

Preface

Currently, as various functional materials and minute electronic devices are produced by the latest nanoscale fabrication technology, it is quite indispensable for scientists and engineers, who continue to challenge the frontier of Nanotechnology, to study and/or rely on authentic first-principles (*ab initio*) calculation methods for correctly understanding electronic configurations and transport properties of nanostructures. However, we know a few practical and tractable calculation methods that accurately describe the relevant physics in nanostructures suspended between semi-infinite electrodes. Indeed, the plane-wave expansion method, a prevailing calculation method in solid-state physics, is not sufficient for determining current flow through nonperiodic nanostructures, because it requires artificial calculation models with three-dimensional periodic geometry. The tight-binding method using a basis set of atomic orbitals is applicable to the analysis for large systems; however, it fails in precise descriptions of electronic states, particularly in the region where tunneling effects dominate.

This book is based on our personal experience with electronic-transport calculations within the schemes of wave-function matching and Green's function matching. For some years, using real-space formalism free from any structural restrictions, we have been developing a first-principles calculation method for electronic-transport properties of nanostructures—overbridging boundary-matching (OBM) method, and we have found that the OBM method is a simple and practical method for doing highly accurate calculations. The book covers this method in a fairly complete fashion, besides introducing other notable real-space calculation methods.

The book consists of two parts: Part I (Chapters 1–5) contains the basic formalism of the real-space finite-difference method with its applications, which lays the vital theoretical foundations of the OBM method

given in Part II. The real-space finite-difference method, in which wave functions and potentials are directly evaluated on real-space grid points instead of using any basis-function sets, has tackled the serious drawbacks of the plane-wave approach, e.g., its inability to describe strictly nonperiodic systems. The *flexibility* of this method allows for highly efficient solutions of electronic ground states of systems in great variety. Then, Part II (Chapters 6–10) focuses on the methods for calculating electronic-transport properties of nanostructures sandwiched between semi-infinite electrodes. Chapters 6–8 are devoted to the formulation of the OBM procedure for wave-function matching and its applications, whereas Chapter 9 deals with some fundamentals of the Green’s function formalism in view of actual practical use. In Appendix B, one sees that when combined with the OBM procedure, the tight-binding method can be a powerful tool for examining transport properties of still larger systems. We attempt to be fairly complete as regards basic schemes, and try to be fairly rigorous with individual subjects.

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