The effect of electron screening on the structure of crystals in degenerate stars

A A Kozhberov
Ioffe Institute, Politekhnicheskaya 26, St. Petersburg, 194021, Russia
E-mail: kozberov@gmail.com

Abstract. The neutron stars crust and white dwarfs consist of a degenerate relativistic electron gas and atomic nuclei arranged into a crystal lattice. The type of lattice that ions form may depend on many parameters, for example, on the external magnetic field, temperature \(T\), and ion number density \(n\). In this paper, we consider the effect of electron background polarization on the type of lattice at \(T = 0\). Two approximations are used to describe this background. If it is described by the Thomas-Fermi model, the influence of polarization is determined only by the parameter \(\kappa_{TF} a\), where \(\kappa_{TF}\) is the Thomas-Fermi wave number, \(a = (4\pi n/3)^{-1/3}\) is the radius of the ion sphere and at \(\kappa_{TF} a \lesssim 1\) the bcc lattice has the lowest energy. On the other hand, if we use the random-phase approximation for the electron dielectric function, the energy of the static lattice will be a function of \(\kappa_{TF}\) and the relativistic electron parameter \(x_r\). In this case, the bcc lattice possesses the lowest energy at \(\kappa_{TF} a < 0.28\) and any \(x_r\), while at higher \(\kappa_{TF} a\) the formation of other lattice in consideration (fcc and hcp) is possible.

1. Introduction
It is known that the properties of terrestrial solids can substantially depend on their crystal structure (e.g., [1]). The question of the type of crystal lattice and its properties may also be relevant for such space objects as neutron stars and white dwarfs. In this paper we are trying to understand what type of lattice forms in these degenerate stars. To solve this problem, we use the widespread Coulomb crystal model for the envelopes description. In this model, ions are considered to be a point-like and with the same charge number \(Z\) (usually \(Z \gg 1\)), while the neutralizing degenerate relativistic electron background is uniform or slightly polarised (e.g., [2]). For the description of the polarised background we use two approximations of the dielectric function \(\epsilon(q)\): the well-known Thomas-Fermi model and the more correct random phase approximation [3].

2. Thomas-Fermi model
If the electron background is uniform, it is thought that the ions form a body-centered cubic (bcc) lattice, since this lattice has the lowest electrostatic energy among all one-component lattices (e.g., [2], see [4] for review). The electrostatic energy of any one-component Coulomb lattice with a uniform background (the Madelung energy) could be written as

\[ U_M = N \frac{Z^2 e^2}{a} \zeta , \]
where $\zeta$ is called a Madelung constant, $a = (4\pi n/3)^{-1/3}$ is the radius of the ion sphere, $n$ is the ion number density, and $N$ is the total number of ions. For the bcc, face-centred cubic (fcc), and hexagonal close-packed (hcp) lattices Madelung constants are

$$
\zeta_{\text{bcc}} = -0.895929255682, \quad \zeta_{\text{fcc}} = -0.895873615195, \quad \zeta_{\text{hcp}} = -0.895838120459.
$$

It is interesting to note that the relative difference ($|\Delta U_M|/U_M$) between the Madelung energies of the hcp and bcc lattice is about 0.0001, while the relative difference between the energies of “spherical” and “cylindrical” (a theoretical model of non-spherical atomic nuclei, which may exist in neutron stars, see [2, 5] for details) Wigner-Seitz cells is less than 0.0003. A comparable difference suggests the importance of studying different lattices. It is just as significant as researching the “nuclear pasta” in the neutron stars.

In many cases, a uniform background approximation works quite well, but it is obvious that the electron number density changes due to the presence of point charges of ions. If the energy of the electron-ion interaction is much smaller than the kinetic energy of electrons, we can restrict ourselves to the linear response approximation. For a strongly degenerate electron gas, the condition $Ze^2/a \ll E_F$ is equivalent to $\kappa TFa \ll 1$, where $E_F \equiv mc^2(\gamma_e - 1)$ is the Fermi energy, $\kappa TF = 2p_F\sqrt{\alpha/(\pi\beta)}$ is the Thomas-Fermi wave number (in general $\kappa \equiv (4\pi^2\partial n_e/\partial p_e)^{1/2}$), $\alpha = e^2/(\hbar\rho)$ is the fine-structure constant, $\beta = x_e/\gamma_e$, $\gamma_e = \sqrt{1 + x_e}$, $x_e \equiv p_F/(mc)$ is the relativistic parameter of the electron, $p_F = h(3\pi^2n_e)^{1/3}$ is the Fermi momentum, $n_e = Zn$ is the electron number density, $m_e$ is its mass and $\mu_e$ is the chemical potential of the electron gas. For a crystal formed by $^{12}$C atomic nuclei, this assumption is valid at $\rho \gg 3000$ g/cm$^3$.

Since ions move slowly or not at all, it is sufficient to use the linear response approximation and the static longitudinal dielectric function $\epsilon(q)$ to describe the electron background [6]. Then, the total energy of a static (all ions are in equilibrium positions $\mathbf{R}_i$) one-component lattice with arbitrary $\epsilon(q)$ is

$$
\frac{U}{Ze^2} = \frac{1}{2} \sum_{l=1}^{N} \sum_{p,p'=(1)}^{N_{\text{cell}}} \frac{d\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} \frac{1 - \delta_{R_l,0} \delta_{pp'}}{q^2 \epsilon(q)} \exp \left[ i \mathbf{q} \cdot (\mathbf{R}_l + \mathbf{x}_p - \mathbf{x}_{p'}) \right] 
+ \frac{1}{2} \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} \left[ \frac{1}{\epsilon(q)} - 1 \right] - \frac{n}{2} \int \frac{d\mathbf{r} d\mathbf{q}}{(2\pi)^3} \frac{4\pi e^{i\mathbf{q} \cdot \mathbf{r}}}{q^2 \epsilon(q)},
$$

(3)

where $\mathbf{q}$ is the wave vector, $\mathbf{x}_p$ is the basis vector, $N_{\text{cell}}$ is the number of ions in the elementary cell. The contribution of the homogeneous component of the electron background to this energy is not taken into account, since it is the same for all lattices.

The dielectric function $\epsilon(q)$ could be described by various ways. The simplest one is to use the Thomas-Fermi (TF) model which gives

$$
\epsilon(q) = 1 + \frac{\kappa^2}{q^2}.
$$

(4)

The Thomas-Fermi model was studied in many papers (e.g., [7, 8, 9] and references therein). Using this approach the electrostatic energy of the bcc and fcc Coulomb lattices with polarized electron background in context of the neutron stars theory were studied in [10]. In [11] it was shown that this model is similar to the phenomenological Yukawa crystal model, which was widely developed in [12, 13, 14, 15] for dusty plasmas. The electrostatic energy in both models is described by the same analytical equation (as a function of $\kappa$), but they have different screening parameters $\kappa$, because in the first case the background is formed by degenerate electrons while in the second case it consist of non-degenerate electrons and ions. According to [15] at zero temperature there is a phase transition between the bcc and fcc lattices at $\kappa a \approx 1.066$. In [15]
this result was found from molecular dynamic simulations and it was checked and improved
($\kappa a \approx 1.065714$) analytically in [11]. In addition to the one-component bcc and fcc lattices,
the hcp and MgB$_2$ lattices was studied in [11] but no new phase transition was discovered and,
moreover, the MgB$_2$ lattice was found unstable against small phonon oscillations. These four
lattices have the lowest electrostatic energies at $\kappa = 0$ and the formation of some other lattices
according to the Thomas-Fermi model is unlikely.

The multi-component crystals via the Thomas-Fermi model were selectively considered in
[16, 17] but by other approaches. It should be noted that the Thomas-Fermi formalism allows us to accurately calculate only
the correction to the total energy, which is proportional to $(\kappa_{TF} a)^2$, as it was done in [10], but
usually this restriction is neglected. So if we consider only a quadratic term the total energy is

$$U = N \frac{Z^2 e^2}{a} (\zeta + \eta_{TF}(\kappa_{TF} a)^2),$$

where $\eta_{TF}$ depends on the type of the lattice:

$$\eta_{TF}^{\text{bcc}} = -0.103732333707, \quad \eta_{TF}^{\text{fcc}} = -0.103795687531, \quad \eta_{TF}^{\text{hcp}} = -0.103809851801.$$ (6)

Thus the phase transition between bcc and fcc lattices will shift to $\kappa_{TF} a \approx 0.93715$. Thus, there is a noticeable difference between the results obtained with the quadratic term and the full equation. One the other hand, both results are mostly outside of the limits of applicability of the theory in use.

3. Jancovici model

A more precise expression for the static dielectric function of a degenerate relativistic electron
gas was obtained by Jancovici in [3] within the random phase approximation (for simplicity, we
call it a Jancovici (J) model). It allows to take into account the dependence on $q$ more correctly:

$$
\epsilon(q) = 1 + \frac{\kappa_{TF}^2}{q^2} \left\{ \frac{2}{3} - \frac{2 y^2 x_r}{3 \gamma_r} \ln (x_r + \gamma_r) + \frac{x_r^2 + 1 - 3 x_r^2 y^2}{6 y x_r^2} \ln \frac{1 + y}{1 - y} \right\} + \frac{2 y^2 x_r^2}{6 y x_r^2} - 1 \frac{1 + x_r^2 y^2}{\gamma_r} \ln \frac{y \gamma_r + \sqrt{1 + x_r^2 y^2}}{y \gamma_r - \sqrt{1 + x_r^2 y^2}} \right\} = 1 + \frac{\kappa_{TF}^2}{q^2} \epsilon_2(q),
$$

where $y = \hbar q/(2 p v) \approx 0.26 q a Z^{-1/3}$. The random phase approximation assumes that $a \ll a_0$, where $a_0 = h^2/(m_e e^2)$ is the Bohr radius, in addition, the zero temperature limit was used ($T \ll E_F/k_B$) and it is correct to use Eq. (7) only in case of $\kappa_{TF} a \ll 1$. In the long waves limit $(y \ll 1)$ Eq. (7) turns to Eq. (4). Thus, the Thomas-Fermi model is a special case of the Jancovici model. The last one is always more correct but the Thomas-Fermi model is simpler and therefore is used more often. The Jancovici model was relatively rare used in the theory of degenerate stars (e.g., [18, 19]). For studying the electrostatic energy it was used only once in [10], where the bcc and fcc lattices were considered. The electrostatic properties of other lattices have never been studied before with this model.

According to [20, 10], the correction to the total energy ($\Delta U \equiv U - U_M$) due to polarization
of the electron background Eq. (3) can be written as:

$$
\frac{\Delta U}{Z^2 e^2} = \frac{1}{2} \sum_{l,p,p'} \int \frac{dq}{(2 \pi)^3} \frac{4 \pi}{q^2} \left[ \frac{1}{\epsilon(q)} - 1 \right] e^{i q (r_l + x_{p} - x_{p'})} - \frac{n}{2} \int dr \int \frac{dq}{(2 \pi)^3} \frac{4 \pi}{q^2} \left[ \frac{1}{\epsilon(q)} - 1 \right] e^{i q r} = \frac{2 \pi \eta N}{N^2_{\text{cell}}} \sum_{m} \sum_{p,p'} \frac{1 - \delta_{G_m,0}}{G_m^2} \left[ \frac{1}{\epsilon(G_m)} - 1 \right] e^{i G_m (x_{p} - x_{p'})},
$$

(8)
where $\mathbf{G}_m$ is the reciprocal lattice vector.

As the Thomas-Fermi approach the Jancovici approach allows us to accurately calculate the correction to the total energy proportional to $(\kappa_{\text{TF}} a)^2$, we can reduce Eq. (8) to

$$U_{21} \equiv U_M + \Delta U_{21}, \quad \frac{\Delta U_{21}}{NZ^2e^2} \equiv \eta_J \frac{(\kappa_{\text{TF}} a)^2}{a} = \frac{2\pi n\kappa_{\text{TF}}^2}{N_c^2} \sum_{m,p,p'} (\delta_{G_m,0} - 1) \epsilon^2_{G_m} e_i G_m(x_p - x_{p'}). \quad (9)$$

The parameter $\eta_J$ can be considered as a function of $x_r$ and $\kappa_{\text{TF}} a$ as it was done in [10] for the bcc lattice but here we consider it as a function of $Z$ and $x_r$. 

![Figure 1](image_url)

**Figure 1.** Dependence $(U_{\text{bcc}}^{21} - U_{\text{fcc}}^{21})a/(NZ^2e^2)$ and $(U_{\text{bcc}}^{21} - U_{\text{hcp}}^{21})a/(NZ^2e^2)$ on $Z$ and $x_r$.

In figure 1A for different $Z$ the dependence $(U_{\text{bcc}}^{21} - U_{\text{fcc}}^{21})a/(NZ^2e^2)$ on $x_r$ is plotted, while in figure 1B the same for $U_{\text{bcc}}^{21}$ and $U_{\text{hcp}}^{21}$. The solid horizontal line shows the difference between the Madelung energies of the bcc and fcc lattices in figure 1A and between the bcc and hcp lattices in figure 1B. At $x_r \gg 1$ the quantities in consideration are negative for any realistic ions ($Z \lesssim 100$). Therefore, at such $x_r$ and $Z$ the bcc lattice possesses the lowest $U_{21}$. However, $(U_{\text{bcc}}^{21} - U_{\text{fcc}}^{21})a/(NZ^2e^2)$ and $(U_{\text{bcc}}^{21} - U_{\text{hcp}}^{21})a/(NZ^2e^2)$ are positive for some $Z$ and at small $x_r$ near the applicability limit of the theory ($\kappa_{\text{TF}} a \ll 1$). For example, at $Z = 12$ and $x_r < 0.657$ the total energy of the fcc lattice is the smallest.

In figure 2 the yellow dots show the range of parameters at which the bcc lattice has the lowest total energy; the blue points for the fcc lattice, and the orange points for the hcp lattice. Each point shows a set of parameters for which investigations were carried out. log$_{10}(x_r)$ and $\kappa_{\text{TF}} a$ are selected as independent parameters (step over log$_{10}(x_r)$ is 0.025, step over $\kappa_{\text{TF}} a$ is 0.01). The results for the bcc and fcc lattices are coincide with the results obtained in [10]. At high $x_r$ the translation between the bcc and fcc lattices takes place at $\kappa_{\text{TF}} a \approx 0.93715$. The hcp lattice has the lowest electrostatic energy at $\kappa_{\text{TF}} a < 1$ only at small $Z$. While the difference between the energies is small, and it is possible that the higher order corrections will lead to the opposite result.

4. Discussions and Conclusions

We used two approaches to study the electron background polarization and its influence on the crystal structure of the neutron stars crust and white dwarfs envelope.
Figure 2. The range of parameters at which one or another lattice has the smallest $U_{2J}$. The yellow dots corresponds to the bcc lattice; the blue points for the fcc lattice, and the orange points for the hcp lattice.

The Thomas-Fermi model shows that at $\kappa_{TF}a < 1.065714$ the bcc lattice forms, while at higher $\kappa_{TF}a$ the fcc lattice is more energetically preferable. According to the more precise model obtained within the random-phase approximation [3] the bcc lattice has the lowest electrostatic energy at $\kappa_{TF}a < 0.28$. At $\kappa_{TF}a \geq 0.28$ the type of the lattice (bcc or fcc) noticeably depends on $x_r$. Formation of the hcp lattice is possible only at small $Z$, which is mostly out of our point of interests, because in degenerate stars $Z \gg 1$. Such noticeable difference between models indicates that the higher-order corrections to the total energy and any improvement of the Coulomb crystal model can radically change the whole picture of phase transitions. Nonetheless, we can conclude that at $\kappa_{TF}a \lesssim 0.1$ the bcc lattice most likely forms in the envelopes of degenerate stars, while for higher $\kappa_{TF}a$ formation of other lattices is not excluded.

In this paper we did not discuss the zero-point vibrations energy ($E_0$). As was obtained in [11] for the Thomas-Fermi model the relation $E_0^{hcp} > E_0^{fcc} > E_0^{bcc}$ holds for any $\kappa_{TF}$ and a rough analysis shows that in the Jancovici model this ratio conserves.

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