Nagaoka ferromagnetism in phosphorene quantum dots

Tanmay Thakur and Bartłomiej Szafran

AGH University of Science and Technology,
Faculty of Physics and Applied Computer Science,
al. Mickiewicza 30, 30-059 Kraków, Poland

Phosphorene, a monolayer form of black phosphorus, is a 2D material with strong anisotropy of the effective masses [1,2] that has been investigated in recent years. We consider a 2x2 array of quantum dots in phosphorene to investigate Nagaoka ferromagnetism - a magnetic ordering promoted in a system where number of electrons are one less than the number of sites. Although the ordering of spins in such system was proved by Nagaoka earlier, an experimental demonstration of this physical phenomenon was shown only recently by Ref. [3] for quantum dots arranged in square array in GaAs. Given than the electrons in phosphorene have large masses as well as large anisotropy, it is not obvious that the magnetic ordering will persist for the square array system in the material. We investigate the robustness of Nagaoka ferromagnetism against the geometry of the arranged dots using a single-band effective mass Hamiltonian [4] to extract the ground state of the system. An exact phase diagram of magnetic ordering as a function of the rectangle parameters is shown and we find the accurate geometry for which the Nagaoka energy gap is the largest. We also discuss the robustness of this ground state against potential detuning and shifting of one quantum dot. We demonstrate that shifting the dot has different impact on the ground state in different directions due to anisotropy, and thus Lieb-Mattis theorem, not Nagaoka theorem, now describes the deformed configuration.

[1] Li, L., Yu, Y., Ye, G. et al., *Nature Nanotech* **9**, 372–377 (2014).
[2] Xia, F., Wang, H. & Jia, Y., *Nat Commun.* **5**, 4458 (2014).
[3] Dehollain, Juan P., et al., *Nature* **579** (7800), 528-533 (2020).
[4] B. Szafran, *Phys. Rev. B* **101**, 23, 235313 (2020).