Quasi two-dimensional models of Dielectric Screening and Excitons: From Atomically thin Materials to van der Waals Heterostructures

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It is well known that electronic screening in bulk semiconductors is well described by a constant, i.e. spatially local, dielectric function. In contrast, for two-dimensional (2D) semiconductors it is crucial to account for the spatial non-locality. In reciprocal space this means that the q-dependence of the dielectric function cannot be neglected. A first order expansion in q of the dielectric function has been widely used in the literature as it leads to an analytical expression for the screened Coulomb interaction in 2D. This strict 2D approach has been used successfully to compute exciton binding energies in atomically thin semiconductors [1–3] . Here we provide a critical assessment of this simplified approach and develop a quasi-2D model with a much broader applicability.
Within the Q2D picture, electrons and holes are described as in-plane point charges with a finite extension in the direction perpendicular to the 2D material. The interaction between these Q2D charges is then screened by a dielectric function which is non-local within the plane and accounts for the finite extension of the charge distributions perpendicular to the layer in a mean field sense. We recently demonstrated that the dielectric function of a general van der Waals heterostructure can be efficiently computed from the Q2D dielectric functions of the individual layers using a multi-scale method which combines quantum accuracy at the single layer level and couples the layers via the Coulomb interaction [4]. The Q2D dielectric functions of more than 50 different 2D materials are available in an open database together with the software for solving the coupled electrostatic equations [5]. From the dielectric function we evaluate the screened interaction between electron and hole charge distributions located within the same layer (direct excitons) or in different layers (indirect excitons) of a heterostructure. The screened interaction is then used in a generalized Mott-Wannier model to compute exciton binding energies in isolated, supported, or encapsulated 2D semiconductors. For isolated 2D materials, the Q2D treatment yields results almost identical to those of the strict 2D model with a linearized dielectric function. For more complex structures, however, the 2D model breaks down and must be replaced by the Q2D description. As an illustration of the latter, we show how the peculiar non-Rydberg exciton series in supported WS2, recently observed experimentally, is well reproduced by the Q2D model.
In summary, the presented Q2D methodology is accurate, yet highly efficient and has the merit of providing a seamless connection between the strict 2D limit of isolated monolayer materials and the more bulk-like screening characteristics of supported monolayers or van der Waals heterostructures.

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[4] The dielectric building blocks and the QEH software can be downloaded from https://cmr.fysik.dtu.dk/vdwh/vdwh.html
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