EXCITON DYNAMICS IN WARM DENSE HYDROGEN

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Insulator-to-metal transition (IMT) in fluid warm dense hydrogen (WDH) is one of the unresolved problems of the last decades. There are a large number of experiments aimed at determining this transition, but they have a large number of disagreements.

At the moment, one of the most used theoretical methods is the Born-Oppenheimer dynamic with finite-temperature density functional theory (FT DFT). It shows the process of hydrogen dissociation at temperatures close to the transition, which, however, cannot explain many effects, such as the difference in the moments when the absorption plateau appears and the optical conductivity is detected [2], or a large isotopic effect [1]. The problem with the formulation of finite temperatures is that it assumes that at the step of ion dynamics, we already have averaging of electronic transitions and we have fractional filling of levels.

However, in this paper we study a separate electronic dynamics, where electronic transitions can occur with longer times than the step of the ion dynamics, so in our approach we can separately observe the moments of electronic excitations, thus getting a much better description of the transition [3].

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