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## Multi-excitons in self-assembled $\text{InAs}/\text{GaAs}$ quantum dots: A pseudopotential, many-body approach

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PACS.71.10.-b – Electron states in low-dimensional structures (superlattices, quantum well structures and multilayers).

PACS.71.70.-b – Optical properties of specific thin films, surfaces, and low-dimensional structures.

**A** – We use a many-body, atomistic empirical pseudopotential approach to predict



the difference in the electron and hole wave functions. It vanishes artificially in single-band effective-mass calculations that use an infinite well depth, such as those in refs. [1, 2, 7]. Second, there is an exchange shift,  $\epsilon_{N \rightarrow N-1}^h$ , given by the second term in brackets in eq. (2). This exchange shift is familiar from theories of band gap renormalization [9] where the existence of high carrier densities during high power photoexcitation acts to reduce the band gap. In addition, since the exchange interaction depends on the spin orientation of the carriers, the exchange contribution (second term in eq. (2)) can split the excitonic transitions.

In the  $N = \text{even}$ , “closed shell” series, the initial state contains no open shells while the final state contains one open shell. This results in one- and four-fold degeneracies for the initial and final states, and hence 4 transitions. These 4 transitions are split by the small electron-hole ex-

same lens-shape, alloyed dot with a 1.1 eV PL peak. Unfortunately, although numerous experiments were conducted on this dot, no multi-exciton spectra were taken since the lowest PL is outside the range of conventional CCD detection equipment, so quantitative comparison awaits a future measurement.

Having obtained the single-particle levels ( $e_0, e_1, \dots, h_0, h_1, \dots$ ) from the pseudopotential method, we then calculate numerically the screened Coulomb and exchange integrals

$$J = \int \int \frac{\psi^*(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi^*(\mathbf{r}_1) \psi(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2, \quad K = \int \int \frac{\psi^*(\mathbf{r}_1) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \psi^*(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2$$

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excitons. For all the transitions shown here, the correlation shift,  $\epsilon^{CI}$ , for the initial state with  $N$  excitons is greater than that for the final  $N - 1$  exciton state. Therefore, all the CI  $n \rightarrow n$  peaks are red shifted with respect to those from the  $(J + K)$  approximation. ii) This  $\epsilon^{CI}$  red shift is larger for the  $2 \rightarrow 1$  transition than for the  $1 \rightarrow 0$  transition and is able to overcome the Coulomb blue shift and “bind” the biexciton. Our calculated binding energy is  $\sim 3$  meV, however, our model QMC calculations suggest that a fully converged value would be  $\sim 2$  meV.