Supplementary Material : A viscous quantum hydrodynamics model based on Dynamic Density Functional Theory

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Appendix

Our viscous QHD formulation requires knowledge of both the direct correlation function $C_{ee}(q)$ and the electronic longitudinal viscosity η_l. In this appendix we describe the methodology used to obtain these quantities.

The radial distribution function for a *classical* system with pair interactions $u(r)$ can be found by solving the equations

$$g(r) = \exp\Big[-\beta u(r) + h(r) - c(r) + B(r)\Big], \tag{1}$$

$$h(r) = c(r) + n_0 \int c(|\mathbf{r}-\mathbf{r}'|)h(r')d\mathbf{r}', \tag{2}$$

which are the closure and the Ornstein-Zernicke equation (OZE), respectively. While these are exact, the bridge function $B(r)$ is not known for a limited number of systems[1]. However, the electron-electron coupling is modest in most physical regimes of interest[2], and we can neglect $B(r)$, which is the so-called hypernetted chain (HNC) approximation, a closed set of equations for $c(r)$ and $h(r) = g(r) - 1$. Here, β is the inverse temperature in energy units, n_0 is the mean density, and $c(r)$ is the direct correlation function. Fast algorithms for solving the HNC equations over a wide range of parameters have been discussed elsewhere[3,4]. When constructing such algorithms, it is essential to remove the long-range character of the functions, choose an iteration cycle beginning with a reasonable initial guess, and solve the OZE in Fourier space. From the self-consistent solution, we can find the direct correlation function through

$$C(q) = \frac{H(q)}{1 + n_0 H(q)}. \tag{3}$$

We can examine the role of strong coupling by comparing the numerical solution of the HNC equations with the analytical solution of their mean-field approximations, obtained with $c_{mf}(r) = -\beta u(r)$.

Of course, we require the correlation functions for the *quantum* system, and under conditions of modest to large degeneracy. The classical HNC scheme is readily modified to treat the quantum case if quantum statistical potentials (QSPs) are used in place of $u(r)$[5]. Such an approach guarantees that $g(r) > 0, \forall r$. Dutta and Dufty[6] have compared the modified Kelbg QSP with the gold standard of PIMC[1]; their results show that over an extremely wide range of physical conditions the QSP and PIMC results are in near perfect agreement, except at very low densities where there is a quite modest deviation. Here, we employ both diffraction and Pauli exclusion potentials, using the Hansen and McDonald[7] form

$$u(r) = \frac{1}{r}\left[1 - \exp\left(\frac{-r}{\lambda_{ee}}\right)\right] + \beta^{-1}(\ln 2)\exp\left(\frac{-r^2}{\pi\lambda_{ee}^2(\ln 2)}\right), \tag{4}$$

where the DeBroglie thermal wavelength is defined as

$$\left(\frac{\lambda_{ee}}{a}\right)^2 = \frac{\Gamma}{\pi r_s} = \frac{2}{\pi}\left(\frac{4}{9\pi}\right)^{2/3}\frac{1}{\theta}. \tag{5}$$

Here a is the Wigner-Seitz radius, $\Gamma = \beta/a$ is the coupling parameter, $r_s = a/a_B$ is the density parameter, a_B is the Bohr radius, and θ is the quantum degeneracy defined as β_F/β where β_F is the inverse of the Fermi temperature.

Results from the HNC-QSP model can be obtained analytically in the mean-field approximation. Numerical results are shown in Fig. 1, where we compare the HNC and mean-field approximations for a range of Γ and $r_s = 2$; as expected, the mean-field result differs from the HNC result when $\Gamma \gtrsim 1$. Moreover, the difference is quite small, further justifying the neglect of $B(r)$.

Figure 2 displays the spatial profile of HM, Kelgb, modified-Kelgb and pure Coulomb potentials. The comparison between these different QSPs show good agreement except at small r for some cases. For $r > 1$, we see some lack of sensitivity of the choice of the potential, suggesting that most QSPs will yield results close to PIMC results. However, we compare our model with PIMC[8] results in Fig. 3; except for very strong degeneracy $\theta = 0.5$, our model is in quite reasonable agreement with PIMC, confirming the results of Dutta and Dufty.

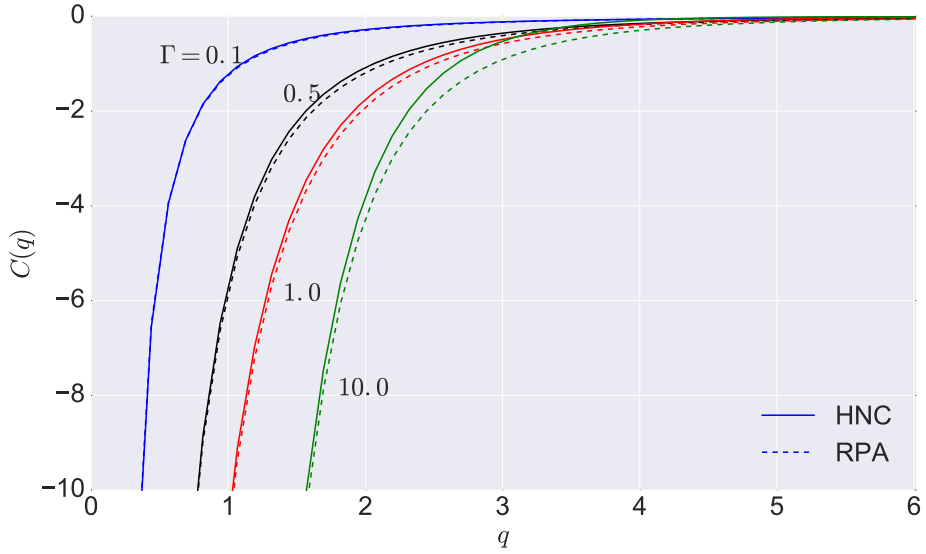

Figure 1. Predicted direct correlation function (DCF). Predictions of the DCF for $r_s = 2$ and $\Gamma = 0.1, 0.5, 1.0, 10$ from the QSP-HNC model and its mean-field approximation.

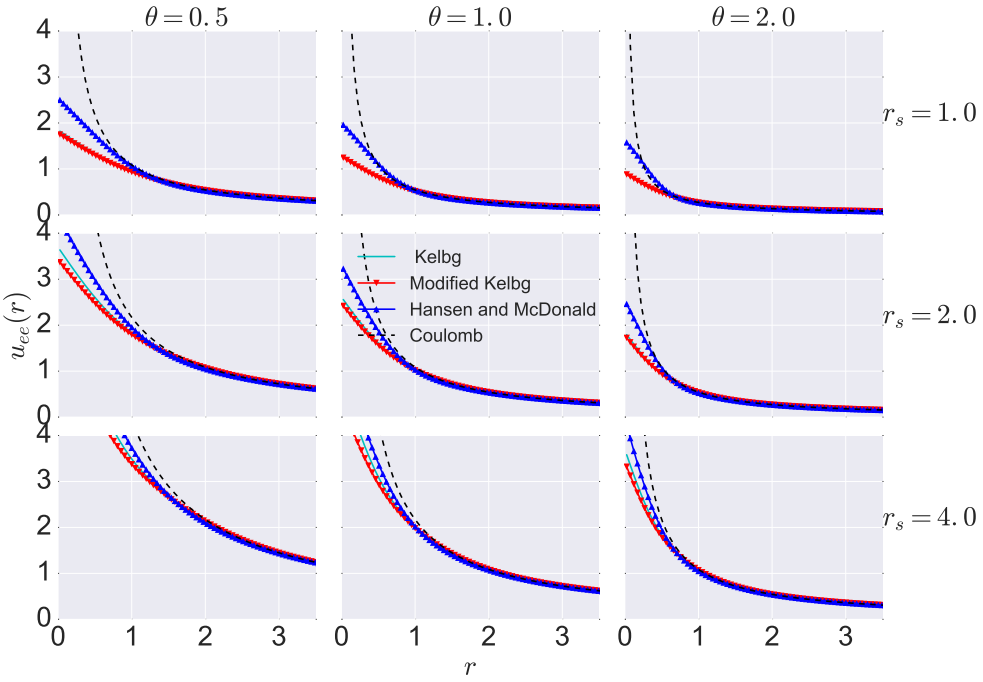

Figure 2. Comparison of quantum statistical potential for different densities and temperature. Electron-electron QSPs obtained with Kelbg[9], modified-Kelbg[6], Hansen and McDonald quantum[7] statistical potentials and the pure Coulomb potential for different values of θ and r_s. There are small r differences at high density.

Next, to determine the longitudinal viscosity $\eta_l = (4\eta/3 + \xi)$ which contains the shear η and bulk ξ viscosities of the electron fluid, we proceed as follows. In the zero-temperature limit, Conti and Vignale[10] suggested that the electron shear

[1] It is worth emphasizing that $g(r)$ here refers to the electron-electron $g_{ee}(r)$, a quantity not readily obtainable from DFT approaches.

viscosity in the units of $na^2\omega_p$ can be approximated by

$$\eta^*_{CV} = \frac{1}{\sqrt{3r_s}} \frac{1}{c_0 r_s^{-3/2} + c_1 r_s^{-1} + c_2 r_s^{-2/3} + c_3 r_s^{-1/3}}, \tag{6}$$

where $c_0 = 60, c_1 = 80, c_2 = -40$, and $c_3 = 62$. In the classical limit, Stanton and Murillo[11] proposed an accurate fit for the

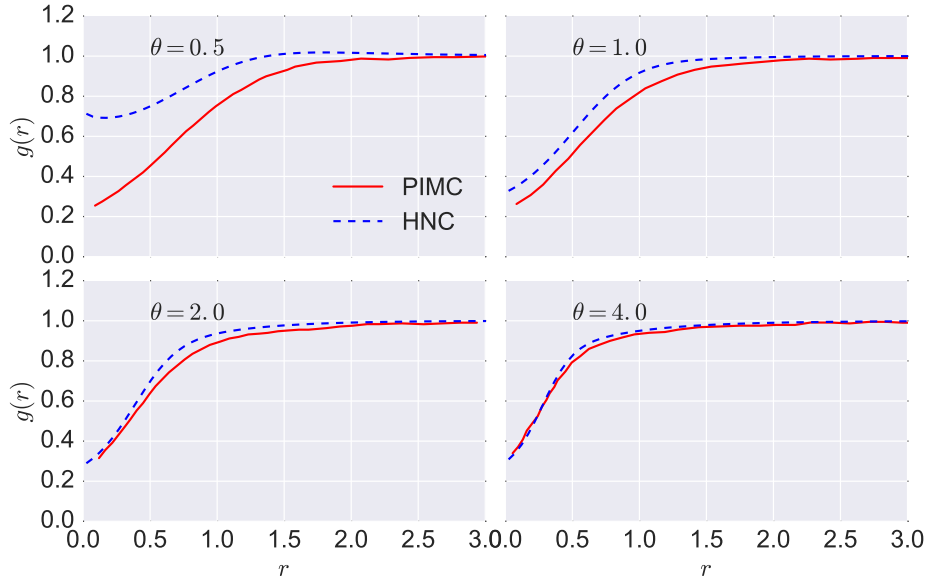

Figure 3. Comparison between HNC-QSP and PIMC for $g(r)$ at four values of the degeneracy parameter $\theta = T/E_F$. The QSPs used are the Hansen and McDonald[7] forms and the PIMC is from Brown[8].

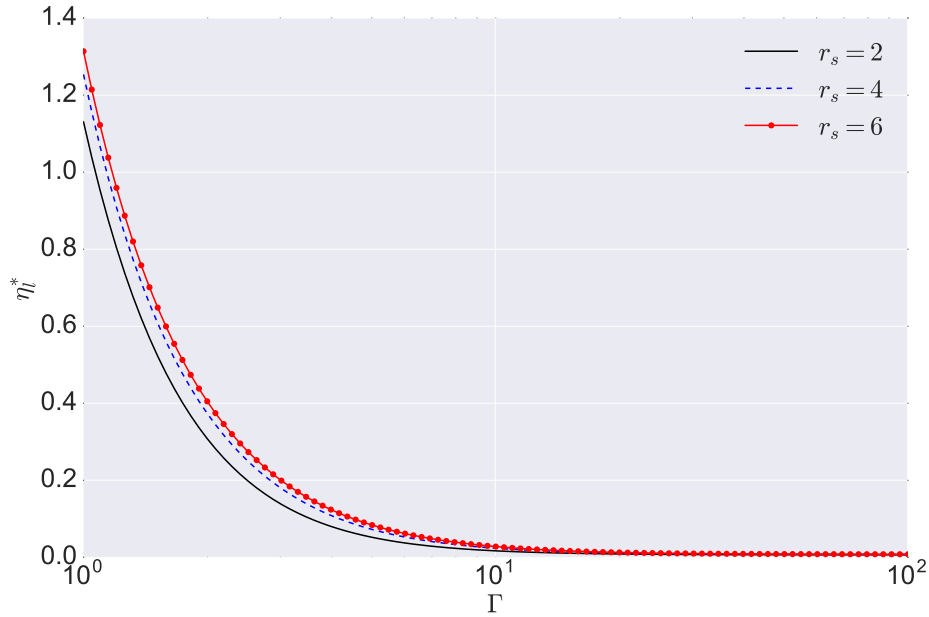

Figure 4. Electronic viscosity. We show the viscosity (8) as a function of the coupling parameter Γ for different values of r_s.

electron viscosity:

$$\eta^*_{SM} = \frac{5\sqrt{3\pi}}{18\Gamma^{5/2}\ln\Lambda_\eta}, \tag{7}$$

where the coupling parameter is defined as $\Gamma = \beta/a$, and Λ_η is the effective Coulomb logarithm for viscosity, for which a numerical solution is given in Ref.[11]. In our calculation, we use the Thomas-Fermi length as the screening length. We obtain the viscosity in both the zero- and finite- temperature limits by interpolating the two formulas (6) and (7) as

$$\eta^*_l = \frac{4}{3}\frac{\eta^*_{CV} + \theta\eta^*_{SM}}{1+\theta}, \tag{8}$$

where the degeneracy parameter is $\theta = T/T_F$, and T_F is the Fermi temperature. Note that the bulk viscosity ξ has been shown to vanish identically both in quantum[12] and classical fluids[13]. The result of the interpolation for the viscosity is shown in Fig. 4 as a function of the coupling parameter.

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