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Paramagnetic-to-diamagnetic transition in dense liquid iron and its influence on electronic transport properties

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Abstract

The electronic transport properties of warm dense liquid iron are important properties for understanding the magnetic field generation in Earth-like and other solid planets. Here we investigate the electrical and thermal conductivity with spin-polarized simulations based on density functional theory over a significant pressure and temperature range using the Kubo-Greenwood formalism [1]. We find that a paramagnetic state is stable in the liquid up to high temperatures at ambient pressure. It is shown that the overestimation of results from exploding wire experiments by more than 30% that occurs in spin-degenerate simulations is reduced to 10% or less when spin polarization is taken into account. Direct comparisons between spin-polarized and spin-degenerate simulations reveal that the spin effects on the conductivities enter via changes in both ionic and electronic structure. Along the 3700 K isotherm, we explore the persistence of magnetic fluctuations toward high densities, and beyond 20-50 GPa the liquid becomes diamagnetic, which suggests the existence of a continuous paramagnetic-to-diamagnetic transition. This transition exerts a significant influence on the transport properties of liquid iron and is potentially of high relevance for dynamo processes in Mercury and Mars.

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References

[1] Korell, J.-A., French, M., Steinle-Neumann, G., and Redmer, R.: Paramagnetic-to-Diamagnetic Transition in Dense Liquid Iron and its Influence on Electronic Transport Properties, Phys. Rev. Lett., Vol. 122, 086601, 2019.