# BIM_HNC: FORTRAN 90 Modified Hypernetted Chain Code for Binary Coulomb Systems

A. Diaw and M.S. Murillo

## 1 Introduction

Strongly coupled plasmas, such as those characteristic of white dwarf and neutron star interiors, have a liquid-like structure [1]. Such a structure is revealed in the prominent oscillations in the radial distribution functions $g_{ij}(r)$ among the species $i$ and $j$. Such correlations impact the equation of state and transport properties of these plasmas, but they are non-trivial to calculate.

Correlations in weakly coupled plasmas are well described by the well-known screening properties of Debye-Hückel theory. For moderately coupled plasmas another approach is needed, and one typically uses an integral equation approach. Among such approaches, the hypernetted chain approximation (HNC) works very well for Coulomb systems. For very strongly coupled systems, HNC itself becomes inaccurate and the so-called bridge functions are needed. Here, we have an example HNC code that employs empirical bridge functions for the case of a binary ionic mixture (BIM). The full method is described in the paper by Diaw and Murillo [Astrophysical Journal, under review, 2016].

## 2 Binary Ionic Mixture HNC

We start with Ornstein-Zernike for a multicomponent systems:

$$h_{\alpha\beta}(r) = c_{\alpha\beta}(r) + \sum_{\lambda} n_{\lambda} \int c_{\alpha\lambda}(|\mathbf{r}-\mathbf{r}'|) h_{\lambda\beta}(r') d\mathbf{r}', \tag{1}$$

with the exact expression of the radial distribution functions $g_{\alpha\beta}(r)$ as

$$g_{\alpha\beta}(r) = \exp\left[ -\frac{v_{\alpha\beta}(r)}{k_B T} + h_{\alpha\beta}(r) - c_{\alpha\beta}(r) + B_{\alpha\beta}(r) \right], \tag{2}$$

where the Coulomb pair potentials $v_{\alpha\beta}(r)$ between species $\alpha$ and $\beta$ reads

$$v_{\alpha\beta}(r) = \frac{Z_\alpha Z_\beta e^2}{r}, \tag{3}$$

$e$ is the electric charge, $k_B$ is the Boltzmann constant, $T$ is the temperature, $c_{\alpha\beta}(r)$ are the direct correlation functions, $h_{\alpha\beta}(r) = g_{\alpha\beta}(r) - 1$ are the total pair correlation functions, and $B_{\alpha\beta}(r)$ are the Bridge functions.

The essential ingredient of HNC algorithms is removing the long range character of the potential through a transformation, as detailed by [2, 3]. Then, given some guess for the direct correlation function $c_{\alpha\beta}(r)$, (2) with $B_{\alpha\beta}(r)$, and the OZE equations in (1) are iterated, using the HNC in Fourier space as

$$\tilde{h}_{\alpha\beta} = \tilde{c}_{\alpha\beta} + \sum_\lambda n_\lambda \tilde{c}_{\alpha\lambda}\tilde{h}_{\lambda\beta}, \tag{4}$$

which is algebraic matrix equation. Here $n_\lambda$ is the density of $\lambda$-species. While this equation is trivially inverted for the binary case, which is the case we have considered so far, extra coding is needed for the arbitrary number of species case. From the self-consistent solution obtained, the direct correlation functions needed for transport result.

Iyetomi, Ogata and Ichimaru [5] has provided a very accurate fit to MC data for the OCP case. This result was extended to single species Yukawa using MD by [6]. In the main text above we have used these results to approximately estimate the BIM bridge functions The bridge function for the binary plasma reads

$$B_{ij}(r) = -0.0464\Gamma_{ij}^{1.336} \exp\left(-0.64\frac{b_1}{b_0}r^2\right), \tag{5}$$

where

$$\Gamma_{ij} = Z_i Z_j \Gamma, \quad \Gamma = \frac{e^2}{a_{\rm WS} k_B T}, \tag{6}$$

$a_{\rm WS} = (3/4\pi n)^{1/3}$ is the Wigner-Seitz radius, $n$ is the total density and

$$b_0 = 0.258 - 0.0612\ln\Gamma_{ij} + 0.0123(\ln\Gamma_{ij})^2 - \Gamma_{ij}^{-1}, \tag{7}$$

$$b_1 = 0.0269 + 0.0318\ln\Gamma_{ij} + 0.00814(\ln\Gamma_{ij})^2. \tag{8}$$

The length units are normalized with the Wigner-Seitz radius $a_{\rm WS}$. The temperature enters through the coupling parameter $\Gamma_{ij}$ and the density through $a_{\rm WS}$.

## Instructions to run the code

The main code is written as a FORTRAN 90, and can be compiled with gfortran.

1. download main file bim-hnc.f90 and the input file bim.in

2. Compile and run gfortran -o bim-hnc bim-hnc.f90 ./bim-hnc
3. The input file contains successively:
   $\Gamma = e^2/a_{WS}k_BT$ : the coupling parameter,
   $n_2/n$: the ratio of species "2" density over the total density $n = n_1 + n_2$.
   $Z_1$: species "1" charge
   $Z_2$: species "2" charge
   Bridge_status: status of the bridge. The bridge is ON if 0, turned off if equal 1.
4. The output file, rdfs.out, contains the spatial coordinate $r/a_{WS}$ and the radial distribution functions ( $g_{11}$, $g_{12}$, $g_{22}$), respectively.

Thats it.

## 3 Outlook

We are releasing this code to make our publication reproducible, show the algorithms we employed so that they can be copied and extended, and to allow the community to improve upon this initial version. Here are some of the ways the code could be improved:

- Convert the code to other languages, such as C and Python.
- Implement FFTs, rather than computing Fourier transforms directly. Note that the algorithm alternates between physical and Fourier space.
- Extend to more than the Coulomb potential. An easy and obvious extension to toward Yukawa mixtures.
- Add more species. This is important to most of the astrophysical settings of interest. Key here is the inversion of the Ornstein-Zernike matrix of equations.
- Employ modern nonlinear solvers. The underlying algorithm is fairly old [2], and does not employ modern approaches and/or libraries from the solvers community. It is worth exploring methods developed for other systems (e.g., Lennard-Jones) to see if they can be adapted [4] to the astrophysical problems.

## References

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