Erratum: Spontaneous Symmetry Breaking in Single and Molecular Quantum Dots [Phys. Rev. Lett. 82, 5325 (1999)]

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In our recent Letter on spontaneous symmetry breaking in quantum dots (QD's), we displayed in Fig. 4 addition energies $\Delta\varepsilon(N) = E(N+1) - 2E(N) + E(N-1)$, where $E(N)$ is the N-electron ground-state total energy, calculated with the spin-and-space unrestricted Hartree-Fock (sS-UHF) method. Subsequent to the publication of our Letter, we have performed further systematic sS-UHF calculations, with the use of larger harmonic-oscillator bases and an implementation of an extensive search for energy minima. While the behavior and magnitudes of $\Delta\varepsilon$ shown in Fig. 4 of our Letter are maintained, as well as our finding pertaining to the prevalent violation of Hund's first rule, our improved calculations yield in certain instances different spin polarizations $P \equiv N\uparrow - N\downarrow$, where $N\uparrow$ and $N\downarrow$ ($N\uparrow + N\downarrow = N$) are the number of electrons with up and down spins, respectively.

In Fig. 1 below, we display our new results for $\Delta\varepsilon$ in a single QD with GaAs parameters, i.e., $\kappa = 12.9$, $\hbar\omega_0 = 5$ meV, and $m^* = 0.067m_e$ (corresponding to the top curve in Fig. 4 of our Letter). The results of our calculations (solid dots) for the spin polarization given in the inset of Fig. 1 exhibit violation of Hund's rule (open squares) for $N = 4$, 8, 9, 14, 15, 16, 18, and 22 (note that this violation appears already for $N = 4$); however, as noted in our Letter, the addition energies display maxima at closed shells (i.e., at $N = 6$, 12, and 20), as well as at the midshell closures (i.e., at $N = 4$, 9, and 16). In general, the non-Hund ground-state minima are accompanied by energetically close spin isomers obeying Hund's rule, and vice versa (e.g., for $N = 17$ the energy difference between the Hund, $P = 3$, and the non-Hund, $P = 1$, isomers is 0.05 meV).

For the corresponding case of a quantum dot molecule with $\kappa = 12.9$, $d = 70$ nm, and $V_b = 10$ meV (third curve from the top in Fig. 4 of our Letter), our improved calculation yields $P = 0$ for $N = 14$ (unlike the earlier value of $P = 2$), with all the other spin polarizations remaining unchanged.

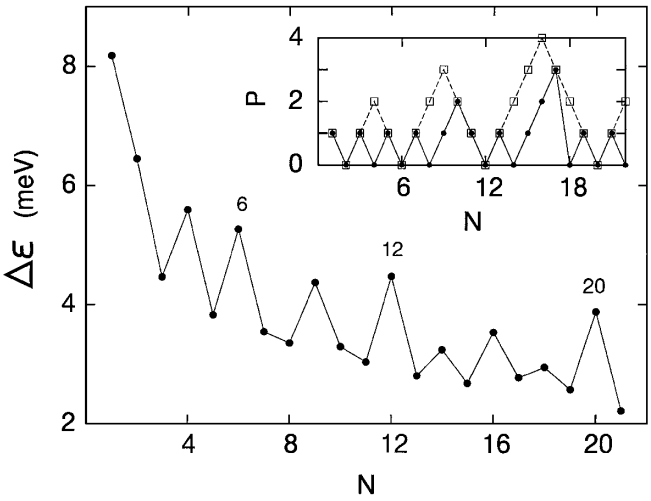

FIG. 1. sS-UHF results for the addition energies ($\Delta\varepsilon$ vs N) of a single QD ($\hbar\omega_0 = 5$ meV, $\kappa = 12.9$, $m^* = 0.067m_e$). The inset displays the calculated (solid dots) spin polarizations, $P \equiv N\uparrow - N\downarrow$, as well as those (open squares) expected from Hund's first rule.

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