MICROSCOPIC DIELECTRIC RESPONSE FUNCTION IN EMICONDUCTOR QUANTUM DOTS

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The dielectric response function is of paramount importance in nanoscience, as it is needed in the description of the charge impurity screening and electron-electron, electron-hole Coulomb interactions in a nanosystem. It has been found both theoretically [1, 2] and experimentally [3] that the averaged dielectric constants of small (1-5 nm) quantum dots (QD) are significantly reduced from their bulk values. Originally, this reduction was attributed to the band gap increase inside the quantum dot. According to this theory, the dielectric response at the interior of the quantum dot (e.g., at the center of the dot) should be reduced compared to its bulk value. However, recently, Delerue *et al.* [4] have argued that the influence of the quantum dot boundary should only be felt close to the surface. Hence screening away from it should be bulklike, and therefore the reduction in the averaged dielectric constant is only due to surface bond breaking, not due to the opening of the band gap. They have performed empirical tight-binding calculations for test cases that validated their arguments for the averaged macroscopic response functions (e.g., under a uniform external electric field). This controversy raises a serious question: What is the correct *microscopic* dielectric function to be used in a nanosystem?

We have investigated this issue by studying the microscopic response function using plane wave *ab initio* calculations. Indeed, we find that the microscopic response function $\chi(\mathbf{r}_1, \mathbf{r}_2)$ is identical to the bulk value when both $\mathbf{r}_1$ and $\mathbf{r}_2$ are within the quantum dot (cf. Fig. 1). We also provide a model which allows to accurately approximate the quantum dot microscopic dielectric function $\chi(\mathbf{r}_1, \mathbf{r}_2)$ from its bulk values without doing explicit calculations (Fig. 2), reproduces the overall dielectric constant reduction for a quantum dot compared to its bulk value.

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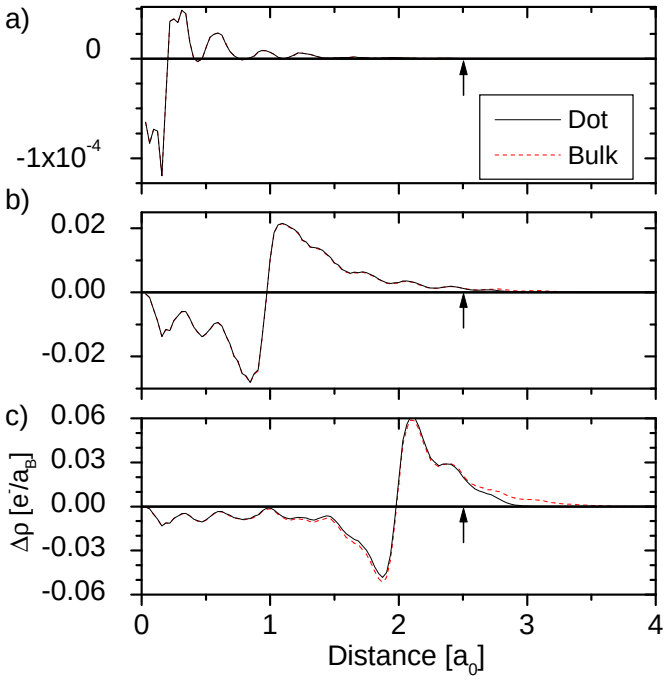

FIG. 1: Direction-averaged change in the change density, $\Delta\rho(\mathbf{r})$, for a 933-atom GaAs dot and bulk under different perturbations. a) δ perturbation. b) Coulomb perturbation truncated at a_0. c) Coulomb perturbation truncated at $2a_0$. The solid (dashed) line shows the dot (bulk) results. The arrow indicates the dot surface.

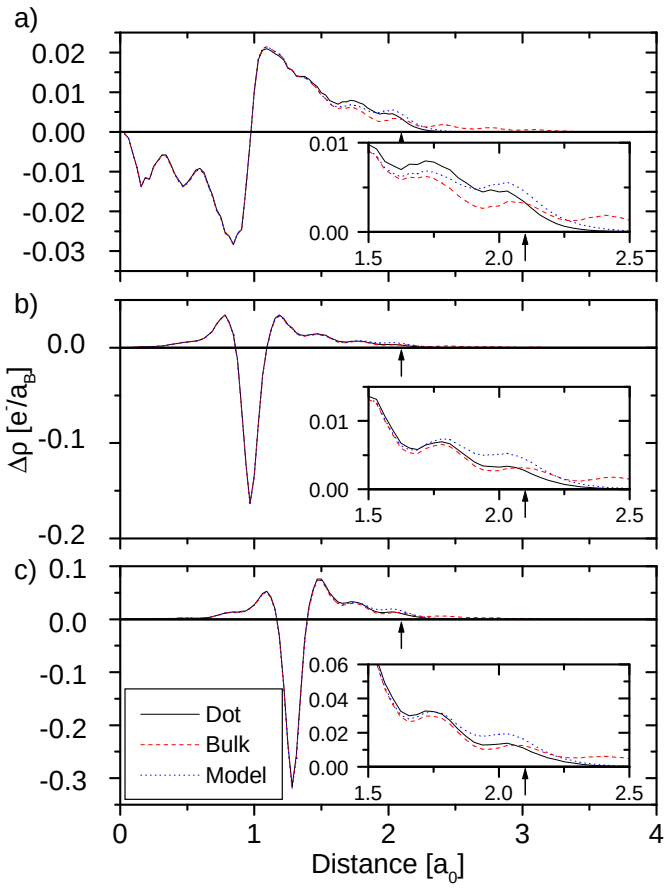

FIG. 2: As in Fig. 1, but with a 465-atom GaAs dot under a a) Coulomb perturbation truncated at a_0; b) $\delta(r_2 - a_0)$ perturbation; c) $\delta(r_2 - 1.3a_0)$ perturbation. The dotted line is the application of the model. The insets show a closeup of the region close to the dot surface.