Directly calculating electrical conductivities of dense hydrogen from molecular dynamics

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The transport properties are important in warm and hot dense matter in which the Coulomb interaction is dominated in the scattering process[1, 2]. Density functional theory (DFT) is considered as an effective method to investigate the transport properties, but the dynamical collisions between particles are missed. Here we use an electron force field (eFF) method based on molecular dynamics (MD) to include the electronic quantum effects to investigate the transport properties of warm dense hydrogen. The eFF method can be regarded as the development of wave packets molecular dynamics and it has been successfully used to describe the thermodynamics of hydrogen, Auger process in diamondoids, the equation of states for dense lithium. The most important point of eFF method is assuming that each electron is considered as a Gaussian wave packet controlled by position and size while ions are still charged points. The electrical conductivity is calculated via the correlation of electrical current. The results show that electronic quantum effects are important for the transport properties in warm dense hydrogen such as diffusion coefficient and electrical conductivity, which are much smaller than the results from DFT calculations.

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[2] J. T. Su and W. A. Goddard III, Phys. Rev. Lett. **99**, 185003 (2007).