

Diffusion and Coulomb Separation of Ions in Dense Matter

M. V. Beznogov^{1,*} and D. G. Yakovlev²

¹*St. Petersburg Academic University, 8/3 Khlopina Street, St. Petersburg 194021, Russia*

²*Ioffe Physical Technical Institute, 26 Politekhnicheskaya, St. Petersburg 194021, Russia*

(Received 23 July 2013; published 14 October 2013)

We analyze diffusion equations in strongly coupled Coulomb mixtures of ions in dense stellar matter. Strong coupling of ions in the presence of gravitational forces and electric fields (induced by plasma polarization in the presence of gravity) produces a specific diffusion current which can separate ions with the same A/Z (mass to charge number) ratios but different Z . This Coulomb separation of ions can be important for the evolution of white dwarfs and neutron stars.

DOI: [10.1103/PhysRevLett.111.161101](https://doi.org/10.1103/PhysRevLett.111.161101)

PACS numbers: 95.30.Qd, 26.60.Gj, 52.25.Fi, 52.27.Gr

Introduction.—In this Letter we consider diffusion in a multicomponent plasma of ions in dense stellar matter. This diffusion can greatly affect the composition of matter, particularly in cores of white dwarfs and envelopes of neutron stars. It produces redistribution of ions (heavier ions move to the star's center) and extra energy release that reheats the star and affects its thermal evolution. For example, we can mention gravitational settling of ^{22}Ne in carbon-oxygen (^{12}C – ^{16}O) cores of white dwarfs (see, e.g., Refs. [1–5]) which is thought to reheat old white dwarfs and helps explain observational data. Diffusion of ions affects also chemical evolution and nuclear burning in envelopes of neutron stars (e.g., Refs. [6–8]). Transport properties are important also in dusty plasmas with their numerous applications (e.g., Ref. [9]).

Diffusion equations are well studied in physical kinetics for the case when the ions constitute almost ideal plasma [10,11]. However, the ion plasma in white dwarfs and neutron stars is typically strongly coupled by Coulomb forces. The diffusion coefficients of ions in strongly coupled Coulomb plasma have been extensively studied in the literature, mainly by molecular dynamics simulations (e.g., Refs. [12–14]). Here we address a delicate problem of diffusion currents in strongly coupled Coulomb plasma of ions.

Diffusion currents.—Consider a plasma which consists of electrons and a mixture of ion species $j = 1, 2, \dots$, with atomic numbers A_j and charge numbers Z_j . Let n_j be the number density of ions j . The electron number density is $n_e = \sum_j Z_j n_j$ (due to charge neutrality).

It is convenient to introduce (e.g., Ref. [15]) the Coulomb coupling parameter Γ_j for ions j ,

$$\Gamma_j = \frac{Z_j^2 e^2}{a_j k_B T} = \frac{Z_j^{5/3} e^2}{a_e k_B T}, \quad (1)$$

where T is the temperature, k_B is the Boltzmann constant, $a_e = (4\pi n_e/3)^{-1/3}$ is the electron-sphere radius, and $a_j = a_e Z_j^{1/3}$ is the ion-sphere radius (for a sphere around a given ion, where the electron charge compensates the ion

charge). Therefore, Γ_j is the ratio of a typical electrostatic energy of the ion to the thermal energy. If $\Gamma_j \ll 1$ then the ions constitute an almost ideal Boltzmann gas, while for $\Gamma_j \gtrsim 1$ they are strongly coupled by Coulomb forces (constitute either Coulomb liquid or solid). One component ion plasma solidifies at $\Gamma \approx 175$. We restrict ourselves to the gaseous or liquid ion plasma.

The diffusion currents in almost ideal plasma are well defined [10,11] but the case of nonideal plasmas requires special attention. We introduce these currents in the spirit of Landau and Lifshitz [16]. Consider the matter which is slightly off thermodynamic equilibrium because of the presence of forces F_α [which act on all particles α —electrons ($\alpha = e$) and ions ($\alpha = j$)] and number density gradients ∇n_α . For simplicity consider isothermal matter (no temperature gradients $\nabla T = 0$, and hence no deviations from thermal equilibrium). The forces F_α and gradients ∇n_α induce (weak) gradients of chemical potentials $\nabla \mu_\alpha$ of particles α . Let us introduce

$$\tilde{F}_\alpha = F_\alpha - \nabla \mu_\alpha = e_\alpha \mathbf{E} + m_\alpha \mathbf{g} - \nabla \mu_\alpha, \quad (2)$$

where we set $F_\alpha = e_\alpha \mathbf{E} + m_\alpha \mathbf{g}$ (e_α and m_α being electric charge and mass of particles α , respectively). The force F_α is produced by gravitational acceleration \mathbf{g} (that can be treated as a constant in the local approximation) and the electric field \mathbf{E} due to weak plasma polarization in the gravitational field.

Note that

$$\sum_\alpha n_\alpha \tilde{F}_\alpha = \rho \mathbf{g} - \nabla P, \quad (3)$$

where $\rho = \sum_\alpha m_\alpha n_\alpha$ is the mass density of the matter and $\nabla P = \sum_\alpha n_\alpha \nabla \mu_\alpha$ (as prescribed by thermodynamics [17]), P being the (total) pressure. The electric field drops off the sum because of electric neutrality but it is most important for driving different particle species (e.g., Refs. [7,8]).

If particles α are in mechanical equilibrium, then $\tilde{F}_\alpha = 0$. This condition is exactly the same as the condition of chemical equilibrium used in Ref. [8]. If the plasma is in

hydrostatic equilibrium as a whole, then $\sum_{\alpha} n_{\alpha} \tilde{\mathbf{F}}_{\alpha} = 0$ and $\rho \mathbf{g} = \nabla P$. Hydrostatic equilibration ($\rho \mathbf{g} = \nabla P$) in neutron stars and white dwarfs is established over milliseconds—minutes [18] but diffusive motion of ions can last over gigayears (Gyrs) (see, e.g., Ref. [5]). This diffusion is studied by standard methods of physical kinetics [10,11] assuming $\rho \mathbf{g} = \nabla P$.

In the diffusion problem, a deviation of particles α from mechanical equilibrium in matter can be conveniently measured by the vector

$$\mathbf{d}_{\alpha} = \frac{\rho_{\alpha}}{\rho} \sum_{\beta} n_{\beta} \tilde{\mathbf{F}}_{\beta} - n_{\alpha} \tilde{\mathbf{F}}_{\alpha}, \quad (4)$$

where $\rho_{\alpha} = m_{\alpha} n_{\alpha}$ is the partial mass density of particles α . Clearly, $\sum_{\alpha} \mathbf{d}_{\alpha} = 0$.

Let $\mathbf{J}_{\alpha} = \rho_{\alpha} \mathbf{V}_{\alpha}$ be the diffusive flux of particles α (\mathbf{V}_{α} being the diffusion velocity of particles α [10,11]). Phenomenological transport equations can be written as

$$\mathbf{J}_{\alpha} = \Phi \sum_{\beta \neq \alpha} m_{\alpha} m_{\beta} D_{\alpha\beta} \mathbf{d}_{\beta}, \quad (5)$$

where $D_{\alpha\beta}$ [$\text{cm}^2 \text{s}^{-1}$] can be called a generalized diffusion coefficient of particles α relative to β , and Φ is a normalization function to be chosen later. The diffusion coefficients should respect the relation

$$\sum_{\alpha} \mathbf{J}_{\alpha} = 0. \quad (6)$$

In a rarefied, almost ideal plasma, we have $\tilde{\mathbf{F}}_{\alpha} = \mathbf{F}_{\alpha} - n_{\alpha}^{-1} \nabla P_{\alpha}$, where P_{α} is the partial pressure of particles α . Then Eq. (5) reduces to the standard definition of diffusion coefficients in rarefied gases [10,11]. For strongly interacting particles, partial pressures P_{α} are ambiguous, while the definition (5), based on chemical potentials μ_{α} , is not.

While the ions are heavy and slow, the electrons are light and mobile. If we are interested in transport properties of ions, we can describe the electrons by the approximation similar to the Born-Oppenheimer approximation in the theory of molecules [19]. Specifically, we assume that the electron gas is always in the state of mechanical (quasi)equilibrium adjusting itself almost instantly to the motion of multicomponent ion plasma. Since the electrons are light, we can set $m_e \rightarrow 0$. Then from Eq. (4) we have $\mathbf{d}_e = -n_e \tilde{\mathbf{F}}_e$. Therefore, the electron quasiequilibrium implies

$$\mathbf{d}_e = 0, \quad \tilde{\mathbf{F}}_e = -e\mathbf{E} - \nabla \mu_e = 0. \quad (7)$$

It allows us to factorize electrons out in the problem of ion transport (diffusive fluxes of ions are mostly determined by a nonequilibrium state of the ion subsystem [20]). In this case Eqs. (5) and (6) retain their form but indices α and β label only ion species ($j = 1, 2, \dots$). Note that Eq. (5) is strictly valid for nonrelativistic particles, whereas the electrons in dense matter can be relativistic. However, the

factorization works well even for relativistic electrons as long as they can be treated as massless.

In the presence of two ion species ($j = 1, 2$) we have $\mathbf{J}_1 = -\mathbf{J}_2$, $\mathbf{d}_1 = -\mathbf{d}_2$, and $D_{12} = D_{21} \equiv D$. Then kinetic phenomena can be characterized by one diffusion coefficient D ,

$$\mathbf{J}_2 = -\mathbf{J}_1 = \frac{nm_1 m_2}{\rho k_B T} D \mathbf{d}_1. \quad (8)$$

Here we have chosen $\Phi = n/(\rho k_B T)$ ($n = n_1 + n_2$ being the total number density of the ions). Then D corresponds to the standard definition of the diffusion coefficient [10,11] for two-component plasma of ions (as follows from the equations presented below). Let us simplify Eq. (8).

From Eq. (4) we have

$$\mathbf{d}_j = -\frac{\rho_j}{\rho} \nabla P - n_j e Z_j \mathbf{E} + n_j \nabla \mu_j, \quad (9)$$

with $j = 1$ or 2 . Because $\mathbf{d}_1 + \mathbf{d}_2 = 0$, we obtain the expression for \mathbf{E} :

$$e n_e \mathbf{E} = -\nabla P + n_1 \nabla \mu_1 + n_2 \nabla \mu_2. \quad (10)$$

Substituting it into (9) and setting $m_j = A_j m_u$ (m_u being the atomic mass unit), we have

$$\mathbf{d}_1 = \frac{n_1 n_2}{n_e} \left[m_u (Z_1 A_2 - Z_2 A_1) \frac{\nabla P}{\rho} + Z_2 \nabla \mu_1 - Z_1 \nabla \mu_2 \right]. \quad (11)$$

Quite generally, the chemical potential of ions j is $\mu_j = \mu_j^{(id)} + \mu_j^{(C)}$, where (id) and (C) label the ideal gas and Coulomb contributions, respectively (see, e.g., Ref. [15]). Then $\mathbf{d}_1 = \mathbf{d}_a + \mathbf{d}_b + \mathbf{d}_c$, with

$$\mathbf{d}_a = m_u Z_1 Z_2 \frac{n_1 n_2}{n_e} \left(\frac{A_2}{Z_2} - \frac{A_1}{Z_1} \right) \frac{\nabla P}{\rho}, \quad (12)$$

$$\begin{aligned} \mathbf{d}_b &= \frac{n_1 n_2}{n_e} [Z_2 \nabla \mu_1^{(id)} - Z_1 \nabla \mu_2^{(id)}] \\ &= \frac{k_B T}{n_e} (Z_2 n_2 \nabla n_1 - Z_1 n_1 \nabla n_2), \end{aligned} \quad (13)$$

$$\mathbf{d}_c = \frac{n_1 n_2}{n_e} [Z_2 \nabla \mu_1^{(C)} - Z_1 \nabla \mu_2^{(C)}]. \quad (14)$$

In Eq. (13) we have used the well-known relation $\nabla \mu_j^{(id)} = k_B T n_j^{-1} \nabla n_j$.

Combined with (8), these equations give us the expression for \mathbf{J}_2 . It contains three terms labeled by subscripts a , b , and c . The terms a and b are well known while the term c seems new.

(a) Assume that the matter is in hydrostatic equilibrium as a whole. Then in Eq. (12) we have $\nabla P = \rho \mathbf{g}$, so that \mathbf{d}_a describes gravitational sedimentation of the ions 2 (provided their effective ‘‘molecular weight’’ A_2/Z_2 is larger than that, A_1/Z_1 , for ions 1).

(b) The term \mathbf{d}_b is especially simple in the limit of $n_2 \ll n_1$. Then $n_e \approx Z_1 n_1$ and $\mathbf{d}_b = -k_B T \nabla n_2$, which corresponds to ordinary diffusion of ions 2. Generally, \mathbf{d}_b describes diffusive motion of the ions if their number densities are out of equilibrium.

(c) The term \mathbf{d}_c is most important in the regime of strong ion coupling and can be accurately described in the ion-sphere approximation combined with the linear mixing rule (e.g., Ref. [15] and references therein):

$$\mu_j^{(C)} = -0.9 \frac{Z_j^{5/3} e^2}{a_e}, \quad \nabla \mu_j^{(C)} = -0.3 \frac{Z_j^{5/3} e^2}{a_e} \frac{\nabla n_e}{n_e}. \quad (15)$$

Then

$$\mathbf{d}_c = 0.3 \frac{n_1 n_2}{n_e} \frac{Z_1 Z_2 e^2}{a_e} (Z_2^{2/3} - Z_1^{2/3}) \frac{\nabla n_e}{n_e}. \quad (16)$$

The structure of \mathbf{d}_c is similar to that of \mathbf{d}_a : it describes specific (“Coulomb”) sedimentation of ions 2 (provided $Z_2 > Z_1$) due to Coulomb coupling in the gravitational field. Its remarkable feature is that it operates even for ions with $A_1/Z_1 = A_2/Z_2$. Such ions are usually thought to have the same “molecular weights.” Then $\mathbf{d}_a = 0$ (as long as we neglect small mass defects of ions 1 and 2) and one commonly assumes that such ions are not separated. We see that it is not true.

By way of illustration, let us rewrite Eq. (8) under simplifying assumptions which are usually satisfied in the cores of white dwarfs and outer envelopes of neutron stars. Assume that the pressure is provided by strongly degenerate electrons $P = P_e(n_e)$ [which allows us to express ∇n_e in Eq. (16) through ∇P] and the hydrostatic equilibrium is established ($\nabla P = \rho \mathbf{g}$). Then we obtain the diffusion flux in the standard form

$$\mathbf{J}_2 = D \frac{m_1 m_2 n}{\rho n_e} (Z_2 n_2 \nabla n_1 - Z_1 n_1 \nabla n_2) + (\mathbf{u}_a + \mathbf{u}_c) m_2 n_2, \quad (17)$$

where

$$\mathbf{u}_a = \frac{\rho_1 n D}{\rho n_e k_B T} Z_1 Z_2 m_a \mathbf{g} \left(\frac{A_2}{Z_2} - \frac{A_1}{Z_1} \right), \quad (18)$$

$$\mathbf{u}_c = \frac{\rho_1 n D}{n_e k_B T} Z_1 Z_2 \mathbf{g} (Z_2^{2/3} - Z_1^{2/3}) \frac{0.3 e^2}{a_e P \gamma} \quad (19)$$

are the velocities of gravitational settling of ions 2 due to “molecular weight” difference and Coulomb separation, respectively; $\gamma = \partial \ln P / \partial \ln \rho$.

Note that, when the matter is in hydrostatic equilibrium, the gravitational settling of ions 2 is accompanied by “lifting” of ions 1 (with $\mathbf{J}_1 = -\mathbf{J}_2$). Such diffusive motion of ions initiates collisional production of the specific entropy (\dot{S}_{coll}) and the associated thermal energy release at a rate Q [erg cm⁻³ s⁻¹] (e.g., Refs. [10,11])

$$Q = T \dot{S}_{\text{coll}} = \frac{\rho}{\rho_1 \rho_2} \mathbf{J}_2 \cdot \mathbf{d}_1, \quad (20)$$

which is easily computed.

Discussion and conclusions.—Although the diffusion flux (17) has a standard form, it contains a new gravitational settling term (19) due to Coulomb separation. This separation has been predicted by Chang, Bildsten, and Arras [8] who considered equilibrium distributions of ion mixtures including the Coulomb interaction term. Thus we extend their work to nonequilibrium mixtures and show that the Coulomb separation is pronounced in the diffusion flux (17) and drives gravitational settling of ions.

The most pronounced effect occurs at temperatures at which the ions constitute strongly coupled Coulomb liquid. At lower temperatures the ions solidify and diffuse much more slowly [14]. At higher T Coulomb coupling is weak and less efficient (although generally available). The Coulomb sedimentation should be especially important for the mixtures of ions with the same A/Z (for instance, mixtures of ⁴He, ¹²C, and ¹⁶O ions). The traditional gravitational sedimentation (18) in such mixtures is greatly suppressed (can occur only due to mass defects of atomic nuclei [8]). The Coulomb settling in these mixtures (19) is typically much stronger than (18). The ions with larger Z should move to deeper layers. The effect is stronger for a larger difference of Z in the mixture.

Because the effect is primarily driven by gravitational forces, it should be most pronounced in compact stars (white dwarfs, and especially in neutron stars) with strongest gravity. First of all we mean ⁴He–¹²C cores of low mass white dwarfs and ¹²C–¹⁶O cores of more massive white dwarfs, and evolution of similar mixtures in the envelopes of neutron stars. The velocity of sedimentation is given by Eq. (19) using appropriate diffusion coefficients (e.g., Refs. [12–14,20], and references therein).

Figure 1 presents the velocity \mathbf{u}_c in the ¹²C–¹⁶O cores of medium mass and massive white dwarfs and in the ⁴He–¹²C cores of low mass white dwarfs. The adopted temperature range $T \sim (0.5\text{--}5) \times 10^7$ K is appropriate to rather old white dwarfs (e.g., Ref. [21]). The settling velocities are higher for massive white dwarfs (with larger g). The velocity profile throughout the core has a maximum at the core boundary $r = R_{\text{core}}$, where the gravitational acceleration $g(r)$ is the largest. The velocity $\mathbf{u}_c \rightarrow 0$ as $r \rightarrow 0$ because $g(r) \rightarrow 0$ at the star’s center. The maximum velocity in the massive (1.2 M_\odot) white dwarf reaches ~ 100 km Gyr⁻¹, meaning that the ¹²C–¹⁶O separation in the outer core can occur in a few Gyrs. The velocity of Coulomb separation of ¹²C and ¹⁶O ions is typically lower than the settling velocity of ²²Ne ions in the ¹²C–¹⁶O core [1–5], but the fraction of ²²Ne ions is much smaller than the fractions of ¹²C and ¹⁶O. Using Eqs. (19) and (20) we have estimated the thermal energy generation rate $Q(r)$ which accompanies this separation and found it insufficiently high to noticeably reheat old white dwarfs. The profile

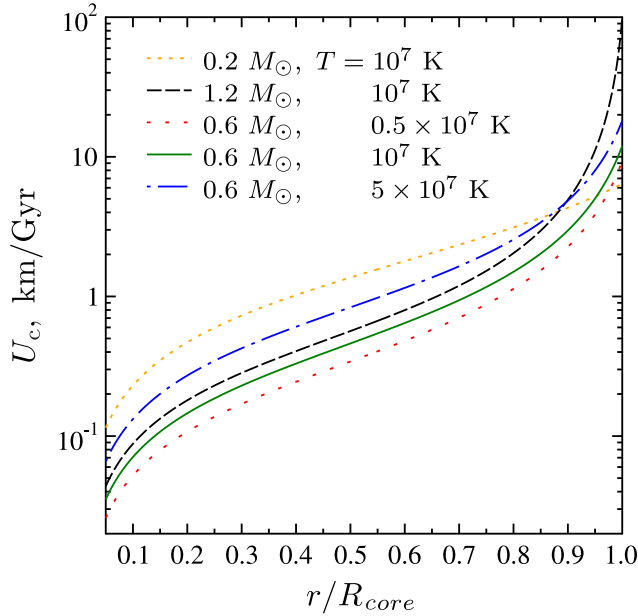


FIG. 1 (color online). Velocity (19) of Coulomb settling in isothermal degenerate cores ($r < R_{\text{core}}$) of white dwarfs of different mass (0.2, 0.6, and $1.2M_{\odot}$, M_{\odot} being the Sun's mass) and internal temperature ($0.5, 1,$ and 5×10^7 K). We show settling of ^{12}C in mixture with ^4He in $M = 0.2M_{\odot}$ star. In other cases it is the settling of ^{16}O mixed with ^{12}C . In all cases we assume that $n_1 = n_2$.

$Q(r)$ has maximum in the outer part of the white dwarf core. Note that our estimates neglect the direct diffusion term [the first term in Eq. (17)] which can enhance $Q(r)$.

The Coulomb separation of ^4He , ^{12}C , and ^{16}O ions can be important in isolated and accreting white dwarfs. It affects chemical composition and, therefore, microphysics of white dwarf core (heat capacity, thermal conductivity, neutrino emission, nuclear reaction rates) as well as chemical, thermal, and nuclear evolution of white dwarfs. Redistribution of ions due to Coulomb separation can affect also vibration properties of stars (asteroseismology).

Coulomb separation of ions with equal A/Z in neutron star envelopes is much stronger than in white dwarfs. Figure 2 plots the sedimentation velocity u_c of ^{12}C ions mixed with ^4He in the outer neutron star envelope versus depth z (measured from the surface) for two effective surface temperatures, $T_s = 1$ and 2 MK. The temperature profile $T(z)$ within the envelope has been determined by solving the heat transport equation for a conserved heat flux emergent from stellar interior (see, e.g., Ref. [8]). The envelope is nonisothermal and the temperature gradient can affect diffusion which we ignore for simplicity. Therefore, the presented curves should be treated as illustrative. For the densities of $\sim 10^5$ – 10^7 g cm^{-3} (a few to a few tens of meters under the surface) the sedimentation velocity can reach a few meters per year. The separation can affect nuclear evolution of the matter in the outer layers of accreting neutron stars. It will change the thermal

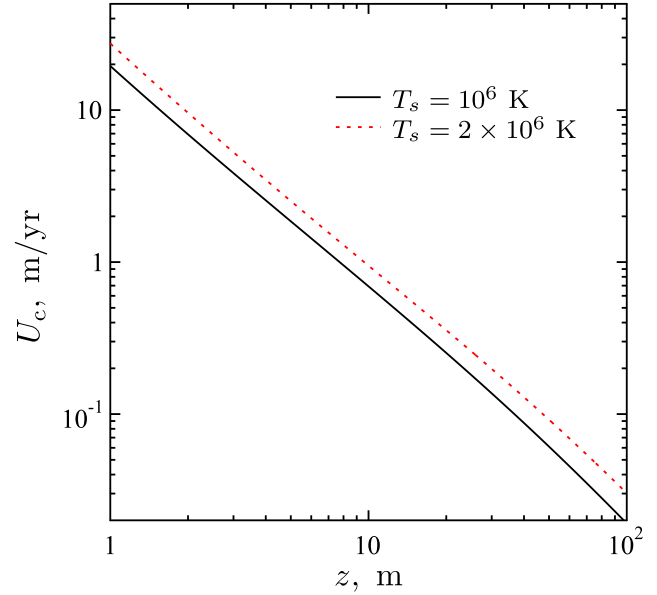


FIG. 2 (color online). Settling velocity of ^{12}C ions mixed with ^4He ($n_1 = n_2$) in the outer envelope of a neutron star (with gravity $g = 2 \times 10^{14}$ cm s^{-2}) versus depth z (measured from the stellar surface) for two effective surface temperatures $T_s = 10^6$ and 2×10^6 K. While z varies from 1 to 100 m, the density increases from $\sim 10^5$ to $\sim 10^9$ g cm^{-3} .

conductivity of this matter, influence the relation between the surface and inner temperatures of neutron stars, and affect cooling of isolated and accreting neutron stars (see, e.g., Refs. [6–8,22–24], and references therein).

Similar Coulomb separation can occur in dusty plasmas which have many applications in science and technology (e.g., Ref. [9]).

We are grateful to A. I. Chugunov and A. Y. Potekhin for useful discussions. D. G. Y. acknowledges support from RFBR (Grants No. 11-02-00253-a and No. 13-02-12017-offi-M), RF Presidential Program NSh 4035.2012.2, and Ministry of Education and Science of Russian Federation (Agreement No. 8409, 2012).

*mikavb89@gmail.com

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