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ORIGINAL ARTICLE

Thermodynamic properties of the magnetized Coulomb crystal lattices

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Abstract It is thought that Coulomb crystals of ions with hexagonal close-packed lattice may form in the crust of strongly-magnetized neutron stars (magnetars). In this work we are trying to verify this prediction assuming that the direction of the magnetic field corresponds to the minimum of the zero-point energy. We also continue a detailed study of vibration modes and thermodynamic properties of magnetized Coulomb crystals in a wide range of temperatures and magnetic fields. It is demonstrated that the total Helmholtz free energy of the body-centered cubic Coulomb crystal is always lower than that of the Coulomb crystal with hexagonal close-packed or face-centered cubic lattice, which casts doubt on the hypothesis above.

Keywords Neutron star · Dense matter · Coulomb crystal · Magnetic field · Thermodynamics

1 Introduction

Matter in white dwarf cores and neutron star crusts is thought to be composed of fully ionized atomic nuclei and degenerate electron gas. At not too low densities ($\rho > 10^4$ g cm^{-3}) and low temperatures ($\Gamma \equiv Z^2e^2/(aT) > 175$, where $a \equiv (4\pi n/3)^{-1/3}$ is the ion sphere radius, n is the number density of ions, Z is the charge number of ions) it will be a good approximation to consider the electron gas as uniform while ions are point-like and arranged into a crystal lattice (e.g., Shapiro and Teukolsky 1983; Haensel et al. 2007). This assumption allows us to use the Coulomb crystal model for description of the envelopes of degenerate stars (e.g. the outer crust of neutron stars at densities below the neutron-drip transition). Properties of Coulomb crystals have been studied in Carr (1961), Pollock and Hansen (1973), Chabrier (1993), Baiko et al. (2001), Baiko (2014) and in several others. In our recent work Kozhberov and Baiko (2015) the electrostatic and thermodynamic properties of one-component hexagonal close-packed (hcp) lattice have been discussed.

One of the unique features of neutron stars is the possible presence of an extremely strong magnetic field. Magnetic fields on the surface of magnetars can reach $B \sim 10^{15}$ G or even more (e.g., Olausen and Kaspi 2014). Unfortunately, the influence of such fields on the internal structure of these stars in general and on Coulomb crystals in particular is studied poorly. For the first time magnetized Coulomb crystals were considered approximately and qualitatively by Usov et al. (1980). Nagai and Fukuyama (1982) and (1983) have studied crystals with the body-centered cubic (bcc), face-centered cubic (fcc), and hcp lattices at zero temperature. Thermodynamic properties of magnetized bcc Coulomb lattice at $T > 0$ have been investigated in Baiko (2009).

Nagai and Fukuyama (1983) have shown that the hcp lattice becomes thermodynamically preferable over the bcc and fcc lattices at $T = 0$ and $r_s < 10\,700$ ($r_s \equiv a/(Z^{1/3}a_0)$ is the standard density parameter and a_0 is the Bohr radius) above certain critical value of the magnetic field. Hence the change of the magnetic field can lead to restructuring of the neutron star crust. However in this work the temperature effects were not taken into account and the direction of the magnetic field was fixed with respect to the crystallographic axes. Even in Usov et al. (1980) it was noted that the crystal rotates relative to the magnetic field to minimize the zero point energy. It was also discussed in Baiko (2009), where

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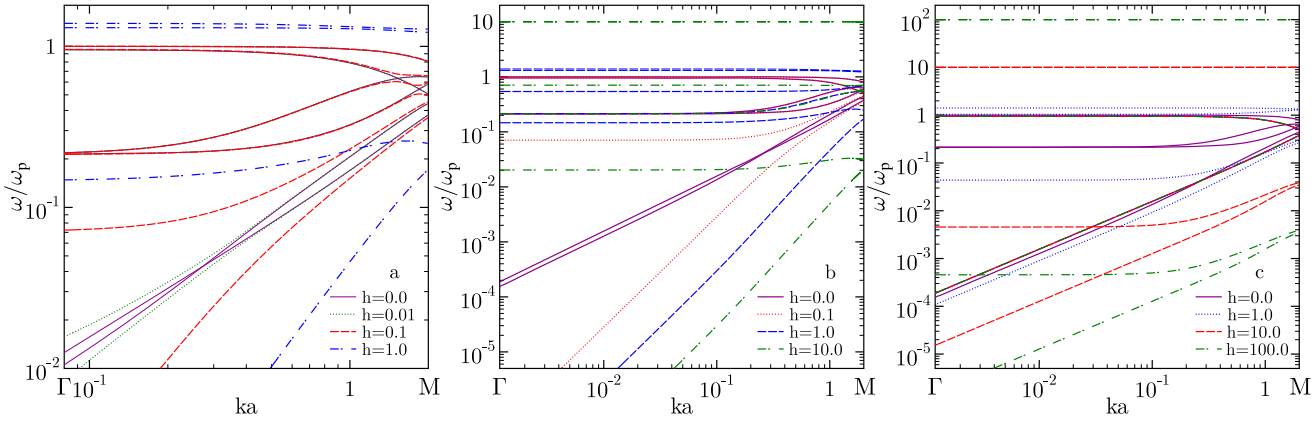

Fig. 1 Dispersion curves of the hcp lattice in the magnetic field. Cartesian coordinate system is directed so that the edge ΓM lies on the axis k_x. In *panel a* and *b* $\mathbf{n} = (1, 1, 0)/\sqrt{2}$, in *panel c* $\mathbf{n} = (0, 0, 1)$. In *panel a* two modes at $h = 1$ are not plotted

the correct configuration of the magnetic field was found for the bcc lattice.

In this work we check the prediction about the phase transition between the hcp and bcc lattices at finite temperature. We study the zero-point energy and the thermal free energy of one-component magnetized hcp and fcc Coulomb lattices. It is shown, that if the direction of the magnetic field corresponds to the minimum of the zero-point energy, the total Helmholtz free energy of the bcc lattice is below the total Helmholtz free energy of the hcp and fcc lattices at any temperature, magnetic field, mass density, and ion type (neglecting anharmonicity and electron polarization effects, which are the same assumptions as those made by Nagai and Fukuyama 1982 and 1983).

2 Phonon spectrum of the hcp lattice in magnetic field

If we choose vector potential as $A_i^\alpha = [\mathbf{B} \times \mathbf{u}_i]/2 = \varepsilon^{\alpha\beta\gamma} B^\beta u_i^\gamma /2$, where $\mathbf{u}_i$ is the i-ion displacement from the equilibrium position (Baiko 2009), the dispersion equation could be written as

$$\det\Big\{D^{\alpha\beta}_{pp'}(\mathbf{k}) - \omega_\nu^2(\mathbf{k},\mathbf{B})\delta^{\alpha\beta}\delta_{pp'} - i\omega_\nu(\mathbf{k},\mathbf{B})\omega_B\varepsilon^{\alpha\gamma\beta}n^\gamma\delta_{pp'}\Big\} = 0, \quad (1)$$

where $D^{\alpha\beta}_{pp'}(\mathbf{k})$ is the dynamic matrix (the equation for the dynamic matrix for any lattice can be found in Kozhberov and Baiko 2012), p and p' enumerate ions in the elementary cell ($p, p' = 1, \ldots, N_{\rm cell}$), Greek indices α, β denote Cartesian components, ν enumerates oscillation modes at given wavevector $\mathbf{k}$ ($\nu = 1, \ldots, 3N_{\rm cell}$). We will measure the ion vibration frequencies $\omega_\nu(\mathbf{k}, \mathbf{B})$ and cyclotron frequency $\omega_B = ZeB/(Mc)$ in units of the ion plasma frequency $\omega_p = \sqrt{4\pi Z^2 e^2 n/M}$, where M is the mass of the ion. At any fixed wavevector $\mathbf{k}$ and the direction of magnetic field $\mathbf{n} \equiv \mathbf{B}/B$ the frequencies satisfy an analogue of the Kohn's sum rule $\sum_\nu \omega_\nu^2(\mathbf{k},\mathbf{B})/\omega_p^2 = N_{\rm cell}(1 + h^2)$, where $h \equiv \omega_B/\omega_p$ ($h \approx B_{15}/\sqrt{\rho_8}$, $B_{15} = B/10^{15}$ G and $\rho_8 = \rho/10^8$ g cm^{-3}).

The hcp lattice has two ions in the elementary cell ($N_{\rm cell} = 2$) for this reason its spectrum consists of six oscillation modes. The frequencies are plotted in Fig. 1 as functions of ka for several directions of the magnetic field. The dependence on the magnetic field in the hcp lattice is more complicated than in the bcc, but near the center of the first Brillouin zone the main features remain the same. Like in the bcc lattice one of the modes, which was acoustic without magnetic field, becomes optic ($\omega \approx$ const if $ka \ll 1$), another one remains linear with respect to k, if $\mathbf{kn} = 0$ (see Fig. 1c) or becomes quadratic with respect to k, if $\mathbf{kn} \neq 0$ (see Fig. 1a and b). The highest mode stays optic. Without field in some directions the modes of the hcp lattice cross each other but in the magnetic field this feature disappears (see Fig. 1a). At $\omega_B \gg \omega_p$ the two highest modes increase $\propto \omega_B$, while the lowest modes (one of the optic modes and the mode with the quadratic or linear dependence over k near the Γ point) decay $\propto \omega_B^{-1}$.

3 The zero-point energy

The energy of zero-point vibrations (E_0) is determined by the average frequency over all phonon modes in the first Brilloun zone: $E_0 = 1.5N\hbar\langle\omega\rangle = 1.5N\hbar\omega_{\rm p}u_1(h, \mathbf{n})$, where $\langle\ldots\rangle$ denotes the averaging over all modes (e.g., $\langle\omega\rangle = (3N_{\rm cell})^{-1}\sum_{\mathbf{k}\nu}\omega_\nu(\mathbf{k},\mathbf{B})$) and $u_1(h, \mathbf{n})$ is called the first frequency moment. Without the field, $u_1 = 0.5133369$ for the hcp lattice, $u_1 = 0.513194$ for the fcc lattice and $u_1 = 0.5113877$ for the bcc lattice. At $h \gg 1$ $u_1(h, \mathbf{n})$ increases proportionally to h because the main contribution

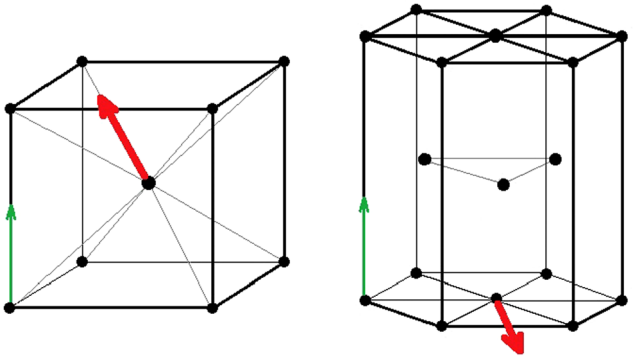

Fig. 2 Elementary cells of the bcc (*left*) and hcp (*right*) lattices. The direction of the magnetic field chosen in Nagai and Fukuyama (1983) is shown by thin arrows, the direction of the magnetic field, which corresponds to the minimum of the zero point energy by thick arrows. For both lattices *z-axis* is directed vertically, *x-axis*—horizontally in the plane of the paper

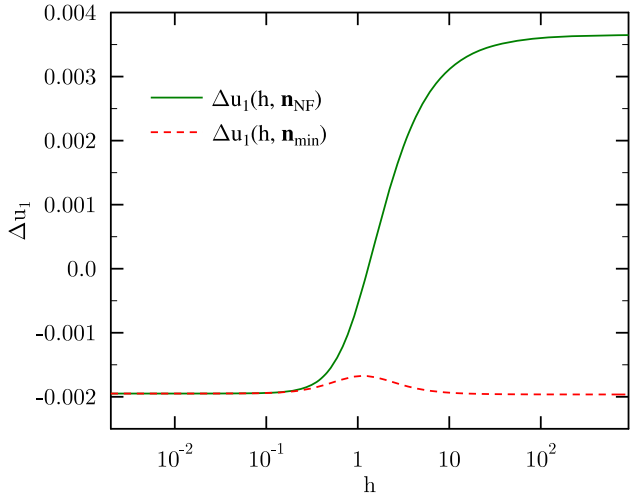

Fig. 3 Dependence of Δu_1 on h

comes from the highest mode. The dependence $u_1(h, \mathbf{n})$ on the direction of the magnetic field $\mathbf{n}$ is relatively weak. The difference between the minimum and maximum values of $u_1(h, \mathbf{n})$ at fixed h is only a few fractions of a per cent (for example, for the hcp lattice it is 0.06% at $h = 1$) but this difference is important in the problem of the most energetically preferable lattice. In the hcp lattice E_0 is minimal in any direction equivalent to $\mathbf{n}_{\min} = (0, 1, 0)$. It could be called the fourth order nearest neighbor and is shown by the thick arrow in the right plane of Fig. 2. At $h > 5$ with accuracy of a few parts in 10^5 $u_1(h, \mathbf{n}_{\min})$ can be fitted as $(0.547352 + 0.527763/h + h)/3$. In the bcc lattice the energy of zero-point vibrations is minimal, if the magnetic field is directed towards one of the nearest neighbors (Baiko 2009), for example, $\mathbf{n}_{\min} = (1, 1, 1)/\sqrt{3}$ (the thick arrow in the left plane of Fig. 2).

If $\mathbf{n} = \mathbf{n}_{\min}$ the zero-point energy of the bcc Coulomb crystal is lower than that of the hcp Coulomb crystal at any h. It is demonstrated in Fig. 3, where $\Delta u_1(h, \mathbf{n}_{\min}) = u_1^{\rm bcc}(h, \mathbf{n}_{\min}) - u_1^{\rm hcp}(h, \mathbf{n}_{\min})$ is plotted by dotted line. In Fig. 2 the directions of the magnetic field ($\mathbf{n}_{\rm NF}$), which were chosen in Nagai and Fukuyama (1983) are shown by thin arrows. $\Delta u_1(h, \mathbf{n}_{\rm NF}) = u_1^{\rm bcc}(h, \mathbf{n}_{\rm NF}) - u_1^{\rm hcp}(h, \mathbf{n}_{\rm NF}) > 0$ at $h \gtrsim 1.293$ (coincides with Nagai and Fukuyama 1983). $\Delta u_1(h, \mathbf{n}_{\rm NF})$ is plotted by the solid line in Fig. 3.

The similar situation occurs in the fcc lattice. The zero-point energy of this lattice reaches minimum, if the magnetic field is directed toward one of the nearest neighbors (e.g., $\mathbf{n}_{\min} = (1, 0, 1)/\sqrt{2}$). For any h $u_1^{\rm bcc}(h, \mathbf{n}_{\min}) < u_1^{\rm fcc}(h, \mathbf{n}_{\min})$, while $\mathbf{n}_{\rm NF} = (0, 0, 1)$ and $u_1^{\rm bcc}(h, \mathbf{n}_{\rm NF}) > u_1^{\rm fcc}(h, \mathbf{n}_{\rm NF})$ at $h \gtrsim 7.29$.

Not all of the average functions depend on $\mathbf{B}$. For example, $u_{\ln} \equiv \langle \ln(\omega) \rangle$ does not, according to the Bohr-van Leeuwen theorem $u_{\ln}(h, \mathbf{n}) = -0.816031$ for the hcp lattice, $u_{\ln}(h, \mathbf{n}) = -0.817908$ for the fcc lattice and $u_{\ln}(h, \mathbf{n}) = -0.831295$ for the bcc lattice (Baiko 2009).

4 The Helmholtz free energy

The total Helmholtz free energy of the Coulomb crystal consists of electrostatic, zero-point and thermal contributions (neglecting anharmonicity and electron polarization effects):

$$\begin{aligned} F &= U_M + E_0 + F_{\rm th} \\ &= N\frac{Z^2e^2}{a}\zeta + N\frac{1.5\sqrt{3}Ze}{a^{1.5}}u_1(h, \mathbf{n}) \\ &\quad + 3NT\left\langle \ln\left(1 - \exp(-\hbar\omega/T)\right)\right\rangle. \end{aligned} \tag{2}$$

The reduced free energy in given as:

$$f \equiv \frac{F}{NT} = \Gamma\zeta + 1.5\frac{u_1(h, \mathbf{n})}{t} + f_{\rm th}(t, h, \mathbf{n}), \tag{3}$$

where $f_{\rm th}(t, h, \mathbf{n}) \equiv F_{\rm th}/(NT)$, $t \equiv T/T_p$, $T_{\rm p} \equiv \hbar\omega_{\rm p}$. The Madelung constant ζ depends on the lattice type only, $\zeta = -0.89583812$, -0.89587362 and -0.89592926 for hcp, fcc and bcc lattices, respectively. Hence among all lattices under consideration the bcc lattice has the lowest electrostatic energy and at $T = 0$ the total Helmholtz free energy of the bcc lattice is smaller than that of the other ones at any magnetic field value, mass density, and type of the ions, if the direction of the magnetic field corresponds to the minimum zero-point energy, but it is not the case for all directions.

For any lattices the thermal contribution changes with $\mathbf{n}$ more noticeably than the zero-point energy. While for both energies the dependence on the direction of the magnetic field has the same scale as the dependence on the lattice type at fixed t and h. For the bcc lattice $f_{\rm th}(t, h, \mathbf{n}_{\rm NF})/$

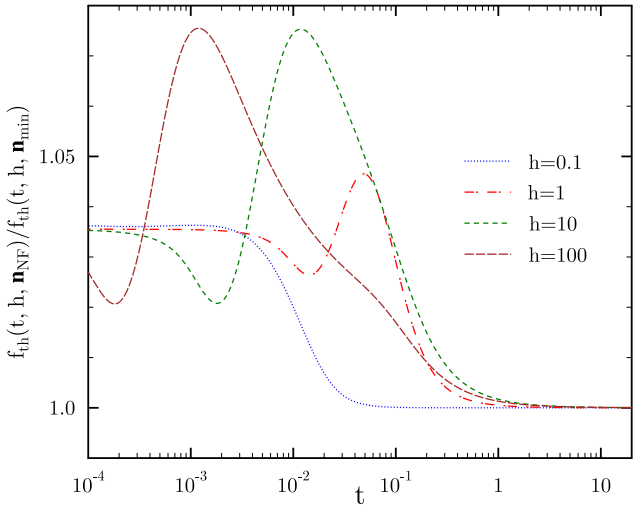

Fig. 4 Ratio between thermal contributions to the free energy of the bcc lattice at different directions of the magnetic field

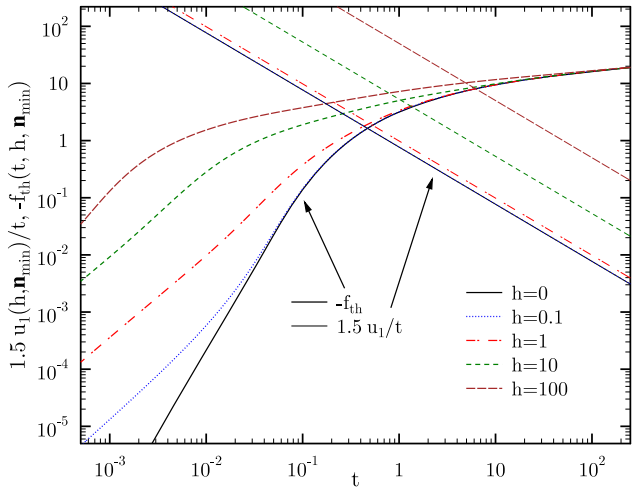

Fig. 5 Thermal and zero-point contributions into the free energy of the hcp lattice

$f_{\rm th}(t,h,\mathbf{n}_{\rm min})$ is plotted in Fig. 4. This ratio is always greater than 1 and, for instance, at $h=10$ it has a maximum of $\approx$1.075 at $t=0.012$.

In Fig. 5 we plot $1.5u_1(h,\mathbf{n}_{\rm min})/t$ and $-f_{\rm th}(t,h,\mathbf{n}_{\rm min})$ of the hcp lattice as functions of t for different h. At high temperatures ($T > T_p\sqrt{1+h^2}$) the thermal contribution behaves as $F_{\rm th} \simeq 3NT(u_{\rm ln} - \ln t) - 1.5N\hbar\omega_p u_1(h,\mathbf{n})$ and consequently the total Helmholtz free energy doesn't depend on the magnetic field and could be rewritten as $F \simeq NT\Gamma\zeta + 3NT(u_{\rm ln} - \ln t)$. Hence, among all considered lattices at high temperatures the bcc lattice has the smallest $F_{\rm th}$ and F (Kozhberov and Baiko 2015).

At $T \ll T_p/\sqrt{1+h^2}$ $f_{\rm th} \propto T^{3/2}$ due to the lowest mode which is $\propto k^2$. Since the lowest mode at $h \gg 1$ does not change its shape and only reduces $\propto B$, the thermal contribution $f_{\rm th} \propto B^{3/2}$. For this reason in Fig. 4 the curves with

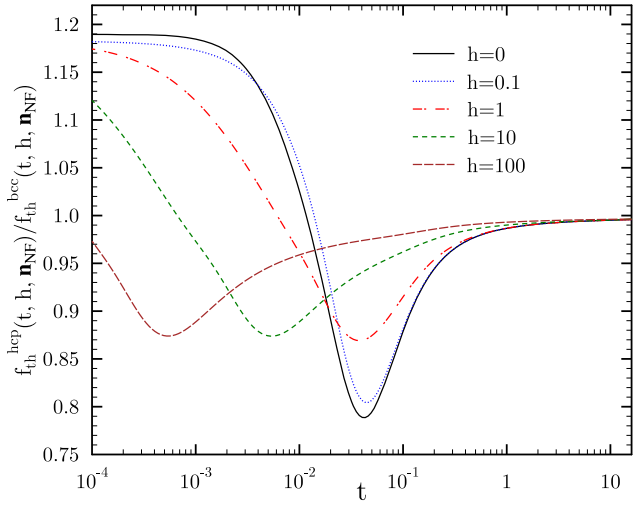

Fig. 6 Ratio between thermal contributions to the free energy of the hcp and bcc lattices

$h = 10$ and $h = 100$ at low temperatures differ from each other only by a temperature shift by a factor of 10. In contrast to the bcc lattice the hcp lattice has the optic mode, which decreases proportionally to B^{-1} and therefore, the $T^{3/2}$-limit is reached at a lower temperature at the same h.

In Fig. 6 we compare the thermal contribution to the free energy of the bcc and hcp lattices at similar direction of the magnetic field ($\mathbf{n} = \mathbf{n}_{\rm NF}$). At $T \gg T_p\sqrt{1+h^2}$ the ratio $f_{\rm th}^{\rm hcp}(t,h,\mathbf{n}_{\rm NF})/f_{\rm th}^{\rm bcc}(t,h,\mathbf{n}_{\rm NF})$ tends to $(u_{\rm ln}^{\rm hcp} - \ln t)/(u_{\rm ln}^{\rm bcc} - \ln t)$, which never exceeds 1. Only at $T \lesssim T_p/\sqrt{1+h^2}$ $f_{\rm th}^{\rm hcp}(t,h,\mathbf{n}_{\rm NF}) < f_{\rm th}^{\rm bcc}(t,h,\mathbf{n}_{\rm NF})$, but at such low temperatures the thermal contribution is significantly smaller than the zero-point energy and therefore can be omitted in Eq. 2. We can assume that $f_{\rm th}^{\rm bcc}(\Gamma,t,h,\mathbf{n}_{\rm NF}) < f_{\rm th}^{\rm hcp}(\Gamma,t,h,\mathbf{n}_{\rm NF})$ at any temperatures where the thermal contribution cannot be ignored. The same inequality holds true for $\mathbf{n} = \mathbf{n}_{\rm min}$. Thus at $\mathbf{n} = \mathbf{n}_{\rm min}$ the total Helmholtz free energy of the bcc lattice is less than the total Helmholtz free energy of the hcp lattice at any physical conditions.

The same comparison could be done for the fcc lattice. In Fig. 7 we present the difference between $f^{\rm fcc}(\Gamma,t,h,\mathbf{n}_{\rm min})$ and $f^{\rm bcc}(\Gamma,t,h,\mathbf{n}_{\rm min})$ as a function of t at several values of h and Γ. At high temperatures $f^{\rm fcc}(\Gamma,t,h,\mathbf{n}) - f^{\rm bcc}(\Gamma,t,h,\mathbf{n})$ tends to the constant $3(u_{\rm ln}^{\rm fcc} - u_{\rm ln}^{\rm bcc}) + \Gamma(\zeta^{\rm fcc} - \zeta^{\rm bcc})$, at low temperatures the main contribution comes from the zero-point energy and this difference is $\approx 1.5(u_1^{\rm fcc}(h,\mathbf{n}) - u_1^{\rm bcc}(h,\mathbf{n}))/t$. As one can see, $f^{\rm fcc}(\Gamma,t,h,\mathbf{n}) - f^{\rm bcc}(\Gamma,t,h,\mathbf{n}) > 0$ at $\mathbf{n} = \mathbf{n}_{\rm min}$ and any Γ,t,h. This means that under assumptions stated above formation of the bcc lattice in magnetized matter is always thermodynamically preferred over the fcc and hcp lattices.

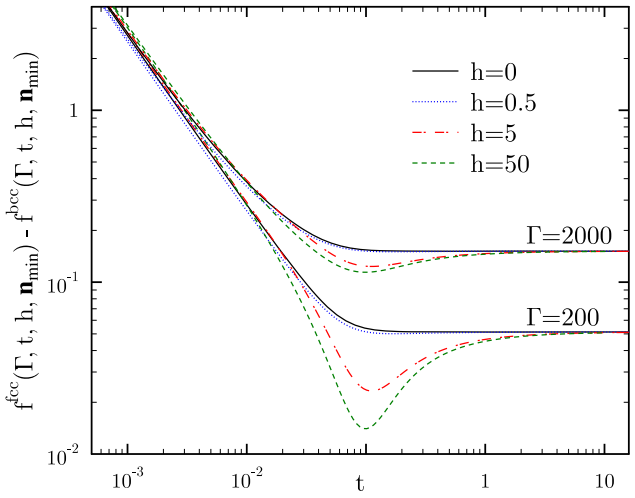

Fig. 7 Ratio between total Helmholtz free energies of the fcc and bcc lattices

Notice that we neglect electron polarization effects, as it was done in Nagai and Fukuyama (1982), Baiko (2009), Baiko and Yakovlev (2013). Previously these effects were discussed for zero magnetic field only in Pollock and Hansen (1973), Baiko (2002) and will be considered in detail for the magnetized Coulomb crystal in our next paper.

5 Conclusions

It follows from the results of Nagai and Fukuyama (1983) that formation of Coulomb crystals of ions with the hexagonal close-packed lattice may be expected in highly-magnetized neutron star crust, which underlines the importance of such systems for astrophysics. We have studied some phonon and thermal properties of one-component magnetized Coulomb crystals to determine, which of the lattices: bcc, fcc or hcp has the lowest total Helmholtz free energy. It was shown that at fixed t and h the dependence on the direction of the magnetic field has the same scale as the dependence on the lattice type and cannot be neglected in our problem. At any temperature, mass density, ion charge, and ion mass, the bcc lattice possesses the lowest total Helmholtz free energy if the magnetic field is directed with respect to the crystallographic axes in such a way that the zero-point energy is minimized. However, it is not the case for other magnetic field directions.

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