Chapter 12
Heterostructures: Basic Formalism

12.1 Overview

The starting point of any theory of electronic states in semiconductor nanostructures is to explain the origin of the discrete energy states, such as is evident in an optical spectrum or in the tunneling current through a resonant-tunneling device (Fig. 12.1).

![Fig. 12.1](image)

**Fig. 12.1** (a) Absorption spectra at 2 K for GaAs quantum wells. Reprinted with permission from [170]. ©1974 by the American Physical Society. (b) Current and conductance characteristics at 77 K for a GaAs double-barrier structure. Reprinted with permission from [171]. ©1974, American Institute of Physics

The theory of Wannier–Luttinger–Kohn for the effective equation satisfied by a Bloch electron in the presence of a slowly-varying perturbation was applied early on to graded semiconductors [172] and to semiconductor inversion layers [173]. With the growth of atomically-sharp heterojunctions using molecular-beam epitaxy and metal-organo chemical vapor deposition techniques in the 1970s, the same theory was applied to the latter case even though the perturbation is no longer slowly
varying [170, 174–176]. An equivalent problem would be to describe the electronic states in colloidal nanocrystals [177]. In all cases, linear dimensions could be as small as 1–10 nm. The fact that the Wannier–Luttinger–Kohn theory leads to an effective Schrödinger equation for an external potential indicates how this might work for a nanostructure. Thus, the external potential, due to the difference in band edges, would be a confining one leading to a problem similar to the particle-in-a-box problem in textbook quantum mechanics. There are, nevertheless, at least three differences. First, the mass is now the effective mass. Second, as we have seen before, a treatment of the valence band requires a multiband description. Third, contrary to the earlier cases, the material properties (e.g., effective masses and Kane parameters) are now position dependent and do not generally commute with spatial differential operators that appear in the Wannier-like equation. Hence, a proper theory should be able to account for all three effects right from the start.

Nevertheless, there have been three main approaches to the theory of the electronic structure of semiconductor nanostructures. The simplest approach is the one-band or particle-in-a-box model [170, 177, 178]. Another is the envelope-function theory of Bastard [175, 176, 179]. They typically require an ad hoc solution to the operator-ordering problem refered to above. Finally, the third approach is the more recent first-principles envelope-function theory of Burt and Foreman [34, 153, 180, 181]. The latter differs primarily from the previous two in attempting to derive the effective Hamiltonian from first principles. A number of review articles have appeared both on the early theories [95, 182–184] and on the more recent ones [185, 186].

The application of the theory has been to many different types of nanostructures; in particular, to quantum wells (QW’s), superlattices, quantum wires and nanowires, and quantum dots. Quantum wells and superlattices are layered materials where one dimension is on the nanoscale. Quantum wires and nanowires display two-dimensional quantum confinement, the term nanowires being often associated with free-standing wires. Finally, quantum dots display three-dimensional quantum confinement with many analogies to atomic systems. Much of the explicit presentation of the theory in this book will be done for the case of QW’s for simplicity and concreteness; the theory carries over trivially to the other cases with higher degree of quantum confinement. Excellent reviews are available specifically for the quantum-wire [187] and quantum-dot [188] problems.

### 12.2 Bastard’s Theory

Bastard’s theory was developed in two articles and expanded in his book [7, 175, 179].

#### 12.2.1 Envelope-Function Approximation

The basic envelope-function model used was to assume that, in each layer of a heterostructure (here labeled A and B), the wave function can be expanded in terms of