

Montag, 01.07.2019 um 15:15 Uhr
Ort: Seminarraum 87, Wilhelm Klemm-Straße 10

On-situ control of quantum states by carrier capture in 2D materials

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The monolayers of transition metal dichalcogenides (TMDC) have attracted wide attention due to their two-dimensional (2D) character and interesting optical and electronic properties [1]. Hybrid 2D-0D systems can be formed, e.g. by means of strain [2], resulting in bound states with specific spectral characteristics and well localized in space: A superposition of these could generate quantum states which, if controllable, could pave the way for on-situ quantum computing.

In order to populate localized states, the carrier capture by emission of optical phonons can be exploited. Adopting a recently introduced Lindblad single-particle approach, which combines computational affordability and ability of catching most of the relevant features of the carrier capture [3], in this work we study the phonon-induced capture from an electronic wave packet in a MoSe₂ monolayer into the localized states of a 0D potential. The resulting combination of non-trivial spatio-temporal dynamics and locality of the carrier capture induces oscillations of the captured spatial distribution thanks to the formation of quantum coherences: These can be controlled by changing the orientation between wave packet and elliptical 0D potential [4] (see Fig. 1), or exploiting more wave packets. These oscillations define a spatial qubit: We will discuss how to control the latter in the case of the 0D confinement potential resulting from a nanobubble, similar to those formed when a monolayer is put on a substrate [5].

Our results show that the carrier capture allows the generation and on-situ control of spatial qubits, which may guide future experiments in the field of quantum information processing.

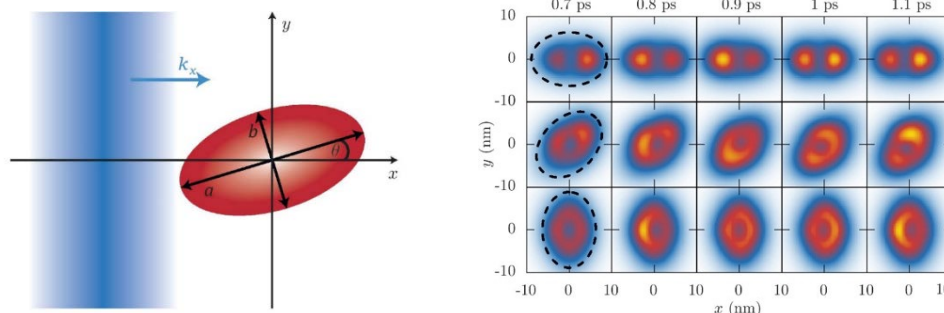


Fig. 1: Sketch of a wave packet impinging on a 0D potential (left) and induced spatio-temporal oscillations of the captured distribution (right) for different relative oscillation (top to bottom, dashed black line indicating the 0D potential).

[1] T. Mueller, and E. Malic, *npj 2D Mater. Appl.* **2**, 29 (2018).

[3] R. Rosati, D. E. Reiter, and T. Kuhn, *Phys. Rev. B* **95**, 165302 (2017).

[5] C. Carmesin et al., *Nano Lett.* **19**, 3182 (2019).

[2] J. Kern et al., *Adv. Mater.* **28**, 7101 (2016).

[4] R. Rosati, F. Lengers, D. E. Reiter, and T. Kuhn, *Phys. Rev. B* **98**, 195411 (2018).