Efficient computation of low frequency opacity in WDM regime

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In investigating the frequency-dependent opacities in plasmas, various approaches are available. They range from experiments to theoretical methods, such as Density Functional Theory based Molecular Dynamics (DFT-MD), or many-body expansion of the grand canonical partition function. As for MD simulations, they are quite demanding in terms of numerical resources, so, for sufficiently hot plasmas, the average-atom approximation is used [1]. Although this significantly speeds up the calculation, a well-known problem inherent to this approximation is the divergence of the free-free opacity at low frequencies in the Kubo-Greenwood formalism. Ziman's approach makes it possible to correct this problem, at the cost of having to calculate the energy-dependent transport cross-section [2]. The phase shifts that enter this cross section may be tricky to correctly compute over large energy and angular number domains. They also greatly vary from element to element.

Here we present a robust method for calculating these phase shifts based on the Calogero [3] equation. This allows us to compute the frequency-dependent opacity, which we compare with ab-initio simulations for various elements. We also explore different approximations in order to speed up the calculations.

References

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