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Diffusive currents and Coulomb separation of ions in dense matter

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Abstract. We derive diffusive currents in strongly coupled Coulomb ion mixtures in dense stellar matter. Coulomb coupling in the presence of gravity and electric fields, induced by gravity owing to plasma polarization, creates a specific diffusion current which separates ions with the same $A/Z$ (mass to charge number ratios) but different $Z$. This Coulomb separation can be important in white dwarfs and neutron stars.

1. Introduction
We consider diffusion of ions in a multicomponent ion plasma of white dwarfs (WDs) and neutron stars (NSs). As an example we can mention gravitational settling of $^{22}$Ne in $^{12}$C–$^{16}$O cores of WDs (see, e.g., [1–5]). This settling is thought to reheat old WDs and delay their cooling in accordance with observations. Diffusion of ions affects also chemical evolution and nuclear reactions in the envelopes of NSs (e.g., [6–8]).

Diffusion formalism is well developed for almost ideal plasma of ions [9, 10]. However, the ions in WDs and NSs are usually strongly coupled by Coulomb forces. The diffusion coefficients of ions in such plasmas have been thoroughly investigated, mainly by molecular dynamics simulations (e.g., [11–14]). We derive a new expression for diffusive currents. Our first results on this subject were published in [15].

2. Diffusion currents of ions
Let a plasma be composed of electrons and a mixture of ion species $j = 1, 2, \ldots$ (whose atomic numbers are $A_j$ and charge numbers are $Z_j$). Let $n_j$ denote the number density of ions $j$. Then the electron number density is $n_e = \sum_j Z_j n_j$ because of charge neutrality.

The state of ions $j$ can be described (e.g., [16]) by the Coulomb coupling parameter $\Gamma_j$,

$$\Gamma_j = Z_j^2 e^2 / (a_j kT) = Z_j^{5/3} e^2 / (a_ekT),$$

where $T$ is the temperature, $k$ is the Boltzmann constant, $a_e = (4\pi n_e / 3)^{-1/3}$ is the electronsphere radius, and $a_j = a_e Z_j^{1/3}$ is the ion-sphere radius (for a sphere around an ion $j$, containing an electron charge which compensates the ion charge). If $\Gamma_j \ll 1$ then the ion species $j$ form nearly ideal Boltzmann gas, while for $\Gamma_j \gg 1$ they form either Coulomb liquid or solid. One component plasma of ions solidifies at $\Gamma \approx 175$. We consider gaseous or liquid ion plasma only.
The diffusion currents in nearly ideal plasma are well studied [9, 10]. However, the case of non-ideal plasmas requires special treatment. We introduce diffusion currents for non-ideal plasma following [17]. Let the plasma slightly deviate from thermodynamic equilibrium under the action of forces $F_\alpha$ [on all particles $\alpha$, electrons ($\alpha = e$) and ions ($\alpha = j$)] and gradients of number density $\nabla n_\alpha$. For simplicity, we assume thermal equilibrium ($\nabla T = 0$). The forces $F_\alpha$ and gradients $\nabla n_\alpha$ create weak gradients of chemical potentials $\nabla \mu_\alpha$ of particles $\alpha$. Let $\tilde{F}_\alpha = F_\alpha - \nabla \mu_\alpha = e_\alpha E + m_\alpha g - \nabla \mu_\alpha$, where $F_\alpha = e_\alpha E + m_\alpha g$ (with $e_\alpha$ and $m_\alpha$ being electric charge and mass of particles $\alpha$, respectively). In stars, the force $F_\alpha$ is produced by gravity $g$ (that can be treated as locally constant) and by the polarization electric field $E$.

Notice that $\sum_\alpha n_\alpha \tilde{F}_\alpha = \rho g - \nabla P$, where $\rho = \sum_\alpha m_\alpha n_\alpha$ is the mass density of the plasma, $\nabla P = \sum_\alpha n_\alpha \nabla \mu_\alpha$ [18], and $P$ is the total plasma pressure; the $E$ field drops off due to electric neutrality.

If particle species $\alpha$ are in hydrostatic balance, then $\tilde{F}_\alpha = 0$. If the plasma is in hydrostatic equilibrium as a whole, then $\sum_\alpha n_\alpha \tilde{F}_\alpha = 0$ and $\rho g = \nabla P$. Hydrostatic equilibration ($\rho g = \nabla P$) in NSs is established in milliseconds and in WDs in a few minutes [19] but the diffusion of ions can take Gyrs (see, e.g., [3]). This diffusion can be analyzed assuming $\rho g = \nabla P$.

A deviation of particles $\alpha$ from hydrostatic equilibrium in a mixture can be measured by
\[ d_\alpha = \frac{\rho_\alpha}{\rho} \sum_\beta n_\beta \tilde{F}_\beta - n_\alpha \tilde{F}_\alpha, \] (2)\[ \text{where } \rho_\alpha = m_\alpha n_\alpha \text{ is the mass density of these particles } \alpha. \] Evidently, $\sum_\alpha d_\alpha = 0$.

Let $J_\alpha = \rho_\alpha V_\alpha$ be the diffusive flux of particle species $\alpha$, and $V_\alpha$ the diffusion velocity of these particles [9, 10]. Phenomenological relations for the diffusive currents can be written as
\[ J_\alpha = \Phi \sum_{\beta \neq \alpha} m_\alpha m_\beta D_{\alpha \beta} d_\beta. \] (3)\[ \text{Here, } D_{\alpha \beta} [\text{cm}^2 \text{ s}^{-1}] \text{ is a generalized diffusion coefficient of particles } \alpha \text{ relative to } \beta; \Phi \text{ is a normalization function to be specified later. The diffusion coefficients obey the relation } \sum_\alpha J_\alpha = 0. \] (4)

In a rarefield, nearly ideal plasma, $\tilde{F}_\alpha = F_\alpha - n_\alpha^{-1} \nabla P_\alpha$, where $P_\alpha$ is the partial pressure of particle species $\alpha$. Then (3) reproduces the standard definition of diffusion coefficients in rarefied plasmas [9, 10]. For strongly coupled plasmas, partial pressures $P_\alpha$ are ambiguous, while the definition (3) is not.

Since the electrons are light and mobile they are always in hydrostatic quasiequilibrium responding almost instantly to the motion of the ions; it is sufficient to set $m_e \to 0$. Then from (2) one has $d_e = -n_e \tilde{F}_e$. This electron hydrostatic quasiequilibrium implies
\[ d_e = 0, \quad \tilde{F}_e = -eE - \nabla \mu_e = 0. \] (5)\[ \text{It allows one to exclude electrons from the ion transport problem. In this case (3) and (4) retain their form but indices } \alpha \text{ and } \beta \text{ run only over ion species } (j = 1, 2, \ldots). \text{ Strictly speaking, (3) is valid for non-relativistic particles, while the electrons in stars can be relativistic. However, the results are applicable even in this case as long as the electrons can be considered as massless.} \]

In a binary ion plasma ($j=1, 2$) $J_1 = -J_2$, $d_1 = -d_2$, and $D_{12} = D_{21} = D$. Therefore, there is actually one diffusion coefficient $D$,
\[ J_2 = -J_1 = \frac{nm_1 m_2}{\rho kT} D d_1. \] (6)
Here we set \( \Phi = n/(\rho kT) \) \((n = n_1 + n_2\) is the total number density of the ions). Then \( D \) becomes the standard diffusion coefficient \([9, 10]\) for a binary plasma of ions.

Now we simplify (6). From (2) we obtain

\[
d_j = -\frac{\rho_j}{\rho} \nabla P - n_j e Z_j E + n_j \nabla \mu_j,
\]

where \( j = 1 \) or \( 2 \). Because \( d_1 + d_2 = 0 \), we have \( e n_e E = -\nabla P + n_1 \nabla \mu_1 + n_2 \nabla \mu_2 \). Substituting this into (7) with \( m_j = A_j m_u \) \((m_u\) being the atomic mass unit), we get

\[
d_1 = \frac{n_1 n_2}{n_e} \left[ m_u (Z_1 A_2 - Z_2 A_1) \frac{\nabla P}{\rho} + Z_2 \nabla \mu_1 - Z_1 \nabla \mu_2 \right].
\]

It is well known \((e.g., [16])\) that \( \mu_j = \mu_j^{(id)} + \mu_j^{(C)} \), where upperscripts \((id)\) and \((C)\) label the ideal gas and Coulomb contributions, respectively. Then \( d_1 = d_a + d_b + d_c \), with

\[
d_a = m_u Z_1 Z_2 \frac{n_1 n_2}{n_e} \left( \frac{A_2}{Z_2} - \frac{A_1}{Z_1} \right) \frac{\nabla P}{\rho},
\]

\[
d_b = \frac{n_1 n_2}{n_e} \left[ Z_2 \nabla \mu_j^{(id)} - Z_1 \nabla \mu_j^{(id)} \right] = \frac{kT}{n_e} (Z_2 n_2 \nabla n_1 - Z_1 n_1 \nabla n_2),
\]

\[
d_c = \frac{n_1 n_2}{n_e} \left[ Z_2 \nabla \mu_j^{(C)} - Z_1 \nabla \mu_j^{(C)} \right].
\]

In (10) we have made use of the well known relation \( \nabla \mu_j^{(id)} = kT n_j^{-1} \nabla n_j \).

Combined with (6), these equations define the diffusion current \( J_2 \). It consists of three terms labeled by subscripts \( a, b \) and \( c \). The terms \( a \) and \( b \) are known but the term \( c \) is new.

(a) Consider the matter which is in hydrostatic equilibrium as a whole \((\nabla P = \rho g)\). Then \( d_a \) describes gravitational sedimentation of the ion species 2 \((provided their effective \"molecular weight\" \( A_2/Z_2 \) is larger than \"molecular weight\" \( A_1/Z_1 \) for ion species 1).

(b) The term \( d_b \) has especially transparent form in the limit of \( n_2 \ll n_1 \). Then \( n_e \approx Z_1 n_1 \) and we obtain \( d_b = -kT R_j \nabla n_2 \) which corresponds to ordinary diffusion of ion species 2. Therefore, \( d_b \) describes diffusive motion of the ions if their number densities deviate from equilibrium ones.

(c) The term \( d_c \) is most important in the regime of strong ion coupling. In this case it can be accurately described in the ion-sphere approximation supplemented by the linear mixing rule \((e.g., [16])\):

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

\[
d_c = 0.3 \frac{n_1 n_2}{n_e} \frac{Z_1 Z_2 e^2}{a_e} \left( Z_2^{2/3} - Z_1^{2/3} \right) \nabla n_e.
\]

The structure of \( d_c \) is similar to that of \( d_a \): it describes the specific \"Coulomb\" sedimentation of ion species 2 \((provided Z_2 > Z_1)\) under the effect of Coulomb coupling in gravitational field. Its most interesting feature is that it separates even the ions with \( A_1/Z_1 = A_2/Z_2 \). Such ions possess the same \"molecular weights.\" Then \( d_c = 0 \) \((as long as we neglect small mass defects of ions 1 and 2)\) and it is widely thought that the ions are not separated. This is seen to be not true.

For illustration, let us rewrite (6) for the degenerate cores of WDs and outer envelopes of NSs. To this aim, we assume that \( \nabla P = \rho g \) and the pressure is provided by degenerate electrons,
\[ P \approx P_c(n_e), \] which allows us to express \( \nabla n_e \) in (13) through \( \nabla P \). Then the diffusion flux can be expressed in the standard form

\[ J_2 = D \frac{m_1 m_2 n}{\rho n_e} (Z_2 n_2 \nabla n_1 - Z_1 n_1 \nabla n_2) + (u_a + u_c) m_2 n_2. \] (14)

In this case

\[ u_a = \frac{\rho n D}{\rho n_e k_B T} Z_1 Z_2 m_a g \left( \frac{A_2}{Z_2} - \frac{A_1}{Z_1} \right), \] (15)

\[ u_c = \frac{\rho n D}{n_e k_B T} Z_1 Z_2 g \left( Z_2^{2/3} - Z_1^{2/3} \right) \frac{0.3 c^2}{a_e P \gamma} \] (16)

are the velocities of gravitational settling of ion species 2 under the effects of “molecular weight” difference and Coulomb separation, respectively; \( \gamma = \partial \ln P/\partial \ln \rho \).

Let us remark that, when the matter is in hydrostatic equilibrium, the gravitational settling of ion species 2 is accompanied by “lifting” of ion species 1 (with \( J_1 = -J_2 \)). This diffusive motion of ions generates the collisional production of the specific entropy \( \dot{S}_{\text{coll}} \) which leads to the thermal energy release with the rate \( Q \) [erg cm\(^{-3}\) s\(^{-1}\)] (e.g., [9, 10])

\[ Q = T \dot{S}_{\text{coll}} = J_2 \cdot d_1 \rho / (\rho_1 \rho_2) \] (17)

that is easily computed.

### 3. Observational consequences and summary

Although the diffusion flux (14) retains its standard form, it contains a new settling term (16) owing to Coulomb separation. That separation was predicted by Chang et al. [8] who analyzed equilibrium distributions of ion mixtures including the Coulomb interaction term. We extend their work to non-equilibrium ion mixtures and show that the Coulomb separation affects the diffusion flux (14) and gravitational settling of ions.

The strongest effect occurs at temperatures at which the ions form strongly coupled Coulomb liquid. At lower temperatures ions solidify; in the solid state they diffuse but much slower [13]. At higher temperatures, Coulomb coupling is available but less efficient. The Coulomb liquid is most important for the mixtures of ions with the same \( Z \approx A/\sqrt{Z} \) sedimentation is most important for the mixtures of ions with the same \( Z \approx A/\sqrt{Z} \). At higher temperatures, Coulomb coupling is available but less efficient. The Coulomb liquid is most important for the mixtures of ions with the same \( Z \approx A/\sqrt{Z} \). At higher temperatures, Coulomb coupling is available but less efficient. The Coulomb liquid is most important for the mixtures of ions with the same \( Z \approx A/\sqrt{Z} \). At higher temperatures, Coulomb coupling is available but less efficient. The Coulomb liquid is most important for the mixtures of ions with the same \( Z \approx A/\sqrt{Z} \). At higher temperatures, Coulomb coupling is available but less efficient. The Coulomb liquid is most important for the mixtures of ions with the same \( Z \approx A/\sqrt{Z} \).

The effect is basically regulated by gravity. It is most pronounced in compact stars (WDs, and NSs) with the strongest gravity. First of all we mean \(^4\)He–\(^{12}\)C cores of low mass WDs and \(^{12}\)C–\(^{16}\)O cores of more massive WDs, and similar mixtures in the envelopes of NSs. The velocity of sedimentation is given by (16) with appropriate diffusion coefficients (e.g., [11–13, 20]).

Figure 1 shows \( u_c \) in the \(^{12}\)C–\(^{16}\)O cores of medium mass and massive WDs and in the \(^4\)He–\(^{12}\)C cores of low mass WDs. The adopted temperate range \( T \approx (0.5 - 5) \times 10^7 \) K is appropriate to old isolated WDs [21]. The settling velocities are higher for massive WDs (with larger \( g \)). The velocity profile throughout the WD core has a maximum at the core boundary \( r = R_{\text{core}} \). We have \( u_c \to 0 \) as \( r \to 0 \) because \( g(r) \to 0 \) at the star’s center. The maximum velocity in 1.2 \( M_\odot \) WD reaches \( \sim 100 \) km Gyr\(^{-1}\); the \(^{12}\)C–\(^{16}\)O separation in the outer core occurs in a few Gyrs.

The velocity of Coulomb separation of \(^{12}\)C and \(^{16}\)O ions is typically lower than the settling velocity of \(^{22}\)Ne ions in the \(^{12}\)C–\(^{16}\)O core [1–5] but the fraction of \(^{22}\)Ne ions is much smaller than the fractions of \(^{12}\)C and \(^{16}\)O. Using (17) and (16) we have estimated the thermal energy generation rate \( Q(r) \) which accompanies this separation and found it insufficient to noticeably reheat old WDs. The profile \( Q(r) \) has a maximum in the outer part of the WD core.
The Coulomb separation of $^4$He, $^{12}$C and $^{16}$O ions can be important in isolated and accreting WDs. It affects chemical composition and, consequently, heat capacity, thermal conductivity, neutrino emission, nuclear reaction rates as well as chemical, thermal and nuclear evolution of WDs. Coulomb separation of ions may affect also asteroseismology of WDs.

Coulomb separation of ions with equal $A/Z$ in NS envelopes is much stronger than in WDs. Figure 2 plots the sedimentation velocity $u_c$ of $^{12}$C ions mixed with $^4$He in the outer NS envelope at $\rho = 10^6 \text{ g cm}^{-3}$ as a function of the mean Coulomb coupling parameter [16]. The solid line is a result of a computation based on numerical calculation of $\mu^C_j$ [22] which is applicable for arbitrary coupling. SC stands for the approximation of strong coupling; this line represents velocity (16). WC represents the approximation of weak coupling. Details of general and weak coupling calculations will be discussed elsewhere. The envelope is non-isothermal and the temperature gradient can affect diffusion which we ignore for simplicity. For the densities of $\sim 10^5 - 10^7 \text{ g cm}^{-3}$ (from a few to a few tens of meters under the surface) the sedimentation velocity can reach several meters per year. The separation can affect nuclear evolution of the matter in the outer layers of accreting NSs. It will change the thermal conductivity of this matter, influence the relation between the surface and inner temperatures of NSs and affect cooling of isolated and accreting NSs (e.g., [6–8, 23–25]).

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Figure 1: (Color online) Velocity (16) of Coulomb settling in degenerate cores ($r < R_{\text{core}}$) of WDs with masses $M = 0.2$, 0.6, and $1.2 \, M_\odot$ ($M_\odot$ being the Sun’s mass) and internal temperatures 0.5, 1, and $5 \times 10^7 \text{ K}$. We show settling of $^{12}$C in mixture with $^4$He in the $0.2 \, M_\odot$ WD. In other cases it is settling of $^{16}$O mixed with $^{12}$C. In all cases we assume $n_1 = n_2$.

Figure 2: (Color online) Settling velocity of $^{12}$C ions mixed with $^4$He ($n_C/n = 0.4$) in the outer neutron star envelope ($\rho = 10^6 \text{ g cm}^{-3}$, $g = 2 \times 10^{14} \text{ cm s}^{-2}$) versus mean Coulomb coupling parameter $\Gamma = (n_C \Gamma_C + n_{He} \Gamma_{He})/n$. See explanation in the text.
References