Interactions of Electron Spin with Phonons: Spin Relaxation and Decoherence in Materials from First Principles

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Combining density functional theory with many-body approaches has enabled quantitative studies of electron interactions and dynamics in materials. Yet treating the electron spin with these first-principles methods remains challenging. Spin interactions with atomic vibrations (phonons) are particularly important as they set an intrinsic limit to the performance of spintronic and spin-based quantum devices.

In this talk, I will present a rigorous framework to compute spin-phonon interactions and phonon-induced spin relaxation and decoherence in condensed matter [1,2]. Our method unifies the treatment of two key spin-phonon processes – spin scattering off phonons and spin precession altered by phonons, commonly known as Elliott-Yafet and Dyakonov-Perel mechanisms. This scheme computes the phonon-dressed vertex correction of the spin susceptibility, with a treatment analogous to the anomalous electron magnetic moment in QED, by solving numerically a spin-phonon Bethe-Salpeter equation. These calculations rely on *ab initio* electron-phonon interactions including spin-orbit coupling [3,4].

I will show accurate predictions of spin relaxation times of electron and hole carriers in key semiconductors for quantum technologies (Si, Ge and GaAs) and in 2D materials. Both spin relaxation and spin precession will be analyzed, showing that the spin-phonon interactions lead to a colossal renormalization of electron spin dynamics in solids. I will conclude by discussing open questions and ongoing work, including: (i) spin relaxation in magnetic materials and semiconducting qubits, (ii) computing higher-order spin-phonon processes, (iii) relating our formalism with calculations based on the density matrix, and (iv) making our new methods available in our open-source Perturbo code [4].

References

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