

Effective Potential Kinetic Theory for Strongly Coupled Plasmas

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Abstract.

The effective potential theory (EPT) is a recently proposed method for extending traditional plasma kinetic and transport theory into the strongly coupled regime. Validation from experiments and molecular dynamics simulations have shown it to be accurate up to the onset of liquid-like correlation parameters (corresponding to $\Gamma \approx 10 - 50$ for the one-component plasma, depending on the process of interest). Here, this theory is briefly reviewed along with comparisons between the theory and molecular dynamics simulations for self-diffusivity and viscosity of the one-component plasma. A number of new results are also provided, including calculations of friction coefficients, energy exchange rates, stopping power, and mobility. The theory is also cast in the Landau and Fokker-Planck kinetic forms, which may prove useful for enabling efficient kinetic computations.

INTRODUCTION

Strongly coupled plasmas are highly charged [1], dense [2, 3, 4], or cold [5] ionized matter in which the Coulomb potential energy at the average interparticle spacing exceeds the average kinetic energy of particles. For a one-component plasma (OCP), this can be quantified using the Coulomb coupling parameter

$$\Gamma \equiv \frac{Z^2 e^2 / a}{k_B T} \sim \frac{\langle \text{potential energy} \rangle}{\langle \text{kinetic energy} \rangle} \quad (1)$$

where Ze is the charge, $a = (3/4\pi n)^{1/3}$ is the average interparticle spacing, T is the temperature and k_B is Boltzmann's constant. The OCP is a model plasma in which one species moves in the presence of an inert neutralizing background. Strong coupling corresponds to $\Gamma \gtrsim 1$. Standard Boltzmann-based theories break down in this situation because many-body correlations strongly influence particle dynamics.

The effective potential theory (EPT) provides a method for extending plasma theory into the strongly coupled regime by relaxing the assumptions underlying the Boltzmann equation: binary interactions and molecular chaos [6, 7, 8]. The binary approximation is relaxed, somewhat, by treating particle interactions as occurring via the potential of mean force, rather than the bare Coulomb potential or the Debye-Hückel potential [6]. The potential of mean force is obtained by taking two scattering particles at fixed positions and averaging over the positions of all other particles. It is related to the radial density distribution function [9]. The theory relaxes the molecular chaos assumption by treating the excluded volume (or Coulomb hole) in repulsive interactions using a modified version of Enskog's kinetic equation for hard spheres [8].

Comparison with molecular dynamics simulations (MD) and measurements from ultracold plasma experiments have revealed that the theory is accurate well into the strongly coupled regime, breaking down when the system exhibits liquid-like behaviors. A number of processes have been considered, including self-diffusion [6] and viscosity [10] of the OCP, mutual diffusion in mixtures [11, 12] and temperature equilibration [6]. Experimental tests have been made using ultracold neutral plasmas for energy relaxation rates [5, 6] and diffusion [13]. Recently, EPT was also applied to determine ionic transport properties in dense plasmas, including the warm dense matter regime characterized by densities near those of solids and temperatures from several to hundreds of electron volts [14]. This was achieved by applying a recent quantum hypernetted chain approximation [15, 16] to determine the effective potential, including novel dense plasma effects such as electron degeneracy and pressure ionization.

Here, we first briefly review these previous results and comparison with MD simulations for self-diffusion and viscosity of the OCP. We then show that the theory can be cast in the form of Landau [17] or Fokker-Planck [18] kinetic equations. This may be important for incorporating the theory into kinetic simulations in a variety of applications, including inertial confinement fusion (ICF) [19], which are typically based on a Fokker-Planck type equation because it is numerically much more efficient to evaluate than the Boltzmann equation. Finally, we compute the friction force density and energy exchange density between two Maxwellian distribution functions flowing at an arbitrary speed relative to one another. We find identical results whether the Boltzmann or Landau/Fokker-Planck (LFP) form of the kinetic equation is used. These results are used to discuss the accuracy of each approach, with regard to the predicted transport coefficients, and are also used to calculate the stopping power and mobility of a fast projectile in an OCP.

EFFECTIVE POTENTIAL THEORY

Kinetic Theory

The kinetic theory basis for EPT has been detailed in [7], which provides a connection with the BBGKY hierarchy. Kinetic theory of an increased collision frequency arising from the excluded volume associated with strong Coulomb repulsion has been detailed in [8]. The later aspect stems from a modification of Enskog's kinetic equation for hard spheres. In this section, we briefly review the results of these previous works, which will be used in the applications and modifications presented in the subsequent sections.

Considerations from the Boltzmann Equation

The EPT is based on a binary collision approximation, which is the basis of the Boltzmann collision operator [20]

$$C_B^{s-s'} = \int d^3v' d\Omega \sigma_{ss'} u [f_s(\hat{\mathbf{v}}) f_{s'}(\hat{\mathbf{v}}') - f_s(\mathbf{v}) f_{s'}(\mathbf{v}')] \quad (2)$$

where $(\mathbf{v}, \mathbf{v}')$ are the initial velocities of colliding particles and $(\hat{\mathbf{v}}, \hat{\mathbf{v}}')$ are the post-collision velocities (s and s' denote species). Here, $\mathbf{u} = \mathbf{v} - \mathbf{v}'$ is the relative velocity vector ($u = |\mathbf{u}|$), $\sigma_{ss'}$ is the differential scattering cross section and $d\Omega = d\phi d\theta \sin\theta$ is the solid angle. The input to Eq. (2) is the differential scattering cross section, which can be determined from the classical dynamics of a binary collision once the interaction force has been specified. Namely, it follows from the scattering angle $\theta = \pi - 2\Theta$, where

$$\Theta = b \int_{r_o}^{\infty} dr r^{-2} \left[1 - \frac{b^2}{r^2} - \frac{2\phi_{ss'}(r)}{m_{ss'} u^2} \right]^{-1/2}. \quad (3)$$

Here, $m_{ss'} \equiv m_s m_{s'} / (m_s + m_{s'})$ is the reduced mass, b is the impact parameter, r_o is the distance of closest approach, and $\phi_{ss'}$ is the interaction potential between binary scatterers. Nominally, this is the bare interaction potential (the Coulomb potential for a plasma), but in EPT this is taken to be the potential of mean force.

Potential of Mean Force

The main premise of EPT is that particles interact not in isolation, but rather in a “sea” of background particles. The potential of mean force is the potential obtained when taking two particles at fixed positions and averaging over the positions of all other particles [9]

$$\begin{aligned} \mathbf{F}_{12} &= \int \left[-\nabla_{\mathbf{r}_1} U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \right] \frac{e^{-U/k_B T}}{\mathcal{Z}} d\mathbf{r}_3 \dots d\mathbf{r}_N \\ &= -k_B T \nabla_{\mathbf{r}_1} \ln g(|\mathbf{r}_1 - \mathbf{r}_2|) \equiv -\nabla_{\mathbf{r}_1} \phi(\mathbf{r}_1 - \mathbf{r}_2). \end{aligned} \quad (4)$$

This is the potential we are interested in. Here $\mathcal{Z} = \int \exp(-U/k_B T) d\mathbf{r}_N$ is the configurational integral and $U \equiv \sum_{i,j} v(|\mathbf{r}_i - \mathbf{r}_j|)$. This depends only on the bare interaction potential of the particles v_{ij} , which is the Coulomb potential.

The main assumption here is that, for the purposes of calculating the interaction potential, the system is in thermodynamic equilibrium. Of course, a system undergoing transport is not in strict equilibrium, and may actually be far from equilibrium. However, the dynamical aspects of the theory do not depend on equilibrium, only this part

about calculating the interaction potential. The main physical aspect that this misses is the influence of the wake that arises around particles traveling faster than the thermal speed. This may lead to some error for large projectile speeds, but since a very small fraction of particles satisfies this condition, it has been found to be a negligible correction for near-equilibrium transport processes. Nevertheless, future work could address the use of a dynamically screened potential.

A convenient feature of Eq. (4) is that the potential of mean force depends only on the radial distribution function

$$\frac{\phi_{ss'}}{k_B T} = -\ln[g_{ss'}(r)]. \quad (5)$$

Since $g(r)$ determines the thermodynamic quantities of a system, many approximations have been developed to approximate this. In the weakly coupled limit, the potential of mean force is the Debye-Hückel potential [7]. Applying the Debye-Hückel potential as the effective potential leads to the results of traditional plasma kinetic theories [21, 22, 23]. However, strong coupling is dominated by many-body correlation effects, so we require an approximation that calculates $g(r)$ across coupling regimes. For this, we use the hypernetted chain approximation [24]

$$g_{ij}(r) = \exp\left[-\frac{v_{ij}(r)}{k_B T} + h_{ij}(r) - c_{ij}(r)\right] = \exp\left(-\frac{\phi_{ij}(r)}{k_B T}\right) \quad (6)$$

$$\hat{h}_{ij}(k) = \hat{c}_{ij}(k) + \sum_{s=1}^N n_s \hat{h}_{is}(k) \hat{c}_{sj}(k) \quad (7)$$

where $h_{ij}(r) = g_{ij}(r) - 1$. The first of these equations is the HNC approximation and the second is the Ornstein-Zernicke equation. This is a well-established approximation that is accurate for Coulomb systems in the regime we are interested in here (comparisons with MD simulations can be found in [6, 7]).

Considerations from the Enskog Equation

The Enskog kinetic equation treats dense gases of hard spheres, accounting for physics beyond the Boltzmann equation associated with the finite size of particles [20]. This includes the excluded volume of space that spheres can occupy because they cannot overlap with other spheres, and that collisions occur between the surfaces of spheres rather than their centers (a nonlocal aspect of the collision). In reference [8], we applied a modified version of these concepts to the strongly coupled plasma. Although Coulomb interactions are soft, the radial distribution function at strongly coupled conditions has a steep rise separating the Coulomb hole at close interaction from the rest of the plasma. The steepness of this slope allows one to identify an effective particle diameter. This was used in analogy with Enskog's hard sphere diameter to derive an increased collision frequency associated with the excluded volume. Details will be left to [8], but the main result is that the collision frequency is increased by a factor

$$\chi \approx 1 + 0.6250b\rho + 0.2869(b\rho)^2 \quad (8)$$

where $b\rho \approx \pi n \bar{\sigma}^3 / 3$ and $\bar{\sigma}$ is the particle diameter, which is determined from the location where $g(r = \bar{\sigma}) = 0.87$. When calculating a transport coefficient, this correction is accounted for by multiplying the collision frequency obtained from the Boltzmann equation by Eq. (8). For $\Gamma \lesssim 1$, $\chi \approx 1$, while for $\Gamma \approx 1 - 100$, $\chi \approx 1.2 - 1.4$. Thus, this predicts a 20-40% increase in the collision frequency in the strongly coupled regime (see figure 7 of [8]).

Transport Theory

Macroscopic transport properties can be obtained from Eq. (2) using any of the standard methods, such as Chapman-Enskog [25] or Grad [26]. In either case, transport coefficients can be expressed in terms of oft-cited Ω -integrals (see [20]). To facilitate the connection with weakly coupled plasma theory, these can alternatively be written in the form [6]

$$\Omega_{ss'}^{(l,k)} = \frac{3}{16} \frac{m_s}{m_{ss'}} \frac{v_{ss'}}{n_{s'}} \frac{\Xi_{ss'}^{(l,k)}}{\Xi_{ss'}}, \quad (9)$$

where

$$\Xi_{ss'}^{(l,k)} = \frac{1}{2} \int_0^\infty d\xi \xi^{2k+3} e^{-\xi^2} \bar{\sigma}_{ss'}^{(l)} / \sigma_o \quad (10)$$

is a “generalized Coulomb logarithm” associated with the $(l, k)^{\text{th}}$ collision integral. These are so named because $\Xi^{(1,1)} \rightarrow \ln \Lambda$ and $\Xi^{(l,k)}/\Xi^{(1,1)} \rightarrow \text{constants}$ (independent of Λ) in the weakly coupled ($\Gamma \ll 1$) limit. Here

$$\nu_{ss'} \equiv \frac{16 \sqrt{\pi} q_s^2 q_{s'}^2 n_{s'}}{3 m_s m_{s'} \bar{v}_{ss'}^3} \Xi_{ss'} \quad (11)$$

is a reference collision frequency,

$$\bar{\sigma}_{ss'}^{(l)} = 2\pi \int_0^\infty db b [1 - \cos^l(\pi - 2\Theta)] \quad (12)$$

is the l^{th} momentum-transfer cross section, $\sigma_o = (\pi q_s^2 q_{s'}^2)/(m_{s'}^2 \bar{v}_{ss'}^4)$ is a reference cross section, and $\bar{v}_{ss'}^2 = 2k_B T_s/m_s + 2k_B T_{s'}/m_{s'}$. The only input to these equations is the interaction potential $\phi_{ss'}(r)$. We now have a closed system of equations by using the hypernetted chain equations to solve for $\phi_{ss'}$ and using this to compute the transport coefficients, which are expressed in terms of Eq. (10). Examples are given in the next section.

TRANSPORT COEFFICIENTS FOR THE ONE-COMPONENT PLASMA

Self-diffusion

To demonstrate the accuracy of the EPT, we compare predictions for the self-diffusion coefficient and the viscosity coefficient of the OCP with MD simulation results. In a one-component system, the self-diffusion coefficient is a measure of the rate at which a particle is displaced in time from its initial position. The self-diffusion coefficient can be obtained from mutual diffusion coefficient of Chapman-Enskog theory by setting the two species to be identical ($s = s'$). The result at first order in the expansion can be expressed as [6, 20]

$$[D^*]_1 = \frac{1}{\chi} \frac{\sqrt{\pi/3}}{\Gamma^{5/2}} \frac{1}{\Xi^{(1,1)}}, \quad (13)$$

in which $D^* \equiv D/(a^2 \omega_p)$ and ω_p is the plasma frequency, and χ accounts for the Enskog correction factor. Retaining second order in the expansion provides [20]

$$[D_{ss'}]_2 = [D_{ss'}]_1 / (1 - \Delta), \quad (14)$$

where

$$\Delta = \frac{(2\Xi^{(1,2)} - 5\Xi^{(1,1)})^2 / \Xi^{(1,1)}}{55\Xi^{(1,1)} - 20\Xi^{(1,2)} + 4\Xi^{(1,3)} + 8\Xi^{(2,2)}}. \quad (15)$$

MD computations were performed using the Green-Kubo relations, as described in [6] and [10]. Results of a comparison for the self-diffusion coefficient are shown in figure 1. The EPT predictions in this figure include the modified Enskog factor from equation 8. The results show excellent agreement between EPT and MD for $\Gamma \lesssim 50$. The prediction of traditional (Landau-Spitzer) theory is shown as the dashed line. This theory breaks down near $\Gamma \approx 1$. Beyond $\Gamma \gtrsim 50$, it is known that the plasma transitions to a liquid-like state [27, 28]. Beyond this point particles spend most of the time trapped in nearest-neighbor potential wells. The EPT approach likely fails in this regime because there is no longer a significant separation of time scales between the interaction and the time between interactions.

Viscosity

Shear viscosity of the OCP can be expressed in dimensionless units as $\eta^* = \eta/(mna^2 \omega_p)$. The EPT evaluation was computed from the Chapman-Enskog relation [20]

$$\eta_1^* = \frac{1}{\chi} \frac{5 \sqrt{\pi}}{3 \sqrt{3} \Gamma^{5/2} \Xi^{(2,2)}} \quad (16)$$

where χ accounts for the Enskog correction factor. MD computations were evaluated using the Green-Kubo formula, as described in [10].

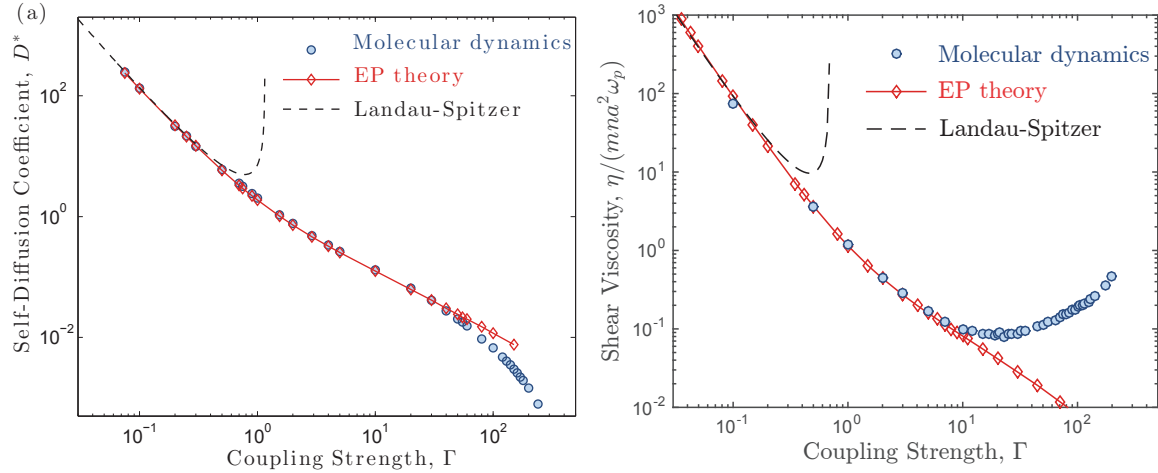


FIGURE 1. Comparison between MD, EPT and standard (Landau-Spitzer) plasma theory for self-diffusion (left) and shear viscosity (right) of the OCP.

Figure 1 shows excellent agreement between the EPT and MD for $\Gamma \lesssim 10$. This is a slightly reduced domain of validity as compared with self-diffusion. One striking feature is that the MD computation shows that viscosity has a minimum at $\Gamma \approx 17$. The EPT theory does not capture this behavior and, unlike with diffusion, the disagreement becomes dramatic for $\Gamma \gtrsim 20$. The reason for this is that viscosity (unlike diffusion) is influenced by contributions from both particle momenta and particle potential energy. At sufficiently strong coupling $\Gamma \gtrsim 20$, the potential contributions dominate. Since EPT is based on a collision model, it does not capture any of the potential contribution. In [10] each contribution was separated, and it was shown that EPT tracks well the kinetic contribution even beyond Γ of 20. Since diffusion is completely determined from the particle momenta, this feature does not arise in the diffusion comparison.

OTHER FORMS OF THE KINETIC EQUATION

The EPT theory above was presented as an extension of the Boltzmann equation. However, it is also interesting to consider whether the theory can be cast in the form of other kinetic equations and, if so, whether the results are accurate. In particular, the most common kinetic equations used in plasma physics are cast in either the Landau or Fokker-Planck form. These forms are often significantly easier to solve numerically in kinetic simulations because the distributions functions are local functions of velocity phase-space (i.e., only the distribution functions $f_s(\mathbf{v})$, rather than $f_s(\mathbf{v} + \Delta\mathbf{v})$, arise). Here, we first recall that the Boltzmann collision operator [Eq. (2)] can be written in either the Landau form or Fokker-Planck form by taking a small scattering angle expansion. Since scattering angles are large in strongly coupled plasmas, one may conclude that this expansion will corrupt the accuracy of the EPT predictions. However, we discuss in the following section why, despite this expansion, one may still find sufficiently accurate results for many transport properties of interest.

Landau Form

The Landau form of the kinetic equation [17]

$$C_L^{s-s'} = -\nabla_{\mathbf{v}} \cdot \int d^3v' Q_L \cdot \left(\frac{\nabla_{\mathbf{v}'}}{m_{s'}} - \frac{\nabla_{\mathbf{v}}}{m_s} \right) f_s(\mathbf{v}) f_{s'}(\mathbf{v}') \quad (17)$$

can be derived from a small scattering angle expansion of Eq. (2) [29]. Here, Q_L is a tensor kernel. To highlight the salient physics of the small scattering angle expansion, the computation of Q_L will be repeated below. Defining the relative velocity vector $\mathbf{u} \equiv \mathbf{v} - \mathbf{v}'$, conservation of momentum and energy imply

$$\Delta\mathbf{u} = u[\sin\theta \cos\phi \hat{x} + \sin\theta \sin\phi \hat{y} - 2\sin^2(\theta/2)\hat{u}] \quad (18)$$

where θ is the scattering angle. Momentum conservation $m_s \hat{\mathbf{v}} + m_{s'} \hat{\mathbf{v}}' = m_s \mathbf{v} + m_{s'} \mathbf{v}'$ can be written $\Delta \mathbf{u} = (m_s/m_{s'}) \Delta \mathbf{v} = -(m_{s'}/m_{s'}) \Delta \mathbf{v}'$, so small scattering angles imply $\Delta \mathbf{v} \ll \mathbf{v}$ and $\Delta \mathbf{v}' \ll \mathbf{v}'$.

Carrying out this small scattering angle expansion to second order, Eq. (2) can be written

$$C^{ss'} = \left[\frac{\partial f_s}{\partial \mathbf{v}} \cdot -\frac{m_s}{m_{s'}} f_s(\mathbf{v}) \frac{\partial}{\partial \mathbf{v}} \right] \frac{\langle \Delta \mathbf{v} \rangle^{s-s'}}{\Delta t} + \left[\frac{1}{2} \frac{\partial^2 f_s}{\partial \mathbf{v} \partial \mathbf{v}} : + \frac{1}{2} \frac{m_s^2}{m_{s'}^2} f_s(\mathbf{v}) \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : - \frac{m_s}{m_{s'}} \frac{\partial f_s(\mathbf{v})}{\partial \mathbf{v}} \cdot \frac{\partial}{\partial \mathbf{v}} \right] \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle^{s-s'}}{\Delta t} \quad (19)$$

where

$$\frac{\langle \Delta \mathbf{v} \rangle^{s-s'}}{\Delta t} = \frac{m_{s'}}{m_s} \int d^3 v' f_{s'}(\mathbf{v}') \{ \Delta \mathbf{u} \} \quad (20)$$

is the coefficient of dynamical friction, and

$$\frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle^{s-s'}}{\Delta t} = \frac{m_{s'}^2}{m_s^2} \int d^3 v' f_{s'}(\mathbf{v}') \{ \Delta \mathbf{u} \Delta \mathbf{u} \} \quad (21)$$

is the coefficient of velocity diffusion. These will arise in the Fokker-Planck representation. Here, the $\{ \dots \}$ have been defined as $\{ \Delta \mathbf{u} \} \equiv \int d\Omega d\mathbf{b} \sigma u \Delta \mathbf{u} = \int d\phi db bu \Delta \mathbf{u}$. This can also be expressed in the form

$$\{ \Delta \mathbf{u} \} = -u \mathbf{u} \bar{\sigma}_{ss'}^{(1)}(u) \quad (22)$$

where $\sigma_{ss'}^{(1)}$ is defined in Eq. (12). The full tensor term is $\{ \Delta \mathbf{u} \Delta \mathbf{u} \} = u[(u^2 \mathcal{I} - \mathbf{u}\mathbf{u}) \bar{\sigma}_{ss',1} + \mathbf{u}\mathbf{u} \bar{\sigma}_{ss',2}]$ where $\bar{\sigma}_{ss',1}(u) \equiv \pi \int db b \sin^2(2\Theta)$ and $\bar{\sigma}_{ss',2}(u) \equiv 8\pi \int db b \cos^4 \Theta$. However, note that $\bar{\sigma}_{ss',1} = 4\pi \int d\theta \sigma \sin \theta \sin^2(\theta/2) \cos^2(\theta/2) = \bar{\sigma}_{ss'}^{(1)}[1 + \mathcal{O}(\theta^2)]$, and that $\bar{\sigma}_{ss',2}$ is higher order by $\mathcal{O}(\theta^2)$ than $\bar{\sigma}_{ss'}^{(1)}$. So, consistency with the small scattering angle expansion in Eq. (19) implies

$$\{ \Delta \mathbf{u} \Delta \mathbf{u} \} \simeq u(u^2 \mathcal{I} - \mathbf{u}\mathbf{u}) \bar{\sigma}_{ss'}^{(1)}. \quad (23)$$

The Landau form, Eq. (17), can be derived by casting Eq. (19) in the form of a total divergence (in velocity). The two key relations to note in carrying out this calculation are

$$\frac{\partial}{\partial \mathbf{v}} \cdot \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle}{\Delta t} = 2 \frac{m_{s'}}{m_s} \frac{\langle \Delta \mathbf{v} \rangle^{ss'}}{\Delta t} \quad \text{and} \quad \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle^{ss'}}{\Delta t} = 2 \frac{m_{s'}}{m_s} \frac{\partial}{\partial \mathbf{v}} \cdot \frac{\langle \Delta \mathbf{v} \rangle^{ss'}}{\Delta t}. \quad (24)$$

Rather than detail the algebraic steps of the derivation, we provide an outline. Considering each of the five terms in Eq. (19): leave the second and fourth terms as is, and write the first, third and fifth terms as a total divergence minus the remainders. Adding the results and using the relations from Eq. (24) gives

$$C^{ss'} = \frac{1}{2} \frac{\partial}{\partial \mathbf{v}} \cdot \left[-\frac{m_s}{m_{s'}} f_s(\mathbf{v}) \frac{\partial}{\partial \mathbf{v}} \cdot \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle}{\Delta t} + \frac{\partial f_s}{\partial \mathbf{v}} \cdot \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle}{\Delta t} \right]. \quad (25)$$

Noting that

$$\frac{\partial}{\partial \mathbf{v}} \cdot \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle}{\Delta t} = \frac{m_{s'}^2}{m_s^2} \int d^3 v' \frac{\partial f_{s'}(\mathbf{v}')}{\partial \mathbf{v}'} \cdot \frac{u^2 \mathcal{I} - \mathbf{u}\mathbf{u}}{u^3} u^4 \bar{\sigma}_{ss'}^{(1)} \quad (26)$$

and applying this relation to the first term in Eq. (25), we arrive at the Landau form of Eq. (17), in which

$$Q_L^{ss'} \equiv \frac{1}{2} \frac{m_{s'}^2}{m_s} u(u^2 \mathcal{I} - \mathbf{u}\mathbf{u}) \bar{\sigma}_{ss'}^{(1)}(u). \quad (27)$$

Finally, we note that Landau's original equation is obtained by inserting the momentum cross section associated with the weakly coupled limit $\bar{\sigma}_{ss'}^{(1)} = 4\pi q_s^2 q_{s'}^2 \ln \Lambda / (m_{s'}^2 u^4)$ (see [7]) into Eq. (27). An EPT evaluation will need to compute this using Eq. (12).

Fokker-Planck Form

Similarly, the Fokker-Planck form of the kinetic equation

$$C_{FP}^{ss'} = -\frac{\partial}{\partial \mathbf{v}} \cdot \left(f_s \cdot \frac{\langle \Delta \mathbf{v} \rangle^{ss'}}{\Delta t} \right) + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : \left(f_s \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle^{ss'}}{\Delta t} \right) \quad (28)$$

can be obtained from the small scattering angle expansion of the Boltzmann equation [18]. This can be obtained directly from Eq. (25) by writing the second term as a total divergence (minus the remainder), then applying Eq. (24) to both the first term and this remainder term. Since the Landau and Fokker-Planck equations are equivalent, we will simply refer to this as Landau-Fokker-Planck (LFP) in the next section.

OTHER TRANSPORT PROCESSES

Friction Force Density

The analysis of transport properties above was concerned with the near equilibrium processes that are well-described by the Chapman-Enskog solution of the Boltzmann equation. Here, we consider a direct calculation of the friction force density and energy exchange density, first for arbitrary distribution functions, and later for Maxwellian distribution functions flowing relative to one another at an arbitrary speed. The former analysis is used to show why one can expect similar results for many transport coefficients whether the Boltzmann or LFP form of the kinetic equation is used. The latter calculation provides a means to estimate transport rates in situations where the distribution functions are far from equilibrium. A couple of examples are provided, including stopping power and mobility.

The friction force density between species s and s' can be computed from the momentum moment of the collision operator describing the interaction between these two species:

$$\mathbf{R}^{ss'} \equiv \int d^3 v m_s \mathbf{v} C(f_s, f_{s'}). \quad (29)$$

Here, we will consider only the Coulomb collisional interaction. If C is taken to be the Boltzmann collision operator, Eq. (29) can be rearranged to the form [23]

$$\mathbf{R}^{ss'} = m_{ss'} \int d^3 u \{ \Delta \mathbf{u} \} \int d^3 v' f_s(\mathbf{u} + \mathbf{v}') f_{s'}(\mathbf{v}') \quad (30)$$

where f_s and $f_{s'}$ are the yet unspecified distribution functions.

We first point out an interesting result: The momentum moment of the LFP collision operator is identical to the momentum moment of the Boltzmann collision operator, i.e., Eq. (30). Starting from Eqs. (17) and (27), this can be shown as follows. First, integrating by parts shows $\mathbf{R}^{ss'} = m_s \int d^3 v \mathbf{J}^{ss'}$ where $C_L^{ss'} = -\nabla_{\mathbf{v}} \cdot \mathbf{J}^{ss'}$. This can be expressed fully as

$$\mathbf{R}^{ss'} = \frac{m_{ss'}^2}{2} \int d^3 v \int d^3 v' u \bar{\sigma}_{ss'}^{(1)}(u) (u^2 \mathbf{I} - \mathbf{u}\mathbf{u}) \cdot \left[\frac{f_s(\mathbf{v})}{m_s} \frac{\partial f_{s'}(\mathbf{v}')}{\partial \mathbf{v}'} - \frac{f_{s'}(\mathbf{v}')}{m_s} \frac{\partial f_s(\mathbf{v})}{\partial \mathbf{v}} \right]. \quad (31)$$

Next, note that

$$u \bar{\sigma}_{ss'}^{(1)}(u) (u^2 \mathbf{I} - \mathbf{u}\mathbf{u}) \cdot \frac{\partial f_{s'}(\mathbf{v}')}{\partial \mathbf{v}'} = \frac{\partial}{\partial \mathbf{v}'} \cdot [u \bar{\sigma}_{ss'}^{(1)}(u^2 \mathbf{I} - \mathbf{u}\mathbf{u}) f_{s'}(\mathbf{v}')] - 2u \mathbf{u} \bar{\sigma}_{ss'}(u) f_{s'}(\mathbf{v}'). \quad (32)$$

Substituting this relation and the analogous one for the second term in Eq. (31), then noting that the surface terms vanish since $f(\mathbf{v} \rightarrow \infty) \rightarrow 0$, one arrives at Eq. (30).

It is, perhaps, somewhat surprising that despite the small scattering angle expansion, the LFP form leads to identical results for the friction and energy exchange rates (which will be shown below) as those calculated from the Boltzmann equation. This implies that first-order estimates of transport coefficients, such as diffusion, are going to be identical from each theory. However, a full Chapman-Enskog or Grad type solution requires moments beyond second order, and these will differ somewhat when calculated from the Boltzmann versus LFP forms. It was long ago pointed out in the neutral gas literature that similar transport coefficients are obtained from the Chapman-Enskog solution of the Boltzmann or Fokker-Planck equations (commonly cited as within a few percent [20]). This gives evidence

that even in systems where large-angle collisions dominate, the LFP equation can provide an accurate description of transport. In weakly coupled plasmas, next-order corrections to transport coefficients are often large (commonly on the order of 50%). However, the small angle scattering expansion is valid in this limit and the results of Boltzmann versus LFP are nearly identical. In a strongly coupled plasma, we have shown that the next to leading order corrections become negligible (see figure 9 of [7]). Thus, spanning from weak to strong coupling, it seems that EPT predictions based on the Boltzmann versus LFP forms of the kinetic equation are likely to lead to similar predictions for the transport coefficients, with the largest deviation expected near $\Gamma \sim 1$. However, more work needs to be done to quantify exactly what the differences are for the various transport coefficients.

Flowing Maxwellians

Next, we evaluate Eq. (30) for the case where each distribution function is Maxwellian with an arbitrary flow shift. This is a convenient model for understanding aspects of transport between species that are flowing relative to one another. It can also provide an accurate description of some physical circumstances, such as ions drifting relative to electrons. It is also a useful model for a number of other processes, including stopping power, mobility and runaway electron generation.

For flowing Maxwellian distributions

$$\int d^3v' f_s(\mathbf{u} + \mathbf{v}') f_{s'}(\mathbf{v}') = \frac{n_s n_{s'}}{\pi^{3/2} \bar{v}_{ss'}^3} \exp\left[-\frac{(\mathbf{u} - \Delta\mathbf{V})^2}{\bar{v}_{ss'}^2}\right] \quad (33)$$

where $\Delta\mathbf{V} \equiv \mathbf{V}_s - \mathbf{V}_{s'}$ is the differential flow velocity. Putting this into Eq. (30), and applying a spherical coordinate system aligned so that $\hat{z} = \Delta\hat{V}$, such that $\mathbf{u} = u[\sin\theta' \cos\phi' \hat{x} + \sin\theta' \sin\phi' \hat{y} + \cos\theta' \Delta\hat{V}]$, then evaluating the θ' and ϕ' integrals leads to the expression

$$\mathbf{R}^{ss'} = -n_s m_s \bar{v}_{ss'} \Delta\mathbf{V} \quad (34)$$

where

$$\bar{v}_{ss'} = \frac{16\sqrt{\pi} q_s^2 q_{s'}^2 n_{s'}}{3m_s m_{s'} \bar{v}_{ss'}^3} \bar{\Xi}_{ss'}(\Delta\bar{V}) \quad (35)$$

is a velocity-dependent ($\Delta\bar{V}$) collision frequency and

$$\bar{\Xi}_{ss'}(\Delta\bar{V}) = \frac{3}{16} \frac{1}{\Delta\bar{V}^3} \frac{1}{2} \int_0^\infty d\xi \xi^2 \frac{\bar{\sigma}_{ss'}^{(1)}(\xi)}{\sigma_o} \left[(2\xi\Delta\bar{V} + 1)e^{-(\xi+\Delta\bar{V})^2} + (2\xi\Delta\bar{V} - 1)e^{-(\xi-\Delta\bar{V})^2} \right] \quad (36)$$

is a velocity-dependent generalization of the Coulomb logarithm from Eq. (10). Here, we have defined $\Delta\bar{V} \equiv \Delta\mathbf{V}/\bar{v}_{ss'}$ for notational convenience. The slow flow limit ($\Delta\bar{V} \ll 1$) returns $\bar{\Xi}_{ss'}(\Delta\bar{V}) = \Xi_{ss'}^{(1,1)}$ from Eq. (10), which is the previously known result (see equation 7 of [23]).

Weakly coupled limit: To connect with known results from plasma physics, we express the weakly coupled limit of Eq. (36). In this limit, $\bar{\sigma}_{ss'}^{(1)}/\sigma_o \simeq (4/\xi^4) \ln \Lambda$ where $\Lambda \equiv m_{s'} \bar{v}_{ss'}^2 \lambda_D / (q_s q_{s'})$ (see reference [7], which gives the details for obtaining this limit). Putting this into Eq. (36) gives

$$\bar{\Xi}_{ss'}(\Delta\bar{V}) = \ln \Lambda \frac{3\sqrt{\pi}}{4\Delta\bar{V}^3} \frac{1}{2\sqrt{\pi}} \int_0^\infty \frac{d\xi}{\xi^2} \left[(2\xi\Delta\bar{V} + 1)e^{-(\xi+\Delta\bar{V})^2} + (2\xi\Delta\bar{V} - 1)e^{-(\xi-\Delta\bar{V})^2} \right]. \quad (37)$$

This can be written in a simple way by noting that

$$\frac{1}{2\sqrt{\pi}} \int_0^\infty \frac{d\xi}{\xi^2} \left[(2\xi\Delta\bar{V} + 1)e^{-(\xi+\Delta\bar{V})^2} + (2\xi\Delta\bar{V} - 1)e^{-(\xi-\Delta\bar{V})^2} \right] = \psi(\Delta\bar{V}^2) \quad (38)$$

where

$$\psi(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{x}} dt \sqrt{t} e^{-t} = \operatorname{erf}(\sqrt{x}) - \frac{2}{\sqrt{\pi}} \sqrt{x} e^{-x} \quad (39)$$

is the Maxwell integral. With this, we have

$$\bar{\Xi}_{ss'}(\Delta\bar{V}) \rightarrow \frac{3\sqrt{\pi} \ln \Lambda}{4 \Delta\bar{V}^3} \psi(\Delta\bar{V}^2) \quad (40)$$

in the weakly coupled limit. If the flow is slow ($\Delta\bar{V} \ll 1$), $\bar{\Xi}_{ss'} \rightarrow \ln \Lambda$ in this limit.

Stopping Power

One application in which the friction between a fast and slow distribution is important is the stopping power of fusion products in ICF. An EPT computation of stopping power can be obtained from Eqs. (34) and (36). Note that in the absence of pressure gradients or external fields, the steady-state momentum balance equation is $\nabla \cdot (m_s n_s \mathbf{V}_s \mathbf{V}_s) = \mathbf{R}^{ss'}$. For a relative drift in the \hat{x} direction, this implies the stopping power is

$$\frac{dE_s}{dx} = \sum_{s'} R^{ss'} / n_s \quad (41)$$

where $E_s = \frac{1}{2} m_s V_s^2$. In many situations one is interested in the stopping of a single particle in a background plasma. This limit is obtained from Eq. (41) simply by taking the temperature of the test species (s) to zero (giving the limit of a delta function in velocity-space for this single particle distribution).

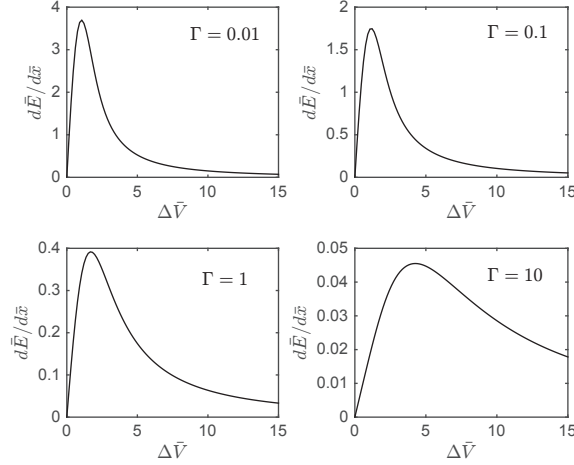


FIGURE 2. Stopping power for the OCP at four values of the coupling strength, computed from Eq. (42).

In an application, one must sum the interaction between each species combination to get the total stopping power. Here, we evaluate Eq. (41) for the OCP. Physically, this represents a single particle stopping on a background of identical particles. In figure 2 this is plotted at coupling strengths of $\Gamma = 0.01, 0.1, 1$ and 10 in the natural units suggested by Eq. (41)

$$\frac{d\bar{E}_s}{d\bar{x}} = \Delta\bar{V} \bar{\Xi}_{ss'}(\Delta\bar{V}) \quad (42)$$

where $\bar{E}_s = E_s / (\frac{1}{2} m_{ss'} \bar{v}_{ss'}^2)$ and $\bar{x} = x / (\bar{v}_{ss'} / \nu_o)$ and $\nu_o = 16 \sqrt{\pi} q_s^2 q_{s'}^2 n_{s'} / (3 m_s m_{ss'} \bar{v}_{ss'}^3)$ is the reference collision frequency, not including the velocity-dependent generalized Coulomb logarithm. The figure shows an interesting feature, that the peak of the stopping power curve shifts to a higher flow speed, and the width of the peak broadens significantly, in the strongly coupled regime.

Mobility

Mobility is a closely related quantity to stopping power. It is usually defined as

$$\mu_{ss'} \equiv \frac{\Delta V}{R^{ss'} / n_s} \quad (43)$$

where ΔV is the differential flow that arises from a background force. It is also assumed that this flow has reached a terminal constant speed (so the applied force directly balances the friction force in the momentum balance). Often times “mobility-limited flow” scenarios are characterized as ones in which $\Delta\bar{V} \ll 1$, in which case $\mu_{ss'} = 1 / (m_s \nu_{ss'})$ is a constant. However, the term can also applied more generally via a velocity-dependent mobility via Eq. (43) [1]. This velocity-dependent mobility can be directly related to the stopping power as $\mu_{ss'} = \Delta V / (dE_s / dx)$. This can also be expressed as $(m_{ss'} \nu_o / 2) \mu_{ss'} = 1 / \bar{\Xi}_{ss'}(\Delta\bar{V})$. Thus, the mobility coefficient predicted by EPT is directly related to Eq. (36).

Energy Exchange Density

The energy exchange density between species s and s' can be computed from the energy moment in the rest frame of the species s

$$Q^{s-s'} \equiv \int d^3v \frac{1}{2} m_s v_r^2 C(f_s, f_{s'}). \quad (44)$$

in which $\mathbf{v}_r \equiv \mathbf{v} - \mathbf{V}_s$. For the Boltzmann collision operator, this can be rearranged to the form [23]

$$Q^{s-s'} = m_{ss'} \int d^3u \{\Delta \mathbf{u}\} \cdot \int d^3v' \left(\mathbf{v}' + \frac{m_{ss'}}{m_{s'}} \mathbf{u} \right) f_s(\mathbf{u} + \mathbf{v}') f_{s'}(\mathbf{v}') - \mathbf{V}_s \cdot \mathbf{R}^{ss'}. \quad (45)$$

(Note that this expression corrects a typo in equation 6 of [23], where $m_{s'} \leftrightarrow m_s$ in the second term).

We next note that the exact same expression as Eq. (45) is obtained from Eq. (44) whether the Boltzmann or LFP collision operator is used. This can be shown in an analogous way as was done for the friction coefficient in the previous section. First, one integrates by parts to show that $Q^{ss'} = m_s \int d^3v \mathbf{v} \cdot \mathbf{J}^{ss'} - \mathbf{V}_s \cdot \mathbf{R}^{ss'}$. Next, apply Eq. (32) and the analogous form with $\mathbf{v}' \leftrightarrow \mathbf{v}$ and $s \leftrightarrow s'$. Simplifying the result leads directly to Eq. (45). This demonstrates the interesting feature pointed out in the last section: The momentum and energy moments of the Boltzmann collision operator are identical to the LFP collision operator.

Flowing Maxwellians

For flowing Maxwellian distributions, note that

$$\int d^3v' \mathbf{v}' f_s(\mathbf{u} + \mathbf{v}') f_{s'}(\mathbf{v}') = \frac{n_s n_{s'}}{\pi^{3/2} \bar{v}_{ss'}^3} (v_{T_{s'}}^2 \mathbf{V}_s + v_{T_s}^2 \mathbf{V}_{s'} - v_{T_{s'}}^2 \mathbf{u}) \exp\left[-\frac{(\mathbf{u} - \Delta \mathbf{V})^2}{\bar{v}_{ss'}^2}\right]. \quad (46)$$

Inserting this and Eq. (33) into Eq. (45) gives

$$Q^{s-s'} = \frac{m_{ss'} n_s n_{s'}}{\pi^{3/2} \bar{v}_{ss'}^3} \int d^3u \exp\left[-\frac{(\mathbf{u} - \Delta \mathbf{V})^2}{\bar{v}_{ss'}^2}\right] \left[\left(\frac{v_{T_{s'}}^2 \mathbf{V}_s + v_{T_s}^2 \mathbf{V}_{s'} - v_{T_{s'}}^2 \mathbf{u}}{\bar{v}_{ss'}^2} + \frac{m_{ss'}}{m_{s'}} \mathbf{u} \right) \cdot \{\Delta \mathbf{u}\} - \mathbf{V}_s \cdot \mathbf{R}^{ss'} \right]. \quad (47)$$

Noting that

$$\frac{m_{ss'}}{m_{s'}} - \frac{v_{T_{s'}}^2}{\bar{v}_{ss'}^2} = \frac{2m_{ss'}(T_s - T_{s'})}{m_s m_{s'} \bar{v}_{ss'}^2} \quad (48)$$

and carrying out the angular integrals of u leads to

$$Q^{ss'} = -3 \frac{m_{ss'}}{m_s} n_s \tilde{\nu}_{ss'} (T_s - T_{s'}) - \frac{v_{T_s}^2}{\bar{v}_{ss'}^2} \Delta \mathbf{V} \cdot \mathbf{R}^{ss'} \quad (49)$$

in which $\mathbf{R}^{ss'}$ is provided in Eq. (34), and

$$\tilde{\nu}_{ss'} = \frac{16 \sqrt{\pi} q_s^2 q_{s'}^2 n_{s'}}{3 m_s m_{ss'} \bar{v}_{ss'}^3} \tilde{\Xi}_{ss'}(\Delta \bar{V}) \quad (50)$$

is a velocity-dependent collision frequency where

$$\tilde{\Xi}_{ss'} = \frac{1}{8 \Delta \bar{V}} \int_0^\infty d\xi \xi^4 \frac{\bar{\sigma}_{ss'}^{(1)}(\xi)}{\sigma_o} \left[e^{-(\xi - \Delta \bar{V})^2} - e^{-(\xi + \Delta \bar{V})^2} \right] \quad (51)$$

is a different velocity-dependent generalization of the Coulomb logarithm that is associated with the energy exchange. Finally, we note that in the slow flow limit, $\Delta \bar{V} \ll 1$, $\tilde{\Xi}_{ss'} \rightarrow \Xi_{ss'}^{(1,1)}$ from Eq. (10), and that the second term in Eq. (45) is $O(\Delta \bar{V}^2)$, thus returning a familiar result (see equation 8 from [23]).

OUTLOOK AND PERSPECTIVES

The effective potential concept has proven a useful method for extending plasma theory into the strongly coupled regime. The results to date have focused on classical plasmas, such as the OCP, and ion transport in warm dense matter [14]. However, one may envision applying the concept to a broader class of problems. In plasma physics, extensions of the theory to strongly magnetized systems [30], and to treating electron transport in warm dense matter via a quantum extension of the theory may be interesting avenues to explore. Outside of plasma physics, applying the concept to transport in dense neutral gases may also lead to interesting insights. This paper provided a version of the theory in the form of a Landau-Fokker-Planck equation. This may lead to a useful avenue for incorporating the theory into kinetic simulations, but more work needs to be done to test the accuracy of this approximation in comparison to the Boltzmann-based version.

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