Transport coefficients of the classical one-component plasma

B. Bernu and P. Vieillefosse
Laboratoire de Physique Théorique des Liquides, Université Pierre et Marie Curie, 4 Place Jussieu, 75230 Paris Cedex 05, France
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We present molecular-dynamics computations of the thermal conductivity, and two viscosities of the classical one-component plasma in a rigid, uniform background. The Kubo formulas are proved for the Coulomb case, and it is shown that some care has to be taken in defining the Kubo currents in order to avoid divergences arising from the long range of the Coulomb interactions.

I. INTRODUCTION

The static and dynamical properties of the one-component plasma (OCP) have been studied extensively.[1-3] In the strong-coupling regime, the transverse and longitudinal viscosity coefficients η and $\zeta+\frac{4}{3}\eta$ have been calculated by choosing a two-parameter Gaussian form for the memory functions associated with the correlation functions of transverse and longitudinal currents and by determining the parameters by comparison with the exact short-time behavior.[3] Wallenborn and Baus, on the other hand, have obtained[4] the viscosity coefficients in the framework of a kinetic theory. The two calculations are in agreement in showing that the viscosity η (Refs. 3 and 4) exhibits a minimum as a function of the temperature and that ζ (Ref. 3) is negligible compared to η, but discrepancies remain, particularly at high temperatures. Moreover the thermal conductivity has not yet been estimated. We have therefore computed these three coefficients through molecular-dynamics (MD) computer simulations. Some care has to be taken in defining the Kubo currents (in particular the energy current) in order to avoid divergences and ambiguities arising from the long range of the Coulomb interactions.

Let us recall that the OCP consists of point particles of mass m and change e, interacting by a e^2/r potential and moving in a uniform and rigid background of opposite charge, in such a way that the total charge is zero. We choose as units of length and time the quantities r_0 and ω_p^{-1} defined by

$$\tfrac{4}{3}\pi\rho r_0^3=1, \quad \omega_p^2=4\pi\rho e^2/m \ ,$$

where ω_p is the plasma frequency and ρ is the number density. Coupling between particles is characterized by the parameter $\Gamma=\beta e^2/r_0$ (where $\beta=1/k_BT$). Classical mechanics can be used as soon as the de Broglie thermal wavelength is small compared with r_0, i.e.,

$$(2\pi\Gamma/r_s)^{1/2}\ll 1 \quad (r_s=me^2r_0/\hbar^2) \ .$$

We are interested in the strong-coupling domain $1<\Gamma<155$, where $\Gamma=155$ corresponds to the fluid-solid transition.[12] A hydrodynamic description is valid only in this domain of strong coupling.[5] A crude calculation allows us to underline this point. Taking the square of the distance of closest approach of thermal particles as an estimate of the cross section, $(\beta e^2)^2$, we obtain the mean free path $\lambda=1/\rho(\beta e^2)^2$ and the collision time $\tau=\lambda\sqrt{\beta m}$,

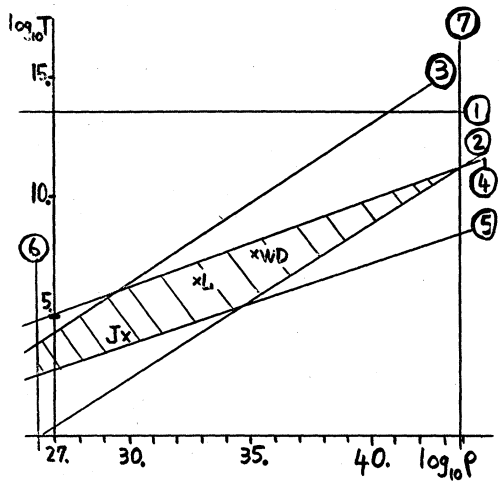

FIG. 1. Diagram $\log_{10}T$ (T in K)-$\log_{10}\rho$ (ρ in m^{-3}). The straight lines give the helium case:
(1) The temperature upper limit (UL) of the nonrelativistic zone for the ions.
(2) The temperature lower limit (LL) of the nonquantum zone for the ions.
(3) The temperature LL of the nonquantum zone for the electrons.
(4) The temperature UL of the strong-coupling zone ($\Gamma=1$).
(5) The temperature LL of the fluid zone ($\Gamma=155$).
(6) The density LL of the small electronic screening zone.
(7) The density UL of the zone in which the nuclear core has no effect. The points correspond to the interior of Jupiter (J), the white dwarfs (WD), laser implosion experiments (L).

with $\omega_p\tau = \Gamma^{-3/2}$; for small values of Γ, the collision time is great compared with the period of plasma oscillations and we are in a kinetic regime, where the hydrodynamic description is invalid, because local equilibrium is not achieved.

The OCP can be applied in a first approximation as a model of various astrophysical situations, in particular of white dwarfs and also to laser-fusion experiments, where the system is essentially one composed of protons and electrons. We show on a T-ρ diagram (Fig. 1) the borders of the domain in which our approximations are valid and the points corresponding to different experimental situations.

In Sec. II, we established the formulas giving the kinetic coefficients by defining the Kubo currents which occur in the Coulombic case. In Sec. III, we present the results of our MD calculations. A brief, preliminary account of this work has been published elsewhere.[6]

II. MICROSCOPIC EXPRESSIONS FOR THE TRANSPORT COEFFICIENTS

Outside equilibrium, the OCP is a locally charged system, which leads to the presence of a macroscopic electric field in the hydrodynamic equations and obliges us to rederive the Kubo formulas giving the transport coefficients. These have already been established for the viscosity coefficients[3] and we are interested here primarily in the thermal conductivity.

A. Kubo formulas for the transport coefficients

1. *Thermodynamic fluctuations*

The system in local equilibrium is described by the number density $\rho(\vec{r})$, the internal energy density $\epsilon(\vec{r})$, and the local velocity $\vec{v}(\vec{r})$; other thermodynamic quantities are s, the entropy per particle; T, the temperature; μ, the chemical potential; P, the pressure; and e, the energy per particle; the deviation of a quantity f from its equilibrium value, is denoted by δf:

$$\delta f(\vec{r}) = \frac{1}{V}\sum_{\vec{k}} \delta f_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \quad \text{and} \quad \delta f_{\vec{k}} = \int d\vec{r}\, \delta f(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} .$$

The probability of having a thermodynamic fluctuation described by $\delta\rho$, $\delta\epsilon$, and $\vec{v}$ is proportional to $e^{\delta S/k_B}$, where δS is the corresponding entropy deviation; for small deviations, δS will be taken to second order. Per unit volume,

$$\delta\rho s = \frac{1}{T}\delta\epsilon - \frac{\mu}{T}\delta\rho + \tfrac{1}{2}\left[\delta\left(\frac{1}{T}\right)\delta\epsilon + \delta\left(-\frac{\mu}{T}\right)\delta\rho\right] . \tag{1}$$

Taking s and p as variables,

$$\delta\rho s = \frac{1}{T}\delta\epsilon - \frac{\mu}{T}\delta\rho - \frac{1}{2}\frac{\rho}{c_p}\delta s^2 - \frac{1}{2}\frac{K_s}{T}\delta p^2 . \tag{2}$$

$c_p = T\,\partial s/\partial T\big|_p$ is the specific heat at constant pressure and $K_s = \rho^{-1}\,\partial\rho/\partial p\big|_s$ is the adiabatic compressibility. The first term in (2) corresponds to the transformation of internal energy into macroscopic kinetic and potential energies:

$$\delta\epsilon = -(\tfrac{1}{2}\rho m v^2 + E^2/8\pi) . \tag{3}$$

The electric field $\vec{E}$ is given by Poisson's equation $\operatorname{div}\vec{E} = 4\pi e\delta\rho$. The second term (2) does not contribute after integration, because of particle number conservation.

We obtain for the total entropy deviation

$$\delta S = -\frac{\rho m}{2TV}\sum_{\vec{k}} \vec{v}_{\vec{k}}\cdot\vec{v}_{-\vec{k}} - \frac{1}{2V}\sum_{\vec{k}\neq 0}\left\{|\delta s_{\vec{k}}|^2\left[\frac{\rho}{c_p} + \frac{4\pi e^2}{k^2}\frac{1}{T}\left(\frac{\partial\rho}{\partial s}\Big|_p\right)^2\right]\right.$$
$$\left. + 2\delta s_{\vec{k}}\delta p_{-\vec{k}}\frac{4\pi e^2}{k^2}\frac{1}{T}\frac{\partial\rho}{\partial s}\Big|_p\frac{\partial\rho}{\partial p}\Big|_s + |\delta p_{\vec{k}}|^2\left[\frac{K_s}{T} + \frac{4\pi e^2}{k^2}\frac{1}{T}\left(\frac{\partial\rho}{\partial p}\Big|_s\right)^2\right]\right\} . \tag{4}$$

The electric field term, which is crucial for the stability of the system,[3] introduces a coupling between entropy and pressure. We deduce from (4) the correlation functions of the entropy with the entropy, the pressure, and the velocity:

$$\langle\delta s_{\vec{k}}\delta s_{-\vec{k}}\rangle = \frac{Vk_B}{\Delta}\left[\frac{K_s}{T} + \frac{4\pi e^2}{k^2}\frac{1}{T}\left(\frac{\partial\rho}{\partial p}\Big|_s\right)^2\right] , \tag{5}$$

$$\langle\delta s_{\vec{k}}\delta p_{-\vec{k}}\rangle = \frac{-Vk_B}{\Delta}\frac{4\pi e^2}{k^2}\frac{1}{T}\frac{\partial\rho}{\partial s}\Big|_p\frac{\partial\rho}{\partial p}\Big|_s , \tag{6}$$

$$\langle\delta s_{\vec{k}}\vec{v}_{-\vec{k}}\rangle = 0 , \tag{7}$$

with

$$\Delta = \frac{\rho}{c_p}\frac{K_s}{T} + \frac{4\pi e^2}{k^2}\frac{1}{T}\left[\frac{\rho}{c_p}\left(\frac{\partial\rho}{\partial p}\Big|_s\right)^2 + \frac{K_s}{T}\left(\frac{\partial\rho}{\partial s}\Big|_p\right)^2\right] . \tag{8}$$

Obviously, these formulas, obtained for thermodynamic fluctuations, are valid only at small $\vec{k}$. The correlation functions in ρ, T, $\vec{v}$ variables can be found in Ref. 3.

2. *Hydrodynamic limit of the correlation functions*

Solution of the hydrodynamic-flow equations gives the behavior of the different correlation functions in the small $\vec{k}$ and ω limit. The strong-coupling assumption allows us to consider the plasma frequency as sufficiently small (compared to the collision frequency).

The linearized equations of conservation of particle number, momentum, and energy are

$$\partial_t \delta\rho + \rho \operatorname{div} \vec{v} = 0 , \tag{9}$$

$$m\rho\, \partial_t \vec{v} = -\vec{\nabla}\delta p + \rho e\vec{E} + \eta\Delta\vec{v} + (\zeta + \tfrac{1}{3}\eta)\vec{\nabla} \operatorname{div} \vec{v} \tag{10}$$

$$\rho T \partial_t \delta_s = \lambda \operatorname{div}\vec{\nabla}\delta T , \tag{11}$$

where λ is the thermal conductivity.

By taking the Fourier transform for the space variable and the Laplace transform for the time variable, and solving the resulting system of three linear equations, we obtain $\tilde{\delta s}(\vec{k}, \omega)$ as a linear function of the deviations at the initial time $t=0$, $\delta s_{\vec{k}}$, $\delta p_{\vec{k}}$, and $\vec{v}_{\vec{k}}$; by multiplying by $\delta s_{-\vec{k}}$ and taking the average on the initial time fluctuations, with the help of the formulas that we have obtained in the preceding paragraph, we get the entropy correlation function

$$\langle \tilde{\delta s}(\vec{k}, \omega)\delta s(-\vec{k}, t=0)\rangle = \sigma_{ss}\langle \delta s_{\vec{k}}\delta s_{-\vec{k}}\rangle + \sigma_{sp}\langle \delta p_{\vec{k}}\delta s_{-\vec{k}}\rangle + \vec{\sigma}_{s\vec{v}} \cdot \langle \vec{v}_k \delta s_{-\vec{k}}\rangle . \tag{12}$$

The σ functions exhibit poles for $z \equiv -i\omega = \alpha$, β, and β^*:

$$\alpha = -D_T\left(1 - \frac{1}{\rho^2}\frac{\partial p}{\partial s}\bigg|_\rho \frac{\partial \rho}{\partial T}\bigg|_p\right)k^2 ,$$

$$\beta = i\omega_p\left(1 + \frac{k^2}{2m\omega_p^2}\frac{\partial p}{\partial \rho}\bigg|_s\right) - \frac{1}{2}bk^2 , \tag{13}$$

where

$$D_T = \lambda/\rho c_p \quad \text{and} \quad b = (\zeta + \tfrac{4}{3}\eta)/m\rho ; \tag{14}$$

in the neutral fluid case the poles would have been

$$\alpha' = -D_T k^2 \quad \text{and} \quad \beta' = i\left(\frac{1}{m}\frac{\partial p}{\partial \rho}\bigg|_s\right)^{1/2} k \tag{15}$$

with a damping term of the sound mode which we have not written.

There are two differences between the neutral and Coulomb cases. First, the sound mode goes into a plasmon mode in the OCP case, which is not surprising. Secondly and more unexpectedly, the thermal diffusion mode introduces a coefficient which is no longer simply D_T, but a modified quantity. We shall see nevertheless that the Kubo formulas for the thermal conductivity are unchanged because the change in the thermal diffusion coefficient is exactly compensated by the change in the static fluctuations of entropy. When $\vec{k}$ goes to zero, the thermal diffusion mode remains only in σ_{ss} (σ_{sp} and $\sigma_{s\vec{v}}$ tend to zero):

$$\sigma_{ss} \underset{\vec{k}\to 0}{\sim} 1/(z-\alpha) . \tag{16}$$

On the other hand, from (5), we obtain

$$\langle \delta s_k \delta s_{-k}\rangle \underset{\vec{k}\to 0}{\sim} Vk_B \frac{1}{T}\left(\frac{\partial \rho}{\partial p}\bigg|_s\right)^2 \Big/ \left[\frac{\rho}{Tc_p}\left(\frac{\partial \rho}{\partial p}\bigg|_s\right)^2 + \frac{1}{\rho T^2}\frac{\partial \rho}{\partial p}\bigg|_s \left(\frac{\partial \rho}{\partial s}\bigg|_p\right)^2\right] = \frac{Nk_B c_p}{\rho^2}\left(1 - \frac{1}{\rho^2}\frac{\partial p}{\partial s}\bigg|_\rho \frac{\partial \rho}{\partial T}\bigg|_p\right)^{-1} . \tag{17}$$

Thus finally we find that

$$\lim_{\omega\to 0}\lim_{k\to 0} \frac{i\omega}{k^2}\left[-i\omega\langle \tilde{\delta s}(\vec{k}, \omega)\delta s_{-\vec{k}}\rangle - \langle \delta s_{\vec{k}}\delta s_{-\vec{k}}\rangle\right] = \lim_{z\to 0}\lim_{k\to 0} -\frac{1}{k^2}\frac{z\alpha}{z-\alpha}\langle \delta s_{\vec{k}}\delta s_{-\vec{k}}\rangle = \frac{Nk_B\lambda}{\rho^3} . \tag{18}$$

Introducing the entropy current through the relation $\partial_t \delta s + \operatorname{div} \vec{j}_s = 0$, we obtain the Kubo formula

$$\lambda = \frac{\rho^3}{Nk_B}\int_0^{+\infty} dt\, \langle j_{ls}(\vec{k}=0, t)\, j^*_{ls}(\vec{k}=0, t=0)\rangle , \tag{19}$$

where j_{ls} is the longitudinal component of $\vec{j}_s$. The entropy current is related to the energy and particle currents $\vec{j}_\epsilon$ and $\vec{j}$ by

$$\rho T\vec{j}_s = \vec{j}_\epsilon - (e + p/\rho)\vec{j} . \tag{20}$$

To conclude the discussion of the thermal conductivity, we note that as $\vec{k}\to 0$ the dynamics eliminate the coupling between entropy and pressure,

which the static fluctuations had introduced.

A similar analysis in ρ, T, $\vec{v}$ variables leads to the Kubo formulas for the viscosity coefficients [Ref. 3, Eqs. (36) and (55)]:

$$\eta=\lim_{\omega\to 0}\lim_{\vec{k}\to 0}\frac{m\rho}{k^2}\left(i\omega+\frac{\omega_0^2}{\tilde{c}_t(\vec{k},\omega)}\right), \tag{21}$$

$$\zeta+\frac{4}{3}\eta=\lim_{\omega\to 0}\lim_{\vec{k}\to 0}\frac{m\rho}{k^2}\,\mathrm{Re}\frac{\omega_0^2}{\tilde{c}_l(\vec{k},\omega)}, \tag{22}$$

where $\omega_0^2=k^2/\beta m$; $\tilde{c}_t$ and $\tilde{c}_l$ are the Laplace transforms of the transverse and longitudinal current correlation functions; Re indicates the real part.

$$c_t(\vec{k},t)=(k^2/2N)\langle\vec{j}_t(\vec{k},t)\cdot\vec{j}_t^{\,*}(\vec{k},0)\rangle, \tag{23}$$

$$c_l(\vec{k},t)=(k^2/N)\langle j_l(\vec{k},t)\,j_l^{*}(\vec{k},0)\rangle. \tag{24}$$

After some transformations, we find

$$\eta=\frac{\beta\rho}{2N}\int_0^{+\infty}dt\,\langle\vec{A}_t(k=0,t)\cdot\vec{A}_t^{\,*}(k=0,t=0)\rangle, \tag{25}$$

$$\zeta+\frac{4}{3}\eta=\frac{\beta\rho}{N}\int_0^{+\infty}dt\,\langle\vec{A}_l(k=0,t)\vec{A}_l(k=0,t=0)\rangle, \tag{26}$$

$\vec{A}_t$ and A_l being the transverse and longitudinal parts of the Kubo current:

$$\vec{A}(\vec{k},t)=i(m/k)\,\partial_t\vec{j}(\vec{k},t). \tag{27}$$

As we have seen the Kubo formulas are not modified for the OCP; but the currents must be carefully defined because of the long range of the Coulomb potential.

B. Kubo currents

1. *Specific difficulties of the Coulomb case*

If we simply replace the potential $v(r)$ by e^2/r (or

$$V^{-1}\sum_{\vec{k}\neq 0}\frac{e^{i\vec{k}\cdot\vec{r}}4\pi e^2}{k^2},$$

to take account of the background) in the usual formulas giving the Kubo currents, ambiguities and divergences appear. As an example, consider the case of the entropy current; the usual definition of the energy density for a system of particles interacting by a potential $v(r)$

$$\epsilon(\vec{r})=\sum_i\left(\frac{1}{2}mv_i^2+\frac{1}{2}\sum_{j\neq i}v(r_{ij})\right)\delta(\vec{r}-\vec{r}_i) \tag{28}$$

leads to a longitudinal entropy current j_{ls}

$$\rho T j_{ls}(\vec{k},t)=\sum_i e^{-i\vec{k}\cdot\vec{r}_i}\left\{\vec{k}\cdot\vec{v}_i\left[\frac{1}{2}mv_i^2+\frac{1}{2}\sum_{j\neq i}v(r_{ij})-\left(e+\frac{p}{\rho}\right)\right]-\frac{1}{4}\sum_{j\neq i}r_{ij}v'(r_{ij})\frac{1-e^{-i\vec{k}\cdot\vec{r}_{ij}}}{i\vec{k}\cdot\vec{r}_{ij}}(\vec{k}\cdot\vec{r}_{ij})[\vec{r}_{ij}\cdot(\vec{v}_i+\vec{v}_j)]\right\}, \tag{29}$$

where $v'(r)=dv/dr$, $\vec{r}=\vec{r}/r$, and $\vec{k}=\vec{k}/k$. When k goes to zero

$$\rho T j_{ls}(k=0,t)=\sum_i v_{i\alpha}\left\{\vec{k}_\alpha\left[\frac{1}{2}mv_i^2-\left(e+\frac{p}{\rho}\right)\right]+\frac{1}{2}\sum_{j\neq i}\vec{k}_\beta f_{\alpha\beta}(\vec{r}_{ij})\right\}, \tag{30}$$

$$f_{\alpha\beta}(\vec{r})=v(r)\delta_{\alpha\beta}-rv'(r)\vec{r}_\alpha\vec{r}_\beta. \tag{31}$$

In calculating the initial time value of the Kubo integrant $\lambda(0)$ [$\lambda=\int_0^{+\infty}dt\,\lambda(t)$], we find that this quantity diverges when the volume goes to infinity essentially because the integral $\int_V d\vec{r}\,f_{\alpha\beta}(\vec{r})$ is diverging at large distances.

Moreover, the term $rv'(r)\vec{r}_\alpha\vec{r}_\beta$ is not well defined. In fact, in the case of a long-range potential, it is necessary to consider the system to be periodically repeated in space in order to remove the bondary problems at the walls of the box which contains the system, and there are several ways to construct a periodic function with $rv'(r)\vec{r}_\alpha\vec{r}_\beta$.

Finally, let us remark that when k is small, we can substitute 1 for $(1-e^{-i\vec{k}\cdot\vec{r}})/i\vec{k}\cdot\vec{r}$ in the expression of $\rho T\vec{j}_s(\vec{k},t)$ only if the potential range d is small compared to $L=V^{1/3}$. Indeed, because of $rv'(r)$, the largest values of r are of the order of d; the smallest value of $\vec{k}$ being of the order of L^{-1}, it is necessary that d/L should be small compared to 1. In the Coulomb case the condition is no longer satisfied.

These remarks have led us to consider again the problem at its beginning, i.e., at the definition of the energy density $\epsilon(\vec{r})$.

2. *Entropy current*

We take $E^2/8\pi$ for the potential-energy density, $\vec{E}$ being the electric field of the charged particles and of the background. We must, of course, subtract the infinite self-energy, which is a single

sum over the particles:

$$\epsilon(\vec{r}) = \sum_i \frac{1}{2} m v_i^2 \delta(\vec{r} - \vec{r}_i) + \frac{E^2}{8\pi} - \epsilon_{\text{self}}(\vec{r}) , \tag{32}$$

$$\operatorname{div} \vec{E} = 4\pi e \left(\sum_i \delta(\vec{r} - \vec{r}_i) - \rho \right) . \tag{33}$$

By taking the Fourier transform, we obtain

$$\epsilon(\vec{k}) = \sum_i e^{-i\vec{k}\cdot\vec{r}_i} \left(\frac{1}{2} m v_i^2 - \frac{1}{2} \sum_{j \neq i} \frac{1}{V} \sum_{\vec{k}' \neq 0, \vec{k}} \frac{4\pi e^2}{k'^2 (\vec{k} - \vec{k}')^2} \vec{k}' \cdot (\vec{k} - \vec{k}') e^{-i\vec{k}'\cdot\vec{r}_{ij}} \right) \tag{34}$$

The longitudinal energy current, defined by,

$$j_{1\epsilon}(\vec{k}) = \vec{k} \cdot \vec{j}_\epsilon(\vec{k}) = -ik^{-1} \partial_t \epsilon(\vec{k}) \tag{35}$$

is

$$j_{1\epsilon}(\vec{k}) = \sum_i e^{-i\vec{k}\cdot\vec{r}_i} \vec{v}_i \cdot \left(\vec{k} \tfrac{1}{2} m v_i^2 + \sum_{j \neq i} \frac{1}{V} \sum_{\vec{k}'} \vec{w}_1(\vec{k}, \vec{k}') e^{-i\vec{k}'\cdot\vec{r}_{ij}} \right) \tag{36}$$

with

$$\vec{w}_1(\vec{k}, \vec{k}') = \frac{4\pi e^2}{k} \left(\frac{\vec{k}'}{k'^2} - \frac{\vec{k}' \cdot (\vec{k} - \vec{k}')}{k'^2 (\vec{k} - \vec{k}')^2} (\vec{k} - \vec{k}') \right), \quad \vec{k}' \neq 0, \vec{k}$$

$$= 0 , \quad \vec{k}' = 0$$

$$= (4\pi e^2 / k^2)(\vec{k}/k) , \quad \vec{k}' = \vec{k} . \tag{37}$$

By taking the limit $k \to 0$, we obtain finally for the energy current the same expression as in the general case (30), but with the following function $f_{\alpha\beta}(\vec{r})$:

$$f_{\alpha\beta}(\vec{r}) = \frac{2}{V} \sum_{\vec{k} \neq 0} \frac{4\pi e^2}{k'^2} (\delta_{\alpha\beta} - \vec{k}'_\alpha \vec{k}'_\beta) e^{-i\vec{k}'\cdot\vec{r}} . \tag{38}$$

When the volume goes to infinity, the discrete sum becomes an integral over $\vec{k}'$,

$$f_{\alpha\beta}(\vec{r}) \underset{V \to \infty}{\sim} (e^2/r)(\delta_{\alpha\beta} + \vec{r}_\alpha \vec{r}_\beta) , \tag{39}$$

which coincides with (31). This expression is valid only for distances such that $r \ll V^{1/3}$, where the discrete character of the sum over $\vec{k}'$ in (38) does not appear. Finally, divergences are removed because

$$\int_V d\vec{r} f_{\alpha\beta}(\vec{r}) = 0 . \tag{40}$$

3. Kubo currents for the viscosities

In the same way, we obtain the current $\vec{A} = i \partial_t m k^{-1} \vec{j}(\vec{k}, t)$ by calculating the accelerations from the energy,

$$\epsilon(\vec{k} = 0) = \sum_i \left(\frac{1}{2} m v_i^2 + \frac{1}{2} \sum_{j \neq i} \frac{1}{V} \sum_{\vec{k} \neq 0} \frac{4\pi e^2}{k'^2} e^{-i\vec{k}'\cdot\vec{r}_{ij}} \right) . \tag{41}$$

A direct calculation leads to

$$A_\alpha(\vec{k}) = \sum_i e^{-i\vec{k}\cdot\vec{r}_i} \left(m \vec{k}_\beta v_{i\alpha} v_{i\beta} + \frac{1}{2} \sum_{j \neq i} \frac{1}{V} \sum_{\vec{k}'} w_{2\alpha}(\vec{k}') e^{-i\vec{k}'\cdot\vec{r}_{ij}} \right) , \tag{42}$$

where $\vec{w}_2$ is defined by

$$\vec{w}_2 = \frac{4\pi e^2}{k} \left(\frac{\vec{k}'}{k'^2} + \frac{\vec{k} - \vec{k}'}{(\vec{k} - \vec{k}')^2} \right), \quad k' \neq 0, \vec{k}$$

$$= (4\pi e^2 / k^2)\vec{k} , \quad k' = 0, \vec{k} . \tag{43}$$

By taking the limit $k \to 0$,

$$A_\alpha(k \to 0) = \sum_i m v_{i\alpha} v_{i\beta} \vec{k}_\beta + \frac{1}{2} \sum_{j \neq i} \vec{k}_\beta f'_{\alpha\beta}(\vec{r}_{ij}) - \vec{k}_\alpha p V(E_i, N) \tag{44}$$

with

$$f'_{\alpha\beta}(\vec{r}) = \frac{1}{V} \sum_{\vec{k}' \neq 0} \frac{4\pi e^2}{k'^2} (\delta_{\alpha\beta} - 2\vec{k}'_\alpha \vec{k}'_\beta) e^{-i\vec{k}'\cdot\vec{r}} . \tag{45}$$

We have subtracted the mean value $\vec{k}_\alpha pV$,[7,8] corresponding to the momentum flow through the surface bounding the system and occurring as a source term in the momentum-conservation equation; it affects only the component $\vec{k} = 0$. On the other hand, pV is a function of the internal energy E_i and the particle number N; in statistical en-

sembles where these quantities are not fixed their fluctuations must be taken into account. We introduce the momentum flow tensor $\tau_{\alpha\beta}$ by $A_\alpha = \vec{k}_\beta \tau_{\alpha\beta}$

$$\tau_{\alpha\beta} = \sum_i m v_{i\alpha} v_{i\beta} + \frac{1}{2}\sum_{i\neq j} f'_{\alpha\beta}(\vec{r}_{ij}) - \delta_{\alpha\beta} pV \ . \quad (46)$$

We deduce from (25) and (26) the longitudinal viscosity in the form

$$\zeta + \frac{4}{3}\eta = \frac{\beta}{V}\int_0^{+\infty} dt\, \langle \tau_{\alpha\alpha}(t)\tau_{\alpha\alpha}(0)\rangle$$

(no summation over α) (47)

and for the transverse one

$$\eta = \frac{\beta}{V}\int_0^{+\infty} dt\, \langle \tau_{\alpha\beta}(t)\tau_{\alpha\beta}(0)\rangle$$

(no summation over α and β; $\alpha \neq \beta$) . (48)

We have taken into account the space isotropy. We also introduce

$$p = \frac{\beta}{V}\int_0^{+\infty} dt\, \langle \tau_{\alpha\alpha}(t)\tau_{\beta\beta}(0)\rangle$$

(no summation over α and β; $\alpha \neq \beta$) (49)

$$I = \frac{\beta}{V}\int_0^{+\infty} dt\, \langle \tau_{\alpha\beta}(t)\tau_{\gamma\delta}(0)\rangle \vec{k}_\alpha \vec{k}_\beta \vec{k}_\gamma \vec{k}_\delta \ . \quad (50)$$

By taking $\vec{k} = (\sin\theta,\ 0,\ \cos\theta)$ and averaging over θ, we obtain

$$I \equiv \zeta + \tfrac{4}{3}\eta = \tfrac{11}{15}(\zeta + \tfrac{4}{3}\eta) + \tfrac{4}{15}p + \tfrac{8}{15}\eta \ . \quad (51)$$

From which, we deduce,

$$\zeta = \tfrac{1}{3}(\zeta + \tfrac{4}{3}\eta) + \tfrac{2}{3}p$$

$$= \frac{\beta}{9V}\int_0^{+\infty} dt\, \langle \tau_{\alpha\alpha}(t)\tau_{\beta\beta}(0)\rangle \ . \quad (52)$$

A direct calculation of $\tau_{\alpha\alpha}$ yields

$$\tau_{\alpha\alpha} = 2(E_k - \langle E_k\rangle) + E_p - \langle E_p\rangle \ , \quad (53)$$

where E_k and E_p are the kinetic and potential energies. This result, which can be generalized for all homogeneous potentials, simply expresses the bulk viscosity ζ as a function of the energy fluctuations.

III. NUMERICAL METHOD

A. Molecular dynamics applied to the OCP

We have computed the Kubo currents appearing in the different autocorrelation functions as a function of time using the molecular-dynamics method, which has already proved very successful in the study of collective modes in the strongly coupled OCP.[2] The system is assumed to be isolated (the total energy and the number of particles are constant and the velocity of the center of mass is taken equal to zero). The N particles are enclosed in a periodically repeating cubic box. Therefore the expressions for the Kubo currents are precisely those we have obtained in Sec. II. We need the position and the velocity of every particle as a function of time. The trajectory of each of the N particles (and all of its images) are computed by Verlet's algorithm[9]:

$$\vec{r}_i(t+\Delta t) = -\vec{r}_i(t-\Delta t) + 2\vec{r}_i(t) + \Delta t^2[\vec{F}_i(t)/m] + o(\Delta t^4) \ , \quad (54)$$

$$\vec{V}_i(t+\Delta t) = \vec{V}_i(t-\Delta t) + 2\Delta t[\vec{F}_i(t)/m] + o(\Delta t^3) \ , \quad (55)$$

where $\vec{F}_i(t) = m(d\vec{V}_i/dt)(t) = m(d^2\vec{r}_i(t)/dt^2)$ is the force acting on i owing to all particles $j \neq i$ and their images. The time step Δt must be (i) sufficiently small to ensure good conservation of the total energy and momentum of the system. (ii) Sufficiently large to limit the accumulation of the round-off errors in computations and yield the longest trajectories in phase space. A reasonable choice is $\Delta t \simeq \frac{1}{20}\tau$, where τ is the time characterizing the evolution of the particles. For weak coupling $\tau \sim r_0/V = \sqrt{\Gamma}\omega_p^{-1}$ (where V is the thermal rms velocity), and for very strong coupling, $\tau \sim 2\pi\omega_p^{-1}$. Thus

$$\Delta t \simeq \tfrac{1}{20}\sqrt{\Gamma}\omega_p^{-1} \quad \text{if } \Gamma < 40 \ ,$$

$$\Delta t \simeq 0.3\omega_p^{-1} \quad \text{if } \Gamma > 40 \ .$$

B. Ewald sums

The computation of the forces and Kubo currents for a periodic system introduces slowly converging sums over definite sets of images. These must be treated by the familiar technique of Ewald sums. To calculate the forces,[1] it is easiest first to express the potential E_p and then to differentiate $\vec{F}_i = -\vec{\nabla}_i E_p$. The calculation of Kubo currents is complicated by the presence of angular terms. The detailed calculation is explained in the Appendix.

We write the currents as

$$\vec{A}(\vec{k}) = \sum_i \left(m(\vec{k}\cdot\vec{v}_i)\vec{v}_i + \frac{1}{2}\sum_{j\neq i}\frac{e^2}{L}\vec{S}_2(\vec{r}_{ij})\right) - PV\vec{k} \ ,$$

(56)

$$j_{1\epsilon}(\vec{k}) = \sum_i \left((\vec{k}\cdot\vec{v}_i)\frac{1}{2}mv_i^2 + \sum_{j\neq i}\frac{e^2}{L}\vec{v}_i\cdot\vec{S}_1(\vec{r}_{ij}) \right), \tag{57}$$

and the potential energy is

$$E_p = \frac{e^2}{2L}\sum_{i,j\neq i}\vec{k}\cdot\vec{S}_0(\vec{r}_{ij}) , \tag{58}$$

where $V = L^3$ is the volume of one cell

$$\vec{S}_\beta(\vec{r}) = \sum_{\vec{\lambda}\neq 0}\frac{e^{2i\pi\vec{\lambda}\cdot\vec{r}/L}}{\pi\lambda^2}[\vec{k} - \beta(\vec{k}\cdot\vec{\lambda})\vec{\lambda}] ,$$
$$\vec{k} = \vec{k}/||\vec{k}||, \quad \vec{\lambda} = \vec{\lambda}/||\vec{\lambda}||, \quad \vec{\lambda} = (n_1, n_2, n_3) . \tag{59}$$

We find for $\vec{S}_\beta(\vec{r})$ the formula (A3) of the Appendix which depends on a dimensionless convergence parameter α. We choose $\alpha = 5.6$, which allows us to restrict ourselves in the first sum over $\vec{\lambda}$ to the $\vec{\lambda}$ vector which minimizes $||\vec{r}_{ij}/L + \vec{\lambda}||$, i.e., to the image of particle j which is closest to i. The error thus introduced is of the order of 10^{-7}. We calculate the second sum in (A3) by changing the sums on i and j with the sum on $\vec{\lambda}$.[10] We calculate the bulk viscosity from the formula (53) where $E = E_k + E_p$ is constant

$$\zeta = \frac{\beta\rho}{9N}\int_0^\infty \langle [E_k(t) - \langle E_k\rangle][E_k(0) - \langle E_k\rangle]\rangle\, dt. \tag{60}$$

The Kubo currents are computed at times $n\Delta t$ where n and Δt are given in Table I. The autocorrelation functions are estimated as usual from

$$F(t) = \langle C(t)C(0)\rangle = \frac{1}{T}\int_0^T C(t+\tau)C(\tau)\, d\tau$$
$$= \frac{1}{M}\sum_{i=1}^{M} C(i_\tau + i)C(i) , \tag{61}$$

with $t = i_\tau n\Delta t$.

TABLE I. N is the number of particles in each cell. Δt is the time step in units of ω_P^{-1}. n is the Kubo currents computed at times $n\,\Delta t$. n_{run} is the number of runs. N_0 is the number of steps for each run. T is the evolution time of one run, in units of ω_P^{-1}.

Γ	N	Δt	n	n_{run}	N_0	T
1	128	0.04	6	4	10 000	400
10.4	250	0.03	8	5	10 000	300
100.4	250	0.3	1	4	1 800	540

TABLE II. Relaxation time defined for $t\omega_P \ll 1$, in units of ω_P^{-1}, of the autocorrelation functions of η, ζ, λ.

Γ	1.0	10.0	100.0
η	0.9	1.4	2.4
ζ	0.45	0.9	1.1
λ	1.2	1.3	2.0

IV. RESULTS

We now discuss our results, first qualitatively, then quantitatively.

A. Qualitative results

The autocorrelation functions decrease rapidly and exhibit in some cases oscillations with frequencies ω_p or $2\omega_p$. At short times ($t\omega_p \ll 1$), we can approximate each autocorrelation function by a Gaussian $C(t) = C(0)\exp(-t^2/\tau^2)$. The corresponding relaxation times are given in Table II. Here we see that $\tau_{100} > \tau_{10} > \tau_1$. The relaxation times are of the same order of magnitude for η and λ, but are two times smaller for ζ.

The autocorrelation functions for η (Fig. 2) do not exhibit any clear oscillations for $t\omega_p < 20$ at $\Gamma = 1$, 10, 100. At $\Gamma = 100$ we observe a "long tail." At $\Gamma = 10$ the decrease is significantly faster, which accounts in part for the minimum in η as function of Γ.

The autocorrelation functions for ζ (Fig. 3) exhibit very pronounced oscillations at a frequency near $2\omega_p$.

The autocorrelation functions for λ (Fig. 4) exhibit pronounced oscillations at $\Gamma = 10$ and 100, roughly at the plasma frequency. The function decreases slowly at $\Gamma = 1$ and this contributes to the relatively high value of λ at lower coupling.

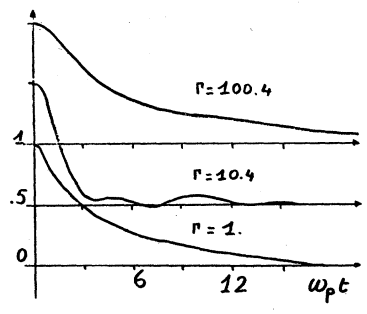

FIG. 2. Autocorrelation functions for the transverse viscosity η.

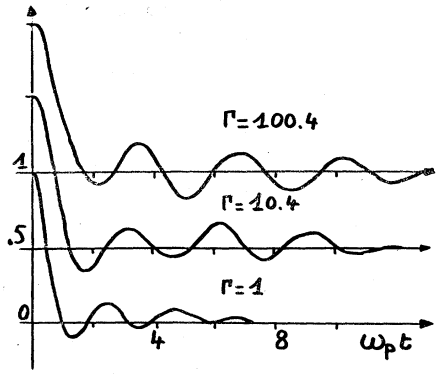

FIG. 3. Autocorrelation functions for the bulk viscosity ζ.

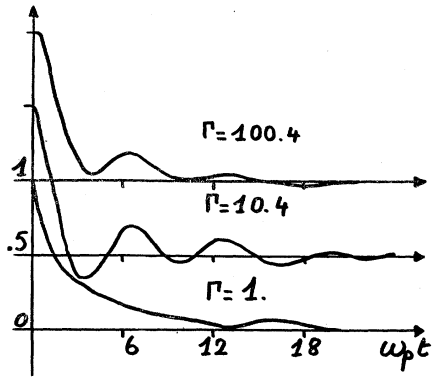

FIG. 4. Autocorrelation functions for the thermal conductivity λ.

B. Quantitative results

We study the variation of the transport coefficients in units which are independent of temperature. Then their variation as a function of Γ is proportional to their variation as a function of $1/T$, at fixed density ρ. We choose the following units: $m\omega_p\rho r_0^2$ for the viscosities: $\eta = m\omega_p\rho r_0^2\eta^*$, $\zeta = m\omega_p\rho r_0^2\zeta^*$. $k_B\omega_p\rho r_0^2$ for the thermal conductivity: $\lambda = k_B\omega_p\rho r_0^2\lambda^*$.

η^* and λ^* exhibit pronounced minima as functions of Γ (and hence of T). At low temperatures (high Γ) η^* and λ^* decrease with T, as in the case of simple neutral liquids. At higher temperatures (small Γ), they increase with T as in the case of gases. For η^* and λ^* the minimum is around $\Gamma = 10$. ζ is always very small compared to η. ζ/η is less than 2% at the three Γ values which we have investigated. ζ increases as function of T. The values of $\eta^*(\Gamma)$, $\zeta^*(\Gamma)$, and $\lambda^*(\Gamma)$ are given in Table III.

C. Interpolation of transport coefficients

Our intention now is to give an idea of the variation of the transport coefficients as functions of Γ for $1 < \Gamma < 155$.

First we note that the integrals of the normalized autocorrelation functions do not vary strongly with Γ. We have therefore fitted these quantities to the following formulas:

$$\eta^*(\Gamma)/\eta_\Gamma^*(0) = \Gamma^{3/2}/(2.5\Gamma - 2.2)\,, \tag{62}$$

$$\zeta^*(\Gamma)/\zeta_\Gamma^*(0) = \Gamma^{1/2}/(0.11\Gamma + 1.5)\,, \tag{63}$$

$$\lambda^*(\Gamma)/\lambda_\Gamma^*(0) = (0.23\Gamma + 3.4)/\Gamma^{1/2}\,. \tag{64}$$

Then we express $\eta_\Gamma^*(0)$, $\zeta_\Gamma^*(0)$, and $\lambda_\Gamma^*(0)$ in terms of equilibrium distribution functions:

$$\eta_\Gamma^*(0) = (1/3\Gamma)[1 - \tfrac{1}{5}\Gamma I_1(\Gamma)] \tag{65}$$

$$\zeta_\Gamma^*(0) = (1/18\Gamma)[1 - 3Nk_B/2C_v(\Gamma)]\,, \tag{66}$$

where $C_v(\Gamma)$ is the specific heat at constant volume, and I_n is an integral involving the pair distribution function:

$$I_n(\Gamma) = \int_0^\infty x^n[g(x) - 1]\,dx, \quad x = \frac{r}{r_0}\,.$$

These quantities can be easily computed using the static properties of the OCP.[1] The results agree very well with the MD values of the autocorrelation functions at $t = 0$.

The correlation of $\lambda_\Gamma^*(0)$ is more complicated because it involves the three-particle distribution function:

TABLE III. $\lambda(0)$, $\eta(0)$, $\zeta(0)$ are the values of the autocorrelation functions at time $t = 0$; the units are $k_B\omega_E^2\rho r_0^2$ for $\lambda(0)$ and $m\omega_E^2\rho r_0^2$ for $\eta(0)$ and $\zeta(0)$.

Γ	$\lambda(0)$	λ	$\eta(0)$	η	$\zeta(0)\times10^{-3}$	$\zeta\times10^{-3}$	ζ/η
1.0	0.870 ± 0.09	2.90 ± 0.6	0.340 ± 0.03	1.040 ± 0.21	4.3 ± 0.2	2.6 ± 0.6	2.5×10^{-3}
10.4	0.350 ± 0.02	0.66 ± 0.16	0.068 ± 0.07	0.085 ± 0.017	1.5 ± 0.1	1.8 ± 0.5	2.0×10^{-2}
100.4	0.338 ± 0.006	0.88 ± 0.17	0.041 ± 0.04	0.18 ± 0.03	0.27 ± 0.02	0.21 ± 0.06	1.2×10^{-3}

TABLE IV. $\eta_\Gamma(0)$, $\zeta_\Gamma(0)$ [respectively, $\lambda_\Gamma(0)$] are given in units of $m\omega_p^2\rho r_0^2$ (respectively, $k_B\omega_p^2\rho r_0^2$). $\eta(\Gamma)$, $\zeta(\Gamma)$ [respectively, $\lambda(\Gamma)$] are given in units of $m\omega_p\rho r_0^2$ (respectively, $k_B\omega_p\rho r_0^2$).

Γ	$\eta_\Gamma(0)$	$\eta(\Gamma)$	$\zeta_\Gamma(0)$ $\times10^{-3}$	$\zeta(\Gamma)$ $\times10^{-3}$	$\lambda_{\Gamma sp}(0)$	$\lambda_{sp}(\Gamma)$
1	0.36	1.2	4.4	2.7	0.95 ± 0.08	3.4
2	0.20	0.2	3.6	3.0	0.75 ± 0.15	2.0
4	0.12	0.12	2.6	2.7	0.68 ± 0.20	1.5
10	0.069	0.096	1.5	1.8	0.49 ± 0.35	0.88
20	0.054	0.1	1.0	1.2		
40	0.046	0.12	0.6	0.64		
70	0.043	0.15	0.4	0.36		
100	0.042	0.17	0.3	0.24		
120	0.042	0.19	0.2	0.15		

$$\lambda_\Gamma^*(0)=\frac{1}{3\Gamma}\left(\frac{5}{2}+4\Gamma^2I_1^2+\frac{3\Gamma^2}{2}I_0^2+\frac{4\Gamma^2}{\pi}\int_0^\infty\frac{dq}{q^2}S(q)+\frac{3\Gamma^2}{(8\pi)^2}\int d\vec{x}\,d\vec{x}'u_3(\vec{x},\vec{x}')\frac{5+(\vec{x}\cdot\vec{x}')^2}{xx'}\right). \tag{67}$$

where $q=kr_0$, $x=r/r_0$, $S(q)$ is the static structure factor, and $u_3(\vec{x},\vec{x}')$ is the Ursell function for three particles.

The evaluation of this expression on a cubic lattice shows that the contribution of the structure-dependent terms vanishes. We therefore compute the values of $\lambda_\Gamma^*(0)$ only for Γ less than 10. Indeed for $\Gamma>10$, the computational errors are multiplied by Γ^2 and become larger than $\lambda_\Gamma^*(0)$ itself. For small Γ, we compute the three-particle term using the superposition approximation[3,11]:

$$\lambda_{\Gamma sp}^*(0)=\frac{1}{3\Gamma}\left(\frac{5}{2}+\frac{4}{\pi}\Gamma^2(I+J+K)+\frac{3}{2}\Gamma^2I_0\right), \tag{68}$$

$$I=\int_0^\infty\frac{dq}{q^2}S(q), \tag{69}$$

$$J=3\int_0^\infty dq\,q^2(S(q)-1)\left[\tilde{u}(q)^2-\tfrac{2}{3}\tilde{u}(q)\tilde{w}(q)+\tilde{w}(q)^2\right], \tag{70}$$

$$K=3\int_0^\infty dq\,(S(q)-1)[\tilde{u}(q)+\tilde{w}(q)], \tag{71}$$

$$\tilde{u}(q)=\int_0^\infty dx\,x^2\frac{g(x)-1}{x}\frac{\sin qx}{qx}, \tag{72}$$

$$\tilde{w}(q)=\int_0^\infty dx\,x^2\frac{g(x)-1}{x}\left(\frac{\sin qx}{(qx)^3}-\frac{\cos qx}{(qx)^2}\right), \tag{73}$$

where $g(x)$ is the radial pair distribution function.

We give in Table IV the values of $\eta_\Gamma^*(0)$, $\zeta_\Gamma^*(0)$, and $\lambda_{\Gamma sp}^*(0)$ and the corresponding values of $\eta^*(\Gamma)$ $\zeta^*(\Gamma)$, and $\lambda^*(\Gamma)$ taken, respectively, from (62), (63), and (64) at various Γ.

V. CONCLUSION

We have shown that the presence of a macroscopic electric field in the hydrodynamic equations does not change the Kubo formulas for the transport coefficients. Nevertheless, the different currents must be defined with some care, on account of the long range of the Coulomb potential.

The results, obtained for the viscosities ζ and η confirm the predictions of Vieillefosse and Hansen[3]; the ratio ζ/η is always less than 2×10^{-2}; η exhibits a pronounced minimum as a function of T, but the precise position of this minimum cannot be predicted from our limited numerical data. Especially at small Γ, these are in better agreement with the results obtained by the kinetic theory of Wallenborn and Baus[4] (Fig. 5). The bulk viscosity ζ increases as a function of temperature.

The thermal conductivity, like η, exhibits a minimum as a function of temperature, but the variation with T is weaker.

As an illustration, we give in Table V the absolute values of dynamic and kinematic viscosities, and thermal conductivity for white dwarfs and a hydrogen plasma under typical laser implosion conditions.

Finally, from our data we find that for a hydrogen plasma at $T=10^7$ K and $\rho=5\times10^{28}$ ions/cm^3, the ionic thermal conductivity is $\lambda_i=2\times10^6$ W m^{-1} K^{-1}. Under these conditions the electron

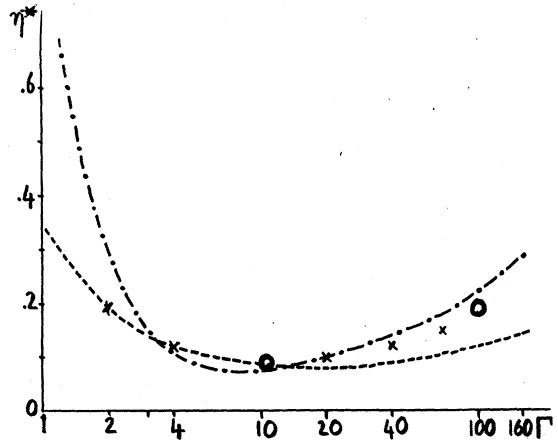

FIG. 5. Comparison between different results for the reduced transverse viscosity η^*; VH (Ref. 3): dashed line, WB (Ref. 4): dash-dot line, present calcuation: circles for the exact values and cross for the fit.

TABLE V. Values of dynamic and kinematic viscosities, and thermal conductivity for white dwarfs (WD) and a hydrogen plasma under typical laser implosion conditions (LI).

	T (K)	ρ (m^{-3})	η (kg $m^{-1}s^{-1}$)	$\eta/\rho m$ ($m^2 s^{-1}$)	λ ($W m^{-1}K^{-1}$)	$\lambda/k_B\rho$ ($m^2 s^{-1}$)
WD	3×10^7	1.5×10^{35}	2×10^2	2×10^{-7}	7×10^5	7×10^{-4}
LI	2×10^6	6×10^{32}	1.7	1.7×10^{-6}	4×10^4	4×10^{-2}

gas is highly degenerate and a simple calculation in the framework of the Lorentz gas model[13] leads to an electronic thermal conductivity $\lambda_e = 2\times10^{10}$ $W m^{-1} K^{-1}$, which is considerably larger than the ionic conductivity.

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APPENDIX

Calculation of $\vec{S}_\beta(\vec{r})$ by the Ewald method:

$$\vec{S}_\beta(\vec{r}) = \sum_{\vec{\lambda}\neq 0} \frac{e^{2i\pi\vec{\lambda}\cdot\vec{r}}}{\pi\lambda^2}\left[\vec{k} - \beta(\vec{k}\cdot\vec{\lambda})\vec{\lambda}\right].$$

r, ρ are in units of $L(V=L^3)$:

$$\vec{S}_\beta(\vec{r}) = \int d\vec{\rho}\, w(\vec{\rho})\,\vec{g}(\vec{\rho}+\vec{r})$$

$$w(\vec{\rho}) = \sum_{\vec{\lambda}}{}' \delta(\vec{\rho}-\vec{\lambda}) - 1$$

$$\vec{g}(\vec{\rho}) = \frac{1}{2\rho}\left[(2-\beta)\vec{k} + \beta\vec{\rho}(\vec{k}\cdot\vec{\rho})\right].$$

We split $\vec{S}_\beta(\vec{r})$ into two parts by introducing a convergence function η.[11]

$$\vec{S}_\beta(\vec{r}) = \int d\vec{\rho}\, w(\vec{\rho})\,\vec{g}(\vec{\rho}+\vec{r})\eta(\vec{\rho}+\vec{r}) + \int d\vec{\rho}\, w(\vec{\rho})\,\vec{g}(\vec{\rho}+\vec{r})[1-\eta(\vec{\rho}+\vec{r})]. \quad \text{(A1)}$$

The convergence function $\eta(\rho)$ for a potential r^{-n} is chosen to be

$$\eta(\vec{\rho}) = \frac{1}{\Gamma(\frac{1}{2}n)}\Gamma(\tfrac{1}{2}n, \alpha^2\rho^2) = \frac{1}{\Gamma(\frac{1}{2}n)}\int_{\alpha^2\rho^2}^{+\infty} dt\, e^{-t}t^{n/2-1},$$

$$1-\eta(\vec{\rho}) = \frac{1}{\Gamma(\frac{1}{2}n)}\int_0^{\alpha^2\rho^2} dt\, e^{-t}t^{n/2-1}.$$

If we choose the same convergence function $\Gamma(\frac{1}{2}, \alpha^2\rho^2)$ as for the Coulomb potential, divergences appear because of the angular integrations. To eliminate these divergences, we must choose $\eta(\rho) = \Gamma(\frac{3}{2}, \alpha^2\rho^2)$ which corresponds to a potential r^{-3}. Hence, we have

$$\eta(\vec{\rho}) = \frac{4}{\sqrt{\pi}}\int_0^{\alpha\rho} du\, e^{-u^2}u^2$$

$$1-\eta(\vec{\rho}) = \operatorname{erfc}(\alpha\rho) - (2\rho\alpha/\sqrt{\pi})e^{-\alpha^2\rho^2}.$$

The second term in (A1) is rapidly convergent:

$$\vec{S}_{\beta 2}(\vec{r}) = \sum_{\vec{\lambda}} \vec{g}(\vec{r}+\vec{\lambda})\left[\operatorname{erfc}(\alpha\|\vec{r}+\vec{\lambda}\|) + \frac{2\alpha\|\vec{r}+\vec{\lambda}\|}{\sqrt{\pi}}e^{-\alpha^2\|\vec{r}+\vec{\lambda}\|^2}\right] - (3-\beta)\frac{\pi}{\alpha^2}\vec{k}. \quad \text{(A2)}$$

The first term is transformed by using Parseval's theorem

$$\vec{S}_{\beta 1}(\vec{r}) = \int d\vec{\rho}\, w(\vec{\rho})\vec{f}(\vec{\rho}+\vec{r}) = \int d\vec{k}'\,\tilde{w}(\vec{k}')\vec{\tilde{f}}(\vec{k}')$$

$$\vec{f}(\vec{\rho}+\vec{r}) = \eta(\vec{\rho}+\vec{r})\,\vec{g}(\vec{\rho}+\vec{r})$$

$$\tilde{w}(\vec{k}') = \sum_{\vec{\lambda}'\neq 0}\delta(\vec{k}'-\vec{\lambda}), \quad \lambda_\alpha = \pm1, \pm2, \ldots \ (\alpha = 1,2,3),$$

and we obtain after a lengthy but straightforward calculation

$$\vec{\tilde{f}}(\vec{k}') = \frac{\exp(-\pi^2k'^2/\alpha^2 - 2i\pi\vec{k}'\cdot\vec{r})}{\pi k'^2}\left[\left(1-\frac{\pi^2k'^2}{\alpha^2}(2-\beta)\right)\vec{k} - \beta\left(1+\frac{\pi^2k'^2}{\alpha^2}\right)(\vec{k}'\cdot\vec{k})\vec{k}'\right],$$

where $\vec{\tilde{f}}(\vec{k}')$ is rapidly convergent and

$$\vec{S}_{\beta 1}(\vec{r}) = \sum_{\vec{\lambda}\neq 0} \vec{f}(\vec{\lambda}) .$$

Finally we have $\vec{S}_{\beta}(\vec{r}) = \vec{S}_{\beta 1}(\vec{r}) + \vec{S}_{\beta 2}(\vec{r})$,

$$\vec{S}_{\beta}(\vec{r}) = \sum_{\vec{\lambda}} \frac{1}{2}\left[(2-\beta)\vec{k} + \beta\left(\frac{\vec{r}+\vec{\lambda}}{\|\vec{r}+\vec{\lambda}\|}\cdot\vec{k}\right)\frac{\vec{r}+\vec{\lambda}}{\|\vec{r}+\vec{\lambda}\|}\right]\left(\frac{\operatorname{erfc}(\alpha\|\vec{r}+\vec{\lambda}\|)}{\|\vec{r}+\vec{\lambda}\|} + \frac{2\alpha}{\sqrt{\pi}}\, e^{-\alpha^2\|\vec{r}+\vec{\lambda}\|^2}\right) - (3-\beta)\frac{\pi}{\alpha^2}\vec{k}$$
$$+ \sum_{\vec{\lambda}\neq 0} \frac{\exp(-\pi\lambda^2/\alpha^2 - 2i\pi\vec{\lambda}\cdot\vec{r})}{\pi\lambda^2}\left[\left(1 - \frac{\pi^2\lambda^2}{\alpha^2}(2-\beta)\right)\vec{k} - \beta\left(1+\frac{\pi^2\lambda^2}{\alpha^2}\right)(\vec{k}\cdot\vec{\lambda})\vec{\lambda}\right]. \qquad \text{(A3)}$$

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