Spin dynamics and exchange interactions from the first- and second-principles calculations

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Magnetic ordering and related phenomena are of essentially quantum and essentially many-body origin and require strong enough electron-electron interactions [1]. Also, they are very sensitive to the details of electronic structure of specific materials [2]. This makes a truly microscopic description of exchange interactions a challenging task. Usually, one cannot use any natural perturbation parameters related with the strength of interactions. Long ago we suggested a general scheme of calculations of exchange interactions responsible for magnetism based on the "magnetic force theorem", when one considers a response of a system on small rotations of spins with respect to a (collinear) ground state magnetic configuration [3,4]. It was formulated originally as a method to map the spin-density functional to effective classical Heisenberg model, the exchange parameters turned out to be, in general, essentially dependent on initial magnetic configuration and not universal [5]. However, they are directly related to the spin-wave spectrum and, thus, can be verified experimentally [6]. Now it is the standard scheme used for many different classes of magnetic materials, from dilute magnetic semiconductors [7] to molecular magnets [8]. This approach also lies in the base of "ab initio spin dynamics" within the density functional approach [9].

It is well known now that this scheme is, in general, insufficient for strongly correlated systems and should be combined with the mapping to the multiband Hubbard model and use of, say, dynamical mean-field theory to treat the latter [10,11]. Our original approach can be reformulated for this "second-principle" method, the results are expressed in terms of Green's functions and (local) electron self-energy [12,13]. It can be also generalized to the case of relativistic magnetic interactions, such as Dzyaloshinskii-Moriya interactions [14]. Very recently, we have extended this scheme to the case of time-dependent Hamiltonians which opens a way to a consequent microscopic theory of laser-induced spin dynamics in strongly correlated systems [15].

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