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Modeling Spin Fluctuations and Magnetic Excitations from Time-Dependent Density Functional Theory TOMMASO GORNI, IURI TIMROV, ANDREA DAL CORSO, STEFANO BARONI, SISSA, Trieste — Harnessing spin fluctuations and magnetic excitations in materials is key in many fields of technology, spanning from memory devices to information transfer and processing, to name but a few. A proper understanding of the interplay between collective and single-particle spin excitations is still lacking, and it is expected that first-principle simulations based on TDDFT may shed light on this interplay, as well as on the role of important effects such as relativistic ones and related magnetic anisotropies. All the numerical approaches proposed so far to tackle this problem are based on the computationally demanding solution of the Sternheimer equations for the response orbitals or the even more demanding solution of coupled Dyson equations for the spin and charge susceptibilities. The Liouville-Lanczos approach to TDDFT has already proven to be a valuable alternative, the most striking of its features being the avoidance of sums over unoccupied single-particle states and the frequency-independence of the main numerical bottleneck. In this work we present an extension of this methodology to magnetic systems and its implementation in the QUANTUM ESPRESSO distribution, together with a few preliminary results on the magnon dispersions in bulk Fe.

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