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Self-consistent inclusion of classical large-angle Coulomb collisions in plasma Monte Carlo simulations

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ABSTRACT

Large-angle Coulomb collisions allow for the exchange of a significant proportion of the energy of a particle in a single collision, but are not included in models of plasmas based on fluids, the Vlasov–Fokker–Planck equation, or currently available plasma Monte Carlo techniques. Their unique effects include the creation of fast 'knock-on' ions, which may be more likely to undergo certain reactions, and distortions to ion distribution functions relative to what is predicted by small-angle collision only theories. We present a computational method which uses Monte Carlo techniques to include the effects of large-angle Coulomb collisions in plasmas and which self-consistently evolves distribution functions according to the creation of knock-on ions of any generation. The method is used to demonstrate ion distribution function distortions in an inertial confinement fusion (ICF) relevant scenario of the slowing of fusion products.

1. Introduction

Large-angle Coulomb collisions affect the distribution of energy in plasmas by allowing the transfer of a significant proportion of the energy of a particle in a single collision. It is well known that their importance relative to the small-angle Coulomb collisions which dominate interactions in classical plasmas is $\mathcal{O}(1/\ln\Lambda)$ [1], where $\ln\Lambda$ is the Coulomb logarithm.

Their effects are therefore expected to be important in the $2 \lesssim \ln\Lambda \lesssim 5$ regime, which includes high intensity laser–plasma interactions at solid density [2], degenerate plasmas [3], and stellar cores [4,5]. This regime also includes inertial confinement fusion (ICF) [6,7], as an igniting ICF hotspot will have conditions [8] of areal density and temperature of $\sim$0.3 g/cm^2 and $\sim$10 keV respectively, which correspond to small values of $\ln\Lambda$ for a typical hotspot radius of tens of microns.

Wide ranging experimentally detectable consequences of large-angle collisions have been described; for the shape and evolution of distribution functions [9–12], for fusion reactivities or as a diagnostic in both ICF and magnetic confinement fusion (MCF) [13–20], for plasma properties such as particle stopping and temperature equilibration [21–23], and for 'athermal' fusion [24,25]. Non-Maxwellian distributions caused by large-angle collisions have been experimentally observed on JET (the Joint European Torus) [26].

A consequence of the inclusion of large-angle collisions is the generation of high energy 'knock-on' ions; these are fast particles generated by collisions between high energy fusion reaction products and thermal ions in the plasma in which the thermal ions can gain many times their initial kinetic energy, distorting the fuel ion distributions from thermal

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equilibrium in the process. The knock-ons may be more likely to fuse themselves (in what are known as reaction-in-flight fusion events), and can go on to generate further knock-ons. These processes must be fully understood in order to use Coulomb collision-induced knock-ons as a diagnostic.

The inclusion of the effects of large-angle Coulomb collisions in plasmas is a long-standing challenge [1,27,28], and we present a new method which applies to plasmas with $\ln\Lambda \gtrsim 2$. Although there are other methods which can include the effects of large-angle collisions and knock-ons, the approach presented has unique strengths as it self-consistently evolves ion distribution functions under the influence of large-angle collisions, but is less computationally intensive than molecular dynamics (MD) simulations.

Large-angle collisions involve a large transfer of energy or momentum *per collision*, as opposed to small-angle collisions. These two types of collision are also known as 'close' and 'remote' collisions respectively due to the relationship between impact parameter, b, and scattering angle, θ, of $b = b_\perp \cot\left(\frac{\theta}{2}\right)$. Here, $b_\perp = \frac{q_i q_j}{4\pi\epsilon_0}\frac{1}{m_{ij} v_{ij}^2}$ and q is the charge, m_{ij} is the reduced mass, v_{ij} is the relative velocity, and the species are denoted by i and j.

The most commonly used plasma theories are based on the Vlasov–Fokker–Planck (VFP) equation, and are only applicable in classical plasmas with $\ln\Lambda \gg 1$ as they either ignore large-angle Coulomb collisions [12], approximate them by over-counting the effects of small-angle collisions in $\ln\Lambda$ [27], or have to be expanded to higher orders to recover some of their effects [29,22]. Current computational methods invoke the small-angle approximation [30–33], and are not applicable to large-angle collisions.

Though small-angle collisions are important for the overall exchange of energy in plasmas with $2 \lesssim \ln\Lambda \lesssim 5$, the impact of fewer large-angle collisions with larger transfers of energy *per collision* can distort distribution functions. This can indirectly change the rate of exchange of energy between two plasma species as the rate of energy transfer is dependent upon their distribution functions. That the changes in energy per collision are discontinuous is also important; continuous loss models fail for large-angle scattering [34]. These problems typically manifest when one species has a much higher average energy than another, as is the case with the slowing down of alpha particles during burn in fusion plasmas.

Analytical theories which include the effects of large-angle collisions via the Coulomb logarithm for plasmas in thermal equilibrium have been developed, including those of Baalrud [35], Brown, Preston, and Singleton (BPS) [36], and Gericke, Murillo, and Schlanges [37]. These have been benchmarked against MD simulations [38–40], and produce the correct results for properties such as temperature equilibration [41]. The MD simulations used to benchmark these theories do not include quantum mechanical effects *ab initio*, so electron interactions are usually modified at short distances [42,39,43,41] to prevent them becoming infinitely bound to ions. However, Dimonte and Daligault [38] presented purely classical results, using only the assumption of like charges in a neutralising background, and found agreement with the classical BPS theory for temperature equilibration [36]. This is strong evidence that these analytical theories are including the effects of classical ion–ion large-angle collisions. However, they involve an integration over assumed Maxwell–Boltzmann distribution functions, and are not designed to give any information about the creation of knock-ons due to large-angle collisions, or the distortion to ion distribution functions caused by them.

Several semi-analytical approaches to calculating the effects of large-angle collisions for non-thermal distributions have been developed. In one, which shall be referred to as the Ryutov theory, the Rutherford cross-section is directly integrated, and a source term for knock-on ions found [10,44,19,16]. This requires assumptions about the initial ion distribution functions, and uses a cut-off in impact parameter between close and remote collisions which is either a multiple of $b_\perp$, or is imposed by computational limits. An initial non-Maxwellian fuel ion distribution is calculated from the knock-on source term, and is subsequently evolved according to a small-angle-only VFP equation. Knock-ons of higher order are ignored, so the Ryutov theory only includes the first generation of knock-on ions. Other semi-analytical approaches only model the athermal part of the distribution function. This approach is usually limited by the assumption that there is no feedback on the bulk distribution function [24], or by the assumption of a steady state athermal distribution [25].

MD simulations are able to model any distribution function, and can resolve the hard collisions which are responsible for knock-on ions. Though MD calculations make few assumptions, they are computationally intensive and typically use a maximum of tens of thousands of particles [39,45]. We find that millions of simulation particles are required to resolve the distortion to the tails of ion distribution functions caused by large-angle Coulomb collisions, and that an alternative method of calculation of their effects, adopting a Coulomb logarithm benchmarked by MD simulations, is therefore desirable.

In the Monte Carlo based method developed here, a cut-off in impact parameter is used to separate out large- and small-angle Coulomb collisions and all ion–ion interactions have a chance of generating knock-ons. The rate of generation of knock-on ions is benchmarked against Ryutov's theory.

The strength of the approach presented is that it includes knock-ons of any generation, and it allows distribution functions to evolve self-consistently according to those knock-ons and to other changes due to fusion reactions. As a demonstration of the application of this method, the effects of the distortions to ion distribution functions on the source neutron spectra of the hotspot in a burning ICF capsule are calculated.

Large-angle collisions between electrons and ions, and electrons and electrons, are omitted from the analysis presented as the dynamics of these interactions are modified at the short ranges relevant to large-angle scattering by quantum mechanical effects [46,47]. These effects would not be included by the classical approach presented. Furthermore, the large mass difference between electrons and ions means both that energy exchange between electrons and ions is much less effective than between different species of ion, and that electrons are less likely to maintain a non-Maxwellian distribution