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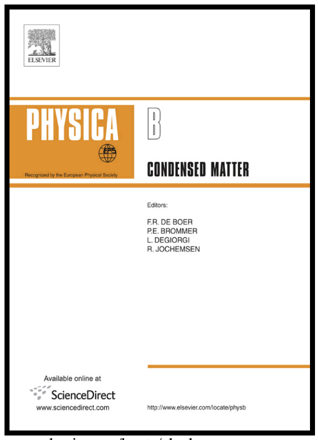

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Interband optical transitions in ellipsoidal shaped nanoparticles

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Abstract

The optical properties of crystalline semiconductor nanoparticles with ellipsoidal shape are investigated and discussed as a function of the shape-anisotropy parameter. The optical transition-matrix elements are calculated in the dipole approximation using perturbation theory and with a direct diagonalization of the appropriate Hamiltonian. The matrix elements involving the ground and first excited states are monotonic functions of the shape-anisotropy parameter, whereas matrix elements involving the highly excited states have zeros and extrema that are reflected in the behaviour of the corresponding transition probabilities. Moreover, some matrix elements involving the excited states have discontinuity. We demonstrate that, nanoparticles with ellipsoidal shape can be grown with the infrared as well as ultraviolet features.

Keywords: nanoparticle, ellipsoidal shape, optical properties, transition-matrix elements

1. Introduction

The electronic and optical properties of crystalline semiconductor structures of various shapes and of nanometer size attract increasing interest [1]. In the regime of strong size quantisation, the optical properties are determined by the transitions between discrete states of electrons and holes confined in a nanoparticle, which signifies a particle of which the extent in each spatial dimension is of order 1 nm. In most early publications, the qualitative and quantitative descriptions of the optical properties apply to spherically shaped nanoparticles, i.e. for spherical quantum dots (see [2] and references therein).

The first study [3] of the optical properties of a spherical quantum dot with infinitely high walls was a theoretical investigation of the direct absorption of light. The optical properties of nanoparticles having cylindrical, ellipsoidal, semiellipsoidal, pyramidal and lens shape were analysed in subsequent works [4-20]. The analysis of both the optical transition-matrix elements and the oscillator strengths in the dipole approximation revealed interesting features induced by the size and shape of a nanoparticle. Specifically, it was shown that the shape anisotropy plays a crucial role in determining the optical properties of nanoparticles. The most stimulating results were obtained in [7] in which a charged particle was considered to be in an ellipsoidally shaped potential well. The appropriate Schrödinger equation for an effective mass was separated in prolate spheroidal coordinates and the obtained one-dimensional equations were solved numerically for an ellipsoid arbitrarily deviating from a sphere, but transitions involving highly excited states have never been considered.

Experiments indicate that small nanoparticles have a nearly spherical shape, whereas large nanoparticles have an ellipsoidal shape [21]. For the growth of nanoparticles with various methods, the energy spectrum and, accordingly, the optical properties vary continuously with the size and shape of nanoparticle. It is important to recognise that nanoparticles of ellipsoidal shape have an advantage with respect to spherical quantum dots, which arises from the additional geometrical characteristics related to the shape-anisotropy parameter. That effect makes possible the tuning of the optical properties of objects of nanometre size. The tuneable control of spectral and optical characteristics of