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Spurious Solutions in the Multiband Effective Mass Theory Applied to Low Dimensional Nanostructures

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Abstract. In this paper we analyze a long standing problem of the appearance of spurious, non-physical solutions arising in the application of the effective mass theory to low dimensional nanostructures. The theory results in a system of coupled eigenvalue PDEs that is usually supplemented by interface boundary conditions that can be derived from a variational formulation of the problem. We analyze such a system for the envelope functions and show that a failure to restrict their Fourier expansion coefficients to small k components would lead to the appearance of non-physical solutions. We survey the existing methodologies to eliminate this difficulty and propose a simple and effective solution. This solution is demonstrated on an example of a two-band model for both bulk materials and low-dimensional nanostructures. Finally, based on the above requirement of small k, we derive a model for nanostructures with cylindrical symmetry and apply the developed model to the analysis of quantum dots using an eight-band model.

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1 Introduction

The electronic structure calculation is among the most fundamental problems in modern science and engineering. While achieving a higher accuracy in the methods for such calculations remains an important issue, our ability to construct simpler computational algorithms that would allow us to obtain reliable results in a more efficient and cost-effective manner is paramount for our progress at the practical level with far reaching ramifications in technological applications.

From a mathematical point of view, most methodologies for the construction of such algorithms are based on effective theories where we attempt to reduce the degrees of freedom and to bridge modelling scales [58, 67]. One such theory, derived with the application of the effective mass theorem [84] and known as the multiband effective mass approximation, provides a fundamental tool in predicting electronic properties of structures. We are interested in the development of an efficient computational tool for predicting electronic properties of quantum heterostructures, that is the low-dimensional (semiconductor) nanostructures where the motion of electrons is restricted, forcing them into a quantum confinement [33–35, 100]. Examples of such structures include quantum wells, quantum wires, or quantum dots, where the motion of electrons is restricted in one, two, or all three directions, respectively. Properties of these small nanocrystals, containing often from a few hundred to a few thousand atoms, are very different from the same material in bulk, which results in a wide range of their current and potential applications, from biological tags for proteins to applications in quantum computing, and to a new generation of optoelectronic devices [63, 65, 66].

The reason for our undertaking stems from the fact that typical characteristic dimensions of nanostructures is ranging between 1 to 100 nm while the characteristic dimensions of atoms are between 0.1 to 0.7nm. Over the last decade, a substantial progress in the development of atomistic methodologies for handling such structures (including the device level) has been achieved and we discuss some of the major highlights of this development in Section 2.2. However, it is widely understood in the research community that in many practical situations atomistic approaches remain computationally prohibitive and the development of simple, often continuum-based, mathematical models and their efficient computational implementations become very important. This is particularly true when we have to account for a multiscale nature of the problem (e.g., [28, 59, 61, 64, 67]) and its multiphysics character where several physical fields, such as mechanical, electric, and/or thermal act simultaneously and we have to deal with coupled problems (e.g., [29, 40–43, 49–58, 75, 76, 82, 83, 90–94, 101]).

Coupled problems arise frequently in the applications to nanoscience and nanotechnology and they bring new challenges at the level of the development of mathematical models and efficient numerical methodologies for their solution. Such problems are intrinsic to the multiband effective mass theory, a major focus of the present paper. In dealing with (nano)crystals we use the fact of crystal symmetry characterized by the transformations which in the bulk case leave the structure, and hence its Hamiltonian