Molecular Dynamics Simulation of Multi-species Neutron Star Crust Conductivity

Accurate knowledge of the thermal properties of the accreting neutron star crust, required to model the time evolution of temperature at all depths in the neutron star crust, is crucial to understanding their non-explosive(quiescent) X-ray emission characteristics, and thereby to unravel the nature of exotic matter in the crust and core of these stars. Apart from the location and strength of the heat sources from various nuclear reaction (see [1] and [2]), the most important determinant of crust thermal profile is the electron thermal conductivity of the crust. The latter is governed by the electron scattering processes off the ionic centers, impurities and defects together with electron interactions with lattice vibration modes.

Calculation of the conductivity at different depths in a neutron star has been complicated by (i) the changing composition due to nuclear reactions and (ii) the uncertainty in the state (amorphous vs. crystalline) of a multi-species, strongly-coupled mixture of nuclei with from a few (~ 10) to more than 300 species of varying nuclear charge Z and mass A ($5 < Z < 55$ and $10 < A < 135$ roughly). Whereas several analytical approaches have been applied to binary mixtures, their extrapolation to 300+ species has never been investigated or verified. A typical example is the so-called "impurity parameter" formalism in which a perfect crystal with a low concentration of impurities substituted at lattice sites can be approximated as being made of two uncorrelated parts: the perfect lattice together with the residual charge. The total electron-ion scattering cross-section is the sum of the Bloch electron-lattice cross-section plus the sum of uncorrelated binary electron-residual impurity collisional cross-sections. However, as the concentration of impurities increases, this splitting is less and less justifiable. Indeed, by performing large-scale parallel Molecular Dynamics simulations of the charge density fluctuations (structure factor) of complex mixtures of nuclei and over a range of densities spanning four orders of magnitude, Los Alamos researchers Sanjib Gupta and Jerome Daligault have shown in [3] that the impurity parameter formalism yields crust conductivities that are an order of magnitude higher than they should be (Figure 1). This has enormous implications for upcoming experimental campaigns that target X-ray transients.

Furthermore, we have verified a microscopic version of the linear mixing rule for the calculation of the structure factor of a complex mixture of nuclei that uses the structure factor of individual species rather than quantities such as conductivity that are integrated over the full range of momentum transfer in electron-ion collisions. This new mixing rule, which can be applied to mixtures of arbitrary complexity (see Figure 2 for an example), can be used not only for calculating the thermal conductivity but also for equation of state and neutrino loss rates, thus drastically reducing the complexity of large astrophysical codes that simulate the thermal structure of neutron stars. We foresee much application of our new mixing rule to prediction of X-ray emissions from transiently accreting neutron stars that will be observed in the future.

[1] Gupta et. al., Astrophysical Journal 662:1188-1197 (2007)
[2] Gupta et. al., Physical Review Letters 101, 231101 (2008)
[3] Daligault and Gupta, Astrophysical Journal 703, 994-1011 (2009)

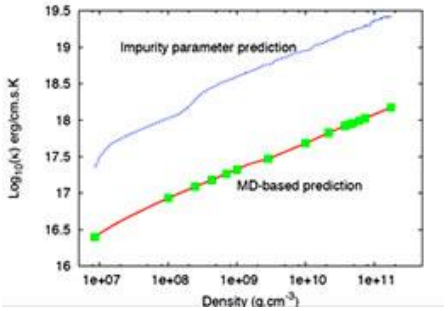

Figure 1: Thermal conductivity as a function of density (g/cc) in the crust of an accreting neutron star. The molecular dynamics (MD) calculations (green squares) are accurately reproduced by the linear mixing rule (red solid line) and are contrasted with the electron-impurity scattering conductivity (blue dotted line) over a range of four orders of magnitude in crust density. The MD conductivity is also less sensitive than the impurity parameter conductivity to sudden crustal composition changes from electron capture reactions triggered by density changes.

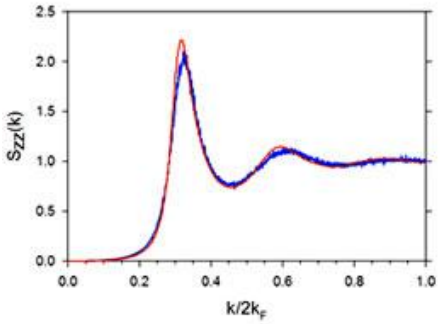

Figure 2: The structure factor obtained with MD simulations (red line) and with the mixing rule formula (blue line) for a realistic mixture of 451 nuclear species at density 2.49 • 10^8 g/cc and temperature 0.5 billion Kelvin in the accreting neutron star crust. This newly discovered microscopic linear mixing rule when expressed as a simple abundance-weighted average of individual species charge-charge structure factors can be applied to a wide range of thermal quantities such as EOS and neutrino loss properties.

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