Quantum mechanics in a comoving frame: an emergence of time-dependent deformation functional theory

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In this talk I introduce a new DFT-like approach to the nonequilibrium quantum many-body problem – a time-dependent deformation functional theory (TDDefFT). One of the main practical motivations to reconsider the basics of conventional time-dependent (current) density functional theory is a so called ultranonlocality problem in nonadiabatic TDDFT. Physically the ultranonlocality is related to a convective motion of the electron fluid: in the nonadiabatic theory the particles at a given point of space retain the memory of their previous positions. As a result the universal density functionals of TDDFT become extremely nonlocal.

The key idea of TDDefFT is to eliminate this source of nonlocality by separating the convective motion, and the motion of quantum particles relatively to the convective flow. Formally this corresponds to the transformation of the exact many-body equations of motion to a comoving Lagrangian frame, i. e. to a local noninertial frame moving with a flow. Within this formalism the convective motion is described by a set of trajectories of infinitesimal fluid elements (the Lagrangian trajectories), while the relative motion is determined by the many-body wave function in the comoving frame. It turns out that the many-body problem in the comoving frame does not contain any external field. The dynamics is completely determined by a fundamental geometric characteristics of the frame – the Green's deformation tensor g_{ij} that plays a role of an effective metric in the Lagrangian space. Hence this many-body problem appears to be universal. It determines the wave function (and thus any observable) as a universal functional of the deformation tensor. In particular, the stress force in the equation of motion for the Lagrangian trajectories, as well as xc potentials in the Kohn-Sham scheme are unique functionals of g_{ij}.

The most interesting property of this approach is that a DFT-like theory emerges in a constructive fashion. It appears as a natural, unavoidable step in solving the quantum many-body problem in a comoving frame. Practically it opens up a possibility to describe nonadiabatic xc effects using local functionals of a new basic variable, the deformation tensor.

References

[1] I. V. Tokatly, Phys. Rev. B **71**, 165104 (2005); *ibid.* **71**, 165105 (2005).
[2] I. V. Tokatly, cond-mat/0612254.