Excitons in twisted hexagonal Boron Nitride bilayers near the quasicrystal limit

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Hexagonal Boron Nitride (hBN) is a two-dimensional material well known for its very strong electron-hole interaction (excitonic) effects [1,2,3]. Recent experiments [3] have shown that, upon twisting, a new luminescence signal appears below the untwisted response. Calculations at the *independent particles* level, close to the quasicrystal limit (twist angle ~30°) [2], also reveal peculiar effects, such as a dependence of the optical response on the axis of twist, as well as real-space localization of conduction (electron) states, but not of valence (hole) states. Theoretical investigations including the – critical – electron-hole interaction would therefore be timely, but they are made delicate by the very large unit cells of the twisted systems. To overcome this difficulty, we generalize a perturbative method to approximate the Bethe-Salpeter Hamiltonian (BSH) in hBN [1] on the basis of a tight-binding model [2]. The resulting BSH is expressed in a basis of real space localized electron-hole pairs, and is both sparse and of a dimension that grows linearly with system size. Coupling this methodology with linear scaling algorithms [4,5], we investigate the optical absorption and excitonic wavefunctions of twisted hBN bilayers close to the quasicrystal limit. Our results [6], supported by first principles many-body calculations for small approximants, confirm the importance of the twist axis in that case, and show that this dependence vanishes for larger approximants close to the quasicrystal limit. We also scrutinize the excitonic wavefunctions responsible for the main absorption features, and highlight the localization characteristics of the electron *and* hole degrees of freedom in the interacting case.

References

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Figures

Figure 1: illustration of the real-space localization of the electron (left) and hole (right) degrees of freedom for the exciton yielding the main peak of a BNNB(11,30) approximant (0.04° from the quasicrystal limit) [2] twisted hBN bilayer.