Towards Collective Excitations in Disordered Systems

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Fundamental collective excitations, such as excitons and magnons, play a central role in the optical, magnetic, dynamical, and spin-transport properties of quantum materials, making them essential for next-generation optoelectronic and spintronic technologies. Recent advances in *ab initio* many-body perturbation theory have provided a unified framework for describing excitonic and magnonic excitations with high accuracy in crystalline materials [1,2].

Beyond crystalline systems, disordered materials offer new opportunities for advancing optoelectronic and spintronic devices. For instance, ultrathin magnetic alloys can support long-lived magnons at terahertz frequencies, opening avenues toward compact magnonic devices [3]. Understanding how disorder modifies collective excitations in these materials is therefore of both fundamental interest and practical importance. However, the stochastic atomic occupations and the resulting loss of translational symmetry prevent the direct application of well-established *ab initio* methods. Currently, first-principles methodologies for investigating collective excitations in disordered systems remain in their infancy.

In this study, we propose an *ab initio* theoretical framework that integrates the Wannier-based coherent potential approximation (WCPA) [4], which efficiently accounts for the effects of disorder, with the *ab initio* Bethe–Salpeter equation (BSE) formalism to investigate magnons in disordered systems. This framework retains a computational cost comparable to that of conventional *ab initio* BSE calculations for crystalline materials, making large-scale first-principles studies of disordered systems computationally feasible.

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