Multiscale quantum-classical micromagnetics: Fundamentals and applications in spintronics

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This talk introduces recently developed [1,2] multiscale and self-consistent computational tool which combines time-dependent nonequilibrium Green function (TDNEGF) algorithms, scaling linearly in the number of time steps and describing quantum-mechanically conduction electrons in the presence of time-dependent fields of arbitrary strength or frequency, with classical description of the dynamics of local magnetic moments based on the Landau-Lifshitz-Gilbert (LLG) equation. Such TDNEGF+LLG approach can be applied to a variety of problems where current-driven spin torque induces the dynamics of magnetic moments as the key resource for next generation spintronics. Previous approaches for describing such nonequilibrium many-body system have neglected noncommutativity of quantum Hamiltonian of conduction electrons at different times and, therefore, the impact of time-dependent magnetic moments on electrons which can lead to pumping of spin and charge currents that, in turn, can self-consistently affect the dynamics of magnetic moments themselves including introduction of non-Markovian damping and magnetic inertia terms into the LLG equation [2]. Thus, TDNEGF+LLG can be viewed as "quantum-classical micromagnetics" which captures numerous effects missed by widely utilized purely classical micromagnetics. We use examples of current- or magnetic-field-driven motion of domain walls within magnetic nanowires (including their annihilation observed in very recent experiments) to illustrate novel insights that can be extracted from TDNEGF+LLG simulations. In particular, TDNEGF+LLG as a nonperturbative (i.e., numerically exact) framework allows us to establish the limits of validity of simpler theories, such as the so-called spin-motive force theory for pumped charge current by time-dependent noncollinear and noncollinear magnetic textures which turns out to be just the lowest order of the result predicted by TDNEGF+LLG.

[1] M. Petrović, B. S. Popescu, U. Bajpai, P. Plecháč, and B. K. Nikolić, Phys. Rev. Applied 10, 054038 (2018).

[2] U. Bajpai and B. K. Nikolić, Phys. Rev. B 99, 134409 (2019).