Ion impact on strongly correlated 2D materials — stopping power and induced collective electronic dynamics

Thursday 23 Sep 17:00

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The energy loss of charged projectiles in correlated materials is of prime relevance for plasma-surface interaction for which we have developed a nonequilibrium Green functions (NEGF) approach. Some particularly interesting effects that occur when a charged plasma particle hits a strongly correlated solid are the correlation induced increase of stopping power at low velocities [1] as well as the creation of doublons (bound correlated pairs of electrons with opposite spins). However, NEGF simulations are possible only for short time durations, due to the unfavorable N_t^3 scaling with the number of discretization time steps. This situation has changed radically with the recently developed G1-G2 scheme [2], which is based on the generalized Kadanoff-Baym ansatz in combination with Hartree-Fock propagators, and allows us to achieve linear scaling with N_t . This enables us to study larger finite systems of varying geometry and to significantly extend the simulation duration which gives access, in particular, to slower projectiles. Furthermore, it enables us to improve the accuracy by using better self-energies that include dynamical screening and strong coupling effects simultaneously [3]. In addition, the systematic increase of the doublon number through multiple projectile impacts [4] is investigated for more realistic setups (e.g. larger systems and random projectile impact points).

[1] Balzer et al., Phys. Rev. B 94, 245118 (2016)

[2] Schlünzen et al., Phys. Rev. Lett. 124, 076601 (2020)

[3] Joost et al., Phys. Rev. B 101, 245101 (2020)

[4] Balzer et al., Phys. Rev. Lett. 121, 267602 (2018)

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Electron mean free path and the Dreicer field in dense semiclassical plasma

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High-energy electrons appear in plasma, for example, in thermonuclear devices, solar flares, laser plasma, energy discharges associated with thunderstorms. One of the important mechanisms for the appearance of such suprathermal electrons is the electron runaway phenomenon in an external electric field. Runaway electrons play a positive role in the case of wake acceleration, inertial confinement fusion (ICF) fast ignition, etc., however, can be a big problem, namely, by its uncontrollability, which leads, for example, to a damage of the walls in the thermonuclear installations. Therefore, an understanding of the runaway mechanism and knowledge of the dynamics of runaway electrons are crucial in order to control this phenomenon. In this work, the phenomenon of electron runaway in dense semiclassical plasma was investigated on the basis of the effective interaction potential, which takes into account the effects of dynamic screening and diffraction [1–2]. Plasma was considered to be fully ionized, i.e. the electron-electron and electron-ion interactions are only taken into account. The calculations were carried out using the method of phase functions. The electron transport cross sections were calculated, and on their basis the mean free path of electrons was determined for various values of the density and coupling parameters. Critical external electric field (the Dreiser field) which is one of the important characteristic of the runaway phenomenon was also investigated. [1] Dzhumagulova K.N. etc. al. Phys. Plasmas. – 2013. – Vol. 20. – p. 042702. [2] Shalenov E.O. etc. al. Phys. Plasmas. – 2018. Vol. 25. – p. 082706. The authors acknowledge support from the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan under Grant number AP08855972.

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Strongly increasing electron-impact-ionization cross section in hot dense plasma by the ion correlation effect and continuous electron decoherence

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There are significant discrepancies between the recent experiment (Berg et al, Phys. Rev. Lett. 120, 055002) and current theoretical calculations on the electronimpact ionization in hot dense plasmas. For the theoretical results are based on structures of the isolated atoms of ions, without considering the influence of hot dense plasmas, we present a model to consider the effects of the ion and free electrons in the selfconsistently calculations of ionic structures, and free electrons decoherence in the electron-impact ionization. The correlation effects due to the interactions between ions and surrounding free electrons, are included by the correlation functions, which are calculated by hyper-netted chain (HNC) approximation. And the effect yields an additional Hermitian potential to the atomic central potential, and will significantly change the atomic structure compared with that of the isolated ion. Due to the partial decoherence caused by random collision with free electrons and ions, we use damped plane waves of the scattered electrons instead of plane waves, which considers the influence of hot dense plasma on the electron collision process. Finally, we study the electron-impact ionization process of Mg7+ in solid-density plasma using the theoretical model, which result in the increase of the ionization cross section by one order of magnitude compared with that of the isolated ion, And the result is an excellent agreement with the experimental result of Berg et al. The model shed some new insights on collisional ionization process, and would be used to study the radiation opacity and the nonequilibrium properties of hot dense plasma. email: yonqhou@nudt.edu.cn

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