1. INTRODUCTION

The thermal conductivity of a dense multi-component plasma (MCP) is critical to the modeling of accreting neutron stars. To this end, we perform large-scale molecular dynamics simulations to calculate the static structure factor of the dense MCP in the neutron star crust from near the photosphere-ocean boundary to the vicinity of the neutron drip point. The structure factors are used to validate a microscopic linear mixing rule that is valid for arbitrarily complex plasmas over a wide range of Coulomb couplings. The microscopic mixing rule in turn implies and validates the linear mixing rule (LMR) for the equation of state properties and also the LMR for the electrical and thermal conductivities of dense MCPs. To make our result as useful as possible, for the specific cases of electrical and thermal conductivities, we provide a simple analytic fit that is valid for arbitrarily complex MCPs over a wide range of Coulomb couplings. We compute the thermal conductivity for a representative compositional profile of the outer crust of an accreting neutron star in which hundreds of nuclear species can be present. We utilize our results to re-examine the so-called impurity parameter formalism as used to characterize impure plasmas.

Key words: dense matter – equation of state – nuclear reactions, nucleosynthesis, abundances – stars: neutron – X-rays: binaries – X-rays: bursts

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2. Another exciting application of accurate conductivities appears in modeling the cooling light curves of transiently accreting neutron stars. In the case of transients with accretion episodes of sufficient duration to heat the crust by deep crustal nuclear reactions (quasi-persistent transients), the thermal relaxation behavior gives us a new observational window into the physics of matter at very high density. Recently, Shterin et al. (2007) and Cackett et al. (2006) have presented detailed analyses of two such quasi-persistent transients, namely KS 1731–260 and MXB 1659–29. Since a critical determinant of the time evolution of surface flux is the thermal diffusion timescale as a function of depth in the neutron star, the conductivity plays an important role in modeling the cooling light curve of transients.

To reduce the uncertainties in modeling the thermal profiles of persistent and transient accretors, we have begun a program of accurately computing the microphysical quantities that influence thermal structure. For the impure ashes from an X-ray burst, it is crucial to ascertain the composition evolution of these ashes with increasing depth in the neutron star crust. It is upon this composition profile that all other thermal structure determinants depend, most notably

1. nuclear heating due to non-equilibrium electron captures, neutron reactions, and pycnonuclear fusion,
2. the thermal conductivity $\kappa$, and

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3. The neutrino emissivity $\epsilon$, from neutrino-pair bremsstrahlung (NPB).

The compositional profile of the outer crust (where there is negligible free neutron abundance) starting with a realistic MCP of XRB ashes was calculated for the first time using global nuclear structure and reaction rate inputs to a large reaction network in Gupta et al. (2007). By a “composition profile” we refer to the changing composition from the top of the crust (X-ray burst ashes) all the way to neutron-drip. This spans four orders of magnitude in density (roughly $10^{7.5}$ to $10^{11.2}$ g cm$^{-3}$) allowing for a large range in Coulomb coupling. It is this compositional profile that we employ in the present work to investigate the resulting crustal microphysics since it has tens to hundreds of abundant species at each depth. Thus, we have an ideal site to explore the physics of strongly coupled MCPs.

In this paper, we perform large-scale molecular dynamics (MD) simulations to calculate the structure factor of the dense MCP in the neutron star crust from near the photosphere-ocean boundary to the vicinity of the neutron drip point. The structure factors are used to validate a microscopic linear mixing rule (MLMR) that is valid for arbitrarily complex MCPs over a wide range of Coulomb couplings. The MLMR in turn implies and validates the mixing rule for the equation of state properties recently proposed for MCPs by Potekhin et al. (2009), and a mixing rule for the electrical and thermal conductivities of MCPs. These mixing rules provide a simple recipe to compute the physical properties of plasma mixtures, such as would be found in terrestrial experiments (e.g., inertial confinement fusion (ICF) plasmas.) In general, the MLMR implies a LMR for any quantity that is an integral of the structure factor, such as the neutrino pair-Bremsstrahlung emissivity. To make our result as useful as possible for the compact object modeling community, we discuss the standard treatments of mixtures, namely the impurity parameter formalism and the LMR.

2. ELECTRONIC PROPERTIES OF IONIC MIXTURES

The section is organized as follows.

1. First, we briefly discuss the principal characteristics of the MCPs found in the crust of accreting neutron stars.
2. We then recall the link between the electronic transport properties and NPB emissivity with the charge-charge structure factor.
3. We discuss the standard treatments of mixtures, namely the impurity parameter formalism and the LMR.
4. Finally, we compare electron scattering in terrestrial metals and neutron star crusts, and comment on the model of electron-ion scattering at the solid–liquid phase boundary as proposed by Baiko et al. (1998).

All the formulae below are expressed in natural (SI) units (in particular $e^2 = q^2 / 4\pi \varepsilon_0$ where $q$ is the electronic charge.) Also, the words “nucleus (nuclei)” and “ion (ions)” are used interchangeably.

2.1. Characterizing the Ionic Mixtures

We consider an unmagnetized, neutral MCP in a volume $V$ at temperature $T$ consisting of a mixture of $N_{sp}$ atomic species of charge $Z_j$ and mass number $A_j$, $j = 1, \ldots, N_{sp}$. The number and mass densities of species $j$ are $n_j$ and $\rho_j$, respectively. The total number density and mass density are $n = \sum_{j=1}^{N_{sp}} n_j$ and $\rho = \sum_{j=1}^{N_{sp}} \rho_j$, respectively. The total electron density is $n_e = \sum_{j=1}^{N_{sp}} Z_j n_j = \langle Z \rangle n$, where $\langle Z \rangle = \sum_{j=1}^{N_{sp}} x_j Z_j$ is the mean ionic charge. We use

$$x_j = n_j / n$$

(1)
to denote the number fraction of the $j$th species. Note that the number fraction is related to the species “abundances” $Y_j$ as traditionally used in the astrophysics literature; therefore the number fraction $x_j$ differs from the usual “mass fraction” $X_j$.

Thus

$$n_j = \rho N_A Y_j = \rho N_A \left( \frac{X_j}{A_j} \right)$$

(2)
Figure 1. Evolution with depth of dimensionless parameters obtained using the crustal composition profile of Gupta et al. (2007). $\Gamma_{\text{eff}}$ is the effective coupling parameter defined in Equation (4), $a/a_B$ is the ratio of the mean interatomic distance to the electronic Bohr radius, $x_r$ is the relativity parameter, $\Theta = T/T_F$ is the degeneracy parameter. The vertical dashes indicate the compositions studied with MD and listed in Table 2. The dots show the ratio $Q_{\text{imp}}$ defined in Equation (24) and $Q_{\text{imp}}$ defined in Equation (24) and $Q_{\text{imp}}$ defined in Equation (24). As discussed in Section 5, $(Z^2_j)$ is less sensitive than $Q_{\text{imp}}$ to composition changes at densities $\sim 10^7$, $2 \times 10^8$, $10^{10}$, and $10^{11}$ g cm$^{-3}$.

(A color version of this figure is available in the online journal.)

where $A_j$ is the mass number of species $j$, $N_\lambda$ is Avogadro’s number, and

$$x_j = \frac{X_j/A_j}{\sum_k (X_k/A_k)}$$  

where the index $k$ denotes summation over all nuclear species in the MCP, including free nucleons. The average inter-particle distance between nuclei is denoted by $a = (3/4\pi n_0)^{1/3}$, whereas the mean distance between electrons is $a_e = (3/4\pi n_e)^{1/3}$. We will occasionally use the compact notations $Z = (Z_1, \ldots, Z_{N_{sp}})$ and $\vec{x} = (x_1, \ldots, x_{N_{sp}})$ to denote the composition. When $N_{sp} = 1$, the system is referred to as a one-component plasma (OCP) and we drop the subscript referring to the particles’ species.

We define several dimensionless parameters to characterize the system, namely:

1. the relativistic parameter $x_r = p_F/m_e c$,
2. the degeneracy parameter $\Theta = T/T_F$,
3. the electron coupling parameter $\Gamma_e = e^2/a_e k_B T$,

where $p_F = \hbar k_F$ is the Fermi momentum, $k_F = (3\pi^2 n_e)^{1/3}$ is the Fermi wavevector and $T_F$ is the Fermi temperature of electrons.

For the typical physical conditions of interest in this paper, the density is in the range $10^8$ g cm$^{-3}$ $\leqslant \rho \leqslant 10^{12}$ g cm$^{-3}$, the temperature is $T \sim 0.5$ GK, and the number of species $N_{sp}$ varies from a few to several hundreds. As illustrated in Figure 1, at these densities and temperatures, $x_r > 1$, $\Theta \ll 1$, and $a/a_B \ll 1$ where $a_B$ is the Bohr radius. As a consequence, atoms are completely pressure-ionized and matter is a dense, MCP composed of bare nuclei neutralized by a relativistic and strongly degenerate gas of delocalized electrons. This paper deals with the scattering of these electrons off the multi-component ionic mixture.

The ions are in general nonrelativistic; we shall also assume hereafter that the ions behave as classical entities, thereby neglecting the quantum nature of the ionic density fluctuations that may occur in the regions where $T > T_p = \hbar \omega_p/k_B$, where $\omega_p$ is the (kinetic) ion plasma frequency.

The nuclei are “strongly coupled” in the sense that their properties are primarily governed by their mutual interactions rather than by purely thermal effects as in an ideal gas.

In the OCP, electron–ion scattering is fairly well understood. The degree of coupling of an OCP is usually characterized by the so-called Coulomb coupling parameter $\Gamma_{\text{OCP}} = Z^2 e^2/a e k_B T$, the ratio of the mean interaction energy $Z^2 e^2/a$ to the thermal energy $k_B T$ of the particles. Neglecting electronic screening, the OCP is known to crystallize into a bcc lattice at $\Gamma_{\text{OCP}} \approx 175$. Below $\Gamma_{\text{OCP}}$ the OCP is in a fluid state whose properties vary from gas-like at small $\Gamma_{\text{OCP}} < 0.1$ to liquid-like when $50 < \Gamma_{\text{OCP}} < \Gamma_{\text{c}}$ (Daligault 2006); in the intermediate regime, $0.1 < \Gamma_{\text{OCP}} < 50$, both potential and kinetic effects play a comparable role in a non-trivial way. As a consequence, models of neutron star crusts based on the OCP usually treat the electron–ion scattering as follows.

1. When $\Gamma > \Gamma_{\text{c}}$, electrons travel in a bcc crystal and electron–ion scattering is interpreted as the scattering of Bloch electrons off the thermal vibrations (phonons) of the ions with respect to the bcc lattice sites.
2. When $\Gamma < \Gamma_{\text{c}}$, electrons scatter off the disordered ionic background characteristic of the fluid state.

Recently Baiko et al. (1998) called into question this canonical picture because it yields discontinuities in the electronic transport properties at melting. In Section 2.2.4, we comment on this controversy regarding the behavior of the electron–ion scattering at the solid–liquid phase boundary of an OCP.

The state of affairs for multi-component mixtures is much less known, and especially for mixtures composed of $N_{sp} \geq 3$ species as encountered in the crust of accreting neutron stars. A common approach used to infer the properties of a mixture is to map the latter onto an effective OCP of coupling $\Gamma_{\text{eff}}$, thereby disregarding the (poorly understood) complexities of the phase diagram and dynamic properties of a true mixture. A suitable definition of the effective coupling is

$$\Gamma_{\text{eff}} = \sum_{j=1}^{N_{sp}} x_j \Gamma_j = (Z^{5/3}) \Gamma_{\text{c}}$$  

where

$$\Gamma_j = (Z^2_j e^2)/(a_j k_B T)$$  

is the coupling parameter for species $j$, $a_j = (3/4\pi n_j)^{1/3}$ being the average inter-particle distance of particles of species $j$, and $(Z^{5/3}) = \sum_j x_j Z_j^{5/3}$. This choice for $\Gamma_{\text{eff}}$ is motivated by the inequality (written here for pure Coulomb interactions; Rosenfeld 1993)

$$-\frac{9}{10} \Gamma_{\text{eff}} \leqslant U_{ex}/nV$$  

$$k_B T,$$

which provides a very good lower bound of the ratio of mean excess (interaction) energy per particle $U_{ex}/nV$ to the thermal energy $k_B T$, and therefore is a lower bound on the effective Coulomb coupling in the MCP.

In the astrophysical literature related to dense plasmas, often a mixture is assumed to crystallize at $\Gamma_{\text{eff}} = 175$ as in the
OCP. Several questions can be raised with regard to the onset of periodic ordering in a true MCP that have not been satisfactorily addressed to date. For instance:

1. Does the system crystallize in a regular, periodic lattice as has often been assumed in the literature?
2. Do the most abundant species make a lattice and the less abundant species contribute to defects in the structure?
3. Is it amorphous with a liquid-like frozen-in structure?

An affirmative answer to questions 1 and 2 above is assumed rather commonly in the literature and consequently, beyond $\Gamma_{\text{eff}} > \Gamma_c$, the total electron–ion scattering cross-section is split into two contributions: (1) the electron–phonon contribution due to the lattice structure and (2) the electron–impurity contribution. We believe that the phase diagram of mixtures such as those existing in the crust of accreting neutron stars is still too poorly known to make any definite statements such as 1 and 2 above. The local composition may also be changed due to phase-separation (demixing) and sedimentation effects, which are still not well understood and are being investigated (Horowitz et al. 1999). Given the complexity of the mixtures, it is, however, not unreasonable to think that, even when $\Gamma_{\text{eff}} > \Gamma_c$, the system will most likely be amorphous, or at the very least be comprised of many defects, and that the existence of Bloch states is questionable. In the following, we shall assume that the composition at any depth in the outer crust of the accreting neutron star is known; in practice, we shall use the outer crust composition from Gupta et al. (2007). In all cases that we considered, when starting from an amorphous structure, the MD simulations performed did not show any evidence for demixing or crystallization over the timescale of the simulations.

2.2. Electron–Ion Scattering in MCPs

We shall focus on electron–ion scattering and ignore the effect of electron–electron (ee) scattering. It was shown in (Potekhin et al. 1999) that ee scattering contributes to conductivity only for very light nuclei with $Z \lesssim 6$ and under non-degenerate conditions. For a pure $^{56}\text{Fe}$ composition in a degenerate plasma at densities $\approx 10^{10}$–$10^{11.5}$ g cm$^{-3}$ (Potekhin et al. 1999) showed that ee collisions could be neglected.

Many of the basic formulae in the following sections can be found, for instance, in Flowers & Itho (1976).

2.2.1. Thermal and Electrical Conductivities

Electron–ion scattering impedes the transport of electronic momentum and energy. The resulting electrical conductivity $\sigma$ and the thermal conductivity $\kappa$ can generally be expressed in terms of the collision frequencies $\nu_\sigma$ and $\nu_\kappa$:

$$\sigma = \frac{n_e e^2}{m_e} \tau_\sigma \tag{7}$$

$$\kappa = \frac{1}{3} \frac{n_e e^2}{m_e c} C_V \tau_\kappa = \frac{\pi^2 k_B^2}{3 m_e^*} T n_e \tau_\kappa \tag{8}$$

where $m_e^* = m_e \sqrt{1 + x_i^2}$ is the effective electron mass, $v_F = p_F / m_e^*$ is the Fermi velocity, and $C_V$ is the heat capacity of the free relativistic electron gas.

The quantities $\tau_\sigma$ and $\tau_\kappa$ describe the typical timescale over which electron–ion collisions degrade the electric and thermal currents. Their inverses, the frequencies $\nu_{\sigma,\kappa} = 1/\tau_{\sigma,\kappa}$, can conveniently be written as the product of a “fundamental” frequency $\nu_0$:

$$\nu_0 = \frac{4\pi (Z^2) e^4 n_i}{p_F^2 v_F} = \frac{4\alpha^2 E_F (Z^2)}{3\pi \hbar} \langle Z \rangle \quad \tag{9}$$

multiplied by a dimensionless quantity $\ln \Lambda_{\sigma,\kappa}$ known as the Coulomb logarithm:

$$\nu_{\sigma,\kappa} = \nu_0 \ln \Lambda_{\sigma,\kappa}. \quad \tag{10}$$

In Equation (9), $\langle Z^2 \rangle$ results form the appropriate normalization $S_{\kappa}(k \to \infty) \to 1$ of the structure factor discussed below in Equation (15), $\alpha = e^2 / \hbar c$ is the fine-structure constant, and $E_F = m_e^* c^2$ is the electron Fermi energy. The fundamental frequency $\nu_0$ can be seen as a frequency of Coulomb collisions associated with the transfer of momentum between electrons and ions; it can be written as

$$\nu_0 = n \left[ 4\pi \left( \frac{(Z^2)^{1/4} e^2}{m_e^* v_F^2} \right)^2 \right] v_F \tag{11}$$

in which the bracketed term can be interpreted as the cross-section for momentum transfer in a binary collision between an electron of velocity $v_F$ and charge $-e$ and a massive ion of charge $(Z^2)^{1/4} e$. The dimensionless Coulomb logarithm contains all the fine details of electron–ion collisions in a plasma, such as charge screening, collective modes, and quantum diffraction effects. In general, $\ln \Lambda_e \neq \ln \Lambda_c$ since the two transport coefficients measure different mechanisms, namely momentum and energy transport. However, when the dominant source of electron–ion scattering is elastic, as in the disordered fluid phase or the high-temperature crystalline phase, the two Coulomb logarithms are equal and the Wiedemann–Franz relation

$$\kappa / \sigma = \frac{\pi^2 k_B^2}{3 e^2} T \quad \tag{12}$$

is satisfied.

A calculation of the Coulomb logarithm that self-consistently treats all the many-body effects occurring in a MCP is in general rather complicated. However, because of the high electron density in neutron stars, the typical electron kinetic energy is very large compared to the electron–ion interaction energy and the average electron–ion correlations are weak. Accordingly, a good approximation can be made by considering the ions and electrons in the plasma as two weakly interacting subsystems, namely an MCP neutralized by a homogeneous negatively charged background and an homogeneous interacting electron gas (i.e., relativistic quantum electronic jellium.) Electrons scatter off the electrostatic potential created by the ionic charge distribution,

$$n_z(r, t) = \sum_{j=1}^{N_e} \sum_{l=1}^{N_i} \delta (r - R_i(t)), \tag{13}$$

where $R_i(t)$ is the position of the $l$th nuclei of the $j$th species at time $t$, and $N_j = n_j V$ is the number of particles of species $j$. In
the (first) Born approximation \(^1\) of the electron–ion interaction and using the fact that the electrons are much heavier than the ions, we obtain (Flowers & Itoh 1976)

\[
\ln \Lambda_{\sigma, k} = \int_0^{2k_F} dkk^3 \frac{v(k)}{\varepsilon_e(k)} \left[ 1 - \frac{x^2}{1 + x^2} \left( \frac{k}{2k_F} \right)^2 \right] S_{\sigma, k}(k),
\]

(14)

with \(v(k) = 1/k^2 \) and \(\varepsilon_e(k)\) is the static dielectric function of the electron jellium.

Equation (14) can be interpreted as follows. The Coulomb logarithm \(\ln \Lambda_{\sigma, k}\) sums all the contributions of collisions characterized by momentum transfer \(k\). The range of integration is limited to \(2k_F\) because the electrons are degenerate and only those electrons near the Fermi surface take part in exchanges of momentum and energy. The electrons behave as if they were scattered independently of each other by the electronically screened electron–ion potential. Because the electrons are much lighter than the nuclei, the energy exchanges \(\hbar\omega\) in inelastic collisions occur in a range over which \(\varepsilon_e(k, \omega) \approx \varepsilon_e(k, 0) = \varepsilon_e(k)\). For relativistic, degenerate electrons, an analytical expression for \(\varepsilon_e\) was obtained by Janovcici (1962) within the random-phase approximation (see Appendix B).

The bracketed term, which describes the kinematic suppression of backward scattering of relativistic electrons, \(\left[ 1 - \frac{x^2}{1 + x^2} \left( \frac{k}{2k_F} \right)^2 \right]\), varies between unity for \(x_i \to 0\) and \(\left[ 1 - (k/2k_F)^2 \right]\) for \(x_i \to \infty\).

The many-body physics of the ionic subsystem is encapsulated in the function \(S_{\sigma, k}(k)\). \(S_{\sigma, k}(k)\) is a functional of the spectrum of charged fluctuations \(\delta n_j(k, t) = n_j(k, t) - \langle n_j(k) \rangle_{\text{eq}}\) in the ionic system

\[
S_{zz}(k, \omega) = \frac{1}{nV \langle Z^2 \rangle} \int d\omega \frac{\delta n_j(k, \omega) \delta n_j(-k, 0)}{2\pi} e^{i\omega t}
\]

(15)

where \(\langle \rangle_{\text{eq}}\) denotes the average of a canonical ensemble at temperature \(T\). In other words, \(S_{\sigma, k}(k)\) self-consistently takes into account all of the separate electron–ion relaxation mechanisms at the level of the Born approximation; it is really an umbrella term for electron–ion, electron–impurity, electron–phonon scattering, and includes multi–phonon processes. We have, from Flowers & Itoh (1976),

\[
S_{\sigma}(k) = \int_{-\infty}^{\infty} S_{zz}(k, \omega) \omega n(z) \right. \right. \left. \left. \left. z = \hbar\omega/k_BT
\]

\[
S_{k}(k) = \int_{-\infty}^{\infty} S_{zz}(k, \omega) \omega n(z) \left[ 1 + \left( \frac{3k_F^2}{\kappa^2} - \frac{1}{2} \right) \right] \right. \right. \left. \left. z^2
\]

where \(n(z) = 1/1 - e^{-z}\). \n
\(^1\) Extensions to higher-order approximations are difficult. An approximate treatment proposed by Yakovlev et al. (1987) prescribes usage of the exact binary cross-section instead of the Born approximation in the integrand of Equation (14). This introduces an additional factor in Equation (14), namely \(R(k) = \sigma(k)/\sigma_0(k)\) where \(\sigma_0\) is the exact differential cross section for a momentum transfer \(k\) and \(\sigma_0\) is the Born approximation. A similar procedure can be applied verbatim to our calculations since the MCP structure factor is not affected. Recently, a similar averaging procedure was used by Itoh et al. (2008); however, the title of that paper is somewhat misleading since it is not actually the second-Born approximation that is performed therein. Such a calculation would involve the higher-order correlation functions of the ionic density Equation (13). However, these higher-order correlations are noticeably absent in the equations of Itoh et al. (2008) for the transport coefficients.

In the special case of a periodic, crystalline structure, the term \(\langle n_j(k) \rangle_{\text{eq}}\) peaks at values of the wavevector \(k\) commensurate with the periodicity of the lattice and subtracts out the elastic Bragg peaks: electron–ion scattering involves Bloch electrons and Equation (14) is obtained by approximating their behavior by means of free particle wave functions.

When the scattering is predominantly elastic in nature, as is expected in the fluid and solid phases at \(T > T_p\) or in a disordered (non-periodic) lattice, we have

\[
S_{\sigma, k}(k) = \int_{-\infty}^{\infty} S_{zz}(k, \omega)
\]

(16)

\[
= \frac{1}{nV \langle Z^2 \rangle} \langle \delta n_j(k, 0) \delta n_j(-k, 0) \rangle_{\text{eq}}
\]

(17)

\[= S_{zz}(k)
\]

(18)

where \(S_{zz}(k)\) is the (charge–charge) structure factor. This leads to

\[
\ln \Lambda_{\sigma, k} = \int_0^{2k_F} dkk^3 \frac{v(k)}{\varepsilon_e(k)} \left[ 1 - \frac{x^2}{1 + x^2} \left( \frac{k}{2k_F} \right)^2 \right] S_{zz}(k).
\]

(19)

In this limit, \(\sigma\) and \(k\) are insensitive to the details of the spectrum of ionic charge fluctuations. These details (ion collective modes and single-particle effects) are present implicitly but in an integrated form via the sum-rule (18).

Until now, we have assumed that the ions are point particles. In this “point-charge” approximation, the only species-dependent term in the integrand of Equation (14) is the charge–charge structure factor \(S_{zz}(k)\). In order to allow for finite nuclear size, one can replace the density (13) with

\[
n_j(k, t) = \sum_{j=1}^{N_j} Z_j F_j(k) \sum_{\omega} e^{-i\hbar Rj(t)},
\]

(20)

where \(F_j(k)\) is the nuclear form factor, which reflects the charge distribution within a nucleus of species \(j\). For instance, assuming uniform proton density in the nuclei,

\[
F_j(k) = \frac{3}{(kR_j)^3} \left( \sin(kR_j) - kR_j \cos(kR_j) \right)
\]

(21)

where \(R_j\) the charge radius of the nuclear species \(j\) which has mass number \(A_j\); we use \(R_j = 1.15A_j^{1/3}\) fm as in Kaminker et al. (1999). Direct MD calculation of the structure factor \(S_{zz}(k)\) with and without the nuclear form factor (21) shows that the finite nuclear size corrections are completely negligible in the outer crust of interest in this paper. (Note that for instance \((F_j(k))^2 = 0.9766\) at the peak of \(S_{zz}(k)\), i.e. at \((k/2k_F) \approx 0.33\), for a typical heavy nucleus having mass number \(A_j \approx 64–100\) or \(A_j^{1/3} \approx 4–4.6\). Accordingly, we neglect finite nuclear size effects in the remainder of this paper.

2.2.2. Neutrino-pair Bremsstrahlung (NPB) Emissivity

In NPB, the electrons are accelerated by the Coulomb field of the crust as in photon Bremsstrahlung but with the emission of a neutrino–antineutrino pair instead of a photon. In the first Born approximation, the neutrino emissivity is
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\[ \epsilon_v = \frac{8\pi G_F(Z^2)e^4C_z^2}{567\hbar^9 e^8}(k_B T)^6 \ln \Lambda_v \] (22)

with the Coulomb logarithm for NPB,

\[ \ln \Lambda_v = \frac{\hbar c}{k_B T} \int_0^{2k_F} dk k^3 \int_0^{\infty} dk' \left\{ \nu(k', k) \right\} S_{zz}(k) R_T(k, k') \]

\[ \approx \int_0^{2k_F} dk k^3 \left\{ \frac{\nu(k)}{\epsilon(k)} \right\}^2 a(k) S_{zz}(k) \] (23)

where \( k = k_0 + k_s \). \( G_F \) is the Fermi weak coupling constant, \( C_z \approx 1.675 \) from the vector and axial-vector constants of the weak interaction, and \( a(k) = \left[ 1 - \frac{2k^2}{4k^2 - 4\alpha \bar{q}} \right] \). The function \( R_T \) describes the thermal broadening of the electron Fermi surface and from Equation (20) of Haensel et al. (1996) this can be approximated as unity for \( T \lesssim 0.6 \) GK typical of models of the neutron star crust at accretion rates characteristic of superburst progenitors (Kaminker et al. 1999).

Thus, in both Equations (14) and (23) the only dependence on the nuclear species present (i.e., on the composition) enters via \( S_{zz}(k) \). Therefore, to tabulate fits to both \( \kappa \) and \( \epsilon_v \) for every nuclear species prior to application of a mixing rule is extremely cumbersome (note that the papers Itoh et al. 2008, 1996 tabulate fit coefficients for only 11 species for conductivities and NPB emissivities, respectively) and also unnecessary from a computational standpoint. The fits to OCP structure factors in Young et al. (1991) are sufficient to cover every one of the \( N_{sp} \geq 100 \) species encountered in the neutron star crust. They can also be used to compute both \( \kappa \) and \( \epsilon_v \) for an MCP of arbitrary complexity using the microscopic mixing rule (MLMR) described in Section 4 which involves only the OCP structure factors and species values. For higher values of \( \Gamma > 225 \) in the neutron star crust we present a simple model for the behavior of the Coulomb logarithm that reduces the evaluation of thermal and electrical conductivity to an analytic formula incorporating crust impurity in a very simple way. We do not present calculations of the NPB neutrino emissivity in this paper, rather we point it out to demonstrate that all such “integral” determinants (i.e., summations over momenta) of crust thermal profile are related to the crust composition via the quantity \( S_{zz}(k) \).

2.2.3. The Standard Treatment of Mixtures in the Crust

For simplicity, we drop the \( \sigma, \kappa, \) and \( \nu \) subscripts in what follows.

The most common approach of electron–ion scattering in the neutron star crust relies on the belief that the MCP is fluid in the upper part of the crust where \( \Gamma_{eff} < 175 \) and consist of a solid, i.e., a crystalline lattice with impurities, in the lower part where \( \Gamma_{eff} > 175 \). Accordingly, in the solid phase, the collision frequency \( \nu = \nu_{e-ph} + \nu_{e-imp} \) is split into the sum of the electron–phonon and the electron–impurity scattering contributions; in the liquid state \( \nu = \nu_{ei} \) where \( \nu_{ei} \) is the electron–ion scattering inverse relaxation time discussed in the next section.

The splitting \( \nu = \nu_{e-ph} + \nu_{e-imp} \) was initially introduced in Flowers & Itoh (1976) to deal with periodic crystals with a small fraction of the lattice sites occupied by impurities. The idea is illustrated in Figure 2. The case of binary mixtures (\( N_{sp} = 2 \)) was discussed in detail in Itoh & Kohyama (1993) for a small concentration of impurity ions (say species "2") of the impurity to electron–ion scattering is equal to its concentration times the binary electron–ion collision frequency between an electron and a “residual” ion of charge \( Z_2 - Z_1 \). This idea was extended to deal with more complex MCPs containing \( N_{sp} \geq 3 \) species, in which case the system is treated as a perfect crystal of charge \( Z \) plus the contribution of uncoupled impurities of charge \( Z_i - (Z) \).

Within this approximation and defining the impurity parameter as

\[ Q_{imp} = \sum_{j=1}^{N_{sp}} x_i(Z_i - (Z))^2, \]

the relaxation frequency can be written as

\[ \nu_{imp} = \nu_{0,imp} \ln A_{imp} \]

where

\[ \nu_{0,imp} = \frac{4\alpha^2 e^2 Q_{imp}}{3\pi\hbar} \frac{1}{(Z)} \]

and

\[ \ln A_{imp} = \int_0^{2k_F} dk k^3 \left\{ \frac{\nu(k)}{\epsilon(k)} \right\}^2 \left[ 1 - \frac{x_i^2}{1 + x_i^2} \left( \frac{k}{2k_F} \right)^2 \right] \]

In \( \ln A_{imp} \) corresponds to Equation (20) with \( S_{zz} \) set to unity to correspond to independent (uncorrelated) electron–impurity collisions.

While the impurity parameter formalism was developed to treat small impurity concentration in an otherwise almost perfect crystal lattice (see Figure 2), it has also been used to characterize electron–ion scattering in complex fluid and amorphous MCPs when \( Q_{imp} \) is large, say \( Q_{imp} \sim 100 \). Such is usually the case when electron–impurity scattering is used to set a lower bound...
on conductivity for the entire crust. However, since \( \Lambda_{\text{imp}} \) is of the order of magnitude as \( \Lambda \), we have

\[
\nu_{\text{imp}} \approx \frac{(Z_j^2) \ln \Lambda}{Q_{\text{imp}} \ln \Lambda_{\text{imp}}} \quad (28)
\]

\[
\approx \frac{(Z_j^2)}{Q_{\text{imp}}} \sim 10 \quad (29)
\]

over the whole outer crust as shown in Figure 1, the impurity parameter can lead to conductivities much higher than the those that would be obtained using the actual structure factors employed in Equation (20). We thus anticipate that \( Q_{\text{imp}} \) is inappropriate for the outer crust (impure liquid metal approaching heterogeneous amorphous solid at high density), and instead we shall justify the usage of \( (Z_j^2) \) from its presence in our expression for the fundamental frequency \( \nu \) in Equation (9). The differences in crust conductivity that would result from these differing prescriptions are discussed in Section 5.

In the liquid state, Potekhin et al. (1999) proposed a different approach to deal with mixtures. In this formalism, one writes

\[
\ln \Lambda \approx \frac{1}{(Z_j^2)} \sum_j x_j Z_j^2 \ln \Lambda \quad (30)
\]

where \( \Gamma_j = Z_j^2 / \Gamma_0 \), \( x_j \) refers to the number fraction as defined in Equation (1), and \( \ln \Lambda \) is the Coulomb logarithm (20) for an OCP of charge \( Z_j \) at coupling \( \Gamma_j \) and relativistic parameter \( x_j \). This prescription for mixtures was also recommended recently in the works of Cassisi et al. (2007) and Itoh et al. (2008) and we corroborate its efficacy in Section 4.

In Sections 4 and 5, we propose and validate with MD simulations a mixing rule for \( \ln \Lambda \) that is slightly modified from Equation (30). We also show that the impurity parameter formalism is inappropriate at large \( Q_{\text{imp}} \).

2.2.4. Discontinuities in Transport Coefficients at Crystallization

The previous expressions tell us that the conductivities and NPB emissivity depend on the scattering of electrons off the fluctuations \( \delta n_r(\mathbf{k}, t) \) in the ionic charge density about the average value \( \langle n_r(\mathbf{k}) \rangle_{\text{eq}} \). However, this average charge density is dependent upon the thermodynamic phase of the system.

1. If the system is fluid, the averaged charge density \( \langle n_r(\mathbf{k}) \rangle_{\text{eq}} = n_e \delta(\mathbf{k}) \) is uniform.

2. If the system is in a crystalline solid state, i.e., comprised of a periodic (Bravais) lattice with the same physical unit, electrons are in Bloch states and \( \langle n_r(\mathbf{k}) \rangle = e^{-2iW(k)/n_e V} \sum_{\mathbf{K}} \delta_{\mathbf{K}, \mathbf{k}} \) depends on \( \mathbf{k} \), where, assuming \( N_p \approx 1, \mathbf{K} \) are reciprocal lattice vectors and \( W(k) \) is the Debye–Waller factor: Bloch electrons do not scatter off the static, wavevector-dependent charge fluctuations (Bragg peak).

Because of this fundamental difference, the formulae of the previous section predict significant (by a factor of 3–5) discontinuities of the electric and thermal conductivities at the melting point (Itoh et al. 1993). Recently, Baiko et al. (1998) argued that this jump in the OCP electronic transport properties upon crystallization is not physical and that the electron transport properties in strongly coupled plasmas should be fairly insensitive to the thermodynamic state of the plasma. Accordingly, they advance that strongly coupled Coulomb liquids are characterized locally by the same long-range order as present in the crystalline solid and although the long-range order does not persist forever as in a solid (the liquid state is fluid), electrons keep traveling in those local crystal-like structures without any significant degradation of their mean velocity. Thus, Baiko et al. (1998) advocate that, in the liquid state, the contribution corresponding to elastic scattering off the incipient crystalline structure must be subtracted from the static structure factor. As intended, this prescription removes the jump in the conductivities at the solid–liquid transition—this prescription was later used in a series of papers to redefine practical fitting formulae for the electron conductivities and NPB (e.g., Cassisi et al. 2007 and references therein; also Horowitz et al. 2008).

The prescription of Baiko et al. (1998) contradicts our current understanding of solid and liquid metals. We instead agree with Itoh et al. (2008) since we believe that the disordered positions and the oscillating and diffusive movement of the ions cannot be ignored in a liquid.

The arguments and conclusions of Baiko et al. (1998) contradict both experimental findings and the contemporary theoretical understanding of liquids: for example, it has been known for a long time that the electrical resistance of most metals in the liquid state just above their melting points are about 1.5–2.3 times larger than those of solid metals (Cusak & Enderby 1960). Even the simplest metals, whose electronic structure do not change appreciably upon melting, show a discontinuity in transport properties at melting, e.g., for sodium \( \sigma_s/\sigma_l \approx 1.05 \) and for aluminum \( \sigma_s/\sigma_l \approx 2.2 \). Interestingly, similar to Baiko et al.’s approach but with the opposite purpose in mind, early theoretical attempts to explain the increase of electrical resistivity upon melting relied heavily on ideas that had proved successful for solid metals. These approaches overlooked the effect of disorder inherent to liquids: for instance, in the “quasi-crystalline” models, the local coordination just above the melting point was treated very similar to that which prevails in the solid phase just below. It was also believed that, as in a solid metal, the resistivity of liquid metals could be divided into two parts: (1) a thermal term, proportional to the mean square amplitude of vibration of the ions, and hence dependent on the temperature \( T \) and (2) a residual term, independent of \( T \) due to defects (e.g., vacancies, dislocations). In 1934, Mott (1934) presented an elegant theory to reconcile these solid-like picture to the increase of electrical resistivity on melting in terms of the entropy change on melting per particle \( \Delta s = (S_l - S_s)/nV \)

\[
\Delta s = 1.5k_B \ln (\sigma_s/\sigma_l). \quad (31)
\]

Using the latent heat of fusion to evaluate \( \Delta s \), Mott’s model yields surprisingly good values of \( \sigma_s/\sigma_l \) (1.68 for sodium instead of 1.45.) It was later realized that Mott’s assumptions do not hold in the light of other facts. Hence Mott’s theory assumes that all the melting entropy is connected with the thermal agitation of the ions and ignored the configurational entropy arising from disorder in the rest positions about which ions are instantaneously vibrating (the so-called “cage effect”). Unfortunately, this argument does not hold: it is indeed known that for all simple metals, the experimental \( \Delta s \) is approximately a universal constant, \( \Delta s \approx 0.8 \pm 0.1 \) (rms), and is chiefly due to the change in configurational entropy (Wallace 1997). The entropy change due to the thermal agitation, the anharmonicities in ionic motions, and the electronic structure are responsible for the small scattering in the universal value. As illustrated in
Table 2 at Table 1, similar findings apply the OCP over a wide range of Figure 3.

Δ electronic screening, namely $\Delta \approx 0.2$ in Equation (14) for liquid metals with effective ionic charges $Z_{\text{eff}} = 1, 2, 3,$ and 4. Its position relative to the main peak in $S_{\text{eff}}(k)$ clearly depends on the valency of the metal ion. In the crust of a neutron star, $(Z) \gg Z_{\text{eff}},$ and consequently the range of integration encompasses all first peaks in $S_{\text{eff}}(k).$ Physically, in neutron star crusts, large momentum transfers (close encounters) significantly contribute to the Coulomb logarithm.

(A color version of this figure is available in the online journal.)

Table 1

| $\kappa$ | $\Gamma_{\text{m}}$ | $\Delta s$ |
|---------|------------------|-----------|
| 0       | 171.8            | 0.8516    |
| 0.2     | 173.5            | 0.8526    |
| 0.4     | 178.6            | 0.8551    |
| 0.6     | 187.1            | 0.8580    |
| 0.8     | 199.6            | 0.8599    |
| 1.0     | 217.4            | 0.8591    |

Notes. $\Gamma_{\text{m}}$ is the coupling parameter $\Gamma_{\text{OCP}}$ at melting. The data were calculated using the equation of state of Hamaguchi et al. (1997).

Table 1, similar findings apply the OCP over a wide range of electronic screening, namely $\Delta s \approx 0.85.$

Finally, we would like to add another argument in disfavor of Baiko et al.’s prescription. If crystallites do indeed exist in the liquid phase as assumed by Baiko et al. (1998), they must be extremely small, smaller than required for a local band structure to be established, because the presence of nuclei would make it impossible for a liquid to supercool. However, all liquid metals can be persuaded to supercool through as much as 20% of their melting temperature (Turnbull & Cech 1950) and MD simulations of the OCP show the same trend (Duligault 2007).

Interestingly, for the multi-component systems found in the crusts of accreting neutron stars, the jump may be much less important than suggested by the calculations of Itoh et al. (1993). However, this is likely not due to the reason proposed by Baiko et al. but because of the lack of long-range order for those complex mixtures and the high degree of impurity-like disorder that those systems possess.

2.2.5. Terrestrial Liquid Metal Compared to the Neutron Star Crust Plasmas

In this section we continue the comparison of electron–ion scattering as occurring in terrestrial liquid metals as opposed to the crust of a neutron star. To make this comparison as quantitative as possible, we shall discuss the different components of the Coulomb logarithm in Equation (14). While this expression applies to both terrestrial liquid metals and to the crusts of accreting neutron stars (under the assumption of the first Born approximation), there are several interesting differences between both systems which we enumerate below.

1. While in the former the number of species is typically of order unity ($N_{\text{sp}} = 1$ in simple metals; $N_{\text{sp}} = 2$–3 in alloys), the number of species in the latter can be several hundred (see Section 3.1) Nevertheless, as shall see, the charge–charge structure factors $S_{\text{eff}}(k)$ is similar in both cases, i.e., characterized by damped oscillations originating from the short-range order of strongly coupled systems. The heights of the peaks increase with the strength of the coupling parameter $\Gamma_{\text{eff}}$ and therefore with depth.

2. While in terrestrial liquid metals electrons are nonrelativistic, electrons in an accreting neutron star crust are relativistic. The main effects of relativity are encapsulated in $\left[1 - \frac{v^2}{c^2} \left(\frac{m}{m_\text{pl}}\right)^2\right]$, which varies from 1 when $v \to 0$ and $1 - (k/2k_p)^2$ when $v \to \infty$ and describes kinematic suppression of backward scattering of relativistic electrons. Relativity also modifies the electronic screening of the ions (see Equation (B2)). The overall effects of relativistic corrections is illustrated in Figures 3 and 4. Figure 3 shows the integrand of Equation (14) for both relativistic and nonrelativistic electrons ($x_F = 0$ in Equation (14)). Relativistic effects are noticeable in large momentum transfer collisions (close encounters) and, as a consequence of the suppression of back-scattering, result in lower scattering cross-sections and consequently higher conductivities. Figure 4 compares the relativistic versus nonrelativistic Coulomb logarithm as a function of depth using the compositional profile of Gupta et al. (2007) discussed in Section 3.1.

3. While in the neutron star crust, ions are fully stripped and all electrons are delocalized electrons and participate in the electronic conduction, $n_e = (Z)n$ with $(Z) \sim 40,$ most electrons in a liquid metal are bound to the nuclei,
A final effect of major importance arises from the magnetic field. In this section, we discuss the MD simulations we performed to base our calculations of crustal properties. To determine the composition profiles at various neutron star depths to validate the LMR. We adopt a fiducial set of physical parameters as input to the simulations. Details for each of the compositions used at depth are given in Table 2 and the spread in the electron Fermi energy, \( \Gamma_F \) the dimensionless TF screening length where \( a \) is the interparticle distance, \( \Delta \) is the dimensionless Fermi wavevector, \( \Gamma \) is the coupling parameter defined by Equation (4).

The mixtures we have simulated discard the less abundant species which would have had less than 10 particles in the simulations. Details for each of the compositions used at depth are given in Table 2 and the spread in \( Z \) is illustrated in Figure 5 for two compositions.

We now use the composition profiles at various neutron star crust depths to validate the LMR. We adopt a fiducial temperature \( T = 0.5 \) GK, and vary the density as in Table 2. Thus, changes in \( \Gamma_{\text{eff}} \) with changing crust depth arise only from composition evolution and a decrease in inter-ionic spacing. At each depth a large number of mass chains \( A \approx 20–100 \) enter the composition as expected from X-ray burst observations between very diverse mass chains. Finally, the accretion rate closely match those expected from X-ray superburst progenitors (\( \sim 0.1 M_{\text{Edd}} \approx 10^{17} g \) s\(^{-1}\)) and therefore we intend the numbers we compute to have practical relevance to the neutron star crust modeling and X-ray observational communities.

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### 3. Molecular Dynamics Simulations of the Neutron Star Crust

In this section, we discuss the MD simulations we performed in order to calculate the structure factors \( S_{\nu \nu}(k) \) of MCPs representative of neutron star crust and to validate the LMR discussed in Section 4.

#### 3.1. Input: A Representative Crust Composition Profile

To base our calculations of crustal \( \kappa \) and \( \epsilon_r \) on a realistic pre-neutron-drip crust compositional profile we have used the compositions of Gupta et al. (2007). Our choice was determined by a number of factors. First, the diversity of species in the starting composition (XRB ashes from Schatz et al. (2001)) is characterized by the “impurity parameter” which has a high value \( Q_{\text{imp}} \sim 100 \), an ideal test-bed for validation of a mixing rule in an MCP. In the outer crust, prior to the onset of neutron reactions, electron captures preserve the high impurity. Only beyond neutron-drip in the inner crust, as demonstrated in the SEC-nucleosynthesis process described in Gupta et al. (2008), do electron-capture-delayed-neutron emissions rearrange abundances between very diverse mass chains. Finally, the accretion rate closely match those expected of X-ray superburst progenitors (\( \sim 0.1 M_{\text{Edd}} \approx 10^{17} g \) s\(^{-1}\)) and therefore we intend the numbers we compute to have practical relevance to the neutron star crust modeling and X-ray observational communities.

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#### 3.2. The MD Procedure

We employ MD simulations to calculate the structure factor (18) at various depths of a neutron star crust. In order to deal with the impure multi-component ionic mixtures typical of neutron star crusts, we have developed a code that allows for the simulation of large charged systems (tens to a few hundred nuclear species) over the long timescales required for the equilibration of such impure MCPs. The code is based on a parallelized implementation of the Particle–Particle–Particle–
Mesh (P³M) algorithm with periodic boundary conditions; high resolution for individual encounters is combined with rapid, mesh-based, long range force calculations. It simulates the classical dynamics of a mixture of nuclei described as point particles interacting through a screened Coulomb interaction. Thus the interaction potential between two nuclei of charge $Z_i$ and $Z_j$ is modeled by the screened Coulomb (Yukawa) potential,

$$v_{ij}(r) = \frac{Z_i Z_j e^2}{r} e^{-k_{sc} r}, \quad (32)$$

where $k_{sc}$ is the inverse screening length. The P³M algorithm can handle any value $k_{sc} \geq 0$ to very high accuracy. In practice, we use the inverse of the relativistic Thomas–Fermi inverse screening length $k_{TF}$ for $k_{sc}$ given by $k_{TF} a_e = 0.185(1 + x_r^{-2})^{1/4}$.

Several technical details of the MD calculations (simulation length, number of particles, time steps, etc) are collected in Appendix A. Here we briefly outline the procedure used to calculate $S_{zz}(k)$. Given a composition at a certain depth, the particles are initially randomly distributed in a cubic box of volume $V = L^3$ with a Maxwellian velocity distribution at the prescribed temperature. After a long equilibration phase, a simulation is performed in which, at each time step $n$, the charge density $n_Z(k; n)$ as in Equation (13) is calculated for values of $k$ commensurate with the simulation box size $L$, namely

$$k = \frac{2\pi L}{L}(n_x, n_y, n_z), \quad ||k|| \leq 2k_F \quad (33)$$

where $n_x, n_y, n_z$ are natural integers. The charge–charge structure factor (18) is calculated at the end of the run using

$$S_{zz}(k) = \frac{1}{N_{run}} \sum_{n=1}^{N_{run}} \sum_{k} \frac{1}{N_k} |n_z(k, n)|^2. \quad (34)$$
Figure 6. Structure factor $S_{zz}(k)$ obtained with MD simulations (red lines) and with the mixing rule formula (40) (blue lines) for the mixtures 1–5 defined in Table 2. (A color version of this figure is available in the online journal.)

3.3. Molecular Dynamics Structure Factors

MD results for the structure factor $S_{zz}(k)$ and corresponding to the crustal compositions of Gupta et al. (2007) listed in Table 2, all at temperature $T = 0.5$ GK, are shown in Figures 6–8 over the range $0 \leq k \leq 2k_F$. Additional data obtained from the MD simulations to test lower temperatures near the photosphere–ocean boundary and potentially high temperatures at different depths are provided in the Appendix C.

The shape of the charge–charge structure factor $S_{zz}(k)$ is typical of the structure factor of liquids. The first peak, which systematically occurs at $k/2k_F \approx 0.33$ and which has a height increasing with the effective Coulomb coupling $\Gamma_{\text{eff}}$, reflects the existence of a dominant short-range order of the particles in
real space. This is illustrated in Figure 9 that shows different pair-distribution functions \( g_{ab}(r) \) for several pairs of species \( a \) and \( b \). The sharp decrease in the pair-distribution functions at small separation, originating from the repulsion between like charges, is responsible for the subsequent maxima and minima of \( S_{zz}(k) \), whose oscillation is strongly damped as \( k \) increases. Eventually, at large \( k \), \( S_{zz}(k) \) approaches unity, in accordance with the normalization in Equation (18). At small \( k \), \( S_{zz}(k) \) probes the long-wavelength static fluctuations in the charge density and approaches zero (as \( k^2 \)) in the \( k \to 0 \) limit as a consequence of charge neutrality and perfect screening.

All the simulations at density larger than \( \sim 10^{10} \) g cm\(^{-3} \) (compositions 9–17 of Table 2) and characterized by \( \Gamma_{\text{eff}} > 260 \) show pronounced short-range structure as seen in the shoulder of the second peak of \( S_{zz}(k) \). Nevertheless, within the timescale of the simulations, we did not witness any clear-cut phase separation or crystallization.

4. VALIDATION OF THE LINEAR MIXING RULE AND PRACTICAL FIT

4.1. Validation of the LMR

A common approximation for the excess (non-ideal) energy \( U_{\text{ex}} \) and free energy \( F_{\text{ex}} \) of strongly coupled ion mixtures is the (empirical) LMR. In terms of the energy per particle and per unit of \( k_B T \), \( u_{\text{ex}} = U_{\text{ex}}/Nk_B T \) and \( f_{\text{ex}} = F_{\text{ex}}/Nk_B T \), the LMR claims that

\[
u_{\text{ex}}(\Gamma_e, \overrightarrow{x}) \approx \nu_{\text{ex,LMR}}(\Gamma_e, \overrightarrow{x}) = \sum_{j=1}^{N_{\text{sp}}} x_j \nu_{\text{ex, OCP}}(\Gamma_j) \tag{35}
\]

\[
f_{\text{ex}}(\Gamma_e, \overrightarrow{x}) \approx f_{\text{ex,LMR}}(\Gamma_e, \overrightarrow{x}) = \sum_{j=1}^{N_{\text{sp}}} x_j f_{\text{ex, OCP}}(\Gamma_j) \tag{36}
\]

where \( \Gamma_j = Z_j^{5/3} \Gamma_e \), and \( u_{\text{ex,LMR}} \) and \( f_{\text{ex,LMR}} \) are the excess free energy of an OCP at coupling \( \Gamma_j \), and \( \overrightarrow{x} = \{x_i\}_{i=1}^{N_{\text{sp}}} \) is the composition vector of species number fractions (see Equation (1)) for the MCP.

To the best of our knowledge, the mixing rules (35) and (36) were obtained empirically and there is no rigorous “derivation” of them. Equation (36) was shown to be very accurate for binary mixtures with both rigid (DeWitt & Slatery 2003) and polarizable background electrons (Chabrier & Ashcroft 1990). Recently, Potekhin et al. (2009) proposed to extend the LMR to
calculation of the equation of state (EOS) of multi-component mixtures. The results derived in the following validate this recent prescription of Potekhin et al. (2009).

The LMRs (35) and (36) suggest a more fundamental, microscopic mixing rule that directly involves the structure factors. To this end, we recall that the excess energy of a screened MCP (i.e., with ions interaction via the screened Coulomb potential (32)) can be obtained from the charge–charge structure factor $S_{zz}(k)$ using (Rosenfeld 1993)

$$u_{ex}(\Gamma_e, \vec{x}) = \frac{\Gamma_e}{\pi} \frac{\langle Z^2 \rangle}{\langle Z \rangle^{1/3}} \int_0^{\infty} dk \frac{k^2}{k^2 + k_{sc}^2} [S_{zz}(k) - 1] - \frac{k_{sc} \langle Z^2 \rangle}{2}.$$  

(37)

The exact Equation (37) together with the accurate approxima-
tion Equation (36) suggest the following MLMR approximation for the MCP structure factor \( S_{zz}(k) \),

\[
S_{zz}(k; \Gamma_e, \mathbf{x}) \approx S^\text{MLMR}_{zz}(k; \Gamma_e, \mathbf{x}) = \frac{(Z)^{1/3}}{(Z^2)} \sum_{j=1}^{N_e} x_j Z_j^{5/3} S^\text{OCP}_j(k; \Gamma_j)
\]

(38)

where \( S^\text{OCP}_j(k; \Gamma_j) \) is the structure factor of the OCP comprised of species \( j \) at coupling \( \Gamma_j \). Indeed, introducing Equation (38) in Equation (37), we obtain the LMR (35) and (36). By introducing Equation (38) in Equation (14), we obtain the LMR for the Coulomb logarithm,

\[
\ln \Lambda \approx \left( \frac{(Z)^{1/3}}{(Z^2)} \right) \sum_{j=1}^{N_e} x_j Z_j^{5/3} \ln \Lambda^\text{OCP}(\Gamma_j, Z_j, x_j),
\]

(39)

where \( \ln \Lambda^\text{OCP}(\Gamma_j, Z_j, x_j) \) is the Coulomb logarithm for an OCP of charge \( Z_j \) at the coupling \( \Gamma_j \) and relativistic parameter \( x_j \) (the explicit dependence on the charge \( Z_j \) comes from the upper limit \( 2k_F = 2(3\pi^2 n_e)^{1/3} = 2(3\pi^2 Z_j n_j)^{1/3} \) of the integral in Equation (14)).

The validity of the MLMR (38) is confirmed by our MD simulations. The structure factors for compositions 1–8 of Table 2, corresponding to \( 8.6 \times 10^6 \) g cm\(^{-3} \) \( \leq \rho \leq 4.8 \times 10^8 \) g cm\(^{-3} \) and \( 70 \leq \Gamma \leq 140 \), are shown in Figures 1 and 2. The blue lines show the results obtained using MD simulations and the red lines show the results obtained with the mixing rule (38). The latter was evaluated with the structure factors for the OCPs obtained by solving the so-called HNC equations (see, e.g., Young et al. 1991). For all the compositions, Figures 1 and 2 show very good agreement between the MD and the mixing rule values. In each case, the position of the peaks is well reproduced and the mixing rule overestimates their heights by at most 10%. (The MLMR is also illustrated in the figures of Appendix C.)

When used in Equation (37) or Equation (14), however, these differences between the MD and MLMR structure factors barely affect the value of the Coulomb logarithm, and in turn the electronic transport properties are unaffected. This is illustrated in Figure 10 that shows the sum \( \ln \Lambda(K) = \int_0^K dk \frac{1}{(\pi k)^2} \left[ 1 + \frac{x^2}{1 + x^2} \right] S_{zz}(k) \) with \( 0 \leq K \leq 2k_F \) obtained with the MD and the mixing rule results. Thus the MLMR provides a very accurate and convenient way of calculating the electronic transport coefficients for complex ionic mixtures in the liquid phase. More generally, all quantities that are functionals of the structure factor such as (37), the electrical and thermal conductivity, and even the NPB emissivities can be obtained to high accuracy from the MLMR.

4.2. Practical Fit to the Coulomb Logarithm of a Mixture

Having validated the LMR, we now provide a simple practical fit to the Coulomb logarithm of an arbitrarily complex liquid or amorphous MCPs. The fit is valid for any effective Coulomb coupling \( \Gamma_j \geq 10 \) and relativistic parameter range \( 1 \leq x_j \leq 1000 \). For the neutron star crust applications in the amorphous state, once the composition as function of depth is known, the conductivity can be calculated very accurately (when compared to numerical MD simulations) without resort to complicated tabulations of fit coefficients or decomposition of conductivity from different scattering processes.
Our prescription is as follows:

\[ \ln \Lambda \approx \frac{(Z_{\text{imp}}/Z)^{1/3}}{(Z^2)} \sum_{j} x_j Z_j^{5/3} \ln \Lambda^{\text{OCP}}(\Gamma_j, Z_j, x_r), \]

where \( \Gamma_j = Z_j^2 e^2 / a_j k_{TF} T \) and \( \ln \Lambda^{\text{OCP}} \) is fitted by the expression

\[ \ln \Lambda^{\text{OCP}}(\Gamma_j, Z_j, x_r) \approx C(Z_j, \Gamma_j, x_r) \frac{1 + 0.177\Gamma_j + 0.00001\Gamma_j^2}{1 + a(x_r)\Gamma_j + b(x_r)\Gamma_j^2} \ln \Lambda^{\text{imp}}(x_r). \]

(41)

In Equation (27),

\[ \ln \Lambda^{\text{imp}}(x_r) = \frac{1 + 396x_r}{0.466 + 394x_r} \]

(42)

\[ \times \frac{1}{2} \left[ (1 + 4\beta^2 q^2) \ln(1 + q^2) - \beta^2 - \frac{1 + 2\beta^2 q^2}{1 + q^2} \right] \]

is obtained by setting \( \epsilon(k) = 1 + k_{\text{TF}}^2 / k^2 \) in Equation (27), where

\[ \beta = \frac{v_{\text{F}}}{c} = \frac{x_r}{\sqrt{1 + x_r^2}}. \]

\[ q = \frac{k_{\text{TF}}}{2k_{\text{F}}} = \frac{0.048196}{\sqrt{\beta}}. \]

\( k_{\text{TF}} \) is the relativistic Thomas–Fermi wavevector, and the functions \( a(x_r) \) and \( b(x_r) \) are given by

\[ a(x_r) = \begin{cases} 
1 + a_1 x_r^{1/3} & x_r < 5 \\
2.22 & x_r \geq 5
\end{cases} \]

(43)

\[ b(x_r) = \begin{cases} 
1 + b_1 / x_r^2 & x_r < 10 \\
2b_2 + b_3 / x_r^3 & x_r \geq 10
\end{cases} \]

(44)

with the parameters \( a_n \) and \( b_n \) as listed in Table 3.

The species dependence is encapsulated in the function

\[ C(Z_j, \Gamma_j, x_r) = \begin{cases} 
1 & Z_j = 1 \\
C_0(Z_j, x_r) + C_1(Z_j, x_r) \Gamma_j & Z_j > 1
\end{cases} \]

(45)

where

\[ C_0(Z_j, x_r) = a_0(x_r) + a_1(x_r) \ln Z_j \]

\[ C_1(Z_j, x_r) = b_0(x_r) + b_1(x_r) \ln Z_j. \]

We fit the coefficients \( a_0(x_r), a_1(x_r), b_0(x_r), b_1(x_r) \) piecewise over disjoint \( \Gamma_j \) and \( x_r \) ranges as follows. For \( 10 \leq \Gamma_j \leq 30, \)

\[ a_0(x_r) = \begin{cases} 
0.973587 - 0.0790899 \ln x_r & x_r < 10 \\
0.806877 & x_r \geq 10
\end{cases} \]

\[ a_1(x_r) = \begin{cases} 
0.652748 + 0.117973 \ln x_r & x_r < 2.5 \\
0.766772 & x_r \geq 2.5
\end{cases} \]

\[ b_0(x_r) = -0.029204 + 0.0367777 \exp(-0.93315 \ln x_r) \]

\[ b_1(x_r) = 0.0853907 - 0.053054 \exp(-0.885854 \ln x_r), \]

(39)

This fit was obtained to match the OCP structure factors of Young et al. (1991) for the range \( 5 \leq \Gamma_j \leq 225 \). However, assuming that the system stays amorphous (no periodic lattice structure), the fit has no restriction on \( \Gamma_j \) as demonstrated in Figure 11.

5. APPLICATION OF THE MLMR TO OBTAIN THERMAL AND ELECTRICAL CONDUCTIVITIES OF SUPERBURST PROGENITORS

Figure 12 shows the thermal conductivity calculated from numerical MD simulations in this paper and accurately reproduced by using the mixing rule prescription of Equation (39). The conductivity of the amorphous outer crust is lower by an order of magnitude from estimates obtained using the impurity parameter formalism, Equation (25). Figure 12 (see also Figure 1) also show that \( (Z^2) \), and as a consequence the conductivity, are less sensitive than \( Q_{\text{imp}} \) to reaction processes that reduce crust impurity abruptly in the outer crust, such as (1) electron captures on very proton-rich nuclei produced in the rp-process (and therefore far away from beta-stability at the top of the crust), (2) charge particle capture and fusion reactions destroying lighter
nuclei, and (3) \( \gamma, n \)- and \( n, \gamma \)-driven rearrangement of abundances in mass chains.

We note that in the limit of a classical amorphous solid, the Coulomb logarithms for electrical and thermal conductivity are equal, i.e., \( \ln \Lambda_e = \ln \Lambda_h \); therefore \( \sigma \) and \( \kappa \) are related by the Wiedemann–Franz law, Equation (12). Thus while we only show a plot of the outer crust thermal conductivity as function of density in Figure 12, the composition-dependent electrical conductivity is related very simply to it.

X-ray burst ash composition differences will exist between one-zone models (Schatz et al. 2001) of an X-ray Burst as opposed to a multi-zone model (Woosley et al. 2004). Our purpose here is not to study all possible compositions in a superburst progenitor, but rather to show the applicability of the MLMR to an arbitrarily complex composition with the heterogeneity expected of X-ray burst ashes. Once composition is known, MD permits us to determine the physical state and heterogeneity expected of X-ray burst ashes. Once composition

![Figure 12. Thermal conductivity as a function of density in the crust of an accreting neutron star with \( M \approx 0.1 M_{\odot} \). The MD calculations (squares) which are accurately reproduced by the LMR (39) (red line) are contrasted with the electron–impurity scattering conductivity as calculated using Equation (25) over a range of four orders of magnitude in crust density. As discussed in Section 5, (\( Z^2 \)), and as a consequence the conductivity, is less sensitive than \( Q_{imp} \) to composition changes at densities \( \sim 10^7, 2 \times 10^9, 10^{10}, \) and \( 10^{11} \) g cm\(^{-3} \).

(A color version of this figure is available in the online journal.)

| Mounting Cash Flow | Fitting Parameters \( a_n \) and \( b_n \), \( n = 1, 2, 3 \), to be Used in Equations (43) and (44) |
|---------------------|-----------------------------------------------|
| \( n \) | \( a_n \) | \( b_n \) |
| 1 | 48.12 | 1.95 |
| 2 | 29.23 | 11.74 |
| 3 | 0.77 | 92.18 |

Table 3

| Simulation Parameters Used for the Mixtures Defined in Table 2 |
|---------------------|-----------------------------------------------|
| Mixture | \( N_{eq} \) | \( N \) | \( N_{run} \) | \( N_{eq} \) | \( N \) |
| 1 | 55 | 9718 | \( 10^3 \) | \( 10^3 \) | 1441 |
| 2 | 50 | 19864 | \( 10^3 \) | \( 10^3 \) | 2464 |
| 3 | 52 | 19851 | \( 10^3 \) | \( 10^3 \) | 2497 |
| 4 | 52 | 19840 | \( 10^3 \) | \( 10^3 \) | 2503 |
| 5 | 50 | 19851 | \( 10^3 \) | \( 10^3 \) | 2497 |
| 6 | 53 | 14862 | \( 10^3 \) | \( 10^3 \) | 2107 |
| 7 | 53 | 19849 | \( 10^3 \) | \( 10^3 \) | 2517 |
| 8 | 52 | 19857 | \( 10^3 \) | \( 10^3 \) | 2517 |
| 9 | 49 | 14847 | \( 10^3 \) | \( 10^3 \) | 2107 |
| 10 | 49 | 19859 | \( 10^3 \) | \( 10^3 \) | 2506 |
| 11 | 52 | 19870 | \( 10^3 \) | \( 10^3 \) | 2869 |
| 12 | 50 | 19875 | \( 10^3 \) | \( 10^3 \) | 3095 |
| 13 | 54 | 19871 | \( 10^3 \) | \( 10^3 \) | 3287 |
| 14 | 50 | 19898 | \( 10^3 \) | \( 10^3 \) | 3350 |
| 15 | 49 | 29888 | \( 10^3 \) | \( 10^3 \) | 4299 |
| 16 | 46 | 39903 | \( 10^3 \) | \( 10^3 \) | 4972 |
| 17 | 24 | 19937 | \( 10^3 \) | \( 10^3 \) | 2143 |

Table 4

| Compositions Used for the MD Calculations Shown in Figures 13 and 14 |
|---------------------|-----------------------------------------------|
| Mixture | \( T (GK) \) | \( \Gamma_{eff} = (Z^{2/3})\Gamma_2 \) |
| 1 | 0.27 | 60 |
| 2 | 0.73 | 49 |
| 3 | 0.81 | 60 |
| 4 | 0.84 | 70 |
| 5 | 0.85 | 81 |
| 6 | 0.85 | 90 |
| 7 | 0.84 | 106 |
| 8 | 0.83 | 142 |

Notes. For a given mixture, the composition is the same as the one given in Table 1. The only difference is in the temperature, and therefore \( \Gamma_{eff} \).

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APPENDIX A

DETAILS OF MD SIMULATIONS

Some technical details of the MD simulations are collected in Table 4, namely

1. \( N_{sp} \) = number of nuclear species;
2. \( N \) = total number of particles in the MD simulations;
3. \( N_{eq} \) = number of particles in equilibrium;
4. \( N_{run} \) = total number of frames used in the run;
Figure 13. Structure factor $S_{zz}(k)$ obtained with MD simulations (blue lines) and with the mixing rule formula (38) (red line) for the mixtures 1–4 defined in Table 5. (A color version of this figure is available in the online journal.)

Figure 14. Same as Figure 13 for composition 5–8 listed in Table 5. (A color version of this figure is available in the online journal.)
3. \(N_{eq}\) = number of time steps used initially to let the system equilibrate;
4. \(N_{run}\) = number time steps of the MD run after equilibration;
5. \(N_k\) = total number of wave-vector norms used to calculated \(S_{zz}(k)\) with \(a_1k \leq 22\); see Equations (33) and (34).

In all the simulations, the time step \(\delta t\) is chosen such that \(\delta t = 0.01/\omega_p\), where \(\omega_p\) is the mean ion plasma frequency. The total energy is very well conserved during the simulation (better than one part in \(10^7\)).

APPENDIX B

RELATIVISTIC DIELECTRIC FUNCTION

The random-phase approximation static dielectric function of the relativistic electron gas in its ground state is (Jancovici 1962)

\[
\epsilon(k) = 1 + \frac{k_{TF}^2}{k^2} \left\{ \frac{2}{3} \sqrt{1 + x^2} - \frac{2x}{3} x \sinh^{-1}x + \sqrt{1 + x^2} \left[ \frac{1}{2} + \frac{x^2 - 3x^2}{6x^2} \ln \left| \frac{1 + x}{1 - x} \right| \right]\right\}
\]

\[
- \frac{1 - 2x^2}{6x^2} \left[ \sqrt{1 + x^2} \sinh^{-1}x + x \sqrt{1 + x^2} \right],
\]

where \(x = k/2k_T\) and \(k_{TF}\) is the (nonrelativistic) Thomas–Fermi (TF) inverse screening length

\[
k_{TF} = \frac{\sqrt{12} \pi m_e n_e}{\hbar k_F}.
\]

APPENDIX C

ADDITIONAL STRUCTURE FACTORS

Figures 13 and 14 shows the charge–charge structure factors \(S_{zz}(k)\) and their mixing rule approximation for some of the compositions of Table 2 but temperatures different than 0.5 GK, as listed in Table 5.