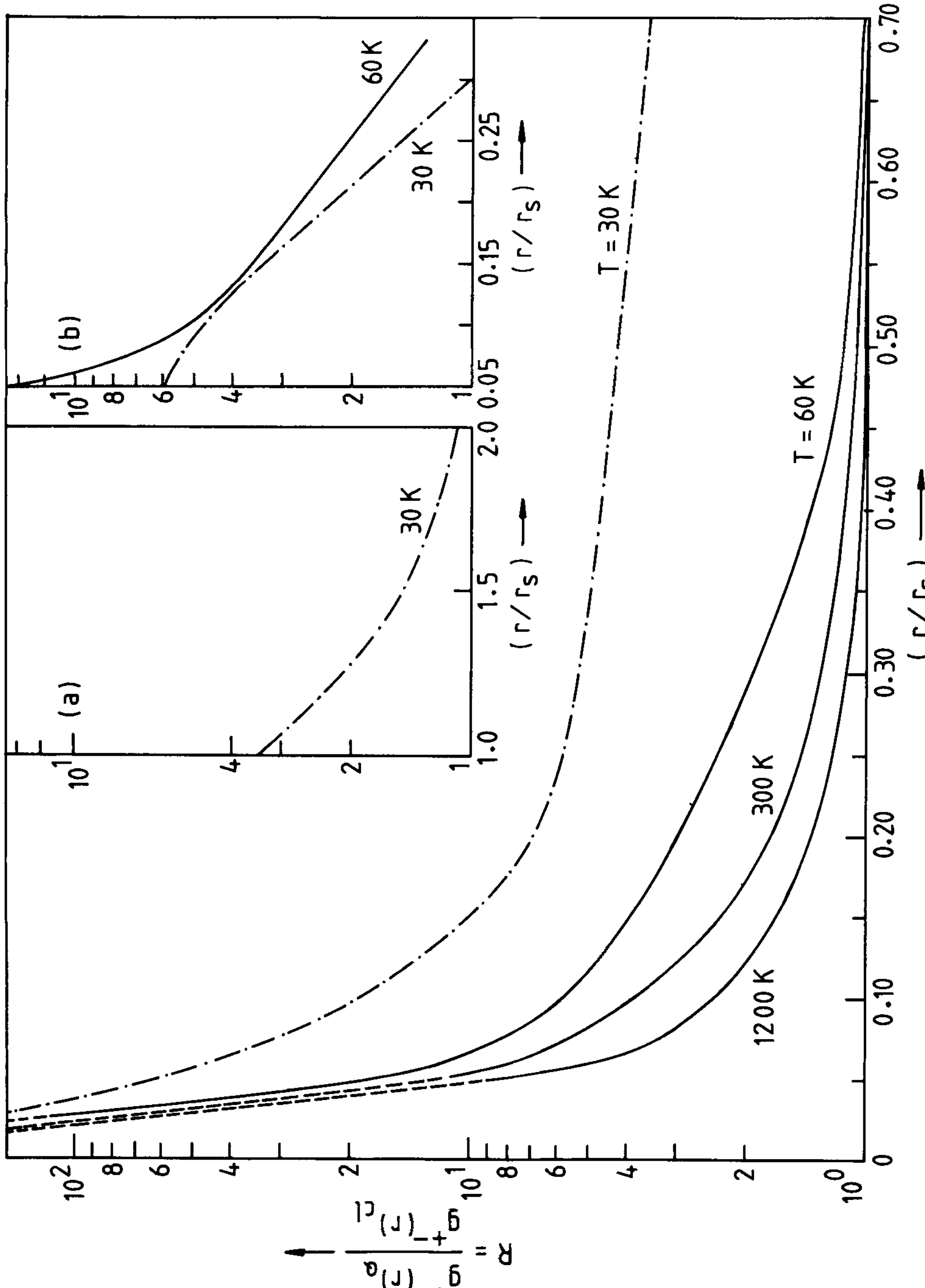

Figure 1. The variation of the temperature dependent ratio R of the quantum mechanical static structure factor, $g^{+-}(r)_Q$, of electrons around a massive positively charged impurity to the classical static structure factor, $g^{+-}(r)_{cl}$, in one component quantum rare plasma with distance r from the impurity expressed in units of r_s, at 1200, 300, 60 and 30 K when the density of electrons $= 10^{15}\,\mathrm{cm}^{-3}$. In inset (a) is shown the variation of R at 30 K for $1{\cdot}0 < r/r_s < 2{\cdot}0$.

In inset (b) are shown the variation of R at 60 and 30 K when the terms having μ^2 as cofactor in the expression of $g^{+}(r)_Q$ have not been taken into account.

4. Conclusions

From our study we conclude that the derived expression of the static structure factor for the electrons around a massive positively charged impurity in a rare plasma taking into account the quantum corrections is quite different from the one given the classical approach. The quantum corrections become increasingly important for distances close to the impurity and at low temperatures when the thermal de Broglie wavelength of electrons becomes a significant fraction of the mean interelectron distance and μ acquires a finite non negligible value.

The results of our work can be checked by performing suitable scattering experiment from a doped semiconductor kept at an appropriate temperature. Explicit values of $g^{\pm}(r)$ for a one component weakly degenerate plasma which can be easily obtained in a doped semiconductor, have been reported in the preceding discussion in order to check these values experimentally. Scattering of low energy photons (0 to $40\,\mu$m) from such a plasma have been performed and reported [9]. Our study may also be useful to assess plasma density in intergalactic space by observing the build up of mobile light mass charge carriers of the plasma around a heavy charged impurity.

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