# Full-potential treatment for multiple-scattering calculation of hot dense plasma opacity

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The calculation of the optical properties of hot dense plasmas with a model that has self-consistent plasma physics is a grand challenge for high-energy density science. It is generally hoped that the development of such a model will reconcile discrepancies between theory and experiments such as the irons opacity problem [1, 2, 3]. Recently, an electronic structure model that uses multiple scattering to solve the Kohn-Sham density functional theory equations has been successfully applied to dense plasmas [4, 5]. A prominent advantage of this approach has over other state-of-the-art methods is that it does not use pseudopotentials; instead, the core electronic states are computed self-consistently. Results from this multiple scattering theory formalism are in good agreement with those obtained with other methods.

The existing implementation of the multiple scattering method is, however, not complete. For example, single-site scattering is treated by first averaging over the true three-dimensional potential then solving the scattering problem in this spherically symmetric average potential. It is expected that the asymmetry of the true potential, arising from the highly disordered nature of a plasma, will have appreciable effects on the plasma's properties such as its equation of state and opacity. Our work seeks to address this issue. We approach the full-potential scattering problem using the Siegert-states formalism [6, 7, 8], which accurately reproduces bound states, while yielding discrete complex-energy free states in contrast to the usual real-energy continuum. Siegert states are thus very convenient for the computation of physical quantities involving summations over complete sets of states. Indeed, the usefulness of Siegert states in the average-atom model has been recently demonstrated [9]. In this poster, we explain how Siegert states may be used for a full treatment of three-dimensional plasma potentials.

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