Importance of Dynamical Electron Correlation in the Stopping Power of Solids for Slow Ions

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The concept of electron correlation permeates many subfields of condensed matter physics, but it is rather difficult to find good examples of its clear manifestation. It is even more difficult to illustrate its importance in dynamical (*i.e.*, time-dependent) processes. Here we report a success in obtaining a clean theoretical formula directly relating dynamical correlation, as characterized by f_{xc} the frequency-dependent exchange-correlation kernel of the time-dependent density-functional theory (TDDFT), with the experimentally observed stopping power, $-dE/dx$, of solids for slow ions.

The nonperturbative theory of scattering of noninteracting electrons by a central potential combined with the density-functional theory (DFT) has proved successful in calculating $-dE/dx$ of an electron gas for slow ions. This scheme accurately reproduces the measured energy loss of slow protons and antiprotons in a variety of solids. To some extent it also successfully accounts for the observed behavior in the energy loss of slow ions with increasing charge Z_1e. This kind of calculations were extended to projectile velocities v approaching the Fermi velocity of the target, but so far only few attempts have been made to include the effect of many-body dynamical correlation that is absent in the existing DFT-based schemes.

We approach the problem of including dynamical correlation in the framework of the TDDFT and have succeeded in deriving a rigorous formula for $-dE/dx$ of an interacting electron gas for ions in the limit of low projectile velocities ($v \rightarrow 0$) [1]. Depending on whether f_{xc} is involved or not, this formula can be rewritten as a sum of two terms: The first one without f_{xc} is shown to yield the conventional result for $-dE/dx$ of noninteracting Kohn-Sham electrons first reported by Echenique *et al.* [2]. The second one represents a new and important result fully incorporating the effect of dynamical correlation through the imaginary part of f_{xc}.

In the spirit of the widely used local-density approximation (LDA), we can think of an appropriate approximation to f_{xc} in such a form as the one proposed by Qian and Vignale [3]. Then our formula enables us to make a reasonably accurate evaluation of the friction coefficient ($-dE/dx$ divided by v in the limit of $v \rightarrow 0$) of an interacting electron gas as a function of the atomic number of the projectile ion Z_1. An example of the results obtained by such calculations for the homogeneous electron gas is shown in Fig. 1 in which the solid and dashed curves correspond, respectively, to the cases with and without dynamical correlation (or the second term in our formula). Here the electron density characterized by the conventional density parameter r_s is taken to be 1.59 which is just the same density as the one for valence electrons in carbon films. In view of the fact that at low velocities the energy loss of ions in solids is due mainly to the stopping power of valence electrons, our present theoretical results can be directly compared with the experimental ones in carbon.

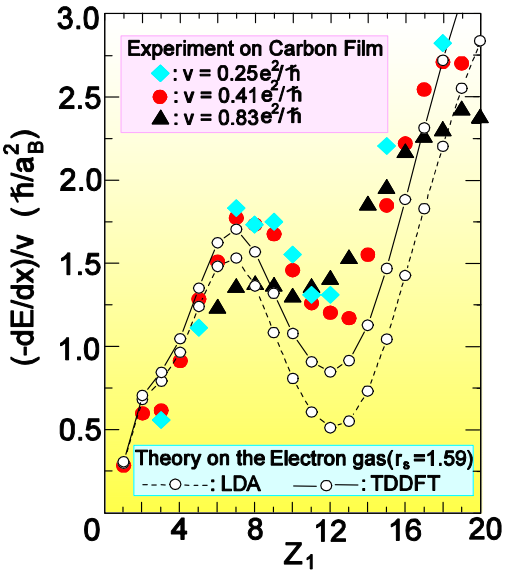

Fig. 1. Comparison between experiment on the stopping power, $-dE/dx$, of carbon films for slow ions (characterized by the atomic number Z_1) with three different values of the velocities v and theory on the same quantity of the homogeneous electron gas with the electron density equivalent to the valence-electron density in carbon in the limit of zero ion velocity ($v \rightarrow 0$).

As can be seen in Fig. 1, experiment exhibits an oscillatory behavior in the friction coefficient with increasing Z_1. This behavior, which is attributed to the shell structure of valence electrons around the ion, is reproduced rather well in the DFT-based calculation (as labeled by LDA), but a better quantitative agreement with experiment is obtained by our theory based on the TDDFT, thanks to the enhancement of $-dE/dx$ by dynamical correlation, or more specifically, the excitonic effect which has recently been revealed to be very important through the accurate calculation of the dynamical structure factor of the homogeneous electron gas [4].

Agreement between theory and experiment becomes unsatisfactory for Z_1 larger than about 20, indicating a need to go beyond the LDA-type approximation in the description of f_{xc}.

References

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