

# Chapter 1

## Introduction to Semiconductor Heterostructures

R. Ferreira

**Abstract** We present an introduction to the physics of semiconductor nanostructures. We review the main assumptions of the  $k \cdot p$  method applied to a bulk crystal and then focus on the envelope function method to describe the electronic states of semiconductor heterostructures.

### 1.1 Introduction

Semiconductor heterostructures have become in the last decades a cornerstone in applicative and fundamental researches on condensed matter. Progresses in the field of semiconductor nano-objects are actually the result of concomitant immense developments in various areas: growth and processing techniques, mastering of materials properties, impressive advances in experimental set-ups and spectroscopic tools, new concepts of structures and devices functioning, the understanding of new physical aspects regarding the coupling of electrons, photons and phonons in low-dimensional systems.

Most such developments are, so to speak, relatively recent, i.e. related to the last two or three decades. The seminal proposal by Esaki and Tsu for band gap engineering by stacking layers of different semiconductors, as well as the early sample realisations, date instead from the 1970s. In the 1980s, systematic optical studies in quantum wells and resonant transport through thin barriers were undertaken. At that time, the main concepts underlying the physics of electrons in semiconductor heterostructures were established. In particular, experimental and theoretical efforts

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R. Ferreira (✉)

Laboratoire Pierre Aigrain, Ecole Normale Supérieure  
24 rue Lhomond, Paris 75231 Cedex 05, France  
e-mail: robson.ferreira@lpa.ens.fr

have permitted to clearly establish quantum confinement and tunnel coupling as key concepts in the field. The appearance of new structures and concepts marked the 1990s. Amongst them we quote (non exhaustively): (i) fabrication and first theoretical modelling of quantum wires and dots, which pushed forward the field of lower (quasi one and zero) dimensional electronic systems; (ii) the exploitation of more and more elaborate stacks of alternating well and barrier layers, like in semiconductor superlattices and periodic structures for quantum cascade lasers (QCL) and (iii) the coming into play of dielectric light confinement altogether with electronic confinement, which launched the field of strong light–matter coupling in semiconductor heterostructures. Quantum dots (QDs), semiconductor microcavities and quantum cascade structures brought to the stage many new aspects of heterostructure physics: the realisation of quasi-atomic structures in a crystalline matrix, the ability to control the light–matter coupling and the study of new elementary quasi-particles (cavity polaritons) in condensed matter, and a new concept (unipolar scheme) for laser light generation in the mid-IR spectral domain. In the last decade the multiple developments of these fields can be observed, as well as the rapid growth of new ones, like nanoacoustics and nanophotonics. A key concept underlying the research efforts in this period is “coherence”. Indeed, many efforts in the semiconductor nanostructure domain have been devoted, in parallel with worldwide studies in many fields, to the realisation of physical systems operating in the (ideally) pure quantum regime, as motivated by the potential implementation of future opto-electronic devices. This has in particular pushed the understanding of decoherence sources in the nano-objects, revealing both the profound influence of the nano-object environment on its electronic and optical properties, as well as many particular aspects of electron–phonon coupling in low-dimensional systems. Additionally, crossing domains have emerged and become mature fields by themselves, like: (a) studies of quantum dots in various kinds of optical (micro-) cavities; (b) studies of strong light–matter couplings in quantum-cascade-like structures (inter subbands polaritons); (c) use of superlattices and quantum dots for the optical generation of acoustic signals. It is finally worth stressing the continuous improvement of the theoretical description of electronic states of nanostructures, in parallel and jointly with advances in sample realisation and experimental studies (we shall come back to this point later on in this chapter; see also Paul Voisin’s contribution in this volume).

Delimiting the field of semiconductor heterostructures is nonsense: in fact, semiconductor nano-objects are today present in numerous areas, and concepts and techniques from many different fields contribute to the advance of nanostructured semiconductor physics. Thus, interdisciplinary concepts and efforts have become a driving force of research nowadays. To illustrate this point, and without aiming to be exhaustive, one can quote: (i) the tremendous developments of the physics of an electron gas confined near a semiconductor heterojunction; (ii) the realisation of structures containing either semiconductor or metallic layers, in the field of spintronics, aiming at developing hybrid devices for the concomitant generation and detection of spin-polarised carriers; (iii) embedding semiconductor-based systems (like QDs and QCL structures) in photonic crystals, aiming at improving/controlling

light–matter coupling and developing light sources with specific characteristics; (iv) the impressive number of transport and optical studies done on carbon nanotubes.

This book aims at presenting an introduction to the physics of semiconductor heterostructures (for a comprehensive review see [1]; see also [2, 3]). This cannot be envisioned without recalling the physics of bulk semiconductors. Indeed, in a rough image, a semiconductor nanostructure is made of juxtaposed pieces of different semiconductors, and, as we will recall, their electronic levels and optical properties retain many fundamental aspects of the corresponding ones for the original materials. The first part is thus devoted to a quick review of bulk properties: the electron Bloch states and the effective mass description of near-edge conduction and valence bands states (see e.g. [4–6]). In the second part we introduce the envelope function method to describe electronic levels in perturbed semiconductors. Indeed, an overwhelming number of studies in semiconductor physics are intimately related to the presence of some kind of perturbation: doping with shallow impurities provide carriers; a d.c. bias triggers a current; the optical characteristics are the response of the crystal to an external e.m. excitation. The building of a theoretical framework allowing the description of electronic levels in perturbed crystals is thus naturally the object of immense efforts from the very beginning of semiconductor physics [7]. The envelope function method appeared as a versatile approach for many cases of interest, namely whenever the perturbation strength is “weak” enough (as compared to typical band energy widths or separations) and “slowly varying” in space (as compared e.g. to the lattice period). The simplest heterostructures are introduced in the third part. We also present an envelope function description of their one-electron states. As we shall see, although the nanostructuring process introduces as a rule a large (in energy) and abrupt (i.e., at the cell size scale) variation of the crystal potential, it can nevertheless be properly tackled by the envelope function method, provided some assumptions, to be discussed later on, are retained in the model.

## 1.2 Electronic States of Bulk Semiconductors

We review in the first part of this paragraph the fundamental concepts related to the formation of energy bands in a semiconductor and the principal characteristics of their electronic states (Bloch functions). The second part is devoted to the  $\vec{k} \cdot \vec{p}$  method.

### 1.2.1 Fundamental Concepts

The key concept in a perfect crystal is *translational invariance*, which characterises the presence of a spatial order at the microscopic level. To describe translational invariance we define a set of lattice vectors: the Bravais ensemble  $\{\vec{R}\}$ . In this way, two points in space differing by a lattice vector are physically equivalent. As a consequence, any physical property (i.e. any observable) of an idealised crystal in

its ground state is invariant under translation by a lattice vector. For instance, the density of electronic charge is a periodic function on the crystal lattice. This is a very fundamental statement, to which any theoretical model aiming at describing the physical properties of a semiconductor should conform, and distinguishes from the very beginning a crystal from an atomic or molecular system in empty space. Strictly speaking, a real sample is finite in size. Nonetheless, the initial assumption of strict periodicity, which applies only for infinite size material, turns out to be a very robust concept in “large enough” systems. Deviations from this infinite-size model for a crystal introduce surface effects, but do not affect its *bulk* properties. Also, interface effects will be of primary importance in nanostructures. For the moment, we keep considering the assumption of translational invariance and shall have the opportunity to come back again to surface and interface effects later on.

From this single assumption, a full set of physical and theoretical results follows. At the outset, it is worth recalling the very useful mathematical concept of *reciprocal lattice*. Indeed, any periodic function in the real lattice can be decomposed in Fourier series within an ensemble of reciprocal lattice vectors  $\{\vec{K}\}$  obeying  $\vec{K} \cdot \vec{R} = 2\pi n$ , with  $n$  an arbitrary integer. We thus possess two equivalent discrete sets of vectors to describe a perfect crystal:  $\{\vec{R}\}$  and  $\{\vec{K}\}$ . The two ensembles share some important properties: (i) the vectors of the ensemble form a periodic lattice in either real or reciprocal spaces, so that each vector can be written in terms of elementary basis vectors  $\vec{R} = i_1\vec{a}_1 + i_2\vec{a}_2 + i_3\vec{a}_3$  and  $\vec{K} = j_1\vec{b}_1 + j_2\vec{b}_2 + j_3\vec{b}_3$ , where  $i_{1,2,3}$  ( $j_{1,2,3}$ ) are integers and  $\vec{a}_{1,2,3}$  ( $\vec{b}_{1,2,3}$ ) are the generating basis in the real (reciprocal) space; (ii) the volume span by the basis vectors form a unitary cell, rigid translations of which within the lattice (i.e. by using the different combinations of  $i_{1,2,3}$  or  $j_{1,2,3}$ ) permits completely filling the space without overlap. The choice of the basis vectors, and thus also of the unitary cells is however arbitrary. There is nevertheless one particular choice that more clearly reflects the symmetry properties of the crystal: this is the Wigner-Seitz cell in real space and its corresponding reciprocal lattice counterpart, the Brillouin Zone (BZ). These particular unit cells, definitions and their constructions in the two spaces are presented and discussed in many workbooks (see e.g. [4, 5]). In the following, we shall implicitly assume the Wigner-Seitz cell in real space and first Brillouin cell in reciprocal space.

Our principal objective is to discuss a method for calculation of electronic states in a semiconductor. This task is of course impossible for a real system, i.e. constituted of a (virtually) infinite number of carriers of either charges: electrons and nuclei. Two approximations are usually invoked to overcome this difficulty: the Born-Oppenheimer and the Hartree-Fock approximations. The first allows disentangling the nuclei and electron motions, whereas the second replaces the true N-electrons problem into an effective one-electron problem. These assumptions, exhaustively discussed in the literature, will not be detailed here. We shall only recall two major consequences of them. (i) The problem of finding the electronic eigenstates of a crystal fits a one-electron problem  $H_{\text{cr}} = T + V_{\text{cr}}(\vec{r})$ , where  $T = \vec{p}^2/(2m_0)$  is the kinetic energy operator ( $m_0$  the bare electron mass) and  $V_{\text{cr}}(\vec{r})$  the effective crystal potential. (ii) However, the true expression of  $V_{\text{cr}}(\vec{r})$  is hardly known: although the

bare interactions are coulombic-like in the original N-body problem, the simplifications brought about by the Born-Oppenheimer and Hartree-Fock schemes considerably influence the profile of the effective crystal potential. A lot of considerable theoretical effort has been put in evaluating its precise form or, equivalently, different matrix elements involving  $V_{\text{cr}}(\vec{r})$ . We shall here instead adopt a more pragmatic strategy, namely, exploit as much as possible the *symmetry properties* of  $V_{\text{cr}}(\vec{r})$  and push as far as possible the description of the crystal eigenstates. As we shall see in the following, we will end up with a semi-phenomenological description of the electronic states in terms of effective parameters, which are ultimately related to different matrix elements involving the eigenstates of  $H_{\text{cr}}$ .

Accounting thus for the two aforementioned approximations, we shall look in the following for the stationary eigenstates of one electron in a static potential  $V_{\text{cr}}(\vec{r})$ . Although not analytically known, the effective potential should comply with translational invariance:  $V_{\text{cr}}(\vec{r} + \vec{R}) = V_{\text{cr}}(\vec{r})$  for any  $\vec{R}$ . Mathematically speaking, this constraint on  $V_{\text{cr}}(\vec{r})$  classes the possible one-electron eigenstates of  $H_{\text{cr}}$  into a very particular kind of solutions: those fulfilling the Bloch condition, namely, any solution  $\Psi(\vec{r})$  verifying  $\Psi(\vec{r} + \vec{R}) = \exp\{i\theta(\vec{R})\} \Psi(\vec{r})$ , where  $\theta(\vec{R})$  is an  $\vec{R}$ -dependent phase. Note that  $\theta(\vec{R})$  should be real to ensure wavefunction normalisation and crystal invariance of any physical property depending upon the electron charge density  $|\Psi(\vec{r})|^2$ . It can also be readily checked that the term  $\exp\{i\theta(\vec{R})\}$  is simply the eigenvalue of the operator  $T_{\vec{R}}$  performing a translation by  $\vec{R}$  in the real space:  $T_{\vec{R}} f(\vec{r}) = f(\vec{r} + \vec{R})$  for any function  $f(\vec{r})$ . More information about this phase can be obtained by the fact that two translation operations in space commute, and thus  $\theta(\vec{R}_1 \pm \vec{R}_2) = \theta(\vec{R}_1) \pm \theta(\vec{R}_2)$ . These results can be cast in the form  $\theta(\vec{R}) = \vec{k} \cdot \vec{R}$ , where  $\vec{k} = (k_x, k_y, k_z)$  is a constant (and so far unspecified) three-dimensional real vector. The  $\vec{k}$  wavevector can thus be used to label the eigenstates:  $\Psi_{\vec{k}}(\vec{r})$ .

In order to proceed, we note that a Bloch state can be written in the form

$$\Psi_{\vec{k}}(\vec{r}) = e^{i \vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r}) \quad (1.1)$$

where  $u_{\vec{k}}(\vec{r})$  is a periodic function over the crystal lattice:  $u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r})$ . It is evident that this form fulfils the Bloch property  $\Psi(\vec{r} + \vec{R}) = e^{i \vec{k} \cdot \vec{R}} \Psi(\vec{r})$  imposed by the existence of translational invariance. Also, one can easily show that the periodic part of the Bloch state is solution of the stationary eigenvalue problem

$$[H_{\text{cr}} + \hbar \vec{k} \cdot \vec{p}/m_0] u_{\vec{k}}(\vec{r}) = [E(\vec{k}) - \hbar^2 \vec{k}^2/(2m_0)] u_{\vec{k}}(\vec{r}) \quad (1.2)$$

The determination of the total eigenstate  $\Psi_{\vec{k}}(\vec{r})$  is replaced by the determination of the periodic solutions  $u_{\vec{k}}(\vec{r})$ . Of course, this cannot be accomplished without knowledge of  $V_{\text{cr}}(\vec{r})$ . However, it is important to realise that such an eigenvalue problem admits more than one solution. Actually, there should be infinity of solutions for a given  $\vec{k}$  value. We need correspondingly a new label (or a new set of labels)

to fully determine the eigenstates. This label is the *band* index,  $n$ . The reason for this name is the following: the eigenfunctions read now as  $\Psi_{n,\vec{k}}(\vec{r})$ , whereas the corresponding energies  $E_n(\vec{k})$  become (quasi-) continuous functions of the (quasi-continuous) variable  $\vec{k}$ , so that  $E_n(\vec{k})$  describes an energy band when  $n$  is kept constant and  $\vec{k}$  is varied inside the first BZ.

Let us now stress the fact that the wavevector labelling the crystal eigenstates can be restricted to the first Brillouin zone. Indeed, two wavevectors differing by a reciprocal lattice vector  $\vec{K}$  have the same Bloch phase (as can be immediately shown by using  $\vec{K} \cdot \vec{R} = 2\pi n$ ). The values that  $\vec{k}$  can assume are usually specified by imposing the so-called Born – von-Karm boundary conditions to the problem: the idealised infinite crystal is replaced by a finite-size sample with periodic eigenstates, i.e.

$$\Psi_{n,\vec{k}}(x + L_x, y, z) = e^{i k_x L_x} \Psi_{n,\vec{k}}(\vec{r}) \equiv \Psi_{n,\vec{k}}(\vec{r}) \quad (1.3)$$

for a translation along the Ox direction over the whole sample size  $L_x = N_x a_x$ , where  $a_x$  is the lattice period along the Ox direction and  $N_x$  the number of crystals sites along this same direction. This restricts the  $k_x$  wavevectors to the ensemble of  $N_x$  values:  $\{2\pi n_x / N_x\}$ ,  $0 \leq n_x < N_x$ . Note that there is thus as many allowed  $k_x$  values as unity cells along the Ox direction, and that  $k_x$  values outside this interval are redundant since they lead to the same Bloch phase: indeed, for  $k'_x = k_x + 2\pi i_x / L_x$  there is  $\exp\{i k'_x L_x\} = \exp\{i k_x L_x\}$  for any integer  $i_x \neq 0$ . The ensemble  $\{2\pi i_x / L_x\}$  is equal to the previously defined reciprocal space wavevectors (here in one dimension). Thus, it results that  $k_x$  can be restricted to values inside the first Brillouin Zone. The same results hold for the two other real space directions, defining analogously  $k_y$  and  $k_z$ . In conclusion, the two principal results that follow the Born – von-Karm assumption are that:

- (i) the non-redundant wavevectors can be restricted to the first Brillouin zone of the crystal lattice;
- (ii) there are as many  $\vec{k}$  allowed wavevectors (and thus one-electron eigenstates *per band*, without considering spin degeneracy) as unity cells in the crystal.

Note that the first result does not follow straightforwardly from the effective eigenvalue problem defining  $u_{\vec{k}}(\vec{r})$ . However, it can be demonstrated that the set of eigensolutions obtained when replacing  $\vec{k}$  by  $\vec{k} + \vec{K}$  in (1.2) is actually  $\vec{K}$ -independent (see e.g. [4, 5]):  $u_{n,\vec{k} + \vec{K}}(\vec{r}) = u_{n,\vec{k}}(\vec{r})$  (except possibly by an absolute constant phase);  $E_n(\vec{k} + \vec{K}) = E_n(\vec{k})$ . As a consequence, both the periodic functions and the energy dispersions (i.e. energy variation as a function of the wavevector) related to Bloch states are periodic functions in the reciprocal space.

Note additionally that the second result (ii) is essential, since it allows recovering extensibility for average physical properties regarding a finite-size sample. It could, actually, surprise us, owing to the sample-dependent nature of the result. Nonetheless, the sample-to-sample variations are meaningless in practice, since for a fixed band  $n$  the energy difference between states related to two consecutive  $\vec{k}$  values is very small (it is actually roughly inversely proportional to the squared inverse of the

characteristic sample size), and thus impossible to be observable in any actual (i.e., macroscopic) sample. That implies that any small (as compared to the BZ) volume  $\Delta_k$  in reciprocal space contains a large number of states:  $\Delta_k \Omega_{\text{cr}} / (2\pi)^3$ , where  $\Omega_{\text{cr}}$  is the crystal volume (a result that can be easily demonstrated by recalling that one state occupies the length  $2\pi/L_x$  of the first BZ of a one-dimensional crystal, and thus a volume  $(2\pi/L_x) (2\pi/L_y) (2\pi/L_z)$  in a three-dimensional crystal). Finally, in any practical calculation involving the whole set of eigenstates of a given energy band, we will be authorized to replace any summation over  $\vec{k}$  as follows:

$$\sum_{\vec{k}} F(\vec{k}) \rightarrow \frac{\Omega_{\text{cr}}}{(2\pi)^3} \int d\vec{k} F(\vec{k}) \quad (1.4)$$

with  $d\vec{k} = dk_x dk_y dk_z$ , provided the function  $F(\vec{k})$  varies “slowly enough” with  $\vec{k}$  (its Fourier transform varies “slowly enough” in real space as compared to the lattice parameter).

Let us now come back to the periodic functions  $u_{n,\vec{k}}(\vec{r})$ . As mentioned, we cannot calculate  $u_{n,\vec{k}}(\vec{r})$  without the knowledge of  $V_{\text{cr}}(\vec{r})$ . However, similar to the existence of Bloch states (and the natural introduction of wavevectors as well as the existence of energy bands) that directly follows from the translational symmetry, one can proceed further and obtain a deeper insight into the crystal eigenstates by considering another very general symmetry property of  $V_{\text{cr}}(\vec{r})$ , namely, the fact that  $V_{\text{cr}}(\vec{r})$  should equally reflect the *local* invariance of the crystal lattice. As far as rotational symmetry is considered, of course, there is no infinitesimal rotational invariance in a crystal, as one finds for an isolated atom (in this latter case the invariance is related to the isotropy of space, whereas a crystal medium is intrinsically anisotropic and physical properties are isotropic only in certain limits and/or under certain conditions). However, it is quite intuitive that there is angular isotropy inside a crystal for *finite* rotations in space. For instance, a cubic lattice with a single atom per site is invariant under an  $n\pi/2$  rotation around any of its principal axis, with  $n$  an arbitrary integer. The stationary eigenstates should reflect this symmetry. Such rotations are better dealt with within the group theory formalism. Without going into the details, one may say, on very general grounds, that the Bloch eigenstates related to high symmetry points in the Brillouin zone should be invariant under a certain number of local transformations that leave invariant the crystal lattice structure. Such local transformations include both finite rotations as well as eventual reflexions through given plans. By high symmetry points we mean particular points (values of  $\vec{k}$ ) of the Brillouin zone, and at these points only the wavefunctions fulfil specific symmetry requirements.

For the sake of this review, we shall concentrate on semiconductors with a particular lattice structure: the so-called zinc-blend lattice. This particular structure includes a large variety of semiconductors that will be considered in the following: III-V (GaAs, InAs, AlAs, ...) and II-VI (CdTe, CdSe, ...) materials. Group IV materials (Ge, Si) have a diamond structure, which corresponds to the zinc-blend structure with two identical atoms per unit cell. Conversely, the zinc-blend structure is the diamond one with two different atoms per unit cell.

It turns out that the  $k = 0$  point of the BZ is particularly important in zinc-blend materials and has been given a particular name: the  $\Gamma$  point. It is a “high-symmetry” point, i.e. the solutions (eigenfunctions) related to this point display well-defined symmetry properties. Let us now quote two important results that will be used in the following:

- (a) It is known from experiments that the fundamental band gap of the semiconductors we will be interested in (like GaAs) occurs at  $k = 0$  and also that most of the optical and low bias transport characteristics of such materials involve electronic states (of the uppermost filled valence band and/or low lying empty conduction band) with small wavevectors, i.e. conduction and valence states near the  $\Gamma$  point. Moreover, other  $k = 0$  edges are energetically far below the uppermost filled valence band or far above the low-lying empty conduction band. As a consequence, in most semiconductors and semiconductor-based heterostructures we will mostly be concerned with a small part of the crystal band structure, in both  $\vec{k}$  and energy axes, namely, with states around  $k = 0$  and pertaining to the topmost valence and low-lying conduction bands. Note however that the remote bands cannot be neglected, as we will see below.
- (b) Group theory analysis (not detailed here) indicates that the  $k = 0$  states around the fundamental interband gap have the following symmetry characteristics (in absence of spin-orbit coupling, to be considered later): there is one low-lying conduction state with “S” orbital symmetry and three uppermost valence states with “P” orbital symmetry. The “practical” meaning of “S” and “P” orbital symmetries will be given later on.

In the following paragraph, we use these two results to discuss the  $\vec{k} \cdot \vec{p}$  method, which is particularly versatile for the description of electronic states with energy around the fundamental band gap and  $\vec{k}$  near the  $\Gamma$  point.

### 1.2.2 The $\vec{k} \cdot \vec{p}$ Method

As mentioned above, we are particularly interested in the description of the states pertaining to a small part of the crystal band structure, in both  $k$  and energy axes, namely, the states around  $k = 0$  and related to the topmost valence and low-lying conduction bands. The  $\vec{k} \cdot \vec{p}$  method is particularly versatile for the description of such electronic states. However, its starting point is actually much more general than focusing in the more interesting but rather small region in energy *versus*  $\vec{k}$  space. Indeed, the structure of the effective eigenvalue problem (1.2) strongly suggests spanning the  $\vec{k} \neq 0$  solutions on the basis of the  $k=0$  solutions, assumed to be known:

$$u_{n,\vec{k}}(\vec{r}) = \sum_{n'} a_{n'}(\vec{k}) u_{n',0}(\vec{r}) \quad (1.5)$$

where  $H_{\text{cr}} u_{n,0}(\vec{r}) = E_{n,0} u_{n,0}(\vec{r})$  with  $u_{n,0}(\vec{r}) = u_{n,\vec{k}=0}(\vec{r})$  and  $E_{n,0} = E_n(\vec{k} = 0)$ . This gives the matrix eigenvalue problem to solve:

$$\left\{ \left[ E_{n,0} - E_n(\vec{k}) + \hbar^2 \vec{k}^2 / (2m_0) \right] \delta_{n',n} + \hbar \vec{k} \cdot \vec{p}_{n',n} / m_0 \right\} a_{n'}(\vec{k}) = 0 \quad (1.6)$$

This method gives in principle exact crystal eigensolutions if one is able to provide a complete set of energy values ( $E_{n,0}$ ) and matrix elements for the momentum operator ( $\vec{p}_{n',n}$ ) associated with the  $k = 0$  states. This is actually impossible to implement and a truncation of the  $k = 0$  ensemble is unavoidable in actual calculations. Before considering such approximations, it is worth stressing at this point one important aspect of the  $\vec{k} \cdot \vec{p}$  formalism. One could envision combining group theory analysis and experiments to obtain detailed information about the *parameters*  $E_{n,0}$  and  $\vec{p}_{n',n}$ : the theory allowing to ascertain which of the numerous matrix elements actually do not vanish, while an ideally complete set of experiments would provide the values of such matrix elements (at least their absolute values) as well as the energy edges  $E_{n,0}$ . In this sense, the  $\vec{k} \cdot \vec{p}$  approach appears as a semi-phenomenological model, in which general considerations based on symmetry arguments are used to push as far as possible the theoretical description, whereas the final determination of ultimate parameters is ensured by experiments. This strategy allows circumventing the very first (and possibly the principal) difficulty underlying the modelling of the one-electron crystal eigenstates, namely, the lack of detailed knowledge of the actual crystal potential  $V_{\text{cr}}(\vec{r})$ .

Different kinds of approximations follow from different truncation schemes and/or treatment of “remote”  $k = 0$  edges (i.e. states with energy  $E_{n,0}$  very far from the energy interval around the fundamental band gap we are interested in). The crudest approximation consists in retaining only the four states (the conduction “S” and the three valence “P” states) mentioned above in the basis: the simplified Kane model. In this case the  $4 \times 4$  hamiltonian matrix (in the basis  $S, P_x, P_y, P_z$ ) reads as:

$$\begin{array}{ccccc} & |S\rangle & |P_x\rangle & |P_y\rangle & |P_z\rangle \\ \begin{array}{l} |S\rangle \\ |P_x\rangle \\ |P_y\rangle \\ |P_z\rangle \end{array} & \begin{array}{l} \lambda_S \\ \Pi^* k_x \\ \Pi^* k_y \\ \Pi^* k_z \end{array} & \begin{array}{l} \Pi k_x \\ \lambda_P \\ 0 \\ 0 \end{array} & \begin{array}{l} \Pi k_y \\ 0 \\ \lambda_P \\ 0 \end{array} & \begin{array}{l} \Pi k_z \\ 0 \\ 0 \\ \lambda_P \end{array} \end{array} \quad (1.7)$$

where  $\lambda_{S,P} = E_{S,P} + \hbar^2 \vec{k}^2 / (2m_0)$ .  $E_S = E_{c,0}$  and  $E_P = E_{v,0}$  are the edges of the conduction and valence band, respectively, which define the interband gap  $E_G = E_S - E_P$ . This matrix has been obtained by making explicit use of the aforementioned symmetry properties of the “S” and “P” orbitals, which in the present case states that only three interband matrix elements do not vanish and they are all equal:  $\langle S | p_x | P_x \rangle = \langle S | p_y | P_y \rangle = \langle S | p_z | P_z \rangle = \Pi$ , where capital P is used to label the three P-like orbitals, while small  $p$  denotes momentum operator. The four eigenenergies are readily obtained as:

$$\begin{aligned}
(\lambda_P - e)^2 &= 0 && \Rightarrow 2 \text{ solutions} \\
(\lambda_P - e)(\lambda_S - e) &= |\Pi|^2 k^2 && \Rightarrow 2 \text{ solutions}
\end{aligned} \tag{1.8}$$

Inserting the obtained solutions back in the matrix eigenproblem allows extracting the expansion coefficients and thus the searched periodic functions (and the full Bloch wavefunction) for any  $\vec{k}$  value. Note that the model lies on two parameters: the interband matrix element of the momentum operator and the interband gap  $E_G = E_S - E_P$ . Their precise values cannot, of course, be inferred from the model itself, but can be extracted from measurements. To illustrate this point, let us consider the eigenstates for energies around the conduction band edge :  $E \approx E_S$ . To the lowest order in the inter-band coupling one has:

$$\begin{aligned}
E(\vec{k}) &\approx E_S + \frac{\hbar^2 \vec{k}^2}{2m_c^*}; & \frac{1}{m_c^*} &= \frac{1}{m_0} + \frac{|\Pi|^2}{E_G} \\
u_{c,\vec{k}}(\vec{r}) &\approx S(\vec{r}) + \frac{\Pi^*}{E_G} \left\{ k_x P_x(\vec{r}) + k_y P_y(\vec{r}) + k_z P_z(\vec{r}) \right\}
\end{aligned} \tag{1.9}$$

The dispersion is parabolic with effective mass  $m_c^* < m_0$ . As a consequence, information on  $|\Pi|$  can be extracted from the electron effective mass (as measured e.g. in cyclotron resonance experiments), while  $E_G$  can be inferred from optical absorption experiments. It turns out that for various zinc-blend semiconductors  $E_P \approx 23$  meV. For GaAs,  $E_G = 1.5$  eV at low temperature and thus  $m_c^*/m_0 \approx 0.07 \ll 1$ .

As crude as it appears (we discuss below its main drawbacks), this model captures two essential features of the crystal electronic states: (i) the near edge dispersions are to a good approximation parabolic with effective masses governed by second order (interband)  $\vec{k} \cdot \vec{p}$  couplings, and (ii) the Bloch functions for mobile electrons are admixtures of conduction and valence band solutions. If, on the one hand, the effect of  $\vec{k} \cdot \vec{p}$  couplings on the effective masses cannot be disregarded ( $m_c^*/m_0 \ll 1$ ), on the other hand the admixtures in the wavefunctions can in many circumstances be neglected, allowing to speak in terms of conduction and valence states as thought pure (i.e. non-admixed) in character: for instance,  $u_{c,\vec{k}}(\vec{r}) \approx u_{c,0}(\vec{r}) = S(\vec{r})$ .

The principal drawback of the simplified Kane model is the occurrence of two valence band dispersions with positive effective mass (and equal to the bare electron one). The corresponding eigenstates are pure valence-band states, thus unaffected by the interband couplings. One can explain this result by invoking a general quantum mechanical argument: the problem of one discrete state (the conduction one) coupled to the states of a degenerate ensemble (the valence ones) can always be reduced to a two levels problem. Indeed, it is always possible to properly hybridize (i.e. linearly combine) the degenerate states in such a way that amongst the states of the new (degenerated and orthonormalized) ensemble only one possesses a nonzero matrix element with the discrete state, all others remaining uncoupled. Actual band structure models account for three essential ingredients not present in the simplified Kane model: spin degeneracy, spin-orbit coupling and interband coupling to states outside the  $\{S, P_x, P_y, P_z\}$  subspace, keeping nonetheless the initial semi-phenomenological strategy of the  $\vec{k} \cdot \vec{p}$  method. We illustrate this point with the Luttinger Hamiltonian that

describes the topmost valence states in diamond-like semiconductors (in this case the low-lying conduction band is treated as a remote band). First point: the consideration of spin enlarges the  $k = 0$  basis to six states:  $P_x \uparrow$ ;  $P_x \downarrow$ ;  $P_y \uparrow$ ;  $P_y \downarrow$ ;  $P_z \uparrow$ ;  $P_z \downarrow$ . Second point: the consideration of the spin-orbit coupling (of the same physical origin as isolated atoms) within this new basis splits the 6-fold degenerate state into a quadruplet (Q) and a doublet (D):

| <i>state</i>  |                    |                                                                                               | <i>energy shift</i> |        |
|---------------|--------------------|-----------------------------------------------------------------------------------------------|---------------------|--------|
| $ Q_1\rangle$ | $ +3/2\rangle$     | $\frac{1}{\sqrt{2}} (P_x + iP_y) \uparrow\rangle$                                             | $+\Delta/3$         |        |
| $ Q_2\rangle$ | $  -1/2\rangle$    | $\frac{-1}{\sqrt{6}} (P_x - iP_y) \uparrow\rangle - \sqrt{\frac{2}{3}} P_z \downarrow\rangle$ | $+\Delta/3$         |        |
| $ Q_3\rangle$ | $ +1/2\rangle$     | $\frac{1}{\sqrt{6}} (P_x + iP_y) \downarrow\rangle - \sqrt{\frac{2}{3}} P_z \uparrow\rangle$  | $+\Delta/3$         | (1.10) |
| $ Q_4\rangle$ | $  -3/2\rangle$    | $\frac{-1}{\sqrt{2}} (P_x - iP_y) \downarrow\rangle$                                          | $+\Delta/3$         |        |
| $ D_1\rangle$ | $ SO; +1/2\rangle$ | $\frac{1}{\sqrt{3}} (P_x + iP_y) \downarrow\rangle + \frac{1}{\sqrt{3}} P_z \uparrow\rangle$  | $-2\Delta/3$        |        |
| $ D_2\rangle$ | $ SO; -1/2\rangle$ | $\frac{-1}{\sqrt{3}} (P_x + iP_y) \uparrow\rangle + \frac{1}{\sqrt{3}} P_z \downarrow\rangle$ | $-2\Delta/3$        |        |

where  $\Delta$  is the spin-orbit energy involving the  $\{P_x, P_y, P_z\}$  states. The states of the lower energy doublet are called “split-off” (SO) states. The linear combinations of orbital and spin components displayed in the previous table are the same as obtained for the three  $P$  states of an isolated atom in the presence of spin-orbit coupling, whose orbital wavefunctions possess well-defined orbital angular momentum components along a given axis, whereas the total wavefunctions possess well-defined total angular momentum components along this same axis. In a crystal the  $k = 0$  orbital states are said to be eigenstates of a pseudo-angular momentum operator, whereas the quadruplet and triplet states are eigenstates of a pseudo-total angular momentum operator. Third point: the inclusion of remote  $k = 0$  states are necessary to obtain a fair description of the energy dispersions (i.e. dependence of the energies with  $k$ ). Indeed, the  $k \cdot \vec{p}$  matrix elements amongst the restricted basis of P-like states vanish. Such couplings involve, as previously mentioned, a number of interband matrix elements and interband energy gaps. However, symmetry analysis shows that only a small number of parameters “effectively” govern the valence band dispersions. To illustrate this point, let us further restrict ourselves to the description of the sole uppermost states (i.e. associated with the quadruplet of  $k = 0$  states). In this case the four dispersions are eigensolutions of the  $4 \times 4$  Luttinger matrix

|                 | $ +3/2\rangle$ | $  -1/2\rangle$ | $ +1/2\rangle$ | $  -3/2\rangle$ |        |
|-----------------|----------------|-----------------|----------------|-----------------|--------|
| $ +3/2\rangle$  | $H_{hh}$       | $c$             | $b$            | $0$             |        |
| $  -1/2\rangle$ | $c^*$          | $H_{lh}$        | $0$            | $-b$            |        |
| $ +1/2\rangle$  | $b^*$          | $0$             | $H_{lh}$       | $c$             | (1.11) |
| $  -3/2\rangle$ | $0$            | $-b^*$          | $c^*$          | $H_{hh}$        |        |

where

$$\begin{aligned}
H_{hh}(\vec{k}) &= \frac{\hbar^2}{2m_0} \left[ (\gamma_1 - 2\gamma_2)k_z^2 + (\gamma_1 + \gamma_2)(k_x^2 + k_y^2) \right] \\
H_{lh}(\vec{k}) &= \frac{\hbar^2}{2m_0} \left[ (\gamma_1 + 2\gamma_2)k_z^2 + (\gamma_1 - \gamma_2)(k_x^2 + k_y^2) \right] \\
c(\vec{k}) &= \frac{\sqrt{3}\hbar^2}{2m_0} \left[ \gamma_2(k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y \right] \\
b(\vec{k}) &= \frac{-i\sqrt{3}\hbar^2}{m_0} \gamma_3 (k_x - ik_y)k_z
\end{aligned} \tag{1.12}$$

are functions of only three adimensional parameters,  $\gamma_{1,2,3}$ : the Luttinger parameters. They incorporate all non-diagonal  $\vec{k} \cdot \vec{p}$  couplings of the valence states with remote bands. Their values have been obtained for a series of materials. For instance, for GaAs there is:  $\gamma_1 = 6.85$ ;  $\gamma_2 = 2.1$ ;  $\gamma_3 = 2.9$ . The labels “hh” and “lh” correspond, respectively, to the “heavy” and the “light” dispersions: for propagation along the Oz axis ( $k_{x,y} = 0$ ), the non-diagonal terms of the Luttinger matrix vanish and one readily obtains two dispersions, related respectively to the  $\pm 3/2$  and to the  $\pm 1/2$  states. Since the hh-related mass ( $m_0/(\gamma_1 - 2\gamma_2)$ ) is larger than the lh-related one ( $m_0/(\gamma_1 + \gamma_2)$ ), the  $\pm 3/2$  states are usually called “heavy” states and the  $\pm 1/2$  ones “light” states. Note however that for  $k_{x,y} \neq 0$ , the non-diagonal terms do not vanish and the corresponding valence state wavefunction contains both heavy and light components.

### 1.3 Envelope Function Model

Let us now introduce the envelope function method to describe electronic levels in perturbed semiconductors. Indeed, as previously mentioned, an overwhelming number of studies in semiconductor physics is related to the modification of the crystal properties due to the presence of some kind of perturbation: doping with shallow impurities provides carriers; a d.c. bias triggers a current; the optical characteristics are the response of the crystal to an external e.m. excitation. The envelope function method is a versatile approach for many cases of interest, namely whenever the perturbation strength is “weak” enough (as compared to typical band energy widths or separations) and “slowly varying” in space (as compared e.g. to the lattice period) [5]. However, our main objective is to show that the envelope function description can be used to describe the electronic states of heterostructures. This is actually not evident *per se*, since, as we shall see, the nanostructuration process introduces as a rule large (in energy) and abrupt (i.e. at the cell size scale) variation of the crystal potential.

For definiteness, let us assume a position-dependent perturbation to the crystal Hamiltonian  $H = H_{\text{cr}} + W(\vec{r})$ . As a starting point, we take advantage of the fact that the Bloch states (eigenstates of  $H_{\text{cr}}$ ) form a complete basis ( $\langle \Psi_{n,\vec{k}} | \Psi_{n',\vec{k}'} \rangle = \delta_{n,n'} \delta_{\vec{k},\vec{k}'}$ ) that can be used to diagonalise the perturbation term. We expand correspondingly the perturbed eigenfunctions within this basis:

$$|\Psi\rangle = \sum_{n, \vec{k}} a_n(\vec{k}) |\Psi_{n, \vec{k}}\rangle \quad (1.13)$$

The coefficients are solutions of the Hamiltonian matrix

$$\sum_{n', \vec{k}'} \left\{ \left[ E_{n'}(\vec{k}') - E \right] \delta_{n, n'} \delta_{\vec{k}, \vec{k}'} + W_{n', \vec{k}'}^{n, \vec{k}} \right\} a_{n'}(\vec{k}') = 0 \quad (1.14)$$

The sum runs over the whole set of Bloch states. Using the definition of Bloch function, the matrix elements of the perturbation reads as:

$$W_{n', \vec{k}'}^{n, \vec{k}} = \int d\vec{r} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}} W(\vec{r}) u_{n, \vec{k}}^*(\vec{r}) u_{n', \vec{k}'}(\vec{r}) \quad (1.15)$$

The main difficulty for the evaluation of this integral (for a given  $W$ , and besides the fact that the  $u$ 's are unknown functions) comes from the fact that it presents terms with completely different spatial behaviours: the product of the two  $u$ 's is rapidly varying (actually this product is periodic on the crystal lattice), whereas the plane wave is slowly varying over a unit cell (for wavevectors near the  $\Gamma$  point, which is of particular interest here). However, this drawback can be turned into an advantage, and serve as the starting point for an important approximation, which is a fundamental aspect of the envelope function method. To illustrate this point, we consider a simpler, one-dimensional version of this same problem:

$$I = \int dx F(x) u(x) \quad (1.16)$$

where  $F(x)$  ( $u(x)$ ) is a slowly (periodic) function.

$$\begin{aligned} I &\equiv \sum_p \int_p dx F(x) u(x) \\ &\approx \sum_p F(x_p) \int_p dx u(x) = \left[ \sum_p F(x_p) \right] \int_0 dx u(x) \\ &\approx \left[ \int dx F(x) \right] \frac{1}{a_0} \int_0 dx u(x) \end{aligned} \quad (1.17)$$

In the first step, the integral over the whole space is exactly replaced by a sum over contributions coming from the different cells (labelled by the integer  $p$  and of spatial period  $a_0$ ). In the second line we take profit of the slow variation of  $F(x)$  over the  $p$ -th unit cell (centred around  $x_p$ ). Since  $u(x)$  is periodic, its integral is the same over any cell, which permits taking its value (evaluated for instance at the central cell) out from the summation. Then, in the last step we use the very notion of an integral

as a limiting of a summation to (approximately) transform the discrete sum into an integral over the whole space. This same procedure can be employed for the original three-dimensional problem:

$$W_{n',\vec{k}'}^{n,\vec{k}} \approx \left[ \int d\vec{r} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}} W(\vec{r}) \right] \int \frac{d\vec{r}}{\Omega_0} u_{n,\vec{k}}^*(\vec{r}) u_{n',\vec{k}'}(\vec{r}) \quad (1.18)$$

Note that we have explicitly assumed that the perturbation potential varies slowly inside one unit cell. This assumption is quite good for a large class of perturbation potentials, for which additionally interband mixings ( $W_{n',\vec{k}'}^{n,\vec{k}}$ ;  $n' \neq n$ ) can be neglected (at least in a first order description of perturbed states). As examples, we quote: (i) weak static electric or magnetic field, which leads to intraband motion of electrons, and (ii) bound and scattering states in the presence of shallow impurities (e.g. donors). Low frequency (as compared with the interband one) electromagnetic fields can also be tackled by this approach (which can be generalised to account for time-dependent effects). On the contrary, an optical excitation near the interband gap does not, of course, belong to this class: however weak, an interband excitation effectively couples valence and conduction band states. Also, the effect of a perturbation on the valence band states deserves a particular treatment, because of the important mixing of the states at  $k \neq 0$  (as e.g. the previously mentioned heavy-light mixings). For the sake of simplicity, let us here restrict ourselves to the simplest one-band description (a multi-band generalisation of the following developments can be found in the literature). In this case, the band index  $n$  is fixed.

The procedure leading to the last equation allows transforming the original integral into the product of two integrals. Its enormous advantage is that it allows decoupling the slowly and rapidly varying terms. Moreover, we can show that the second integral can, for many purposes, be set equal to unity:

$$\int_{\Omega_0} \frac{d\vec{r}}{\Omega_0} u_{n,\vec{k}}^*(\vec{r}) u_{n',\vec{k}'}(\vec{r}) \approx \delta_{n,n'} + O^{(2)}(\vec{k} - \vec{k}') \quad (1.19)$$

where the second term is a second order correction in the one-band model. Finally, one gets

$$W_{n',\vec{k}'}^{n,\vec{k}} \approx \delta_{n,n'} \tilde{W}(\vec{k}' - \vec{k}) \quad (1.20)$$

where the tilde refers to Fourier transform. We endup with the eigenvalue problem:

$$\sum_{\vec{k}'} \left\{ \left[ E_n(\vec{k}') - E \right] \delta_{\vec{k},\vec{k}'} + \tilde{W}(\vec{k}' - \vec{k}) \right\} \alpha_n(\vec{k}') = 0 \quad (1.21)$$

Solving this matrix Hamiltonian is equivalent to solving the operator equation

$$\begin{aligned} \left[ E_n(\vec{k} \rightarrow -i\vec{\nabla}) + W(\vec{r}) \right] F(\vec{r}) &= E F(\vec{r}) \\ F(\vec{r}) &= \sum_{\vec{k}} \alpha_n(\vec{k}) e^{i\vec{k} \cdot \vec{r}} \end{aligned} \quad (1.22)$$

where  $\vec{\nabla}$  is the gradient operator. This can be demonstrated by (i) formally expanding  $E_n(\vec{k})$  in powers of  $\vec{k}$  and using  $(-i\vec{\nabla})^p e^{i\vec{k} \cdot \vec{r}} \rightarrow (\vec{k})^p e^{i\vec{k} \cdot \vec{r}}$ , and (ii) multiplying on the left by  $e^{-i\vec{k}' \cdot \vec{r}}$  and integrating over the whole space. In the simplest case of a parabolic dispersion there is:

$$\begin{aligned} E_n(\vec{k}) &= E_n(0) + \frac{\hbar^2 \vec{k}^2}{2m_n^*} \\ \left[ -\frac{\hbar^2 \vec{\nabla}^2}{2m_n^*} + W(\vec{r}) \right] F(\vec{r}) &= [E - E_n(0)] F(\vec{r}) \end{aligned} \quad (1.23)$$

Finally, the steps leading to this last equation resume in the replacement

$$-\frac{\hbar^2 \vec{\nabla}^2}{2m_0} + W(\vec{r}) + V_{\text{cr}}(\vec{r}) \rightarrow -\frac{\hbar^2 \vec{\nabla}^2}{2m_n^*} + W(\vec{r}) + E_n(0) \quad (1.24)$$

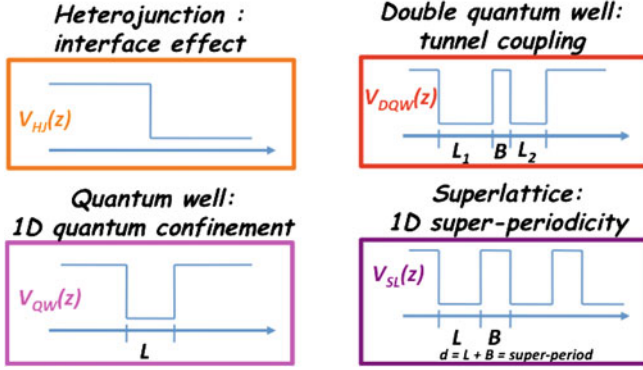
On the left-hand side of this expression, one has the original problem of one electron moving in the crystal with its bare mass and in the presence of the perturbing potential. In the envelope function model the crystal potential is no longer explicitly present but its effect is contained in two effective parameters, the effective mass  $m_n^*$  and the energy edge  $E_n(0)$ , both related to a given band. This constitutes the essence of the envelope function method, namely, incorporating the role of the crystal potential into a few (two in the simple one-band model) effective parameters that can be either separately calculated (via more accurate theories) or inferred from experiments. In this sense, it extends to a perturbed crystal the strategy of the  $\vec{k} \cdot \vec{p}$  method developed to calculate the electronic states of a perfect one.

As previously mentioned, this model has been applied with success to many physical situations of practical interest (calculations of low field electron transport, shallow impurity levels, cyclotron resonance effects). In the last part of this chapter, we indicate how it can also be implemented to describe the electronic levels of nanostructured systems.

In the following, we describe the electronic levels of nanostructured systems within the envelope function approach. To this end, we shall return to the one-band envelope function Hamiltonian and consider an “unperturbed” crystal:  $W(\vec{r}) = 0$ . On very general grounds, a nanostructure is obtained by the juxtaposition of regions of different semiconductors. For simplicity, we shall focus on the case of multilayers, i.e. a nanostructure formed by juxtaposing layers of different semiconductors (we shall not enter into the details of the growth process). Figure 1.1 shows some examples of such structures. The simplest one is, of course, the simple heterojunction (uppermost scheme), where two semi-infinite layers are brought into contact through a common surface (the heterojunction interface). Before discussing the envelope

### A large variety of multi-layers heterostructures:

$$V_{HS}(\vec{r}) = V_{HS}(z) \Rightarrow \text{quasi-1D systems}$$



**Fig. 1.1** Schematic representation of the band alignments related to the formation of four 1D heterostructures: a single heterojunction, a quantum well, a double quantum well and a superlattice

function formalism, it is worth pointing out two important aspects: (i) the two materials are often chosen “not so different”, namely, they usually share the same crystalline structure and energy band sequence and (ii) the interface is assumed to be “ideal”, namely, the materials on either sides of the interface conserve their bulk-like characteristics (crystal symmetry, interatomic bounds). Departures from either assumption do actually lead to new physics in the nanostructures; the consideration of such fine effects is nevertheless beyond the scope of these introductory notes.

The key point in the envelope function analysis is the fact that the energy edges  $E_n(0)$  of different semiconductors have different values. Calculation of the alignment of such bands is a very complex problem. One has, nevertheless been able to infer from experiments the relative alignment of, e.g., the conduction band edges. As a practical example, let us consider the binary GaAs and the ternary  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  (other systems will be discussed in the forthcoming chapters). The ternary has a larger fundamental bandgap than the binary and it is nowadays well established how the energy difference between the two conduction band edges (at the  $\Gamma$  point) varies with the Al content in the ternary. In a multilayer, the edge  $E_n(0)$  related to the same band becomes a position-dependent function,  $E_n(z)$ . More generally, in a nanostructure the edge variation writes  $E_n(\vec{r})$  and the envelope function Hamiltonian for the heterostructure becomes:

$$\left[ -\frac{\hbar^2}{2} \vec{\nabla} \frac{1}{m_n^*} \vec{\nabla} + E_n(\vec{r}) \right] F(\vec{r}) = E F(\vec{r}) \quad (1.25)$$

The kinetic energy term has been rewritten in order to comply with the requirement of current conservation through a given interface (another condition is the continuity of

the envelope wavefunction  $F(\vec{r})$ ). Note that the difference in mass introduces much weaker effects, as compared to those due to the band edge offsets; correspondingly, the effective mass is very often taken to be position-independent.

The different structures in Fig. 1.1 correspond to model systems, which have been extensively studied in the framework of the envelope function method, with the help of the last equation. They allow envisioning many different fundamental physical effects, as the quantum confinement of carriers in a quantum well of nanometric width, the interwell (tunnel) coupling through a thin barrier in a double quantum well system, and the formation of a super-periodicity in superlattice structures. The physics of such structures, as well as of many others, will be discussed in detail in the later chapters. Additionally, more accurate methods will be presented and discussed, allowing a deeper understanding and finer description of the electronic states of electrons in nano-objects and their interactions. Also, other effects will be presented and discussed, as the response of different heterostructures to both external (applied electric bias and electromagnetic fields) and internal (coupling of electrons to lattice ions motions, strains) perturbations. In conclusion, nanostructuration represents nowadays a whole field of research in semiconductor heterostructures, leading to powerful concepts as band engineering, in particular in the field of optoelectronics and aiming at the development of new transport-based devices.

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