Exciton transport in twisted 2D heterostructures: transition between hopping and dispersive regime

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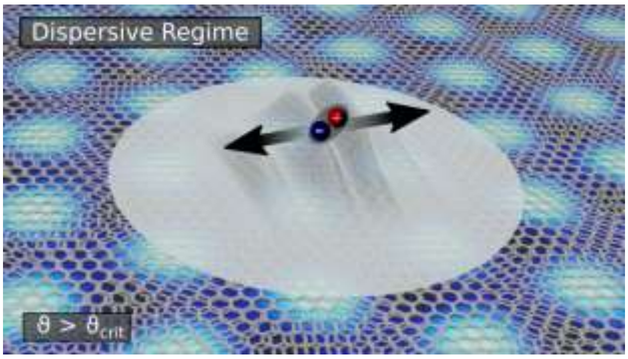
The propagation of excitons in monolayers of transition metal dichalcogenides (TMDs) has been intensively studied, with interesting effects, such as halo formation [1], non-classical diffusion [2], and negative diffusion [3]. Initial studies have investigated how exciton transport changes in twisted TMD bilayers, including Coulomb repulsion and Hubbard-like exciton hopping. In this work, we investigate the twist-angle-dependent transition of the Hubbard-like hopping regime to the dispersive regime of effectively free excitons. We use an exciton Hubbard model in the presence of a Moiré potential and show that the hopping regime occurs up to an angle of θ < 2° [4]. In contrast, at large angles, the Hubbard model fails due to the increasingly delocalised exciton states. Here, the quantum mechanical dispersion of free particles with an effective mass determines the propagation of excitons. Overall, our work provides new microscopic insights into the character of exciton propagation in twisted van der Waals heterostructures.

References

[1] Raul Perea-Causin et al., Nanoletters 19.10 (2019), pp. 7317–7323
[2] Koloman Wagner et al. , Physical Review Letters 127.7 (2021), p. 076801
[3] Roberto Rosati et al., Nanoscale 12.1 (2020), pp. 356–363
[4] Willy Knorr et al., Physical Review Materials 6.12 (2022) 124002

Figures



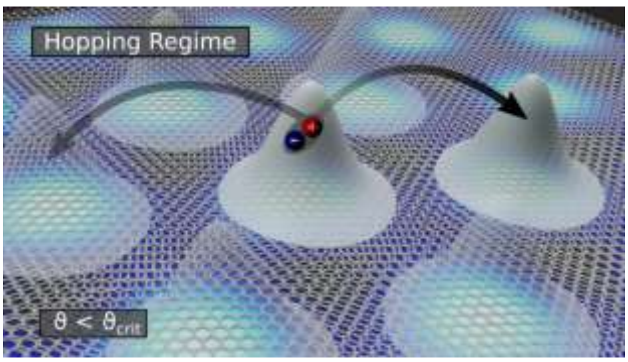


Figure 1: Schematic Illustration of two distringt exciton transport regimes in a moiré potential created in a twisted TMD heterostructure. At small twist angels, we observe Hubbard-like hopping driven
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