Characterization of shell filling of interacting polarons in a quantum dot through their optical absorption

S. N. Klimin, V. M. Fomin, F. Brosens, and J. T. Devreese

Theoretische Fysica van de Vaste Stoffen, Universiteit Antwerpen (U.I.A.), B-2610 Antwerpen, Belgium

The method for calculating the ground-state energy and the optical conductivity spectra is developed for a system of a finite number of interacting arbitrary-coupling polarons in a spherical quantum dot with a parabolic confinement potential characterized by the confinement energy $\hbar\Omega_0$ and with a background charge. The path-integral formalism for identical particles (see, e. g., [1 - 3]) is used in order to account for the fermion statistics. Using a generalization of the Jensen-Feynman variational principle [1, 3], the ground-state energy of a confined N-polaron system is analyzed as a function of N and of the electron-phonon coupling strength α.

In order to describe a system of identical interacting polarons in a quantum dot, a model system is chosen, which consists of N electrons and N_f fictitious particles in a harmonic confinement potential with elastic inter-particle interactions as studied in Ref. [4]. The present approach is applied to both closed-shell and open-shell systems.

In Fig. 1, the total spin S is plotted as a function of the number of electrons in a quantum dot for different values of the confinement energy, of the coupling constant and of the ratio η of the high-frequency and the static dielectric constants. As distinct from the few-electron systems without the electron-phonon interaction, *three* types of spin polarization are possible for the ground state, which can be distinguished from each other using, e. g., capacity measurements.

(i) Except the strong-coupling case and the low-density case, for closed-shell systems $S = 0$, while for open-shell systems S takes a maximal value for a given shell filling, *in correspondence with the Hund's rule*.

(ii) When weakening confinement for a fixed number of electrons, the electron density falls down. Hence, at sufficiently small values of Ω_0, a *spin-polarized* state for a system of interacting polarons in a quantum dot becomes more energetically favorable than a state satisfying the Hund's rule.

(iii) In the strong-coupling case ($\alpha >> 1$ and $\eta << 1$), the total spin of an open-shell system for the ground state can take a *minimal* possible value. This trend to minimize the total spin is a consequence of the

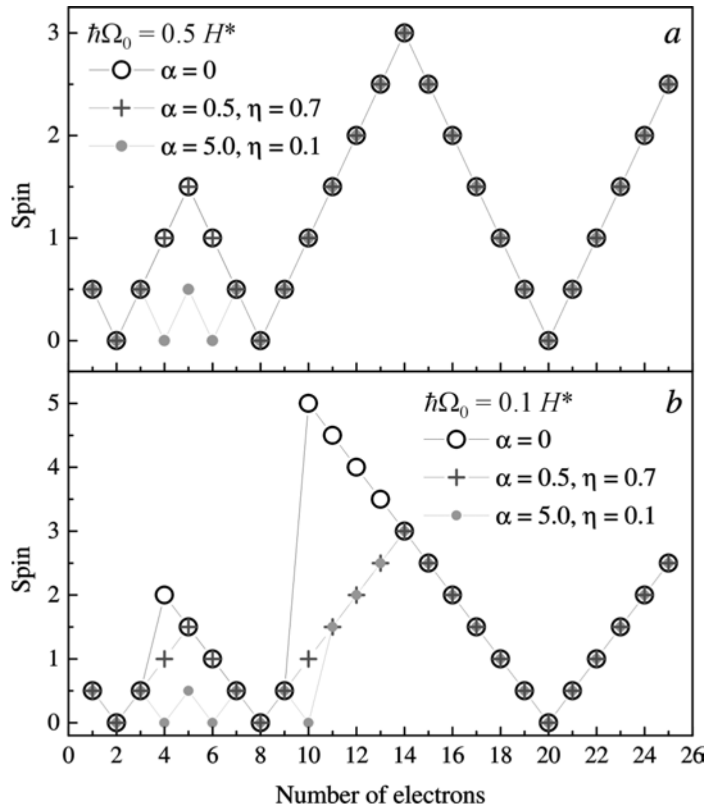

Fig. 1. Total spin of the system of interacting polarons in a quantum dot as a function of the number of electrons for $\hbar\Omega_0 = 0.5\ H^*$ (*a*) and for $\hbar\Omega_0 = 0.5\ H^*$ (*b*). The confinement energy is measured in effective Hartrees $H^* = [m_b/(m_0\varepsilon_\infty^2)] \times$ Hartree.

electron-phonon interaction, presumably due to the fact that the phonon-mediated electron-electron attraction overcomes the Coulomb repulsion.

The parameters from the variational procedure are used as input for the calculation of the optical-conductivity spectrum of the system. The aforesaid ground-state transitions between states with different values of the total spin, which occur when varying the confinement energy, are manifested in the optical absorption spectra, in particular, through the dependence of the first frequency moment of the optical absorption spectra $\langle\omega\rangle$ on the number of electrons. The transitions between the ground state obeying the Hund's rule and the spin-polarized ground state are pronounced in Fig. 2, which represents the function

$$\Theta(N) = \langle\omega\rangle\big|_{N+1} - 2\langle\omega\rangle\big|_{N} + \langle\omega\rangle\big|_{N-1}$$

and the addition energy $\Delta(N)$, respectively. Both $\Theta(N)$ and $\Delta(N)$ exhibit peculiarities at $N = 4$ and at $N = 7$ where the aforesaid transition occurs. Namely, at $N = 4$, $\Theta(N)$ and $\Delta(N)$ have minima, whereas at N = 7, $\Theta(N)$ has a minimum, and $\Delta(N)$ has a kink. Distinguishable peaks appear in $\Theta(N)$ and $\Delta(N)$ at the "magic numbers" $N = 10$ and $N = 20$, which correspond to closed-shell systems. The transition between the spin-polarized ground state and the ground state obeying the Hund's rule thus should be observable using optical measurements. The analysis of the first frequency moment thus provides a specific tool for examining the shell structure of a system of interacting polarons through experimental measurements of the optical absorption in quantum dots.

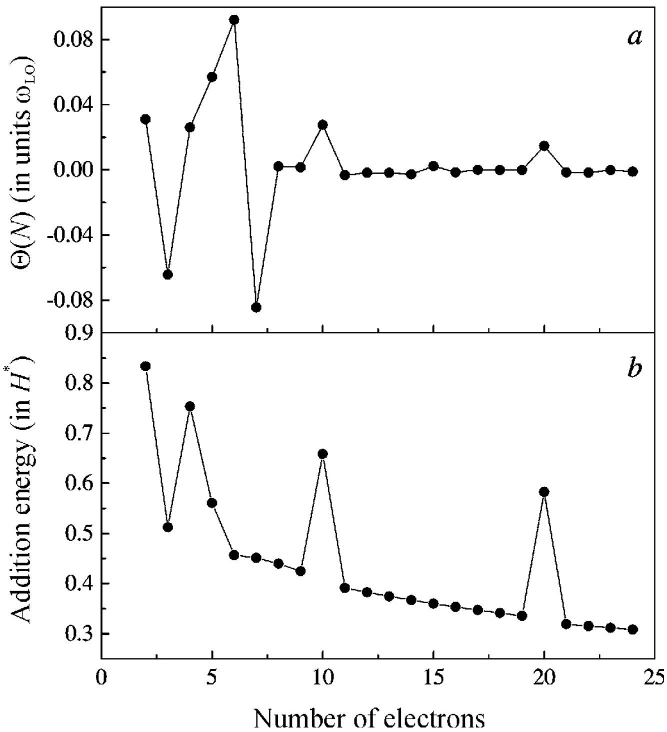

Fig. 2. The function $\Theta(N)$ (*a*) and the addition energy $\Delta(N)$ (*b*) for systems of interacting polarons in a quantum dot with $\alpha = 3$, $\eta = 0.3$ and $\Omega_0 = 0.5\omega_{LO}$ ($\hbar\Omega_0 = 0.0136\ H^*$).

This work has been supported by the GOA BOF UA 2000, I.U.A.P., F.W.O.-V. projects G.0274.01N, G.0435.03, the W.O.G. WO.025.99N (Belgium) and the European Commission GROWTH Programme, NANOMAT project, contract No. G5RD-CT-2001-00545.

[1] L. F. Lemmens, F. Brosens, and J. T. Devreese, Phys. Rev. E **53**, 4467 (1996).

[2] F. Brosens, J. T. Devreese, and L. F. Lemmens, Phys. Rev. E **55**, 227 (1997); **55**, 6795 (1997); **58**, 1634 (1998).

[3] J. T. Devreese, in: *Fluctuating Paths and Fields* (World Scientific, Singapore, 2001), pp. 289-304.

[4] J. T. Devreese, S. N. Klimin, V. M. Fomin, and F. Brosens, Solid State Commun. **114**, 305 (2000).