To Scale or Not to Scale: Self - Capacitance, "Hubbard U" and Quantum Dot Size?

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Abstract

A seminal question to ask regarding quantum dots is how (if at all) its self - capacitance scales with size. What kind of a phenomenology should guide physicists who are involved in studying Coulomb blockade effects and in the practical task of evolving single electron transistors? Answering these issues involves calculating many body effects in quantum dots. We study the electron-electron interaction within a simplified spherical quantum dot using the local density approximation (LDA) and local spin density approximation (LSDA). We experiment with a variety of confining potentials (triangular, harmonic, square well etc.) and with a varying number of electrons (N = 2 to 20). We carry out a detailed study of the scaling behaviour of the "Hubbard U", which is a measure of the capacitive energy, with quantum dot size R ($U \sim 1/R^{-}$). We find that the scaling exponent _ is approximately 1/2 for harmonic confinement and equal to 1 for the square well confinement. We show that the "Hubbard U" depends critically on the shape of the confining potential chosen and size of the quantum dot. It exhibits a weak dependence on the number of electrons. We also examine the relative importance of Coulomb, exchange and correlation terms in the "Hubbard U" and find that correlation plays a relatively more important role at larger size.

REFERENCES

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