Real-space method for excitons in disordered hexagonal Boron Nitride

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Hexagonal Boron Nitride (hBN) is well-known for its large excitonic effects. In the presence of defects, it has attracted attention as a single-photon emitter [1]. More recently, amorphous Boron Nitride has garnered interest for its potential technological applications [2], and twisted hBN has come under active investigation. All these systems share large and complex unit cell structures, if they have one at all. This highlights a need for atomistic simulation methods able to describe excitonic effects in disordered media, a task which is usually very demanding computationally. Indeed, several recent theoretical advances have been proposed in this direction (e.g. [3]). In this work, we extend to the disordered case an approximate method for the construction of the Bethe-Salpeter Hamiltonian (BSH) in real space from a tight-binding Hamiltonian [4]. Under certain perturbative conditions, which are realized in hBN, the BSH can be built by perturbation theory, bypassing the need to diagonalize the single particle Hamiltonian. The resulting BSH is of tight-binding form on a basis of real space localized electron-hole pairs and is sparse, allowing efficient linear scaling algorithms [5,6] to be brought to bear. Combined with a real-space cutoff to neglect weakly bound pairs, this permits the computation of properties of interest in O(N) time, where N is the number of atoms in the unit cell. We demonstrate this by exploring the excitonic properties and optical absorption of hBN in the presence of static disorder, such as the Anderson case (figure 1).

References

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Figures

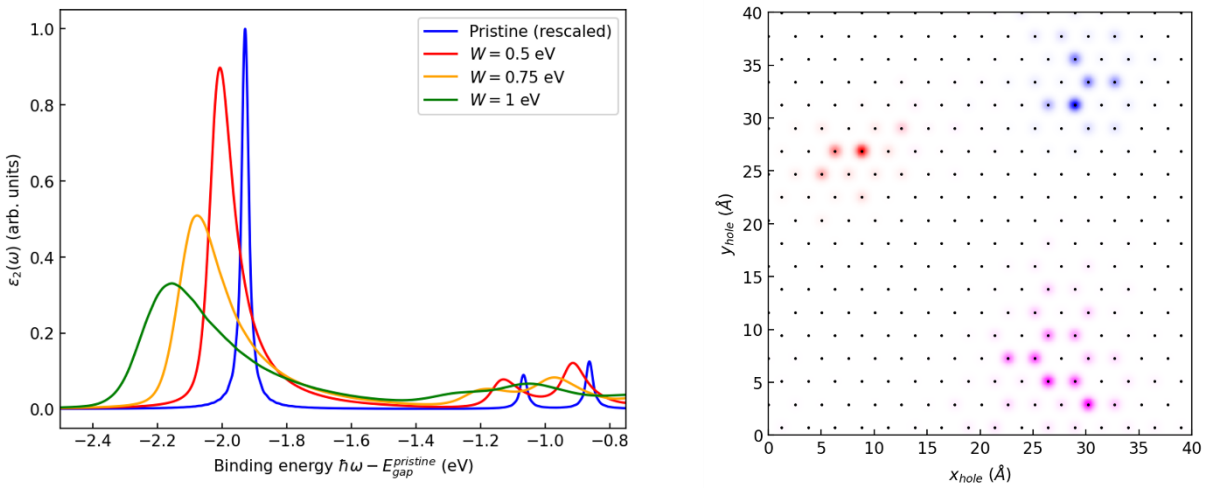

Figure 1: left: absorption spectrum of single-layer hBN in the presence of gradually increasing Anderson disorder. Right: localization of excitonic states under Anderson disorder (hole coordinate).