Unveiling the Berry curvature in the spectral properties in 2D transition-metal dichalcogenides

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The Berry curvature is a relevant geometric quantity in the characterisation of electronic bands in solids, and it is a key concept in the understanding of the topological properties of condensed matter ever since the advent of graphene and topological insulators in 2005 and 2006. However, the concept had been known before but left aside as a curiosity of the quantum-mechanical properties of electrons in solids. This lack of interest in the Berry curvature was most probably due to the absence of its manifestation in the spectral properties of electrons in solids, within conventional band theory. Indeed, in order to uncover its relevance, (local) electric fields beyond those arising from the periodic crystal potential are required, as it is evident when considering the quasi-classical equations of motion of band electrons in the form of the anomalous velocity of Karplus and Luttinger.
However, this does not mean that the Berry curvature is absent in all spectral properties. Indeed, it was observed some years ago that excitons in some semiconducting two-dimensional materials (transition-metal dichalcogenides) do not obey the otherwise extremely successful hydrogen model used in the description of excitons. While non-local screening effects, due to the layered structure of the material, are certainly one reason for the observed deviations, a conceptually more important effect is precisely the role played by the Berry curvature that is non-zero at the direct gap at the K and K' points in the first Brillouin zone. The electric field, which arises from the mutual Coulomb attraction between the electron and the hole that build up the exciton, is precisely the quantity that couples to the (excitonic) Berry curvature, and additional terms arise in the fundamental Hamiltonian, which determines the dynamical and thus spectral properties of the excitons.
In this presentation, we show how the Berry-curvature terms arise in the effective model for excitons in 2D TMDC and discuss their effect on the exciton spectra [1,2], both in the case of neutral and charged excitons (trions) [3]. We show that these terms conspire with the Keldysh potential and that their inclusion provides a better estimate of the screening length in comparison with ab initio calculations.

References

[1] M. Trushin, W. Belzig, and M. O. Goerbig, Phys. Rev. B **94** (2016) 041301(R).
[2] M. Trushin, W. Belzig, and M. O. Goerbig, Phys. Rev. Lett. **120** (2018) 187401.
[3] A. Hichri, S. Jaziri, and M. O. Goerbig, Phys. Rev. B **100** (2019) 115426.