The Transfer Matrix Method and the Theory of Finite Periodic Systems. From Heterostructures to Superlattices

Pedro Pereyra

Dedicated to Pier A. Mello and to the memory of Thomas Brody

Historically, the physics, energy spectrum, and wave functions of superlattices have had different levels of understanding. Unlike the standard approaches, based on theorems for infinite systems, the theory of finite periodic systems (TFPS) constitutes a genuine quantum approach, with closed analytical results. In this theory the finite number of unit-cells is an essential condition, while the number of propagating modes, as well as, the potential profiles (or refractive indices) are arbitrary. In this work, the transfer matrix definitions, symmetry properties, group representations, and relations with the scattering amplitudes are reviewed. The derivation of multichannel matrix polynomials (which reduce to Chebyshev polynomials in the one-propagating mode limit), analytical formulas for resonant states, energy eigenvalues, eigenfunctions, parity symmetries, and discrete dispersion relations for superlattices with different confinement characteristics are reviewed. After showing the inconsistencies and limitations of hybrid approaches that combine the transfer-matrix method with Floquet's theorem, some applications of the TFPS to multichannel negative resistance, ballistic transistors, coupled channels transport, spintronics, superluminal, and optical antimatter effects are revisited. Two high-resolution superlattice related experiments are reviewed: the tunneling time in photonic band-gap and the optical response of blue-emitting diodes. It is shown that the TFPS accurately predicts the experimental results.

1. Introduction

The continuous development of semiconductor devices and their simultaneous reduction to nanometric dimensions, have increased the need for precise and efficient calculations to solve the Maxwell or Schrödinger equations for a variety of systems, among them are the multiple quantum wells (QWs) and superlattices (SLs) whose complexity is intermediate between simple systems that are almost textbook examples and intricate 3D molecular heterostructures that require heavy numerical calculations. Multiple quantum wells (MQWs) and SLs have become important and appealing structures for applications in optical and electronic devices. Different theoretical approaches have emerged to describe optical and semiconductor structures. Some, like the envelope function theory,[1–4] evolved by adjusting known theories (rigorously valid for infinite periodic systems) that work well for large systems, others like the transfer matrix method, closely related to the scattering theory[5] that was useful in other branches of physics, such as nuclear physics, electromagnetism, and elementary particles physics, was adapted and evolved into a rigorous formalism suitable for SLs. The understanding of the effects that the “additional periodicity” of SLs has on the energy spectrum and wave functions has also evolved, from the appearance of minigaps in the bands with continuous dispersion relations to the calculation of truly discrete subbands with discrete dispersion relations and well defined surface state energies. Similarly, the apparent need to assume Bloch-type functions evolved into the real possibility of determining the true eigenfunctions of finite periodic systems.

The development of growing techniques of semiconductor structures such as the metalorganic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE)[6] reached in the 1970s the ability to produce heterolayered structures (first suggested by Kroemer[7]), QWs, MQWs, and SLs.[8–10] It also opened up an intense race in search of better optical devices[11–15] and a new era of artificial and endless growing family of heterostructures with new properties and a new spectrum of application possibilities which settled and expanded the research universe of physics. Finally, new semiconductor SLs have become much more appealing than metallic alloy SLs that had, already, a long history.[16–26] The growth techniques of semiconductor structures have long ago reached the level of atomic-layer precision.

The emerging field of semiconductor SLs, originated in the seminal research papers published in the 1970s, led to the study of a variety of basic properties, including, among others, the electron tunneling,[16,27] semiconductor lasers,[14,28–37] injection current thresholds,[32,38,39] the temperature effect in growing processes,[40] enhancement of charge carries mobility,[41,42] recombination and stimulated emission processes,[43–46] exciton dimensionality,[47–51] impurity effects and photoluminescence,[52]
and photoreflectance.\cite{53,54} In recent years, the field of metallic SLs has also seen a renewed momentum with the emergence of photonic crystals, with an overwhelming amount of theoretical and experimental work published.\cite{55–72} A common feature of these papers is that they end up dealing with infinite or semi-infinite SLs by introducing the approximate Bloch periodicity condition, whose first drawback is the derivation of continuous subbands, i.e., Kronig–Penney\cite{73–75} like bands with dispersion relations that give, at best, the widths of the allowed and forbidden subbands. Almost simultaneously, other fields of interest for the theoretical and experimental physics of periodic systems have grown. Among them are the tunneling time through optical superlattices (OSLs), triggered by direct measurements of tunneling times of photons and optical pulses;\cite{76–79} the blue laser diodes based on GaN SLs in the active region;\cite{51,76–78} with interesting features in the optical response due, particularly, to emissions from surface states. In the 1990s and first years of this century, there has been also much research activity in the field of spintronics,\cite{79–88} as well as the transport properties in magnetic SLs.\cite{89–108} Although quantum dots has become also another hot field, the interest on periodic arrays of quantum dots is scarce. Lately, graphene and 2D systems\cite{109,114} become important fields and most of the theoretical approaches rely on the Bloch theorem.

The field of optical and electronic periodic structures, both experimental and theoretical, is so vast that it is impossible to cover everything. As mentioned in the abstract, we will focus on the theory of finite periodic systems (TFPS) based entirely on transfer matrices and their properties, valid for any number of propagation modes, any number of unit cells, and arbitrary potentials or refractive indices profiles. We explicitly exclude theoretical approaches\cite{71,111–114} that in one way or another are based on the Bloch and Floquet theorem\cite{115} which imply the assumption of infinite or semi-infinite systems\cite{96,99,60,66–72,116–129} where relevant physical variables, such as the transmission or reflection coefficients, cannot be conceived without being inconsistent. Since the exclusion of the theoretical approaches for periodic systems that use transfer matrices and are based on Kramers’ argument to determine their dispersion relations\cite{130} implies neglecting most of the theoretical papers in this branch, we include a section that justifies this decision and show the wrong arguments and show graphically that the derived fields, supposedly periodic, do not meet the periodicity requirement. For this purpose, we will also outline the group structure of the transfer matrices to make clear that it contains a compact and a noncompact subgroup. We will show that the transfer matrices that are compatible with Kramers’ eigenvalue argument and fulfill the Floquet theorem belong to the compact subgroup, are diagonal and imply only transmission coefficients equal to 1, without reflection, and no attenuation of the wave functions.

Often the band energies and Bloch functions were mistaken for the energy eigenvalues and eigenfunctions of finite periodic systems,\cite{111} and a rigorous treatment of the frequency problem in the physical theory of crystals, was considered impracticable,\cite{132} hence, approximation methods like the Born–von Karman cyclic boundary conditions were widely applied. Fairly accurate experiments\cite{113,133–135} and fanciful applications using SLs in mesoscopic and nanoscopic domains stimulated the development of theoretical approaches to account for the fine structure inside energy bands. The full quantization of electrons and photons became a focal characteristic, relevant in a number of attractive applications as the foreseen “zero-threshold lasers,” where the electron–hole transitions couple with a single spontaneous emission mode.\cite{136,137}

The layered characteristic of MQWs and SLs structures makes the quasi-1D scattering approach suitable for studying transport properties in these systems. The transfer matrices method was widely used in the 1940s and 1950s of the last century to study wave propagation and electronic structure in 1D alloys,\cite{5,138–143} and later to study resonant tunneling and transmission coefficients in heterostructures and SLs.\cite{11,51,133–137,144–154}

The application of transfer matrices for 1D local periodic systems was attractive and obvious, especially due to the simple relation that the transfer matrix has for the scattering amplitudes and the multiplicative property of the transfer matrices. The use of these matrices has been so appealing that one of the most important and well-known results, the n-cell transfer matrix, that was first reported by Jones in 1941,\cite{155} and later by Abeles, in 1950 when studying the propagation of electromagnetic waves through layered media,\cite{139,143} was rediscovered many times.\cite{145,146,148–154,156–158} Given the transmission coefficients, the calculation of the Landauer conductance,\cite{159,160} became a common and important goal in the analysis of periodic structures. In 1988, Ram-Mohan et al.,\cite{161} by assuming that when going from layer to layer, the fast-varying periodic parts of the Bloch functions do not differ, developed an algorithm to calculate band structures based on the transfer matrix method together with the envelope function approximation. Griffiths and Steinke\cite{162} used the transfer matrix approach to study the theory of waves propagation in different kind of 1D locally periodic media. Sprung et al.\cite{163} studied the relationship between bound states and surface states in finite periodic systems. In the last years, the TFPS was successfully applied to calculate optical transitions in the active region of (blue) laser devices,\cite{164,165} to study phonon modes in wurtzite,\cite{166} periodic structures, coupled resonators and surface acoustic waves for mode localization sensors,\cite{167} to adjust the coherent transport in finite periodic SLs,\cite{168} transport through ultrathin topological insulator films,\cite{169} to model QW solar cells,\cite{170} to study the expectation values for Bloch functions in finite domains,\cite{171} bound states in the continuum,\cite{172} wave packets (WPs) on finite lattices and through semiconductor and optical-media SLs\cite{173–176} to calculate the magneto-conductance of cylindrical wires in longitudinal magnetic fields,\cite{177} persistent currents in small quantum rings,\cite{178} spin transport through magnetic SLs\cite{103,105,106,108,179} to explain the spin injection through Esaki barriers in ferromagnetic/nonmagnetic structures,\cite{85,180–184} to study properties of metamaterial SLs and the antimatter effect,\cite{185,186} to improve the theoretical approach to study electromagnetic waves through fiber Bragg gratings,\cite{187} to show why the effective mass approximation works well in nanoscopic structures,\cite{188} and many other physical properties and systems.

Unfortunately the use of the transfer matrix method has been a bit patchy, and a coherent summary of the transfer matrix capability, beyond the pure calculation of n-cells transmission coefficients, is lacking. The main purpose of the TFPS has been to use the transfer matrix properties and the physical meaning of this mathematical tool not only for the calculation of the resonant energies and wave functions, but also for determining...
fundamental quantities, such as the energy eigenvalues and the corresponding eigenfunctions for bounded SLs, plus congruous discrete dispersion relations.

We will start in Section 2 with an introductory review of Bagwell’s\textsuperscript{[189]} quasi-1D approach of electrons described by a Schrödinger equation with locally periodic potential, whose solutions, describing $N$-propagating modes along the growing direction $z$, are determined in terms of the transfer matrix $W(z_2, z_1)$ that connects the wave functions and their derivatives at any two points.\textsuperscript{[154,190]} We will then introduce the transfer matrix $M(z_2, z_1)$, which connects wave functions at $z_1$ and $z_2$, and the similarity transformation that relates $M$ with $W$. We will also introduce the transfer matrix in the WKB approximation for systems whose refractive index and potential functions are not piecewise constant.\textsuperscript{[191,192]} Among the important properties that we will first review are the transfer matrix representations determined by physical and symmetry requirements, such as time reversal invariance, spin-inversion symmetry and flux conservation, and then we will review the group structure of the transfer matrices,\textsuperscript{[193,194]} and the relation of transfer matrices with the scattering matrix and the scattering amplitudes.\textsuperscript{[5]} To establish this relation, perhaps the most appealing of the transfer matrix $M$, it will be convenient to define the transfer matrix in the basis of incoming/outgoing functions. We will also show the relation of the scattering amplitudes with the transfer matrix $W$. In Section 3, we review the derivation of the main results of the TFPS: 1) the derivation of the transfer matrix $M_{Nn}$ for a system with $n$ unit cells, provided that the transfer matrix $M$ of a unit cell is known. In this derivation, it is assumed that the number of propagation modes $N$ is arbitrary and that the profile of the potentials or refractive indices is also arbitrary. This leads to determining a generalized recurrence relation for noncommutative polynomials, whose solutions, the $N \times N$ matrix polynomials $P_{Nn}$, define the $N \times N$ matrix blocks of the transfer matrix $M_{Nn}$.\textsuperscript{[154,158]} As mentioned before, in the scalar one propagating mode limit, the polynomials $P_{Nn}$ become the well-known Chebyshev polynomials of the second kind $U_n$, and the $2N \times 2N$ transfer matrix $M_{N0}$ becomes the $2 \times 2$ transfer matrix $M_0$ of Jones and Abeles; 2) given the $n$-unit cells transfer matrix $M_{Nn}$, the second objective has been the calculation of fundamental physical quantities. Although the best-known relation is with the transmission and reflection amplitudes,\textsuperscript{[5]} other basic quantities that are naturally sought when solving the Schrödinger equation, are the eigenvalues and eigenfunctions, which are useful quantities when studying other properties of confined SLs and as important as the transmission coefficients in open SLs. In fact, although resonant levels and resonant properties in open systems were identified many years ago in the resonant behavior of transmission coefficients, and resonant behavior was observed in optical spectra, only in recent years has it been possible to determine analytic and general expressions for the evaluation of eigenvalues and eigenfunctions in confined SLs, the parity symmetries of eigenfunctions, new transition selection rules, and closed expressions for the tunneling time. In this review, we will leave out the detailed derivation of noncommutative polynomials. Similarly, as mentioned before, we will only briefly refer to the branch of periodic systems theory that uses the transfer matrix method combined with Floquet’s theorem, which was first invoked by Jones.\textsuperscript{[195]} In the last sections, we will discuss a few examples where the transfer matrix method and the multichannel TFPS were used as an alternative or as the natural and appropriate description. In Section 8, we will address, first, the application of the transfer matrix method to study the resonant transport properties (transmission coefficients and conductance) in the negative resistance domain of a biased double barrier (DB), whose transverse dimension implies a number of propagating modes and the need of a multichannel approach. We will then review the ballistic\textsuperscript{[197]} and multichannel transport through SLs.\textsuperscript{[158]} The TFPS has been also applied with success to study the transmission of electrons and electromagnetic WPs through semiconductor and optical periodic structures,\textsuperscript{[174–176]} of electromagnetic waves through photonic crystals\textsuperscript{[64,65,188]} and through left-handed SLs.\textsuperscript{[185,186]} Interesting results were also found when studying the spin injection and the transport and manipulation of spin waves in magnetic SLs\textsuperscript{[97,108,198]} We will present only brief summaries and main results here. At the end, in Section 10, we will review the application of TFPS to two different types of problems in which high-resolution experimental results were reported. First, we consider the tunneling time of photons and optical pulses in the photonic band gap of SLs, as an example of application to transport problems, and then the calculation of the optical response of SLs in the active region of a laser diode. This as an example of explicit calculation of energy eigenvalues, eigenfunctions, and transition matrix elements for electrons and holes in the conduction and valence bands.

2. On the Propagating Modes and Transfer Matrices in Quasi-1D Systems

Most of the formulas written here are equally valid for electromagnetic systems and quantum systems. For the sake of simplicity and lack of space, we will mainly discuss in terms of electronic systems, and the few examples given in the next sections are, basically, in the one propagating mode limit.

When we deal with transport through a system of length $l = z_N - z_1$, and transverse cross section $w_x w_y$ connected to perfect leads of equal cross section (see Figure 1), the potential

![Figure 1. A quasi-1D periodic system (GaAs/AlGaAs)$_n$ of period $l$, located between $z_2$ and $z_N$. In the upper panel, arrows indicate right-moving and left-moving waves. Lower panel describes the potential profile along the system with the transverse confining potential $V_C(y)$ and a periodic potential $V_P(y,z)$. $V_b$ is barrier height and $w_x$ is the width along $x$. Reproduced with permission.\textsuperscript{[158]} Copyright 2002, American Physical Society.](image-url)
energy of charge carriers can be modelled by a confining hard wall potential \( V_C(x, y) \) plus a potential \( V_p(x, y, z) \), which we will later require to be periodic, at least along the growing direction \( z \). For simplicity, we will consider \( V_p(x, y, z) \) as a stepwise function of \( z \), extending from \( z_1 \) to \( z_2 \) with discontinuities at \( z = \epsilon_i \) (with \( r = 0, \ldots, m_z \)), and infinite outside \( 0 \leq x \leq w_x, 0 \leq y \leq w_y \). The coordinates \( \epsilon_i \) represent the end points of layer’s and may coincide with the end points of the unit cells. For the periodic systems with \( n \) unit cells along the \( z \) axis, the end points of the unit cells will be at \( z = z_j \) (with \( j = 0, \ldots, n, z_0 = z_1 \), and \( z_n = z_2 \)). When a unit cell contains two discontinuity points, \( m_\epsilon = 2n \). To solve the Schrödinger equation

\[
-\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + (V_C(x, y) + V_p(r)) \Psi(r) = E \Psi(r)
\]

we follow ref. [189] and solve first the Schrödinger equation at the leads

\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \phi_{n,n,y}(x,y) + V_C(x,y) \phi_{n,n,y}(x,y) = E \phi_{n,n,y}(x,y)
\]

which give us the set of orthogonal and normalized functions \( \phi_{n,n,y}(x,y) \). The quantum numbers \( n_x, n_y \), and the spin projections define the channel numbers \( i = \{n_x, n_y, s\} \). For a given Fermi energy \( E \), the (open) channels or propagating modes, in the leads, are those whose threshold energies fulfill the relation

\[
E_{\ell_i} = -\frac{\hbar^2}{2m} \left( \frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} \right) \leq E
\]

with longitudinal wave numbers

\[
k_{l}^2 = \frac{2m}{\hbar^2} E - \pi^2 \left( \frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} \right) \geq 0
\]

and threshold wave numbers determined by the transverse wave number \( k_{T_i} = \sqrt{2mE_{\ell_i}/\hbar} \).

Following Bagwell [189] we can use the set of functions \( \{\phi_i(x, y)\} \) to express the wave function \( \Psi(r) \) as

\[
\Psi(x, y, z) = \sum_i \phi_i(x, y) \tilde{\phi}_i(z) \quad \text{for} \quad \epsilon_\ell < z < \epsilon_{\ell+1}
\]

and substitute into the Schrödinger Equation (1), multiply by \( \phi^*_i(x, y) \) and integrate to obtain the system of coupled equations

\[
\frac{d^2}{dz^2} \tilde{\phi}_i(z) + \left( k^2 - k_{T_i}^2 \right) \tilde{\phi}_i(z) = \sum_j K_{ij}^c(z) \phi^*_j(z) \quad i = 1, 2, \ldots
\]

where \( k = \sqrt{2mE/\hbar}, k_{T_i} = \sqrt{2mE_{\ell_i}/\hbar}, \) and \( K_{ij}^c(z) \) the coupling matrix elements

\[
K_{ij}^c(z) = \frac{2m}{\hbar^2} \int \phi^*_j(x, y) V_p(x, y, z) \phi_i(x, y) dx dy \quad \text{for} \quad \epsilon_\ell < z < \epsilon_{\ell+1}
\]

The set of coupled Equations (6) is infinite, therefore impossible to solve in general. Thus, it is natural to cut it at a finite number \( N = sN \), which we call the number of channels that, depending on the Fermi energy, may include only open channels or open plus some closed channels. For a discussion on the alternatives for choosing the transverse solutions in the leads or inside the system, see ref. [190]. Among all the possibilities, we have either coupled or uncoupled channels.

When the potential function \( V_p(x, y, z) \) is a stepwise function of \( z \), with discontinuities at \( z = \epsilon_i \), and does not couple channels, the matrix \( K(z) \) is diagonal, and the propagating modes are solutions of

\[
\frac{d^2}{dz^2} \tilde{\phi}_i(z) + (k^2 - k_{T_i}^2) \tilde{\phi}_i(z) = K_i^c(z) \tilde{\phi}_i(z), \quad i = 1, 2, \ldots, N
\]

The solutions of these set of equations differ in the threshold wave number \( k_{T_i} \). For energies below \( E_{\ell_i} \), the channels are closed and the solutions are evanescent. When channels are open, the solutions are oscillating functions \( e^{ik_{T_i}z} \) when \( k^2 - k_{T_i}^2 - K_i^c(z) > 0 \), otherwise, the solutions are exponential functions \( e^{\pm k_{T_i}z} \). We shall represent the right and left moving ith propagating mode (with spin \( \sigma \)) as \( \tilde{\phi}_i^\sigma(z) \) and \( \tilde{\phi}_i^{-\sigma}(z) \), respectively. The total wave functions at any point \( \epsilon_\ell < z < \epsilon_{\ell+1} \) in the scattering region, can be written as

\[
\tilde{\phi}(z) = \sum_{i=1}^{N} (a_i \tilde{\phi}_i^\sigma(z) + b_i \tilde{\phi}_i^{-\sigma}(z)) = (a_i, b_i) \left( \begin{array}{c} \tilde{\phi}_i^\sigma(z) \\ \tilde{\phi}_i^{-\sigma}(z) \end{array} \right)
\]

with \( \epsilon_\ell < z < \epsilon_{\ell+1} \)

where \( a_i \) and \( b_i \) are \( N \)-dimensional coefficients and \( \tilde{\phi}_i^\sigma(z) \) and \( \tilde{\phi}_i^{-\sigma}(z) \) \( N \)-dimensional state vectors. To determine the wave function at any point \( z \) within the system, we use the transfer matrix method, which ensures the rigorous fulfillment of the continuity requirements at each discontinuity point \( \epsilon_i \) of the periodic system. The transfer matrix method is a useful tool, particularly simple in the case of decoupled channels. In this case and for piecewise potentials, we will present the two types of transfer matrices that will be used more in this review, the transfer matrices \( M \) and \( W \). After introducing these matrices, we will continue with the case of coupled channels.

2.1. The Transfer Matrices \( M \) and \( W \)

To solve the dynamical equations for SLs, using the transfer matrix method, we need to remember the transfer matrix definitions and some of their properties. There are at least two transfer matrices, generally denoted as \( M \) and \( W \). They both connect state vectors at any two points \( z_1 \) and \( z_2 \), contain the continuity conditions everywhere between \( z_1 \) and \( z_2 \), and are related to each other by a similarity transformation. Given the wave function \( \phi(z) \) of equation (9), we can write it as a vector, either as

\[
\phi(z) = \left( \begin{array}{c} \phi_a(z) \\ \phi_b(z) \end{array} \right) \quad \text{or, as} \quad f(z) = \left( \begin{array}{c} \phi_a(z) + \phi_b(z) \\ \phi_a(z) - \phi_b(z) \end{array} \right)
\]

where \( \phi_a(z) \) and \( \phi_b(z) \) are \( N \)-dimensional vectors with elements \( a_1 \tilde{\phi}_1^\sigma(z), \ldots, a_N \tilde{\phi}_N^\sigma(z) \) and \( b_1 \tilde{\phi}_1^{-\sigma}(z), \ldots, b_N \tilde{\phi}_N^{-\sigma}(z) \), respectively.
respectively, and \( \phi'_0(z) \) and \( \phi'_0(z) \) are their derivatives with respect to \( z \), respectively. If \( z_1 \) and \( z_2 \) are any two points in the system, the transfer matrices \( M(z_1, z_2) \) and \( W(z_1, z_2) \) that connect the state vectors at these points are defined in general by

\[
\phi(z_2) = M(z_1, z_2)\phi(z_1) \quad \text{and} \quad f(z_2) = W(z_1, z_2)f(z_1)
\]  

In the next section, we determine specific transfer matrices that fulfill continuity conditions. It is common to write the transfer matrices in block notation as

\[
M(z_2, z_1) = \begin{pmatrix} a & \beta \\ \gamma & \delta \end{pmatrix} \quad \text{and} \quad W(z_2, z_1) = \begin{pmatrix} \beta & \mu \\ \nu & \chi \end{pmatrix}
\]  

where \( a, \beta, \gamma, \delta, \beta, \mu, \nu, \) and \( \chi \) are \( N \times N \) complex submatrices. There are some constraints between the submatrices \( a, \beta, \gamma, \delta, \beta, \mu, \nu, \) and \( \chi \) that depend on the physical properties and symmetries inherent to the Hamiltonian of the system. The number of free parameters and symmetries of the transfer matrices depend, in general, on the symmetry constraints. We will refer later to these symmetries.

### 2.2. Examples. Transfer Matrices of QW and Rectangular Barrier

The QW and the rectangular barrier (RB) are important structures and building blocks of larger systems, we outline here the calculation of the transfer matrices \( M \) and \( W \) for these structures. When the Schrödinger equation is in the effective mass approximation, and the potential barriers and QWs are determined by the discontinuities in the conduction and valence bands of a heterostructure, the mass \( m \) in the wave numbers \( q \) and \( k \) must be replaced by the corresponding effective mass \( m^* \).

#### 2.2.1. Transfer Matrices for a Rectangular QW

If we have the QW shown in Figure 2 and the particle’s energy is \( E < V_o \), the solutions of the Schrödinger equation in regions I, II, and III are, respectively

\[
\varphi_I(z) = a_1 e^{i k z} + b_1 e^{-i k z}, \quad \text{for} \quad z \leq 0,
\]

\[
\varphi_{II}(z) = a_2 e^{i k z} + b_2 e^{-i k z}, \quad \text{for} \quad 0 < z < a,
\]

\[
\varphi_{III}(z) = a_3 e^{i k z} + b_3 e^{-i k z}, \quad \text{for} \quad a \leq z
\]  

with \( q = \sqrt{2m(V_o - E)/\hbar^2} \) and \( k = \sqrt{2mE/\hbar^2} \). Although the wave functions \( \varphi_I(z) \) and \( \varphi_{II}(z) \) diverge when \( z \to -\infty \) and \( z \to \infty \), respectively, we keep temporarily the coefficients \( b_1 \) and \( a_1 \). Once the transfer matrices are determined, one can take \( b_1 = a_1 = 0 \), if necessary. Before we determine the transfer matrices, it is worth writing the state vectors and some relations that will be used below. For the transfer matrix \( M \) we need the state vectors

\[
\phi(z) = \begin{pmatrix} a_1 e^{i k z} \\ b_1 e^{-i k z} \end{pmatrix}, \quad \phi_{II}(z) = \begin{pmatrix} a_2 e^{i k z} \\ b_2 e^{-i k z} \end{pmatrix}
\]  

For the transfer matrix \( W \), we need the following relation

\[
f(z) = \begin{pmatrix} \phi_{II}(z) \\ \phi_{III}(z) \end{pmatrix} = \begin{pmatrix} e^{i k z} \\ i k e^{i k z} \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = Q(z) \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}
\]  

The well-known procedure to solve the Schrödinger equation that consists in calculating the unknown coefficients by successive replacements in all equations (all the equations that result from the continuity requirements on the wave functions and their first-order derivatives), is done also in the transfer matrix method but in a more efficient and systematic way. At \( z = 0 \), the continuity conditions imply the following equations

\[
a_1 + b_1 = a_2 + b_2
\]

\[
q(a_1 - b_1) = i k (a_2 - b_2)
\]  

which, in matrix representation, can be written as

\[
\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \frac{1}{2k} \begin{pmatrix} k - i q & k + i q \\ k + i q & k - i q \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = M_f(0^+, 0^-) \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}
\]  

The transition matrix that we have here, is a transfer matrix that connects the state vectors \( \phi_I(0^-) \) and \( \phi_{II}(0^+) \). Here and in the following \( z^\pm \) means \( z \pm \epsilon \), in the limit of \( \epsilon \to 0 \). These relations could be used to determine the coefficients \( a_3, b_3, b_2, \) but in the transfer matrix method this is not really the purpose. For the type of quantities of interest, almost all the coefficients are unnecessary and the TMM leaves us with functions that carry the relevant information of the physical processes. As in \( z = 0 \), the continuity conditions at \( z = a \), in matrix representation, take the form

\[
\begin{pmatrix} a_2 e^{i k a} \\ b_2 e^{-i k a} \end{pmatrix} = \frac{1}{2q} \begin{pmatrix} q + i k & q - i k \\ q - i k & q + i k \end{pmatrix} \begin{pmatrix} a_1 e^{i k a} \\ b_1 e^{-i k a} \end{pmatrix} = M_f(a^+, a^-) \begin{pmatrix} a_2 e^{i k a} \\ b_2 e^{-i k a} \end{pmatrix}
\]  

with the transition matrix \( M_f(a^+, a^-) \) equal (when the QW is symmetric) to the inverse of the transition matrix \( M_f(0^+, 0^-) \). To connect the state vector \( \phi_{II}(0^+) \) on the left-hand end of the well with the state vector \( \phi_{II}(a^-) \) on the right-hand end, we need another transfer matrix that propagates the state vector in a constant potential region. It is easy to verify that

\[
\begin{pmatrix} a_2 e^{i k a} \\ b_2 e^{-i k a} \end{pmatrix} = \begin{pmatrix} e^{i k a} & 0 \\ 0 & e^{-i k a} \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = M_a(a^- , 0^+) \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}
\]  

With this matrix, we have all the necessary relations to connect the state vector in region III with the state vector in region I. Indeed, combining (17), (18), and (19), we obtain
$\begin{align*}
\left( a_1 e^{iqa} \\
( b_1 e^{-iqa} \right) &= \left( \frac{1}{4qk} \begin{pmatrix} q + ik & q - ik \\ q - ik & q + ik \end{pmatrix} \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \\
& \times \begin{pmatrix} k - iq & k + iq \\ k + iq & k - iq \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \right) \\
\text{(20)}
\end{align*}$

The sequence of transition and transfer matrices define the QW transfer matrix

$M_p(a^+, 0^-) = M_e(a^+, a^-)M_p(a^-, 0^+)M_l(0^+, 0^-)$

After multiplying, and simplifying, the transfer matrix of the rectangular QW is

$M_w(a^+, 0^-) = \begin{pmatrix} \cos ka & \frac{q^2 - k^2}{2qk} \sin ka \\ \frac{k^2 + q^2}{2qk} \sin ka & \cos ka - \frac{q^2 - k^2}{2qk} \sin ka \end{pmatrix}$

$= \begin{pmatrix} a_0 & b_0 \\ -\beta_a & \delta_a \end{pmatrix}$

(22)

For the calculation of the transfer matrix $W_w$, we can start from the second-order differential equation or, given the solutions and the transfer matrix definition (11), we can obtain the transfer matrix $W_w(a^+, 0^-)$, which satisfies the relation

$f_3(a^+) = W_w(a^+, 0^-) f_1(0^-)$

(23)

The functions $f_1(z)$ and $f_3(z)$, at the lateral barriers of the QW, are

$\begin{align*}
&f_1(z) = \begin{pmatrix} \phi_1(z) \\ \phi'_{1}(z) \end{pmatrix} = \begin{pmatrix} e^{iqa} & e^{-iqa} \\ e^{-iqa} & -e^{iqa} \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = Q_1(z) \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \\
&f_3(z) = \begin{pmatrix} \phi_{11}(z) \\ \phi'_{11}(z) \end{pmatrix} = \begin{pmatrix} e^{iqa} & e^{-iqa} \\ e^{-iqa} & -e^{iqa} \end{pmatrix} \begin{pmatrix} a_3 \\ b_3 \end{pmatrix} = Q_3(z) \begin{pmatrix} a_3 \\ b_3 \end{pmatrix} \\
\text{(24)}
\end{align*}$

Since the continuity conditions at $z = 0$ and $z = a$ are

$f_3(a^-) = f_2(a^-)$ and $f_2(0^-) = f_1(0^-)$

(26)

and the function $f_3(z)$, of equation (15), evaluated at these points is

$f_2(a^-) = Q_2(a^-) \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$ and $f_2(0^-) = Q_1(0^-) \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$

(27)

Equation (23) becomes

$f_3(a^+) = Q_2(a^-)Q_2^{-1}(0^-) f_1(0^-) = W_w(a^+, 0^-) f_1(0^-)$

(28)

Thus

$W_w(a^+, 0^-) = \begin{pmatrix} \cos ka & k^2 \sin ka \\ -k \sin ka & \cos ka \end{pmatrix}$

(29)

Using the relations (24) and (25), for $f_1(z)$ and $f_3(z)$, it is easy to show that

$M_w(a^+, 0^-) = \begin{pmatrix} 1 & 1 \\ q & -q \end{pmatrix}^{-1} W_w(a^+, 0^-) \begin{pmatrix} 1 & 1 \\ q & -q \end{pmatrix}$

(30)

2.2.2. Transfer Matrices of a Rectangular Potential Barrier

Let us now consider the rectangular potential barrier shown in Figure 3. Again, we will assume that $E < V_o$, and the solutions of the Schrödinger equations in each of the three regions are

$q_1(z) = a_1 e^{ikz} + b_1 e^{-ikz}$, for $z \leq 0$

$q_2(z) = a_2 e^{iqa} + b_2 e^{-iqa}$, for $0 < z < b$

$q_3(z) = a_3 e^{ikz} + b_3 e^{-ikz}$, for $z \geq b$

(31)

(32)

(33)

with $k = \sqrt{2mE/\hbar^2}$ and $q = \sqrt{2m(V_o - E)/\hbar^2}$. The fulfillment of the continuity conditions, at $z = 0$ and $z = b$, leads to establish the relation

$\phi_{11}(b^+) = M_l(b^+, 0^-)M_p(b^-, 0^+)M_l(0^+, 0^-)\phi_{11}(0^-)$

(34)

The barrier transfer matrix that connects state vectors at the left- and right-hand sides of the RB is

$\begin{pmatrix} k - iq & k + iq \\ k + iq & k - iq \end{pmatrix} \begin{pmatrix} e^{ib} & 0 \\ 0 & e^{-ib} \end{pmatrix}$

(35)

which after multiplying and simplifying becomes

$M_b(b^+, 0^-) = \begin{pmatrix} \cosh qb + i \frac{k^2 - q^2}{2qk} \sinh qb & -i \frac{k^2 + q^2}{2qk} \sinh qb \\ i \frac{k^2 + q^2}{2qk} \sinh qb & \cosh qb - i \frac{k^2 - q^2}{2qk} \sinh qb \end{pmatrix}$

(36)

$= \begin{pmatrix} a_b & \beta_b \\ \beta_b^* & a_b^* \end{pmatrix}$

In the same way as for the QW, we can determine the transfer matrix $W_b(b^+, 0^-)$ defined by

$f_3(b^+) = W_b(b^+, 0^-) f_3(0^-)$

(37)

Figure 3. The rectangular potential barrier, its potential parameters and the propagating solutions at the left and right sides.
With the continuity conditions at \( z = 0 \) and \( z = b \)
\[
 f_3(b^+) = f_2(b^-) \quad \text{and} \quad f_3(0^+) = f_1(0^-)
\]
(38)
We need now the function
\[
f_2(z) = \begin{pmatrix} \phi_1(z) \\ \phi_2(z) \end{pmatrix} = \begin{pmatrix} e^{z} & e^{-z} \\ q e^{z} & -q e^{-z} \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = Q_2(z) \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}
\]
(39)
that allows us to write the relation
\[
f_2(b^-) = \begin{pmatrix} e^{b} & e^{-b} \\ q e^{b} & -q e^{-b} \end{pmatrix} \frac{1}{Z_2} \begin{pmatrix} q & 1 \\ q & -1 \end{pmatrix} f_2(0^+)
\]
\[
= Q_2(b^-)Q_2^{-1}(0^+)f_2(0^+)
\]
(40)
Therefore
\[
f_3(b^+) = Q_2(b^-)Q_2^{-1}(0^+)f_1(0^-) = W_b(b^+,0^-)f_1(0^-)
\]
(41)
with
\[
W_b(b^+,0^-) = \begin{pmatrix} \cosh qb & q^{-1} \sinh qb \\ q \sinh qb & \cosh qb \end{pmatrix}
\]
(42)
and the relation between this matrix and the transfer matrix \( M_b(b^+,0^-) \) is given by
\[
M_b(b^+,0^-) = \begin{pmatrix} 1 & 1 \\ i k & -i k \end{pmatrix}^{-1} W_b(b^+,0^-) \begin{pmatrix} 1 & 1 \\ i k & -i k \end{pmatrix}
\]
(43)

### 2.3. Coupled Channels and the Transfer Matrix \( W \)

When the propagating modes are coupled, we use the reduction of order method of the theory of differential equations. For this purpose, we need the state vector \( f \), defined before, with elements \( f_j = a_j \phi_j + b_j \psi_j \) and \( f_{j+N} = \phi_j^* \) for \( j = 1, 2, \ldots, N \). Using these functions, the system of coupled equations can be written as
\[
f'(z) = U f(z) \quad \text{for} \quad z_r < z < z_{r+1}
\]
(44)
with
\[
U_r = \begin{pmatrix} 0 & K'(z) - k^2 I_N + k^2 \frac{I_N}{0} \\ 0 & 0 \end{pmatrix}
\]
(45)
a \( 2N \times 2N \) matrix. \( I_N \) is the unit matrix of dimension \( N \times N \) and \( k_T = \text{diag}(k_{T_1}, k_{T_2}, \ldots, k_{T_N}) \). Since \( K' \) is symmetric and real, \( U_r \) corresponds to an infinitesimal symplectic transformation. For details, see ref. [190]. It is simple to verify that the first-order differential Equation (44) has the solution
\[
f(z) = \exp[(z - z_r) U_r] f(z_r) = W(z,z_r)f(z_r),
\]
for \( z_r < z < z_{r+1} \)
(46)
If we define the symmetric matrix
\[
U_r^2 = \frac{2m}{\hbar^2} (V - E I_N) + k_T^2 \quad \text{such that} \quad U_r = \begin{pmatrix} 0 & I_N \\ u_r^2 & 0 \end{pmatrix}
\]
(47)
and expand \( W \) in power series, we obtain, for the transfer matrix \( W(z,z_r) \), the following representation
\[
W^{(1)}(z) = \begin{pmatrix} \cosh zu_r & u_r^{-1} \sinh zu_r \\ u_r \sinh zu_r & \cosh zu_r \end{pmatrix}
\]
(48)
which is well known in the 1D-one channel approaches, with \( u_r \) scalar functions. In ref. [190], the matrix functions \( \cosh(zu_r) \) and \( u_r^{-1} \sinh(zu_r) \) are written as polynomials of degree \( N-1 \) in the matrix variable \( u_r \). In block notation, we write the transfer matrix \( W \) as
\[
W = \begin{pmatrix} \theta & \mu \\ \nu & \chi \end{pmatrix}
\]
(49)
with \( \theta, \mu, \nu, \) and \( \chi \). \( N \times N \) submatrices. For some purposes, it is convenient to deal with the transfer matrix \( M \). Based on the transfer matrix \( W \) and transfer matrix \( M \) definitions, it is easy to show that
\[
M = \begin{pmatrix} \kappa^{-1/2} & \kappa^{-1/2} \\ i \kappa^{1/2} & -i \kappa^{1/2} \end{pmatrix}^{-1} W \begin{pmatrix} \kappa^{-1/2} & \kappa^{-1/2} \\ i \kappa^{1/2} & -i \kappa^{1/2} \end{pmatrix}
\]
(50)
where \( \kappa = \text{diag}(k_{T_1}, k_{T_2}, \ldots, k_{T_N}) \).

Before we review the relation with the scattering amplitudes, we will consider the transfer matrices for potential functions which are not piecewise constant. This means transfer matrices in the WKB approximation, an approximation that works well for an important class of potentials.

### 2.4. Transfer Matrices in the WKB Approximation

Thanks to the atomic-layer precision reached in the growing techniques of heterostructures, the abrupt and ideal transition in the potential profiles can be justified for many real systems, however, in most of the actual systems, the change in the gap energies is gradual and the potential profile at the interfaces is better modeled by continuous functions. In these cases, the transfer matrices in the WKB approximation are suited and convenient. The explicit derivation of these matrices are given in ref. [191]. As can be seen there, the derivation, similar to that of a QW or a barrier, is based on the matrix representation of the continuity conditions, and careful cancellation of zeros of equal order. The main result for the transfer matrix of an arbitrary QW, as the one shown in Figure 4, is
\[
M_w(z_2', z_1') = \begin{pmatrix} \cos \xi & -\sin \xi \\ \sin \xi & \cos \xi \end{pmatrix}
\]
(51)

Figure 4. An arbitrary potential well.
where \( z_1 = z_1 - \epsilon \) and \( z_2 = z_2 + \epsilon \), with \( \epsilon \) infinitesimal, correspond to the classical return points \( z_1 \) and \( z_2 \), and

\[
\xi(z_2, z_1) = \int_{z_1}^{z_2} k(z) dz
\]

The transfer matrix for an arbitrary potential, as the one shown in Figure 5, is

\[
M_b(z_2, z_1) = \begin{pmatrix} \cosh \xi & -i \sinh \xi \\ i \sinh \xi & \cosh \xi \end{pmatrix}
\]

where

\[
\zeta(z_2, z_1) = \int_{z_1}^{z_2} q(z) dz
\]

3. Transfer Matrix Symmetries, Group Structure, and the Scattering Amplitudes

The conservation of flux or current is an important principle, and the most common symmetries underlying the interactions are the time reversal invariance (TRI) and spin-rotation invariance (SRI). These symmetries may not be present, but the requirement of flux conservation (FC) must always hold. This requirement implies that the transfer matrices should always fulfill the pseudo-unitarity condition\(^{[199]}\)

\[
M \Sigma M^t = \Sigma \quad \text{with} \quad \Sigma = \begin{pmatrix} I_N & 0 \\ 0 & -I_N \end{pmatrix}
\]

Here \( I_N \) is the unit matrix of dimension \( N \times N \). In the absence of TRI, the Hamiltonians for both spin-dependent and spin-independent interactions can be diagonalized by an orthogonal transformation, and the system belongs to the orthogonal universality class. The transfer matrices for spin-independent systems of the orthogonal universality class should fulfill the condition (see Refs. \([194, 199]\))

\[
M = \Sigma_x M^t \Sigma_x
\]

where \( \Sigma_x \) is the Pauli matrix of dimension \( 2N \times 2N \). In this case, the transfer matrices can be represented as

\[
M_o = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}
\]

with \( \alpha \alpha^t - \beta \beta^t = I_N \) and \( \alpha \beta^t - \beta \alpha^t = 0 \). Here, the superscript \( T \) stands for the transpose of the matrix. The transfer matrices of the orthogonal class that fulfill both TRI and FC belong to the symplectic group \( Sp(2N, C) \) and satisfy the requirement

\[
M_o \mathcal{F} M_o^t = \mathcal{F} \quad \text{with} \quad \mathcal{F} = \Sigma_x \Sigma_x = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}
\]

Besides the physical symmetries and the requirements on the transfer matrices, the group structure and the possible representations, in terms of linearly independent parameters, are very important properties and we will now refer to this topic briefly. It has been shown in ref. \([194]\) that every transfer matrix \( M_o \) can be written as the product of two matrices \( M_{so} \) and \( M_{on} \) that belong to a compact and a noncompact subgroup, respectively, i.e.

\[
M_o = M_{so} M_{on} = \begin{pmatrix} \mu & \gamma \\ \delta & \nu \end{pmatrix} \begin{pmatrix} \sqrt{I_N + \xi \xi^t} & \xi \\ \xi^t & \sqrt{I_N + \xi \xi^t} \end{pmatrix}
\]

where \( \mu \) and \( \xi \) are unitary and symmetric matrices, respectively. Similarly, if we are dealing with systems of the symplectic class with spin-dependent interactions, the invariance under spin inversion and time reversal, for spin 1/2 particles, imply that the transfer matrices \( M_s \) fulfill the requirement (see ref. \([194]\))

\[
M_s = K^t M_s K \quad \text{with} \quad K = \begin{pmatrix} 0 & \Sigma_y \\ \Sigma_y^t & 0 \end{pmatrix}
\]

\[
\Sigma_y = \begin{pmatrix} 0 & -i \eta \\ i \eta & 0 \end{pmatrix}
\]

These matrices belong to the pseudo-orthogonal \( spO(4N, C) \) group, and decompose also as the product of a compact \( M_{so} \) and a noncompact matrix \( M_{on} \), i.e.

\[
M_s = M_{so} M_{on} = \begin{pmatrix} \nu w & 0 \\ 0 & \Sigma_x^t w^\dagger \Sigma_x \end{pmatrix} \begin{pmatrix} \sqrt{I_N + \eta \eta^t} & \eta \\ \eta^t & \sqrt{I_N + \eta \eta^t} \end{pmatrix}
\]

where \( w \) is a unitary matrix and \( \eta \Sigma_x = \nu (\sinh \lambda) \Sigma_x \nu^t \) is an antisymmetric product, with \( \nu \) a unitary matrix. When the interactions are not time reversal and spin rotation invariants, the systems belong to the unitary class. The transfer matrices fulfill only the FC requirement, and belong to the pseudo-unitary
$spU(2N, C)$ group, and every transfer matrix of this group can also be decomposed as the product of a compact $M_{uc}$ and a non-compact matrix $M_{un}$, i.e.

$$M_u = M_{uc} M_{un} = \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix} \begin{pmatrix} \sqrt{I_N + \zeta^T} & \zeta \\ \zeta^T & \sqrt{I_N + \zeta^T} \zeta \end{pmatrix}$$  \hspace{1cm} (63)

where $w_1$ and $w_2$ are unitary and $\zeta = v_1 (\sinh \lambda) v_2$ an arbitrary square matrix, with $v_1$ and $v_2$ unitary. Notice that, $\det M_u = \det M_{uc} = \det M_{un} = 1$.

### 3.1. Transfer Matrix and the Scattering Amplitudes

To describe transport properties based on transfer matrices, it is worth recalling the well-known relations between the transfer matrices $M$ and $W$, and the scattering matrix $S$. This relation, first derived to our knowledge by Borland\cite{15,199} to show that atomic potentials could be replaced by $\delta$-functions surrounded by two regions of zero potential, is one of the best known within the theoretical and experimental researches that use transfer matrices frequently. For a scattering process as the one sketched in Figure 6, with incident amplitudes $\overrightarrow{\varphi}_{in}$ and $\overrightarrow{\varphi}_{in}$, from the left and the right hand side, respectively, the outgoing amplitudes are $\overrightarrow{\varphi}_{out} = r \overrightarrow{\varphi}_{in} + t \overrightarrow{\varphi}_{in}$ and $\overrightarrow{\varphi}_{out} = r' \overrightarrow{\varphi}_{in} + t' \overrightarrow{\varphi}_{in}$, where $r, t, r'$, and $t'$ are reflection and transmission amplitudes for particles coming from the left and right, respectively. These relations define the scattering matrix $S$, that connects the incoming amplitudes with the outgoing ones, and depends on the scattering amplitudes as follows

$$S = \begin{pmatrix} r & t \\ t & r' \end{pmatrix}$$ \hspace{1cm} (64)

The scattering matrix is an amply studied mathematical and physical quantity. It is well-known that flux conservation implies that the $S$ matrix is unitary and $S' S = I$, while time reversal invariance implies that $S = S^T$. When time reversal symmetry is present, one has to distinguish spin-dependent from spin-indepenent systems. The TRI requirement for spin-independent systems implies that $t' = t^T$ while for spin-dependent and TRI systems, the transmission amplitude should satisfy the condition $t' = \Sigma_i t_i^2 \Sigma_i^T$. These global relations (valid independently of the size of the system, the number of unit cells, the number of propagating modes and the potential profiles), are important and appealing properties of the transfer matrix method and provide the possibility to establish a bridge between mathematically well-defined objects, as the transfer matrices, and physical quantities.

The relation between the $S$ and $M$ matrices, can easily be obtained based on their definitions (It is worth emphasizing that in order to establish the relation between $S$ and $M$, we have to use the same basis of wave functions.)

$$\begin{pmatrix} \overrightarrow{\varphi}^o_{out} \\ \overrightarrow{\varphi}^i_{in} \end{pmatrix} = S \begin{pmatrix} \overrightarrow{\varphi}^i_{in} \\ \overrightarrow{\varphi}^i_{in} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \overrightarrow{\varphi}^o_{out} \\ \overrightarrow{\varphi}^i_{in} \end{pmatrix} = M \begin{pmatrix} \overrightarrow{\varphi}^i_{in} \\ \overrightarrow{\varphi}^i_{in} \end{pmatrix}$$ \hspace{1cm} (65)

When the transfer matrix is of the unitary universality class $M_u$ (in the symplectic and TRI case, one has $\gamma = \beta^*$ and $\delta = \alpha^*$), one obtains the following equations

$$t - \alpha - \beta r = 0 \quad r' - \beta t' = 0 \quad \gamma + \delta r = 0$$ \hspace{1cm} (66)

$$1 - \delta t' = 0$$

whose solutions, using the relations $r r + t' t = 1$ and $r r' + t t' = 0$, are \cite{158}

$$\alpha = (t^T)^{-1}, \quad \beta = (r^T)^{-1}, \quad \gamma = -(t^T)^{-1} r', \quad \text{and} \quad \delta = (t')^{-1}$$ \hspace{1cm} (67)

and

$$t = (\alpha^T)^{-1}, \quad r = -(\delta)^{-1} r', \quad t' = (\delta)^{-1}, \quad \text{and} \quad r' = \beta (\delta)^{-1}$$ \hspace{1cm} (68)

Thus, the transfer matrix of the unitary universality class can be written as

$$M_u = \begin{pmatrix} (t^T)^{-1} & r' (t^T)^{-1} \\ -r (t^T)^{-1} & (t')^{-1} \end{pmatrix}$$ \hspace{1cm} (69)

while a transfer matrix in the orthogonal universality class, takes the form

$$M_o = \begin{pmatrix} (t^T)^{-1} & r' (t^T)^{-1} \\ -r (t^T)^{-1} & (t')^{-1} \end{pmatrix}$$ \hspace{1cm} (70)

It can also be shown that the scattering amplitudes in terms of the transfer matrix $W$ blocks are given by the following relations

$$t = 2 \kappa^{1/2} (\theta^T + \kappa \chi^T \chi^{-1} - i (\mu^T + \kappa^{-1} - 1) \chi^{-1} / 2) = (t^T)^T$$ \hspace{1cm} (71)

$$r = 1 / 2 \mu^{1/2} (\theta - \kappa^{-1} \chi^T + i (\mu \kappa + \kappa^{-1} i \chi) \chi^{-1})$$ \hspace{1cm} (72)

and

$$r' = - \frac{1}{2} \kappa^{1/2} (\theta - \kappa^{-1} \chi^T - i (\mu \kappa + \kappa^{-1} i \chi) \chi^{-1} / 2)$$ \hspace{1cm} (73)

Another important attribute of the transfer matrices that makes them appropriate quantities to describe systems of finite but in principle arbitrary size is the multiplicative property. Indeed, if $M(z_2, z_1)$ connects state vectors at $z_1$ and $z_2$, and $M(z_3, z_2)$ connects state vectors at $z_2$ and $z_3$, the transfer matrix that connects state vectors at $z_1$ and $z_3$ is given by the product

\[ M(z_3, z_1) = M(z_3, z_2) M(z_2, z_1) \]
\[ M(z_3, z_1) = M(z_3, z_2)M(z_2, z_1) \quad (74) \]

This property and the possibility of relating the matrix with the scattering amplitudes, have been broadly used; they constitute the principal components of the transfer matrix approach to the quantum description of finite periodic systems.

It should be noted that the dispersion and transfer matrices contain all the physics of the dispersion processes. This is why a theory based on these quantities is capable of describing physical systems whose geometries allow us not only to define transfer matrices but also to determine, analytically, new results for larger systems. This is the goal of the next section. We will establish a general method and derive general formulas that can be applied directly to determine the physical quantities of specific finite periodic systems. Although most systems belong to the orthogonal universality class, we will assume in the derivations reviewed here that all transfer matrices belong to the unitary universality class. All of our results can be easily adjusted for the other universality classes. For example, for the orthogonal universality class we have just to consider \( \gamma = \alpha^* \) and \( \delta = \alpha^* \).

4. The TFPS, \( N \) Propagating Modes, \( n \)-Unit Cells

The TFPS aims to describe and to determine the physical properties of a layered periodic system based on the transfer matrix method (Most of the content in this section was published in Refs. [156b,158,190]). The multiplicative property of transfer matrices make them suitable quantities to describe systems. As mentioned before, if we put together two identical cells of length \( L/n \) and the transfer matrix of each unit-cell is \( M \), the transfer matrix \( M_2 \) of the resulting system, of length \( 2L/n \), is \( M_2 = MM = M^2 \). It is well established that knowing the unit-cell transfer matrix, we have all the information about the wave functions in the unit cell. In the same way, knowing the transfer matrix \( M_2 \), we have the whole information of the wave functions of the two-unit-cell system, and the possibility of determining other quantities such as eigenvalues or scattering amplitudes, whose formal relations with the transfer matrix remain unchanged. Applying the multiplicative property over and over, we can express the global \((n\)-cell\) transfer matrix as

\[ M_n = M^n = \left( \begin{array}{cc} \alpha & \beta \\ \gamma & \delta \end{array} \right)^n \equiv (\alpha_n, \beta_n, \gamma_n, \delta_n) \quad (75) \]

The relation with the scattering amplitudes is

\[ \begin{align*}
\alpha_n & = (t_n^{-1})^{-1} \\
\beta_n & = (r_n^{-1})^{-1} \\
\gamma_n & = (t_n^{-1})^{-1} \\
\delta_n & = (r_n^{-1})^{-1}
\end{align*} \quad (76) \]

An important leap in the transfer matrix method is precisely, the possibility of analytically determining the matrices \( \alpha_n, \beta_n \), etc., and hence, to deduce analytical expressions for global \( n \)-cell physical quantities. It is clear that for the purpose of numerical evaluations it may be sufficient to diagonalize \( M \) as \( UAU^{-1} \) and to write the \( n \)-cell transfer matrix as \( UAU^nU^{-1} \). However, by doing this, one loses a great deal of the power of the transfer matrix method and spoils the possibility of deriving new expressions for fundamental physical quantities. It is worth mentioning that transfer matrices are frequently used to study structures with few layers as well as in non-periodic structures, such as Fibonacci systems \([156]\) and self-similar fractal structures. \([200]\) Our interest here is mostly periodic structures.

Let us now consider some transfer-matrix properties and derive fundamental relations in this approach. In the following, we will be concerned with \( M_n \), but for an easy notation the sub-index \( n \) will be omitted.

Since

\[ M_n = MM_{n-1} \quad (77) \]

it is clear that

\[ \alpha_n = \alpha \alpha_{n-1} + \beta \gamma_{n-1} \quad (78) \]

\[ \beta_n = \alpha \beta_{n-1} + \beta \delta_{n-1} \quad (79) \]

\[ \gamma_n = \gamma \alpha_{n-1} + \delta \gamma_{n-1} \quad (80) \]

\[ \delta_n = \gamma \beta_{n-1} + \delta \delta_{n-1} \quad (81) \]

with \( \alpha_0 = \delta_0 = I_N \) and \( \beta_0 = \gamma_0 = 0 \). Starting from these relations, one can easily obtain the matrix recurrence relation (MRR)

\[ \beta_n = (\alpha + \beta \delta^* \beta^-1) \beta_{n-1} + (\beta \gamma - \beta \delta^* \alpha) \beta_{n-2} \quad (82) \]

and a similar one for \( \alpha_n \). We also obtain

\[ \gamma_n = (\delta + \gamma \alpha \gamma^{-1}) \gamma_{n-1} + (\gamma \beta - \gamma \delta \gamma^{-1}) \gamma_{n-2} \quad (83) \]

and a similar one for \( \delta_n \). All these relations are three-term recurrence relations with matrix coefficients of dimension \( N \times N \). If we define the matrix-functions

\[ p^{(1)}_{N,n} = \beta^{-1} \beta_n \quad \rightarrow \quad \beta_n = \beta p^{(1)}_{N,n-1} \quad (84) \]

and

\[ \gamma_{N,n} = \gamma^{-1} \gamma_n \quad \rightarrow \quad \gamma_n = \gamma \gamma_{N,n-1} \quad (85) \]

we can write Equations (79) and (80) as

\[ \delta_n = \beta p^{(1)}_{N,n} - \beta \alpha p^{(1)}_{N,n-1} \quad (86) \]

\[ \alpha_n = \beta p^{(2)}_{N,n} - \gamma \delta p^{(2)}_{N,n-1} \quad (87) \]

and Equations (82) and (83), dropping the index \( N \) to simplify notation, become the noncommutative polynomials recurrence relation (NCPRR)

\[ p_i^{(i)} + \zeta_i p_i^{(i-1)} + \eta_i p_{i-2}^{(i)} = 0 \quad \text{for} \quad n \geq 1, \quad i = 1, 2 \quad (88) \]

Here, \( \zeta_1 = -(\beta \delta^{-1} \alpha \gamma + \delta), \quad \eta_1 = (\delta \beta^{-1} \gamma \beta - \gamma \delta), \quad \zeta_2 = -(\gamma \alpha \gamma^{-1} \beta \gamma + \alpha), \]

and \( \eta_2 = (\gamma \beta \gamma^{-1} \beta \gamma - \gamma \delta \gamma^{-1}) \) are the matrix coefficients. The subindex \( N \) has been dropped for simplicity. It is easy to see that the initial conditions are \( p^{(1)}_1 = 0 \) and \( p^{(2)}_0 = I_N \). An important achievement of this theory, extremely important to obtain analytical expressions for the physical quantities, has been the solution of Equation (88). The explicit derivation of the matrix polynomials \( p^{(1)}_n \) and \( p^{(2)}_n \), can be seen in Refs. [154,158,190]. The polynomials in terms of the unit-cell transfer matrix eigenvalues \( \lambda_i \) are
\[ P_{m,n} = \sum_{k=0}^{m \leq 2N} \sum_{l=0}^{k} P_{l,\beta k} q_{m-k} \quad \text{for} \quad m < 2N \] (89)

and

\[ P_{m,n} = \sum_{k=0}^{2N-1 \leq 2N} \sum_{l=0}^{k} P_{l,\beta k} q_{m-k} \quad \text{for} \quad m \geq 2N \] (90)

where

\[ g_m = (-)^m \sum_{l_1 < l_2 < \cdots < l_m} \lambda_{l_1} \lambda_{l_2} \cdots \lambda_{l_m}, \quad \text{and} \quad g_0 = 1 \] (91)

and

\[ q_n = \sum_{i=1}^{2N+n-1} \frac{\omega^{2N+n-1}}{i^{2N+n-1}} \frac{1}{i^{N}} \] (92)

Using these results, we can now write the most general \( n \)-cell transfer matrix \( M_n \) as

\[ M_n = \begin{pmatrix} P_{n,n}^{(2)} - \gamma^{-1} \delta P_{n,n-1}^{(2)} \\ \beta P_{n,n-1}^{(1)} \\ P_{n,n}^{(1)} - \beta^{-1} \gamma P_{n,n-1}^{(1)} \end{pmatrix} \] (93)

By solving the matrix recurrence relation, the TFPS extends the capabilities of describing the transport properties of multichannel systems. From the mathematical point of view, the generalized recurrence relations have special implications which go beyond the purpose of this paper. The matrix representations of the generalized orthogonal polynomials and the noncommutative algebras, are similar to those discussed by Gelfand.\(^{[201]}\)

We will see below that the NCPRR becomes, in the limit \( N = 1 \), the recurrence relation of the well-known Chebyshev polynomials of the second kind.

### 4.1. The Scattering Amplitudes, Transport Coefficients, Landauer Conductance

Given the noncommutative polynomials and using Equations (86) and (87), together with the relation (69), we can write the global multichannel transmission and reflection amplitudes as

\[ t_n = (p_n - p_{n-1} - \gamma^{-1} \delta) \] (94)

\[ t'_n = (p_n - \beta^{-1} \gamma p_{n-1})^{-1} \] (95)

\[ r_n = -(p_n - \beta^{-1} \alpha p_{n-1})^{-1} r_{n-1} \] (96)

\[ r'_n = \beta p_{n-1} - (p_n - \beta^{-1} \alpha p_{n-1})^{-1} \] (97)

These interesting results show that the \( n \)-cell scattering amplitudes can be expressed entirely in terms of single-cell transfer-matrix blocks (or single-cell transmission and reflection amplitudes \( r, t, r', \) and \( t' \)) and the polynomials \( p_n \). For time-reversal invariant and spin-independent systems, \( t_n \) is just the transpose of \( t'_n \), and \( \gamma = \beta^{*}, \delta = \alpha^{*} \). For spin-dependent systems \( t' = k^{*} t' k \) and \( \gamma = k^{*} \beta k, \delta = k^{*} \alpha k \). The previous relations are simple and of general validity at the same time.

Especially simple, in its functional appearance, are the global Landauer multichannel resistance amplitudes \( R_{n,n}^{(i)} = r_{n,n} (t_{n,n})^{-1} \) and \( R_{n,n} = -(t_{n,n})^{-1} r_{n,n} \). These quantities, in terms of the polynomials \( p_{n,n} \), are just

\[ R_{n,n} = R_{n,1} p_{n,n-1} \quad \text{and} \quad R_{n,n} = R_{n,1} p_{n,n-1}. \] (98)

Here, the most important properties, tunneling, and interference phenomena, appear nicely factorized.

A quantity often used in the transport theory is the Landauer multichannel conductance matrix

\[ G_N = \frac{e^2}{h} \sum_{k=1}^{N} \frac{1}{r_{n,n}^{(i)}} t_{n,n}^{(i)} \] (99)

which for the \( n \) cell system becomes

\[ G_{n,n} = \frac{1}{p_{n,1,n}} G_{n,1} \left( \frac{1}{p_{n,n-1}} \right)^{\dagger} \] (100)

So far, we have given a number of non-trivial but extremely appealing relations and results. The \( n \)-cell Landauer resistance amplitude is just the product of the one-cell Landauer resistance amplitude \( R \) and the polynomial \( p_{n,n} \). The polynomial \( p_{n,n} \) has the information on the number of layers \( n \), the number of channels \( N \) and, more importantly, on the complex but precise phase interference phenomena that happens along the \( n \)-periodic structures.

### 5. The TFPS in the One-Propagating Mode Limit, and \( n \)-Unit Cells

So far we have presented a general approach for quasi-1D, multichannel periodic systems. Since the more common systems are well modeled as one propagating mode systems, we will consider in this section the one-propagating mode limit, and given the scalar polynomials \( p_n \), we will deduce general expression for the most common SL configurations. For open systems, which are the best known systems, we will review the resonant energies, eigenfunctions and dispersion relations. For bounded SLs, we will obtain formulas for the evaluation of energy eigenvalues, eigenfunctions, and discrete dispersion relations.

#### 5.1. The Polynomial Recurrence Relation and the Transfer Matrix for \( n \)-Unit Cells in the One-Channel Limit

In the one-propagating mode limit, the functions \( \zeta \) and \( \eta \) defined before become \( \alpha + \delta = TrM \) and \( \delta \alpha - \gamma \beta = detM \), respectively. Thus, for the 1D systems the matrix NCPRR becomes the scalar commutative recurrence relation

\[ p^{(i)}_n + (\alpha + \delta) p^{(i)}_{n-1} + detM p^{(i)}_{n-2} = 0 \quad \text{for} \quad n \geq 1 \quad i = 1, 2 \] (101)

which, for the orthogonal universality class, where \( \alpha = \delta^{*} \), reduces to...
p_n + 2\alpha R p_{n-1} + p_{n-2} = 0 \quad \text{for} \quad n \geq 1 \quad (102)

with \alpha = \text{Re} \alpha (\text{i.e., the real part of } \alpha), \text{and initial conditions } p_{-1} = 0 \text{ and } p_0 = 1. \text{This is precisely the recurrence relation of the Chebyshev polynomials of the second kind } U_n \text{ evaluated at } \alpha R.

In the one-propagating mode limit, the transfer matrix \( M_n \) becomes

\[
M_n = \begin{pmatrix}
U_n - \delta U_{n-1} & \beta U_{n-1} \\
\gamma U_{n-1} & U_n - \alpha U_{n-1}
\end{pmatrix}
\quad (103)
\]

which for the orthogonal universality class, i.e., for the time reversal invariant systems becomes the well-known Jones-Abelès' transfer matrix

\[
M_n = \begin{pmatrix}
U_n - \alpha^* U_{n-1} & \beta^* U_{n-1} \\
\beta^* U_{n-1} & U_n - \alpha U_{n-1}
\end{pmatrix}
\quad (104)
\]

This matrix, reported initially for electromagnetic fields through layered media, has been repeatedly rediscovered and frequently used to calculate transmission coefficients through semiconductor SLs, metallic SLs, photonic crystals, and many other types of periodic systems, even though the theoretical approaches generally also introduce the Floquet theorem which is rigorously valid for \( n = \infty \).

Although the one propagating mode approach is the simplest version in the TFPS, it has been frequently applied to calculate transmission coefficients for different types of systems. When the channel coupling is weak, these matrices may be also useful for a first-order approximation. Other systems as the magnetic SLs are at least two-mode systems.

5.2. Scattering Amplitudes and Transport Properties in the One-Channel Limit

In the particular but very much used 1D one channel case, the transmission amplitude

\[
t_n = \frac{t^*}{p_n t^* - p_{n-1}}
\quad (105)
\]

takes the form

\[
t_n = \frac{t^*}{t^* U_n - U_{n-1}}
\quad (106)
\]

This is an extremely simple function of the Chebyshev polynomials of the second kind, \( U_n(\alpha_R) \) and \( U_{n-1}(\alpha_R) \) (evaluated at the real part of \( \alpha \)), and of the single-cell transmission amplitude \( t \). Using the identity \( U_n U_{n-2} = U_n^2 - 1 \), or alternatively \( |\alpha|^2=1+|\beta|^2 \), it is easy to show that the transmission coefficient \( T_n = |t_n|^2 \) can be written as \[202\]

\[
T_n = \frac{T}{T + U_n^2 - 1}
\quad (107)
\]

with an evident resonant behavior. Here, \( T = |t|^2 \) is the single-cell transmission coefficient. The transmission resonances occur precisely when the polynomial \( U_{n-1} \) becomes zero. Therefore, the \( \nu \)-th resonant energy \( E_{\nu} \) is the solution of

\[
(\alpha_R)_\nu = \cos \frac{\nu\pi}{n}
\quad (108)
\]

with \( \nu = 1, 2, 3, \ldots, n - 1 \). The index \( \nu \) labels the bands and \( \nu \) labels the intraband states. This equation is a dispersion relation for the resonant states, a discrete dispersion relation, at variance with the continuous dispersion relations that result in the hybrid approaches that combine transfer matrices and Bloch functions. We will refer to these approaches below. It is worth mentioning here that 60 years ago some theoretical approaches studying ordered and mainly disordered one-dimensional systems, obtained similar equations for eigenfrequencies of simple linear chains.\[203,204\]

In the one-channel case, the \( n \)-cell Landauer conductance is just

\[
G_n = \frac{1}{(U_{n-1})^2} G
\quad (109)
\]

The zeros of the polynomial determine both the points of divergence of \( G_n \) and the zeros of the resistance \( R_n \). They also determine the resonant energies \( E_{\nu} \), where the global transmission coefficient \( T_n \) is resonant.

Before we continue with the most recent advances of the TFPS that make possible the calculation of basic physical quantities, such as the optical transitions, let us consider a Kronig-Penney-like sequence of square barrier potentials in the conduction band of a (GaAs/AlGaAs)\( n \) SL. It is easy to calculate, using Equation (107) and fixed unit-cell parameters, the transmission coefficients shown in Figure 7. The series of graphs of the transmission coefficient \( T_n \) plotted as a function of the particle’s energy \( E \) and of the number of unit cells \( n \), show that by increasing \( n \) a band structure builds up gradually. It is evident also that when \( n \) is of order 5 the gaps in the band structure begin to look better defined.

6. The TFPS and the Eigenvalues, Eigenfunctions, and Dispersion Relations of SLs

The calculation of eigenvalues and eigenfunctions is one of the most important objectives in solving differential equations of the
dynamical systems. The calculation of energy eigenvalues and the corresponding eigenfunctions of bounded quasi-1D periodic systems is also as important as the calculation of transmission coefficients and resonant states in open systems. Many other properties of the periodic systems, such as transition probabilities, and optical response in semiconductor SLs depend on these quantities. The TFPS, originally oriented to calculate scattering amplitudes and resonant energies defined by the zeros of the Chebyshev polynomial $U_{n-1}$ in open SLs, was expanded and rigorous and compact analytical expressions for the calculation of energy eigenvalues, $E_{\mu,\nu}$ and the corresponding eigenfunctions $\Psi_{\mu,\nu}(z)$ in bounded SLs were derived. We will present here only the main formulas for the three possible configurations in which SLs can be found; either as part of an electronic transport system or as a part of a device where the SL is bounded by cladding layers (symmetric or asymmetric) which impose (finite or infinite) lateral barriers, as sketched in Figure 8. All the results obtained in this section are accurate, free of additional assumptions or approximations and they are based on the transfer matrix method as well as on the general formulas derived in the last section.

We will first consider open SLs as in Figure 8a. We will then review the derivation of analytic expressions for eigenvalues and eigenfunction of confined SLs as functions of the unit-cell transfer matrix elements. In Figure 8b,c, we show examples of confined SLs. For a detailed derivation of the results presented here, see ref. [202]. We will also see that the eigenfunctions of symmetric SLs possess well-defined parity symmetries, and we will derive new selection rules for inter- and intrasubband transition probabilities. For detailed analysis of this issue, see refs. [165,205].

### 6.1. Resonant Energies and Resonant Functions in Open 1D Periodic Systems

We will assume that the $n$-cell system is connected to ideal leads. Even though the results that will be obtained here are valid in general, i.e., for any shape of the single cell potential profile, we will, for specific calculations, consider in this section and the coming ones, SLs with piecewise constant potential, as shown in Figure 1, known also as the Kronig–Penney model.

In open SLs, the resonant behavior of the transmission coefficient has been always recognized as a natural feature in these systems, and, at the same time, the continuous energy spectrum and Bloch functions were assumed as characteristic properties of SLs. In this section, we will present the formulas that allow an exact calculation of the true energies and wave functions for open SLs. Since the characteristics of these results contrast eloquently with the well-established and widely accepted theory, we will present more specific results.

In the previous section, we observed that the resonant transmission occurs when the energy is such that the argument of the Chebyshev polynomial, $\alpha_R$, becomes a zero of the Chebyshev polynomial $U_n(\alpha_R)$. It is known and was recalled in ref. [205] that, for each value of an integer $\mu = 1, 2, \ldots$, the number of zeros of the Chebyshev polynomial $U_n$ is $n$. Thus, the resonant energies for a periodic system with $n$ unit cells are solutions of

$$\alpha_R(\mu,\nu) = \cos \frac{\nu + (\mu - 1)n}{n} \pi$$

(110)

and are characterized by the quantum number $\mu$ that labels the subbands (or cycles in the unit circle) and by the quantum number $\nu$, that labels the intrasubband resonant energies.

Solving this equation, we have the whole set of resonant energies $E_{\mu,\nu}$, with $\nu = 1, 2, \ldots, n - 1$ and $\mu = 1, 2, 3, \ldots$. The function $\alpha_R(\mu,\nu)$ represents the $\nu$-th zero of the $\mu$-th subband. The number of resonant states per subband equals the number of confining wells in the periodic system.

With the resonant energies that can be easily obtained from this relation, we can determine the density of resonant levels for any number of unit cells $n$ from

$$\rho_\mu(E_{\mu,\nu}) = \frac{1/n}{E_{\mu,\nu+1} - E_{\mu,\nu}}$$

(111)

for $\mu = 1, 2, 3, \ldots$ and $\nu = 1, 2, 3, \ldots, n - 1$.

In the continuous limit, the level density becomes

$$\rho(E) = \frac{1}{\pi E} \cos^{-1}(\alpha_R)$$

(112)

which corresponds to the level density of Kronig and Penney.\(^{[73]}\)

In Figure 9a,b, we show the resonant energies and the level density of the resonant states $\rho_\mu(E_{\mu,\nu})$ and $\rho(E)$ for the GaAs($Al_{0.3}Ga_{0.7}As$)/GaAs\(^n\) SL, modeled as a sequence of sectionally constant potentials, with GaAs layer widths of 10 nm in the wells, and $Al_{0.3}Ga_{0.7}As$ layer widths of 3 nm in...
the barrier, whose height is taken as $V_o = 0.23$ eV. For this system, the explicit form of equation (110) is

$$\cos k_o a \cosh q_o b - \frac{k_o^2 - q_o^2}{2k_o q_o} \sin k_o a \sinh q_o b = \cos \frac{\nu + (\mu - 1)n}{n} \pi$$

(113)

where $k_o^2 = 2m_o^*E_o^j/\hbar^2$ and $q_o^2 = 2m_o^*(V_o - E_o^j)/\hbar^2$. In the upper panel of Figure 9, the energy spectrum of the resonant energies inside the first three conduction subbands are shown, for $n = 14$. In the lower panel, the subband-level densities, for $n = 7$ and $n = 70$ (squares and triangles, respectively). As expected, the continuous-level density $\rho(E)$ predicted by the Kronig–Penney is reached when the number of cells $n \to \infty$.

The resonant functions are also in clear contrast with the Kronig–Penney. Here, the transfer matrix definition, the state vector at any point $z$ of the SL, say inside the $j+1$ cell, is determined by and obtained from

$$\phi(z) = M_p M_j \left( \frac{\phi^j(z_j)}{\phi(z_j)} \right) = M_j M_p \left( \frac{\phi^p(z_j)}{\phi(z_j)} \right).$$

(114)

Here, $\phi(z_j)$ and $\phi^p(z_j)$ are the right and left moving wave functions at $z_j$, $M_j$ is the transfer matrix for $j$ full cells, and $M_p$ the transfer matrix $M(z_j, z_o)$, as shown in Figure 8. Assuming that the incidence is only from the left side, we have

$$\phi^j(z_j) = -\frac{\beta_n}{\alpha_n} \phi^j(z_j) = r_n \phi^j(z_j)$$

(115)

Here, $\alpha_n$ and $\beta_n$ are the transfer matrix elements of the whole n-cell system, and $r_n$ the total reflection amplitude. Thus, the wave function at $z$, for any value of the energy $E$, is given by

$$\phi(z) = \frac{\phi(z_o)}{\phi(z_o)} \left[ \left( \frac{\beta_n}{\alpha_n} \right)^j \phi^j(z_j) \right] = \phi(z_o) \left[ \frac{\beta_n}{\alpha_n} \right]^j \phi^j(z_j).$$

(116)

By evaluating this function for $E = E_n^p$, we get the desired $\nu$-th resonant wave function in the $\mu$-th subband, i.e.

$$\psi_{\nu,\mu}^p(z) = \phi(z, E_n^p).$$

(117)

In 1D periodic systems, the resonant wave function $\psi_{\nu,\mu}^p(z)$ is a simple but not trivial combination of Chebyshev polynomials. It is easy to verify that Equation (116) implies

$$\psi_{\nu,\mu}^p(z) = \frac{1}{\alpha_n} \psi^p(z) = t_n \psi(z_o) = \psi(z_n)$$

(118)

$$\psi_{\nu,\mu}^p(z) = \left( 1 - \frac{\beta_n}{\alpha_n} \right) \psi(z_o) = (1 + r_n) \psi(z_o)$$

Here, $t_n$ and $r_n$ are the $n$-cell transmission and reflection amplitudes, respectively.

To make even more compelling the difference with the standard approach, we show in Figure 10 resonant wave functions and a function in the gap. It is clear that, at variance with the Bloch functions, the resonant functions are not periodic. Furthermore, the resonant states are extended wave functions with particle density different from zero throughout and at the ends of the system. This will not be the case, of course, for bounded systems.

6.2. Eigenvalues and Eigenfunctions in Bounded 1D Periodic Systems

An important extension in the TFPS approach has been accomplished when general expressions for the evaluation of
and of length \( L = nL_c \), derived before, gives us

\[
U_{n-1}(\alpha_i - \beta_i) = 0 \tag{122}
\]

Here, the subscript \( l \) refers to the imaginary part. It is clear from this formula that there are \( n - 1 \) of the energy eigenvalues that come from the zeros of the Chebyshev polynomial \( U_{n-1} \), and two other eigenvalues come from the factor \((\alpha_i - \beta_i)\). This is not a trivial result; it is remarkable because they correspond to the well-known Tamm and Shockley\(^{[206,207]}\) localized surface states. The hard walls push upward two of the \( n + 1 \) energy levels of each subband as can be seen in the upper panel of Figure 12.

When the length of the system is \( nL_c + a \), which can be achieved by adding two layers of thickness \( a/2 \) at the ends of the \( n \)-cells SL, the eigenvalue equation changes slightly into

\[
(\alpha_n e^{i\beta_n a} - \alpha_n e^{-i\beta_n a}) + \beta_n - \beta_n = 0 \tag{123}
\]

assuming that the potential in the additional half layers is constant. In terms of the Chebyshev polynomials the eigenvalue equation is

\[
U_n \sin ka + (\alpha_i \cos ka - \alpha_i \sin ka - \beta_j)U_{n-1} = 0 \tag{124}
\]

As for the open systems, the transfer matrix properties and the boundary conditions lead, for the SL of length \( L = nL_c \), to the wave function

\[
\Psi^b(z, E) = A \left[ \left( \alpha_p + \gamma_p \right) \left( \alpha_j - \beta_j \frac{\alpha_n + \beta_n}{\alpha_n + \beta_n} \right) + \left( \beta_p + \delta_p \right) \left( \beta_j - \alpha_j \frac{\alpha_n + \beta_n}{\alpha_n + \beta_n} \right) \right] \tag{125}
\]

Here, \( A \) is a normalization constant. Evaluating this function at \( E = E_{n\mu} \), we obtain the corresponding eigenfunction

\[
\Psi^b_{\mu}(z) = \Psi^b(z, E_{n\mu}) \tag{126}
\]

This is a rigorous solution of the Schrödinger equation for \( 1D \) finite periodic systems, bounded by infinite hard walls. In the case of SL with length \( L = nL_c \), the wave function gets, if the potential in the additional half layers is constant, an overall factor \( e^{i\beta_n a} \), and the term \((\alpha_n + \beta_n)/(\beta_n + \alpha_n)\) is replaced by \((\alpha_n + \beta_n e^{-i\beta_n a})/(\beta_n + \alpha_n e^{i\beta_n a})\).

To plot specific eigenvalues and eigenfunctions, we use parameters of the SL \( \text{GaAs(Al}_{0.3}\text{Ga}_{0.7}\text{As/GaAs)}^{12} \), bounded by hard walls. In Figure 11 and 12, we show in the upper panels the discrete spectra, of the bounded SLs with lengths \( L = nL_c \) and \( L = nL_c + a \), respectively. In both figures, we plot the eigenfunctions \( |\Psi^b_{22}(z)|^2, |\Psi^b_{23}(z)|^2 \), the lower panels in Figure 12 are the surface functions \( |\Psi^b_{212}(z)|^2, |\Psi^b_{213}(z)|^2 \), these functions describe localized particles at the ends of the SL and correspond to the energy levels pushed upward by the hard walls. Notice that because of the overall phase, the envelopes of the eigenfunctions of the SL with length \( L = nL_c + a \) have a sine-like shape, while the envelopes of the eigenfunctions of the SL of length \( L = nL_c \) are cosine-like.
6.3. Eigenvalues and Eigenfunctions for SLs Bounded by Cladding Layers

The SLs bounded by symmetric or asymmetric cladding layers represent an important class of MQW structures, widely used in optical devices. Assuming that $E < V_o$, $V_{lb}$, where $V_o$ is the barrier height, $V_{lb}$ and $V_{rb}$ the left and right cladding layer barrier heights, general formulas for the calculation of the energy eigenvalues and their corresponding eigenfunctions have been obtained. For a symmetric SL of length $L = nL_0$, i.e., of exactly $n$-unit cells, the eigenvalue equation is

$$h_w U_n + f_w U_{n-1} = 0$$  \hspace{1cm} (127)

where

$$h_w = 1, \quad \text{and} \quad f_w = \alpha_i \frac{q_w^2 - k^2}{2q_w k} - \alpha_R - \beta_1 \frac{q_w^2 + k^2}{2q_w k}$$  \hspace{1cm} (128)

When $V_{lb} = V_{rb} \equiv V_w$, $q_w^2 = 2m(V_w - E)/\hbar^2$, and $k$ is the wave vector at $z_j$, and $z_{j-1}$, while $\alpha_R$ and $\alpha_i$ are the real and imaginary parts of the single-cell transfer-matrix element $\alpha$.

Again, as in the previous section, a slightly more realistic and symmetric structure is a SL of length $L = nL_0 + a$. The eigenvalue equation for this system is again Equation (127) but the functions $h_w$ and $f_w$, change. For the system shown in Figure 13, these functions are

$$h_w = \frac{q_w^2 - k^2}{2q_w k} \sin ka + \cos ka$$  \hspace{1cm} (129)

and

Using the transfer matrices introduced in previous sections, it is easy to show that the wave function at any point $z$ in cell $j + 1$ is given by

$$\Psi^j(z, E) = \frac{A}{g_n} \left\{ \left[ (\alpha_p + \gamma_p)\alpha_j + (\beta_p + \delta_p)\beta_j \right] \left( 1 - i \frac{q_w}{k} \right) \right. \right.$$

$$\left. + \left( (\alpha_p + \gamma_p)\beta_j + (\beta_p + \delta_p)\alpha_j \right) \left( 1 + i \frac{q_w}{k} \right) \right\}$$  \hspace{1cm} (131)

Here, $A$ is a normalization constant and

$$g_n = \alpha_n \frac{q_w^2 + k^2}{2q_w k} - \beta_n \frac{q_w^2 - k^2}{2q_w k} - \beta_w$$  \hspace{1cm} (132)
three eigenfunctions in the second subband, for the energies indicated in the graphs.

6.3.1. SLs Bounded by Asymmetric Cladding Layers

When the cladding layers that bound a SL are asymmetric, the eigenvalue equation remains the same, i.e.

$$h_w U_n + f_w U_{n-1} = 0$$  \hspace{1cm} (134)

but now the functions $h_w$ and $f_w$ modify a bit and become

$$h_w = \frac{q_{lw} q_{rw} - k^2}{(q_{lw} + q_{rw})k} \sin ka + \cos ka$$  \hspace{1cm} (135)

and

$$f_w = \frac{q_{lw} q_{rw} - k^2}{(q_{lw} + q_{rw})k} \left( \alpha_l \cos ka - \alpha_R \sin ka \right) - \alpha_l \sin ka - \beta_l \frac{q_{lw} q_{rw} + k^2}{(q_{lw} + q_{rw})k}$$  \hspace{1cm} (136)

with $q_{lw}^2 = 2m(V_{lh} - E)/\hbar^2$ and $q_{rw}^2 = 2m(V_{rh} - E)/\hbar^2$, the wave numbers in the left and right barriers. As a consequence of this asymmetry, the quasi-degeneracy of the surface energy levels is lifted, and the energy levels split. The splitting grows as the asymmetry increases.

The universal formulas reported here, written in terms of Chebyshev polynomials $U_n$ and the single-cell transfer matrix elements, allow us to solve completely the fine structure in the bands, and can easily be applied to calculate intraband states, phototransitions, and other properties of finite periodic systems described either by the electromagnetic or the quantum theories. All the expressions are valid for any profile of the single-cell potential and arbitrary number $n$ of unit cells. In the limit of $n \to \infty$, these formulas reproduce the well-known results of current theories.

At the time these resonant energies and the energy eigenvalues were first obtained it was not yet clear that high-resolution optical response measurements revealed the intrasubband energy levels. In Section 8.2, we will present an example that can be fully explained only with the results obtained in this section.

6.4. Parity Symmetries of the SL Eigenfunctions and the Transition Selection Rules

The parity of the resonant functions and particularly of the eigenfunctions is an important property that was analyzed in ref. [205]. We shall now outline the parity symmetries of the three cases considered in the last section. Since the eigenfunctions depend on the Chebyshev polynomials, their symmetry properties are closely related to the Chebyshev polynomials’ symmetries. It is worth recalling that all the Chebyshev polynomials, which enter in the physical expressions derived here for 1D SLs, are evaluated at $\alpha_R$, the real part of $\alpha$. 

![Figure 13. Quasibounded eigenfunctions $|\Psi_{\mu\nu}(z)|^2$ in the second subband of a GaAs(Al$_x$Ga$_{1-x}$As) SL, with AlAs cladding layers and $n = 12$. These functions are rather similar to the corresponding functions in Figure 5 and 7. For the confining potential height $V_w$ equal to 0.44 eV, indicated in the SL sketch, the repulsion effect is weak and the effect slightly visible. Reproduced with permission.](image-url)
6.4.1. The Parity Symmetries of the Resonant Wave Functions

While the resonant energies were recognized in open systems associated with the resonant behavior of the transmission coefficients defined in Equation (107), there is no reference to resonant wave functions of open SLs. In the previous section, the resonant wave functions are given by

$$
\Psi^r_{\mu,\nu}(z) = \bar{\psi}(z_0) \left[ \left( \alpha_j - \beta_j \frac{\beta_n}{\alpha_n} \right) (\alpha_p + \gamma_p) + \left( \beta^*_j - \alpha^*_j \frac{\beta_n}{\alpha_n} \right) (\beta_p + \delta_p) \right] \bigg|_{E_n}
$$

(137)

In order to determine the space-inversion symmetries of these functions, it is useful to evaluate the resonant functions at two points, symmetric with respect to the middle point of the SL. Since this function is complex, two parity relations were reported in ref. [205]. One for the real part and one for the imaginary part (see Figure 14). Choosing the points $z_n = L/2$ and at $z_o = -L/2$, it is easily found that the real part possess the symmetry

$$
\Re[\Psi^r_{\mu,\nu}(z_n-1)] = \frac{1}{U_n} \Re[\Psi^r_{\mu,\nu}(z_1)]
$$

(138)

The imaginary parts of $\Psi^r_{\mu,\nu}(z_1)$ and $\Psi^r_{\mu,\nu}(z_n-1)$ satisfy the relation

$$
\Im[\Psi^r_{\mu,\nu}(z_n-1)] = -\frac{1}{U_n} \Im[\Psi^r_{\mu,\nu}(z_1)]
$$

(139)

These relations together imply the symmetry (here * stands for complex conjugate)

$$
\Psi^r_{\mu,\nu}(L/2) = U_n \Psi^r_{\mu,\nu}(-L/2)
$$

(140)

which depends on the symmetry of the Chebyshev polynomial $U_n$ evaluated at the resonant energies. From a simple analysis of the Chebyshev polynomials, it was found in ref. [205] that

$$
U_n|_{E_n} = \begin{cases} (-1)^n & \text{for } n \text{ even} \\ (-1)^{n+1} & \text{for } n \text{ odd} \end{cases}
$$

(141)

Therefore

$$
\Psi^r_{\mu,\nu}(L/2) = \begin{cases} (-1)^n \Psi^r_{\mu,\nu}(-L/2) & \text{for } n \text{ even} \\ (-1)^{n+1} \Psi^r_{\mu,\nu}(-L/2) & \text{for } n \text{ odd} \end{cases}
$$

(142)

6.4.2. The Parity Symmetries of Eigenfunctions of Bounded SLs

In this case, we will analyze separately the two cases: bounded SLs of length $L = nL_c$ and bounded SLs of length $L = nL_c + a$.

When the length of the bounded SL is $L = nL_c$, the eigenfunctions are given by

$$
\Psi^b_{\mu,\nu} = A \left[ (\alpha_p + \gamma_p) \left( \alpha_j - \beta_j \frac{\alpha_n + \beta_n}{\alpha_n} \right) + (\beta_p + \delta_p) \left( \beta^*_j - \alpha^*_j \frac{\alpha_n + \beta_n}{\alpha_n} \right) \right] \bigg|_{E_n}
$$

(143)

where $A$ is a normalization constant. The symmetries are obtained also by evaluating the eigenfunctions at two points, symmetric with respect to the center of the SL. Choosing the points at $z = z_1 = -L/2 + k$ and at $z = z_{n-1} = L/2 - k$, the matrix elements are $\alpha_p = \delta_p = 1$ and $\beta_p = \gamma_p = 0$. At $z_1$, $\alpha_j = \alpha$, and $\beta_j = \beta$, while at $z_{n-1}$, $\alpha_j = \alpha_{n-1}$, and $\beta_j = \beta_{n-1}$. The eigenvalue equation implies also that $(\alpha_n + \beta_n)/\alpha^*_n + \beta^*_n = 1$, therefore

$$
\Psi^b_{\mu,\nu}(z_1) = A(\alpha - \beta + \beta^* - \alpha^*)
$$

(144)

Figure 14. Imaginary and real parts of the resonant wave functions of an SL with $n=7$ (left column) and $n=8$ (right column). In accordance with the parity symmetry relations (136) and (135), in the left column (for $n=7$), $\Im[\Psi^r_{1,1}(z)]$ is symmetric and $\Im[\Psi^r_{1,2}(z)]$ is antisymmetric, and in the right column (for $n=8$), $\Re[\Psi^r_{1,1}(z)]$ is antisymmetric and $\Re[\Psi^r_{1,2}(z)]$ is symmetric. Reproduced with permission. Copyright 2017, Elsevier.
Similarly, we have
\[ \psi_{\mu,\lambda}^{b}(z_{n-1}) = A(\alpha_{n-1} - \beta_{n-1} + \beta_{n-1}^* - \alpha_{n-1}^*) \] (145)

Using the relations
\[ \alpha_{n-1} = \alpha_{n}^* - \beta_{n}^* \quad \text{and} \quad \beta_{n-1} = -\alpha_{n}^* - \beta_{n}^* \] (146)
results in
\[ \psi_{\mu,\lambda}^{b}(z_{n-1}) = -A(\alpha_{n} - \beta_{n}^*)(\alpha - \beta^* + \alpha^*) \] (147)
which means
\[ \psi_{\mu,\lambda}^{b}(L/2 - l_{k}) = - (\alpha_{n} + \beta_{n}^*)\psi_{\mu,\lambda}^{b}(-L/2 + l_{k}) \] (148)

Since the imaginary part of \( \alpha_{n} + \beta_{n}^* \), which is proportional to \( U_{n-1} \), is zero, we are left with
\[ \psi_{\mu,\lambda}^{b}(L/2 - l_{k}) = -U_{n}\psi_{\mu,\lambda}^{b}(-L/2 + l_{k}) \] (149)
and the symmetry parities are also related to those of \( U_{n} \) when \( U_{n-1} = 0 \). This means that
\[ \psi_{\mu,\lambda}^{b}(z) = \begin{cases} (-1)^{i+1}\psi_{\mu,\lambda}^{b}(-z) & \text{for } n \text{ even} \\ (-1)^{i}\psi_{\mu,\lambda}^{b}(z) & \text{for } n \text{ odd} \end{cases} \] (150)

When the length of the bounded SL is \( L = n_{l} + a \), the eigenfunctions are given by
\[ \psi_{\mu,\lambda}^{b}(z) = Ae^{-ika/2}(\alpha_{0} + \gamma_{p})(\alpha - \beta e^{-i\alpha}) + (\beta_{p} + \delta_{p})(\beta_{0} - \gamma e^{-i\alpha}) |_{E_{\mu}} \] (151)
where \( A \) is a normalization constant and the eigenvalue equation
\[ \alpha_{e} + \beta_{e} = \alpha_{0} + \gamma_{p} \quad \text{and} \quad \beta_{e} = \beta_{0} - \gamma e^{-i\alpha} \] (152)
and
\[ \psi_{\mu,\lambda}^{b}(L/2) = Ae^{-ika/2}(1 - e^{-i\alpha}) \] (153)

Again, using the eigenvalue equation it is possible to write
\[ \psi_{\mu,\lambda}^{b}(L/2) = -Ae^{-ika/2}(1 - e^{-i\alpha})(\beta_{n} - \alpha_{0}e^{ika}) \] (154)
with the imaginary part of \( \beta_{n} - \alpha_{0}e^{ika} \) equal to zero. It was shown in ref. [205] that this factor has also the symmetries of \( -U_{n} \) when \( U_{n-1} = 0 \). Therefore
\[ \psi_{\mu,\lambda}^{b}(z) = \begin{cases} (-1)^{i+1}\psi_{\mu,\lambda}^{b}(-z) & \text{for } n \text{ even} \\ (-1)^{i}\psi_{\mu,\lambda}^{b}(z) & \text{for } n \text{ odd} \end{cases} \] (155)

6.4.3. The Parity Symmetries of the Eigenfunctions of SLs

Bounded by Cladding Layers, and Selection Rules

It was shown in ref. [205] that when the SLs are bounded by finite lateral barriers, the eigenfunctions possess the same symmetries as the eigenfunctions of SLs bounded by infinite walls (Figure 15 and 16). This means that for a SL of length \( L = n_{l} + a \) the eigenfunction symmetries are
\[ \psi_{\mu,\lambda}^{b}(z) = \begin{cases} (-1)^{i+1}\psi_{\mu,\lambda}^{b}(-z) & \text{for } n \text{ odd} \\ (-1)^{i}\psi_{\mu,\lambda}^{b}(z) & \text{for } n \text{ even} \end{cases} \] (156)

If we write the parity symmetries of the wave functions, in general, as
\[ \psi_{\mu,\lambda}^{b}(z) = s_{\nu,\rho}^{c}\psi_{\mu,\lambda}^{b}(z) \] (157)
\( s_{\nu,\rho}^{c} \) is a sign factor, whose values depend on the type of the SL (i.e., open \( c = 0 \), or confined by hard walls \( c = b \), or finite height walls \( c = gb \)), the quantum numbers \( \mu \) and \( \nu \), and the parity of the number of unit cells \( n \). The possible values are summarized in Table 1.

The wave function parity relations lead to the following selection rules. When the number of unit cells \( n \) is even,
Table 1. Parity symmetry sign \(s_{\nu}^{\mu}\) for resonant (\(f_i\)), bounded (\(b\)), and quasibounded (\(qb\)) SLs, as a function of the parity of the number of unit cells \(n\), and the quantum numbers \(\mu\) and \(\nu\).

| \(s_{\nu}^{\mu}\) | SL length | \(n\) even | \(n\) odd |
|------------------|-----------|-------------|-----------|
| \(s_{\nu}^{\mu}\) | \(n_l\)   | \((-1)^\nu\) | \((-1)^{\nu+1}\) |
| \(s_{\nu}^{\mu}\) | \(n_l\)   | \((-1)^{\nu+1}\) | \((-1)^\nu\) |
| \(s_{\nu}^{\mu}\) | \(n_l + a\) | \((-1)^{\nu+\mu}\) | \((-1)^{\nu+1}\) |

The symmetry selection rules are

\[
\int dz \Psi_{\mu',\nu}^{\mu,\nu}(z) \frac{\partial}{\partial z} \Psi_{\mu',\nu}^{\mu,\nu}(z) \begin{cases} = 0 & \text{when } P[\mu + \nu] = P[\mu + \nu + 1] \\ \neq 0 & \text{when } P[\mu' + \nu'] = P[\mu' + \nu + 1] \end{cases} \tag{158}
\]

Here, \(P[\mu + \nu]\) means parity of \(\mu + \nu\). \(c\) refers to conduction band, \(v\) refers to valence band, and \(q\) stands for quasibounded SL. When \(n\) is odd the symmetry selection rules are

\[
\int dz \Psi_{\mu',\nu}^{\mu,\nu}(z) \frac{\partial}{\partial z} \Psi_{\mu',\nu}^{\mu,\nu}(z) \begin{cases} = 0 & \text{when } P[\nu'] = P[\nu] \\ \neq 0 & \text{when } P[\nu'] = P[\nu + 1] \end{cases} \tag{159}
\]

Similar relations are valid for infrared (intraband) transitions but with additional restrictions \(\mu' \geq \mu\) and, whenever \(\mu = \mu'\) we must also have \(\nu > \nu'\).

The transfer matrix method is one of the most pedestrian methods in the sense that a transfer matrix is built up step by step, that is, layer by layer, and therefore the finiteness of the system is taken into account explicitly, and becomes an intrinsic quality of the method. On the other hand, the Bloch–Floquet theorem that is known to be rigorously valid for infinite systems, implies necessarily the infiniteness as the intrinsic quality. Any attempt to construct an approach based on concepts valid in different domains falls necessarily into inconsistencies and limited predictions. The number of papers that combine the transfer matrix method with the Bloch theorem to study semiconductor, optical, and other types of SLs is really overwhelming.

As mentioned above, faced with the problem of describing the physics of layered periodic structures, whose dynamics are determined by differential equations, it is natural to resort to the transfer matrix method, which is becoming gradually a well-known method and particularly useful as a tool to solve quantum equations of simple structures. When applied to larger systems, the Jones–Abelès transfer matrix (that has been multiple times rediscovered) is also a well-known formula in the literature and highly regarded by its capability of making possible direct calculations of the transmission coefficients. On the other hand, we face the real fact that most physicists have adhered to the mistaken idea that Bloch functions and periodic systems are intimate and inextricable joint concepts that oblige us to invoke the Bloch functions whenever a periodic system appears. Based on the well-established transfer matrix properties and the explicit relations recalled in the first sections, it is easy to show the inconsistency of these approaches. Let us first join some important pieces.

As mentioned above, the group of transfer matrices contains the compact subgroup of transfer matrices whose general representation is of the form

\[
M_{uc} = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix}
\tag{160}
\]

with \(u_i\) \(N\)-dimensional unitary matrices. In the orthogonal universality class \(u_2 = u_1\). In most of the publications dealing with infinite and semi-infinite-layered and periodic systems, where the authors end up invoking the Floquet theorem (see for example, refs. [118–120,122]) the electromagnetic fields and field vectors in the \(n\)-th unit cell, are written, respectively, as

Figure 16. Eigenfunctions of SLs with length \(L=nl_1+a\), bounded by finite walls. According to the parity symmetry relation (153), the eigenfunction \(\Psi_{9,2}^{b}(z)\) and \(\Psi_{7,2}^{b}(z)\) in the left column (for \(n=11\)) are both antisymmetric, while the eigenfunctions \(\Psi_{9,2}^{b}(z)\) and \(\Psi_{7,2}^{b}(z)\) in the right column (for \(n=10\)) are antisymmetric and symmetric, respectively. Reproduced with permission\(^{[205]}\) Copyright 2017, Elsevier.
\[ \mathcal{E}(z, n) = a_n e^{ik_z(z-nl_z)} + b_n e^{ik_z(z-nl_z)} \]
and
\[ \Phi_n(z, n) = \begin{pmatrix} a_n e^{ik_z(z-nl_z)} \\ b_n e^{-ik_z(z-nl_z)} \end{pmatrix} \] (161)

In this case, it is clear that
\[ \Phi_n(z, n) = \begin{pmatrix} e^{ik_zl_z} & 0 \\ 0 & e^{-ik_zl_z} \end{pmatrix} \begin{pmatrix} a_{n-1} e^{ik_z(z-(n-1)l_z)} \\ b_{n-1} e^{-ik_z(z-(n-1)l_z)} \end{pmatrix} \] (162)
\[ = M_{oc} \Phi_n(z, n-1) \]

with \( M_{oc} \) of the compact subgroup. It is worth noticing that while this matrix (that connects fields fulfilling the Floquet theorem) is diagonal, the matrices that connect fields in finite optical structures, even in binary (AB)\( ^n \) SLs, are nondiagonal. An important issue behind this difference, and for the argument discussed below, is the relevance of the wave functions basis. When the relation between a transfer matrix and the \( S \) matrix was derived, we mentioned the importance of using the same basis. This means that whenever we refer to a transfer matrix like
\[ M_n = \begin{pmatrix} a & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} (t')^{-1} & r' \\
\end{pmatrix} \begin{pmatrix} (t')^{-1} \end{pmatrix} \] (163)
the basis of functions is fixed. Due to the importance of this topic and the large number of followers that the P. Yeh’s argument has,[200] we will briefly refer to Yeh’s assumptions and we will see if his most consequential result, the supposedly periodic factor of the so-called electromagnetic Bloch wave (reported in Equation (6.2-9) of Yeh’s book, and copied in our Equation (170) below), is truly periodic, as stated just after equation (6.2-9) in Yeh’s book, or it is not. We will show graphically that the supposed periodic factor does not meet the periodicity requirement. The lack of periodicity, exhibits the drawbacks of the procedure that we criticize and discuss now.

The problem posed in the hybrid approach, when “the solutions for periodic medium in accordance with Floquet theorem” are written as
\[ E_K(x, z) = \mathcal{E}_K(x) e^{-iKz} e^{ikx} \] (164)
where \( E_K(x + \Lambda) = \mathcal{E}_K(x) \), is to find \( K \) and \( \mathcal{E}_K(x) \). We will see below that a correct approach should be to determine the transfer matrix compatible with the Floquet theorem.

Starting from the electromagnetic fields
\[ E(x) = \begin{pmatrix} a_n e^{-ik_z(x-n\Lambda)} + b_n e^{ik_z(x-n\Lambda)} \\ e_n e^{-ik_z(x-n\Lambda + a)} + d_n e^{ik_z(x-n\Lambda + a)} \end{pmatrix} \text{ for } n\Lambda - a < x < n\Lambda \]
\[ = \begin{pmatrix} a_n e^{-ik_z(x-n\Lambda)} + b_n e^{ik_z(x-n\Lambda)} \\ e_n e^{-ik_z(x-n\Lambda + a)} + d_n e^{ik_z(x-n\Lambda + a)} \end{pmatrix} \text{ for } (n-1)a < x < n\Lambda - a \] (165)
for the fields of a two layer unit-cell, Yeh ends up writing the relation
\[ \begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix} \] (166)
with a nondiagonal transfer matrix. The transfer matrix here is the inverse of ours, but this is not an issue. An important step in the attempt to obtain Bloch-type electromagnetic fields has been to write the Bloch waves as
\[ \begin{pmatrix} a_n \\ b_n \end{pmatrix}_K = e^{-iK\Lambda} \begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix}_K \] (167)

Notice that the Bloch vectors, written here with a subindex \( K \), are not the same as the electromagnetic fields in (166). Disregarding this important difference, one believes that the same transfer matrix that relates the electromagnetic field vectors also relates the Bloch vectors in the last equation. This misleading assumption leads to write the Kramers eigenvalue equation
\[ \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix}_K = e^{iK\Lambda} \begin{pmatrix} a_n \\ b_n \end{pmatrix}_K \] (168)

Solving this equation, the eigenvalues
\[ \lambda = e^{iK\Lambda} = \frac{1}{2} (A + D) \pm \sqrt{\left( \frac{1}{2} (A + D) \right)^2 - 1} \] (169)
and the corresponding eigenvectors are obtained. To derive the periodic factor \( E_K(x) \), in a kind of backward step, a second assumption that identifies again the eigenvectors with the electromagnetic waves is made, and leads to Equation (6.2-9) of Yeh’s book for “the Bloch wave in the \( n_1 \) layer of the \( n \)-th unit cell” given by
\[ \mathcal{E}_K(x) e^{-iKz} = \left[ (a_0 e^{-ik_z(x-n\Lambda)} + b_0 e^{ik_z(x-n\Lambda)}) e^{iK(x-n\Lambda)} \right] e^{-iKz} \] (170)
with \( a_0 = B \) and \( b_0 = \lambda_+ - A \), and the additional statement that the “expression inside the square brackets... is periodic.” However, using the same transfer matrix elements given in Yeh’s book, we have plotted the expression inside the square brackets and find that it is not periodic and behaves as shown in Figure 17. For \( n_1 = 1 \) and \( n_2 = 1.2 \), the function in the square bracket behaves as shown in Figure 17a and for \( n_1 = 1 \) and \( n_2 = 2.1 \) has the divergent behavior shown in Figure 17b, as \( x \) grows. This is a consequence of the unjustified assumptions.

It may be important however to see what kind of transfer matrix is compatible with Bloch-type electromagnetic functions. If instead of assuming Equation (168) as if we were looking for vectors, which are known and fixed, we look for the transfer matrix elements \( A_K, B_K, \ldots \) such that
\[ \begin{pmatrix} A_K & B_K \\ C_K & D_K \end{pmatrix} \begin{pmatrix} a_n e^{iK(x+n\Lambda)} \\ b_n e^{-iK(x+n\Lambda)} \end{pmatrix} = \lambda e^{iK\Lambda} \begin{pmatrix} a_n e^{iK(x+n\Lambda)} \\ b_n e^{-iK(x+n\Lambda)} \end{pmatrix} \] (171)
where \( \lambda_+ \lambda_- = 1 = e^{iK\Lambda} e^{-iK\Lambda} \). an obvious solution is 
\( K_+ = -K_-, A_K = \lambda_+, D_K = \lambda_-, \) and \( B_K = C_K = 0 \), thus a Floquet transfer matrix that is compatible with these assumptions is
\[ M_F = \begin{pmatrix} e^{iK\Lambda} & 0 \\ 0 & e^{-iK\Lambda} \end{pmatrix} \] (172)
which belongs to the compact subgroup of transfer matrices and allows Bloch-type electromagnetic fields such that

$$\begin{pmatrix} E^+(z + n\Lambda) \\ E^-(z + n\Lambda) \end{pmatrix} = M^n \begin{pmatrix} E^+(z) \\ E^-(z) \end{pmatrix}$$

(173)

In this way, each component of the electromagnetic waves is a Bloch-type wave function, and can be written as

$$E^+(z + n\Lambda) = e^{iKn\Lambda} E^+(z) = e^{iKn\Lambda} e^{ikz}$$

(174)

$$E^-(z + n\Lambda) = e^{-iKn\Lambda} E^-(z) = e^{-iKn\Lambda} e^{-ikz}$$

(175)

The price to pay for an electromagnetic wave whose amplitude does not vanish from $-\infty$ to $\infty$ is a transmission amplitude $t_B = e^{iKn\Lambda}$ that only modifies the phase and implies, as should be expected, a local transmission coefficient $T_n = 1$.

8. Multichannel Features in DBs, Ballistic Resonant Tunneling Transistors, and Some Other Examples

We will review here, and in the next section, some examples in which the TFPS has been applied. We will start with the calculation of the conductance for a resonant biased double barrier (DB). We will see that the shoulder that is present in the negative resistance domain of numerous experimental results is easily explained by the multichannel conductance calculation for biased DB.\[209] We will then refer to one of the various proposals of ballistic electrons through SLs in resonant tunneling transistors, and we will show also good agreement between the theoretical prediction and the measured transmission coefficients.\[197] We will review also the ballistic multichannel transmission through a 3D periodic array of $\delta$-scatterer centers,\[138] and will see an example of channel coupling and channel interference. In some of the applications of the TFPS the space–time evolution of Gaussian electromagnetic and Gaussian electron WPs through SLs were studied. We will show few results in the published work, among them, evidences of superluminal transmission of electromagnetic waves packets through optical media SLs,\[175] optical antimatter effect in electromagnetic WPs through metamaterial SLs,\[185,186,210,211] $I$–$V$ characteristics in spin injection, spin filter, and spin inversion behavior for spin WPs through homogeneous magnetic SLs.\[179]

8.1. Multichannel Features in the Negative Resistance Domain of Biased DBs

The biased DB is a simple system and the resonant tunneling and negative resistance behavior have been amply and extensively studied, and little or nothing should be added after 50 years of research and applications. However, it turns out that a feature in the negative resistance domain, that appeared in numerous experimental reports,\[196,212–222] has not been well understood, much less predicted. That feature is a shoulder as the one seen, between 0.32 and 0.43 V, in the experimental (black, continuous) curve in Figure 18b) reported by Bowen et al. in ref. [196].

The dot-dashed line in this figure, is a single band simulation, while the dashed line curve is ten bands simulation in a nearest neighbor sp3s$^*$ model.\[223] In ref. [212], the shoulder is considered a consequence of a self-detection; in ref. [222], it is attributed to serial resonance, and, in ref. [221], to oscillations due to the bias field. The shoulder in the conductance and $I$–$V$ characteristics of biased DBs is a good example to test the calculation of these quantities.

In many real systems, the transverse dimensions imply, as mentioned in Section 2, the contribution of several propagating modes. In ref. [209], the transfer matrix method and the multichannel (multi-propagating modes) approach, introduced in Section 2, was applied to study transmission coefficients and
conductance through a DB under the influence of longitudinal and transverse electric fields. Some results published there give an insight to explain what is behind the frequently observed shoulder in the negative resistance domain of DBs. In fact, a simple calculation of the transmission coefficient of a biased DB, with only longitudinal electric field, has the behavior shown in red in Figure 18a, and in the current shown in Figure 18b. For this results, we consider the Schrödinger equation

\[
-\frac{\hbar^2}{2m^*} \nabla^2 \Psi(r) + (V_C(x, y) + V_f(z))\Psi(r) = E\Psi(r)
\]  

(176)

Here

\[
V_f(z) = \begin{cases} 
-f_b z & -l_z < z \leq 0 \\
-f_b z & 0 < z < b \\
-V_o - f_b z & a + b < z < a + 2b \\
-f_b z & a + 2b < z < a + 2b + l_z 
\end{cases}
\]

(177)

where \( f_b \) is the electric force of a bias \( V_B \) potential applied between \( z = -l_z \) and \( z = a + 2b + l_z \), where \( a \) and \( b \) are the well and barrier widths. \( V_C(x, y) \) is a confining hard wall potential, as in Equation (1). After performing variables separation, and neglecting the evanescent channels contribution, one is left with the system of coupled equations

\[
\frac{d^2}{dz^2} \varphi_i(z) + (k_i^2 - k_i^2) \varphi_i(z) = \sum_{j=1}^{N} K_{ij}(z)\varphi_j(z)
\]

(178)

where \( N \) is the number of open channels and

\[
K_{ij}(z) = \frac{2m^*}{\hbar^2} \int_{0}^{w_0} dxdy \varphi_i^*(x, y) V(z)\varphi_j(x, y)
\]

(179)

is the coupling channels matrix. The functions \( \varphi_i(x, y) \) are the eigenfunctions of the infinite square well in the leads. As explained in Section 2, the channel indices \( i, j \) characterize the propagating modes and the transverse momenta \( k_{ij} = \pi y/w_y \). Here, \( w_y \) is the largest transverse width, or the radius when the transverse section is circular. For the DB potential \( U(y, z) \), defined above, the coupling matrix is

\[
K_{ij}(z) = \frac{2m^*}{\hbar^2} (-f_b z + V_o)\delta_{ij}
\]

(180)

Notice that in the absence of a transverse field, no channel mixing exists, and one is left with the system of solvable Airy equations

\[
\frac{d^2}{dz^2} \varphi_i(z) + (k_i^2 - k_i^2) \varphi_i(z) = \frac{2m^*}{\hbar^2} (-f_b z + V_o)\varphi_i(z)
\]

(181)

\( i = 1, 2, \ldots, N \)

As was explained in Section 2.2.1, given the solutions and their derivatives, it is possible and some times convenient to define transfer matrices \( W(z_2, z_1) \), that connects functions and their derivatives. For the DB, the \( N \) channel transfer matrix is a \( 2N \times 2N \) block-diagonal matrix, with blocks of the form

\[
W(z_2, z_1) = \begin{pmatrix} A_i(z_2, k_{1i}) & B_i(z_2, k_{1i}) \\
A'_i(z_2, k_{1i}) & B'_i(z_2, k_{1i}) 
\end{pmatrix}
\]

(182)

where \( A_i(z_2, k_{1i}) \) and \( B_i(z_2, k_{1i}) \) are the Airy functions in channel \( i \). After the similarity transformation, see Equation (43), it is easy to calculate the Landauer conductance

\[
G = \frac{e^2}{h} Tr TI^t
\]

(183)

as well as the current

\[
j = en_e f_u L Tr TI^t
\]

(184)

for a given incoming energy \( E \). In the last equation \( n_e \) is the charge carriers concentration, \( e \) is the electron’s charge, \( \mu_e \) the mobility, \( h \) the Planck’s constant, and \( L = a + 2b + l_z + l \), the distance between the point contacts. In Figure 18a,b, we show the calculated conductance and current for the parameters mentioned in ref.[196] (with \( a \) and \( b \) slightly modified to fit multiples of the lattice constant). By definition, the number of propagating modes (or open channels), is of the order of

Figure 18. Multichannel transmission and conductance of a biased DB. In the right, the experimental and theoretical I-V characteristics of the DB reported in ref. [196]. The transmission coefficient (a) and current (b) calculated for one propagating mode (blue) and for \( N = 26 \) propagating modes (red). The graph (b) shows that the multichannel conductance (present work) reproduces faithfully the shoulder observed in several experiments. Experimental figure: Reproduced with permission.[196] Copyright 1997, American Institute of Physics.
2\sqrt{2m^*E}/\hbar, with \( w \) the transverse width. It is clear the relevance that the finite transverse dimension \( w \) has in the splitting of the propagating modes, whose number is limited also by the energy \( E \). The calculation shows not only the origin of the shoulder in the negative resistance domain of a biased DB observed in the experimental reports but also the ability of the multichannel transfer matrix method to solve faithfully and to explain features that previous theoretical attempts failed to do so. It is evident also from Figure 18a that the propagating modes with higher longitudinal energy transmit at higher bias, but with lower transmission probability, a well-known effect that led to envision new devices where the symmetry of the DB, broken by the bias field, could be restored “not by applying an electric field, but by injecting minority carriers or ballistic electrons.”

8.2. Ballistic Electrons through Heterostructures and SLs

In the 1980s of the last century, when the size of semiconductor devices reached dimensions commensurate with the mean free path of charge carriers, it became natural to think that the carriers’ current is not only less diffusive, but ballistic or quasi-ballistic.

Thus, new structures and devices were proposed, in which ballistic electrons pass resonantly through the quantized energy levels of symmetric DBs or the minibands of SLs located in the base or in the emitter region. The main objectives were to increase the transmission probability and to obtain high peak-to-valley ratios, by restoring the symmetry of DBs or avoiding the loss of periodicity and the ensuing phase coherence in SLs. Among the numerous resonant tunneling transistors with SLs, we will review the three-terminal devices, with anti-reflecting coating, studied experimentally and theoretically by Pacher et al.

Figure 19 shows the schematic band structure of the three-terminal device with the SL studied by Pacher et al. The width of a GaAs valley is \( a = 6.5 \) nm, the width of the Al\(_{0.3}\)Ga\(_{0.7}\)As barrier is \( b = 2.5 \) nm, and the number of unit cells is \( n = 6 \). The width \( b' \) of the first and last barriers, which act as antireflection coating, is \( b' = b/2 \). Pacher et al. calculated and measured the transmission coefficients shown in Figure 20. For the calculation of the transmission coefficient of the uncoated and coated SL, in the 1D one-propagating mode limit, one has first to determine the transfer matrix given by

\[
M_{\epsilon} = M_{\beta} M_{\alpha} M_{\beta}^{-1}
\]

where \( M_{\alpha} \) is the SL transfer matrix

\[
M_{\alpha} = \begin{pmatrix}
U_n - \alpha^* U_{n-1} & \beta U_{n-1} \\
\beta^* U_{n-1} & U_n - \alpha U_{n-1}
\end{pmatrix}
\]

defined in (103) and \( M_{\beta} \) the transfer matrix of a coating layer, defined as

\[
M_{\beta} = \begin{pmatrix}
\alpha_{\beta} & \beta_{\beta} \\
\beta_{\beta} & \alpha_{\beta}
\end{pmatrix}
\]

In these matrices, we have

\[
\alpha = e^{i\alpha k} \left( \cosh q b + i \frac{k^2 - q^2}{2qk} \sinh q b \right)
\]

\[
\beta = -i \frac{k^2 + q^2}{2qk} \sinh q b
\]

\[
\alpha_{\beta} = e^{i\alpha k} \left( \cosh q b' + i \frac{k^2 - q^2}{2qk} \sinh q b' \right)
\]

\[
\beta_{\beta} = -i \frac{k^2 + q^2}{2qk} \sinh q b'
\]

with \( k = \sqrt{2m^*_c E}/\hbar \) and \( q = \sqrt{2m^*_b (V_o - E)}/\hbar \) the wave numbers in the wells and barriers, and \( m^*_c \) and \( m^*_b \) the effective masses and \( V_o = 0.23 \) eV. As mentioned before, the Chebyshev polynomials \( U_n \) are evaluated at the real part of \( \alpha \). After multiplying and simplifying, one can obtain the relevant matrix element of \( M_{\epsilon} \) to determine the transmission coefficient, i.e., the element \( \epsilon_{\alpha} = M_{\epsilon} \alpha \) that can be written in compact form as

\[
\epsilon_{\alpha} = (\alpha^2_{\beta} - \beta^2_{\beta}) U_n - (\alpha^2_{\alpha} - \beta^2_{\beta}) \alpha + 2\alpha_{\alpha} \beta_{\beta} \beta U_{n-1}
\]

\[
= 1 + h_{\beta} U_{n} + f_{\beta} U_{n-1}
\]

Pacher et al. by assuming that \( f_{\beta} U_{n-1} = 0 \), reported a simplified transmission coefficient, denoted as \( T_{SL}^{\text{SLC}} \) in the Equation (1) of ref. [197], plotted it and compared with the transmission coefficient for a SL without coating layers (see graphs in the left panel of Figure 20, with dotted and full curves, respectively). It is worth noticing that the assumption \( f_{\beta} U_{n-1} = 0 \) is correct only for \( b' \approx b/2 \). By applying a DC voltage between the emitter and the base, hot electrons were injected and transmitted through the SL. From the ratio \( I_c/I_E \) of the measured currents at 4.2K, the transmission results shown in the right panel of Figure 20 were obtained.

8.3. Multichannel Conductance through a 3D SL

Multichannel conductance calculations through 1DSIs with coupled channels were published, among others, by Ulloa et al., based on self-consistent numerical calculations, and using the
transfer matrix method in refs. [158,190,209,231]. In most of the latter works, a transverse electric field couples the propagating modes leading to interference and flux transition from one propagating mode to another, clearly observed in the transmission coefficients \( T_{ij} \) and conductance. In ref. [158], 3D SLs with 2D arrays of \( \delta \)-scatterer centers, separated by homogeneous layers of width \( l_c \), as shown in Figure 21, were considered, and the transmission coefficients and conductance \( G_{N,n} = (e^2/h)TrT^t \), defined in Section 4.1, calculated for different values of the number of propagating modes \( N \) and different number of unit cells \( n \). Here, we will review some of the specific formulas and present new results for \( N = 3 \) and \( n = 2, 3, 6 \).

For a periodic potential
\[
V_p(x, y, z) = \gamma (z - \eta l_c) \sum_{i=1}^{N_x} \delta(x - x_i) \delta(y - y_\mu), \quad \kappa = 1, \ldots, n
\]
with confining 2D hard walls, infinite outside \( \{0 \leq x \leq w_x, 0 \leq y \leq w_y\} \), longitudinal lattice parameter \( l_c \) and interaction strength \( \gamma \), the solutions
\[
\phi_i(x, y) = \frac{2}{\sqrt{w_x w_y}} \sum_{(F = n_x^2 + n_y^2)} \sin \left( \frac{n_x \pi x}{w_x} \right) \sin \left( \frac{n_y \pi y}{w_y} \right)
\]
and energies
\[
E_i = \frac{h^2 \pi^2}{2m^*} \left( \frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} \right) \leq E
\]
with \( E \) the incoming particles energy, define the transverse propagating modes labeled by the channel-index \( i \), which is determined by the pairs of quantum numbers \( n_x, n_y = 1, 2, 3, \ldots \). The functions \( \phi_i(x, y) \) constitute a realization of the set of orthonormal functions, mentioned in Section 2, which allow us to obtain the channel coupling matrix
\[
K_{ij} = \frac{8\pi^2 m^*}{h^2} \delta(z - \eta l_c) \sum_{i=1}^{N_x} \sum_{\mu=1}^{N_y} \phi_i^*(x_\nu, y_\mu) \phi_j(x_\nu, y_\mu)
\]
\[
= \delta(z - \eta l_c) G_{ij}
\]
Replacing and integrating the Schrödinger equation upon the variable \( z \) and following the usual procedure with \( \delta \)-potentials, to impose the continuity conditions, one can straightforwardly determine the transfer matrix
\[
M_\delta = \begin{pmatrix} \alpha_\delta & \beta_\delta \\ \beta_\delta & \alpha_\delta \end{pmatrix}
\]
with
\[
\alpha_\delta = I_\delta + \beta_\delta, \quad \beta_\delta = \frac{1}{2i} \begin{pmatrix} \Gamma_{11} & \Gamma_{12} \\ \Gamma_{21} & \Gamma_{22} \end{pmatrix}, \quad \text{and} \quad \Gamma_{ij} = \frac{k_i}{k_j}
\]

To use the polynomials and invariant functions mentioned in previous sections, it is necessary to determine the eigenvalues of the \( 2N \times 2N \) transfer matrix \( M \). A specific procedure to evaluate the matrix polynomials, for this type of transfer matrix, is reported in ref. [158], and we refer the reader to this reference.

Given the transfer matrix and applying the TFPS, we can evaluate the transmission coefficients \( T_{ij} \) and the conductance \( G = (2e^2/h)TrT^t \) for any set of parameters. In Figure 22, we show transmission coefficients and conductance for the three propagating modes, the channels with the lowest energy, and for different number of unit cells. For this figure, we consider \( l_c = 20\text{Å}, \ w_x = 100\text{Å}, \ w_y = 50\text{Å}, \ N_u = 30, \ N_v = 15, \) and

![Figure 20](image1.png)

*Figure 20.* Transmission coefficients. a,b) The left side panel, the theoretical transmission coefficients for SL without (full curves) and with coating layers (dotted curves). In the right-hand side panel the measures transmission coefficients. Reproduced with permission.[197] Copyright 2002, Elsevier.

![Figure 21](image2.png)

*Figure 21.* Schematic representation of a 3D SL with 2D arrays of \( \delta \)-scatterer centers.
\( \gamma = -200 \text{ eV} \). For these parameters, the channel thresholds are: \( E_{T_1} = 0.281 \text{ eV} \), \( E_{T_2} = 0.449 \text{ eV} \), and \( E_{T_3} = 0.954 \text{ eV} \). In Figure 22a,b, the number of unit cells is \( n = 2 \). In Figure 22a, we plot the transmission coefficient \( T_{ii} \) and the conductance \( G \), while in Figure 22b, we plot the transmission coefficients \( T_{ij} \) for channels indices \( i,j = 1,3 \), with the strongest channel coupling. It is clear from this figures that the transition probability \( T_{ij} \) from channel \( j \) to channel \( i \), starts to rise once the energy \( E \) is enough to open the incoming channel \( j \). In Figure 22c,d, we plot the transmission coefficients when the number of units cells are \( n = 3 \) and \( n = 6 \), respectively.

9. Superluminal and Optical Antimatter Effects. Injection, Filter, and Spin Inversion

The TFPS has been applied also to study the space–time evolution of WPs through SL structures. Among the various examples, we shall review first the transmission of electromagnetic waves through normal media and through metamaterial SLs where normal media alternates with left-handed layers. We will then review some topics of spintronics where the transfer matrix method and the TFPS has been applied with success. Specifically, to understand the negative resistance behavior in the \( J-V \) characteristics of spin injection and detection in all-semiconductor contacts, and to show a couple of results of spin WPs through homogeneous magnetic SLs and clear examples of spin filter and spin inversion.

9.1. Electromagnetics Wave Packets through SLs. Evidences of Superluminal Effects

Simanjuntak et al. applied the TFPS to study the space–time evolution of electrons\(^{[174]}\) and of electromagnetic\(^{[175]}\) WPs, and to discuss the presumption of the so-called generalized Hartmann effect\(^{[176]}\). We will briefly review here the time evolution (described by Maxwell equations) of Gaussian WPs with centroids in the allowed and in the photonic bandgaps, which was studied with more detail in ref. \( [175] \). The calculation reviewed here shows that the time spent by the WP with centroid in the photonic gap is half of the time it will require moving with light velocity, a result compatible with the experimental and theoretical results in refs. \( [74,75,232] \), referred to in the last section.

A Gaussian WP of electromagnetic fields, with parallel polarization and normal incidence from the left, was defined as

\[
\Psi_E(z,t) = \int dk e^{-r(k-k_0)z} E(z,k)e^{-i\omega t} \tag{196}
\]

with the packet-peak at \( t = 0 \) located at \( -z_0 \). To determine \( \Psi_E(z,t) \), for any \( t \) and at any point \( z \), one needs the \( k \)-component \( E(z,k) \) outside and inside the SL, which was assumed to contain \( n \) cells of length \( l_i = l_{i_1} + l_{i_2} \), being \( l_{i_1} \) and \( l_{i_2} \) the lengths of dielectric layers with permittivities \( \epsilon_1, \epsilon_2 \), refractive indices \( n_1, n_2 \) and permeabilities \( \mu_1, \mu_2 \). At any point, the electric and magnetic fields contain a right- and a left-moving parts. Hence

\[
E(z,k_i) = A_re^{ik_1z} + A_le^{-ik_2z} = E_r(z,k_i) + E_l(z,k_i) \tag{197}
\]
\[ H(z, k) = \frac{n_i}{\mu c} (E_r(z, k) - E_i(z, k)) \]  

(198)

where \( k_i = n_i k \) (\( i = 0, 1, 2 \)), \( k = \omega/c \), with \( c \) the speed of light in vacuum, and \( n_0 \) the refractive index outside the SL. To use the transfer matrices, it was convenient to define the field vectors

\[ \mathbf{E}(z, k) = \left( E_r(z, k), E_i(z, k) \right) \]  

(199)

and the transfer matrix \( M(z', k) \)

\[ \mathbf{E}(z', k) = M(z', z) \mathbf{E}(z, k) \]  

(200)

Inside the SL, a vector \( \mathbf{E}_{j+1}(z, k) \) at \( z = jl + z_p \) in cell \( j + 1 \) (with \( j = 0, 1, \ldots, (n - 1) \) and \( 0 < z_p < l \)) is related to \( \mathbf{E}(0^-, k) \) at \( z = 0^- \) by

\[ \mathbf{E}_{j+1}(z, k) = M_p(z, jl) M(jl, 0^+) M(0^+, 0^-) \mathbf{E}(0^-, k) \]  

(201)

\[ M_p(z, jl), \] as in Section 6, is the transfer matrix for part of a unit cell, and \( M(jl, 0^+) \) the transfer matrix for the first \( j \)-cells, thus

\[ M(jl, 0^+) = [M(l, 0^+)]^j \]  

(202)

Here, \( M(l, 0^+) \) is the single-cell transfer matrix

\[ M(l, 0^+) \equiv \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} = \begin{pmatrix} \alpha e^{i\theta} & \beta_p \\ \beta_p^* & \alpha_p e^{-i\theta} \end{pmatrix} \]  

(203)

Assuming \( \mu_1 = \mu_2 = \mu_0 = 1 \), the unit cell matrix elements reduce to

\[ \alpha_p = \cos(k_l l) + i \frac{1}{2} \left( \frac{n_2}{n_1} + \frac{1}{n_2} \right) \sin(k_l l), \quad \beta_p = i \frac{1}{2} \left( \frac{n_2}{n_1} - \frac{1}{n_2} \right) \sin(k_l l) \]  

(204)

and, for the transfer matrix elements of \( j \) cells, we have

\[ \alpha_j = U_j(\alpha_p) - \alpha^* U_{j-1}(\alpha_p), \quad \beta_j = \beta^* U_{j-1}(\alpha_p) \]  

(205)

Outside the OSL, the electric field, assuming an incoming wave of unit amplitude at \( z < 0 \), is

\[ E(z, k) = e^{ikz}(1 + r_T) \]  

(206)

Here, \( r_T = -\beta_T/\alpha_T \) is the reflection amplitude, with

\[ \alpha_T = \alpha_{tr} - \frac{i}{2} \left( \frac{n_0}{n_1} + \frac{1}{n_0} \right) \alpha_{ni} + \frac{i}{2} \left( \frac{n_0}{n_1} - \frac{1}{n_0} \right) \beta_{ni} \]  

(207)

\[ \beta_T = -\frac{i}{2} \left( \frac{n_0}{n_1} - \frac{1}{n_0} \right) \beta_{ni} - \frac{i}{2} \left( \frac{n_0}{n_1} + \frac{1}{n_0} \right) \beta_{ni} \]

and the subindices \( r \) and \( i \), as used before, stand for the real and imaginary parts. The electric field in cell \( (j + 1) \) takes the form

\[ E_{j+1}(z, k) = \frac{1}{2} \left[ (\alpha_p + \gamma_p)\alpha_j + (\beta_p + \delta_p)\beta_j \right] \times \left[ 1 + \frac{n_0}{n_1} + \frac{1 - n_0}{n_1} \right] r_T \]

(208)

\[ \frac{1}{2} \left[ (\alpha_p + \gamma_p)\beta_j + (\beta_p + \delta_p)\alpha_j \right] \times \left[ 1 - \frac{n_0}{n_1} + \frac{1 + n_0}{n_1} \right] r_T \]

where \( \alpha_p, \beta_p, \gamma_p, \delta_p \) are the elements of \( M_p(z, jl) \). In the transmitted field region, i.e., at \( z > n_0 l \), the electric field becomes

\[ E(z, k) = \frac{1}{\alpha_T} e^{ikz} \]  

(209)

Using Equation (206), (208), and (209) in Equation (196), we have the WP described by Maxwell equations in space and time. It is worth mentioning that in these equations, the multiple scattering processes are rigorously taken into account. As time develops the WP evolves in a rather complicated but describable way. The actual behavior depends critically upon the OSL parameters and the WP characteristics. To visualize the space–time evolution, crucial snapshots at some specific values of time will be taken. If the WP centroid at \( t = 0 \) and the left edge of the SL is at \( z = 0 \). Important snapshots are at: 1) \( t_0 = 0 \), 2) \( t_a = z_o/\nu_a \), 3) \( t_c = t_b + \tau \), when (according to the phase time prediction) the centroid must be just leaving the SL, and 4) at \( t_b = 2z_o/\nu_a + \tau \), when the reflected (transmitted) WP should be located at \( -z_o \) (or at \( z_o + L \)). The phase time was defined by Bohm[233] and Wigner[234] as the frequency derivative of the transmission amplitude’s phase \( \theta_t \), i.e., as

\[ \tau = \frac{\partial \theta_t}{\partial \omega} \]  

(210)

where \( \theta_t \) is the phase of the transmission amplitude. This is one of various formulas proposed for the theoretical calculation of tunneling times, among them was the Büttiker–Landauer tunneling time.\[235–237\] It was shown in ref. [232], reviewed briefly in the next section, that the phase time describes within the error bars of the experimental results of Steinberg et al.\[74\] and those of Spielmann et al.\[75\]

In ref. [175], the time series was calculated for a specific SL where silica with low (\( n_1 = 1.41 \)) and titanium oxide with high (\( n_2 = 2.22 \)) refractive indices alternate. In Figure 23, some quantities are plotted for the electromagnetic WP through this low-high index superlattice (LHSL). In the upper left panel a) of Figure 23, the phase time \( \tau_b \) is plotted as function of the field wavelength, when the silica and titanium oxide layers widths are \( l_1 = 124.46 \text{ nm}, l_2 = 79.06 \text{ nm} \), respectively. In this phase time spectrum, two regions of almost constant phase time are indicated with red arrows. One in the allowed band and one in the photonic gap. The WPs shown in the other panels are defined in these wavelength regions.

In panels b,c, at the left, the WP centroid is in the allowed band. In these panels, the WP is shown at \( t_0 \) and when it comes back at \( t_b \). The Gaussian envelopes (red curves) are plotted BY assuming that the WP centroid moves with the speed of light outside the SL and inside the SL spends the phase time...
\( \tau_n \approx 7.2 \text{ fs} \), instead of \( \approx 4 \text{ fs} \) that would be required if it were to move with light velocity. The agreement with the assumption that the time spent is \( \tau_n \), is perfect. More details are shown in ref. [175].

In the time series of the panels in the right side of Figure 23, we have the snapshots of the WP defined in the photonic bandgap, with centroid at \( \lambda_0 = 735 \text{ nm} \). The width is adjusted such that the main part of the WP lies in the photonic gap and in a region of almost constant phase time, \( \tau \approx 2.32 \text{ fs} \), which is close to the experimental \( \tau_{\text{ex}} \approx 2.1 \pm 0.2 \text{ fs} \) and the predicted phase time \( \tau \approx 2.3 \text{ fs} \) for a slightly different system with \( n = 5 \). As is well-known, these results imply the striking superluminal velocities. In Figure 23b, we have the WP at \( t_0 \) touching the left-hand edge of the SL. In Figure 23c, the WP at \( t_r = z_0/v_g + \tau \). Because of the phase shift due to the interference between the “arriving” and “leaving” packets, the coincidence is not easy to visualize. But it is much easier to compare the WPs in (a) and (d). In the inset both packets are plotted, and even though the packets coincide there is a phase shift. However, the Gaussian enveloping of the reflected WP at \( t_0 = 2z_0/v_g + \tau \) is also the enveloping of the WP at \( t = 0 \). This coincidence shows that the actual time spent by the WP inside the SL, \( \Delta t = t_r - 2t_0 \), agrees with the phase time prediction.

\[
\frac{\partial c}{\partial \mu} > 0, \quad \frac{\partial \mu}{\partial \varepsilon} > 0
\]  

Here, \( \varepsilon \) and \( \mu \) are the material’s permittivity and permeability, respectively. Smith and Kroll, \[239\] maintain that while a reversed \( k \) resembles a time-reversed propagation toward the source, the work done is nevertheless positive.

Besides the blazing presumption of perfect lenses, \[240\] and problems like the sign selection and directions of motion of
the energy and the electromagnetic field, an overwhelming research activity, from basic to applied science, has developed, with significant advances in manufacturing artificial LHM and structures, as well as in specific calculations for transmission of electromagnetic waves through the left-handed (LH) media.\cite{241-246} Robledo et al.\cite{185,210,211} studied the transmission of electromagnetic waves through LH and the right-handed (RH) structures by using the transfer matrix method and, by applying the TFPS for left- and right-handed superlattices (LRL). It has been explicitly shown that the oblique transmission amplitude

\[
t_l = \left[ \cos(k_l d_1 \cos \theta_1) + \frac{i}{2|n_1|^2 n_2} \left( n_2^2 \cos \theta_1 + n_1^2 \cos \theta_2 \right) \right]^{-1}
\times \sin(|k_1|d_1 \cos \theta_1)
\]

of a single left-handed slab is just the complex conjugate of the transmission amplitude

\[
t_l = \left[ \cos(k_l d_1 \cos \theta_1) - \frac{i}{2|n_1|^2 n_2} \left( n_2^2 \cos \theta_1 + n_1^2 \cos \theta_2 \right) \right]^{-1}
\times \sin(k_1 d_1 \cos \theta_1)
\]

of a similar but right-handed slab. In these equations, \( \theta_1 \) is the incidence angle and \( d_1 \) is the slab width. An important consequence of this property is that the phase time \( \tau \) of a single slab, becomes the negative of the corresponding phase time of a right-handed slab. This implies, in general, negative transmission times, and warnings on possible causality violation.

To follow the space–time evolution of a Gaussian electromagnetic wave packet (GEWP), we plot in Figure 24 the real part of the function \( \Psi_l(z,t) \) defined in (196) for different values of \( t \). The electric fields \( E(z,k) \), outside and inside the negative indices medium, are solutions to the corresponding Maxwell equations. In the time series of Figure 24, the WP is defined with centroid in the middle of a forbidden region of the transmission coefficient of its field components \( E(z,k) \) through a left/right superlattice LRSL with indices \( n_1 = -2.22 \) and \( n_2 = 1.41 \), \( l_1 = l_2 = 140 \) nm, and \( n = 6 \). In a, the WP at \( t = 0 \) and an enveloping Gaussian for reference in panel d). In panel b, the WP at \( t = 0 / \gamma \), when theoretically the centroid is reaching the left side of the SL. To visualize the WP in this panel, its amplitude was slightly amplified. As will be seen in the next figure, because of canceled layer, due to the antimatter effect, the WP gets transmitted slightly before it really reached the SL. In panel c, the WP at \( t_0 = 2 / \gamma \), with the phase time \( \tau_p = 0.9223 \) fs much smaller than the time \( L/c = 5.6 \) nm, it would require if it moves with light velocity. In panel c, the WP should be leaving the SL. It certainly seems that the halves of the WP are already outside the SL. Notice that, in this panel, the reflected WP amplitude is larger than the incoming one. In (d), at \( t_0 = 2 \gamma \), the WP should be back, i.e., under the enveloping curve of the WP at \( t = 0 \), however, the WP centroid is a distance \( \Delta z \) farther because of the optical antimatter effect better visualized in the next figure. Reproduced with permission.\cite{175} Copyright 2007, Elsevier.

**Figure 24.** Space–time evolution of a WP through an LRSL with indices \( n_1 = -2.22 \) and \( n_2 = 1.41 \), \( l_1 = l_2 = 140 \) nm, and \( n = 6 \). In (a), the WP at \( t = 0 \). In (b), the WP at \( t_0 = \gamma \), when theoretically the centroid is reaching the left side of the SL. To visualize the WP in this panel, its amplitude was slightly amplified. As will be seen in the next figure, because of canceled layer, due to the antimatter effect, the WP gets transmitted slightly before it really reached the SL. In panel c, the WP at \( t_0 = 2 / \gamma \), with the phase time \( \tau_p = 0.9223 \) fs much smaller than the time \( L/c = 5.6 \) nm, it would require if it moves with light velocity. In panel c, the WP should be leaving the SL. It certainly seems that the halves of the WP are already outside the SL. Notice that, in this panel, the reflected WP amplitude is larger than the incoming one. In (d), at \( t_0 = 2 \gamma \), the WP should be back, i.e., under the enveloping curve of the WP at \( t = 0 \), however, the WP centroid is a distance \( \Delta z \) farther because of the optical antimatter effect better visualized in the next figure. Reproduced with permission.\cite{175} Copyright 2007, Elsevier.
In other words, we will see the WP at two different points at the same time!

In the left and right columns of Figure 25, we present a set of snapshots of the first 100 fs. In the bottom left panel, at \( t = 13.3 \text{ fs} \), the WP is on its way to the negative indices slab. When the Gaussian peak is not yet half-way to the slab, one can observe the formation, in the neighborhood of the right-hand side of the slab, of a kind of image of the Gaussian WP. If we observe the snapshot at and after \( t = 39.9 \text{ fs} \), it is clear that the transmitted WP starts to be formed before the centroid of the incoming WP reaches the left handed medium. It is interesting to observe the GEWP at \( t = t_\tau = 33.3 \text{ fs} \). At this time, we have two Gaussian WPs. The Gaussian packet in the left, with peak at \( z = -10 \text{ μm} \), is the original GEWP half-way to the slab. The other Gaussian packet contains two halves separated by the dotted red line at the interface between the slab and the semi-infinite medium. The half packet inside the slab moves to the left, and the half packet outside the slab (inside the semi-infinite medium) moves to the right. The former half corresponds to the image of the GEWP, and the other half corresponds, as can be seen in the other panels (for \( t > 33 \text{ fs} \)), to the transmitted Gaussian WP. These graphs are compatible with the phase time prediction and show a way in which the incoming WP, its image and the transmitted one can be seen, at the same time, at different points of the space. Mathematically, this is a natural consequence of the continuity conditions imposed at the interfaces. Through these conditions each part of the system becomes aware of the physical properties of the other parts.

9.3. Exchange Energy and Spin Injection through Esaki Barriers

The ability to inject, manipulate, and detect spin-polarized carriers has been the main goals of semiconductor spintronics. Different proposals by countless research groups have been published. Spin injection and detections represent an important part of the problem, and different in nature to the spin manipulation problem. Despite the big progress, the problem of producing an efficient all-semiconductor all-electrical injection and detection device, remained rather elusive. This problem has slowed down the development of actual devices to control and manipulate the spin-filter and spin-inversion mechanisms.

The theoretical suggestion that larger contact resistance \( R_c \) may increase the ferromagnetic/nonmagnetic (F/N) spin injectors efficiency promoted the research on all-semiconductor Mn-based ferromagnetic semiconductors and opened up the possibility to inject spin-polarized electrons using the Esaki diode \( p^+ (\text{Ga,Mn}) \text{As}/n^+ \text{GaAs} \).

In Figure 26 a and b, low-bias IV characteristics obtained by Shiogai et al. and by Holmberg et al. respectively, are shown. A feature of interest in these graphs is the structure below and around 0.4 eV. This and the negative resistance behavior as a function of bias, lead us to study the injection and detection as a spin tunneling problem through bias and spin-dependent Esaki barriers. To understand the IV characteristics for spin-up and spin-down through a dynamical barrier where, besides the bias potential and build-up interface potential, one has to consider the strong exchange interaction energy and
the impurity states in the gap, we undertake a transfer matrix calculation based on the transfer matrix method. It was shown in ref.[184] that the turning points of the negative magnetoresistance are closely related with the exchange energy. The spin-splitting on the ferromagnetic side leads, naturally, to vanishing of tunneling probabilities at bias threshold points, where the propagating modes become evanescent. In forward bias, the spin up transmission coefficient, $T_E^+$, vanish when the Fermi level, of the $n$ side, aligns with the spin up valence band edge.

In Figure 27a, the band structure at the interface $p^+Ga_{0.95}Mn_{0.05}As/n^+GaAs$ is shown. At this interface, an Esaki barrier is formed with classical return points at $z_L$ and $z_R$. The quantum nature of this contact has been systematically ignored by semi-classical approaches, which generally restrict themselves to recognizing it as a resistor with some numerical value. The physics in this contact, however, is a truly quantum phenomenon. For the accurate calculation of transmission coefficients, the transfer matrix method (TMM) in the WKB approximation was used (details can be seen in ref. [252]). In reverse (injection) and forward (extraction) configurations, the corresponding $4 \times 4$ transfer matrices fulfill the relations

$$\Phi(z_L) = M_I(z_R, z_L) \Phi(z_L) = \left( \begin{array}{c} a \alpha \\ b \gamma \end{array} \right) \Phi(z_L)$$  \hspace{1cm} (214)

and

$$\Phi(z_L) = M_E(z_L, z_R) \Phi(z_L) = \left( \begin{array}{c} a \alpha \\ b \gamma \end{array} \right) \Phi(z_L).$$  \hspace{1cm} (215)

The state vectors

$$\Phi(z) = (\varphi^+_0, \varphi^+_1, \varphi^-_0, \varphi^-_1)^T$$  \hspace{1cm} (216)

in the propagating modes representation, are written in terms of the propagating wave functions ($\sigma$ stands for spin up $\uparrow$ or spin down $\downarrow$)

$$\varphi^+_\sigma(z) = \frac{a_\sigma}{\sqrt{k_\sigma}} e^{ik_\sigma z} \chi_\sigma$$ \hspace{0.5cm} and \hspace{0.5cm} $$\varphi^-_\sigma(z) = \frac{b_\sigma}{\sqrt{q_\sigma}} e^{-ik_\sigma z} \chi_\sigma$$  \hspace{1cm} (217)

and the evanescent functions

$$\varphi^+_\alpha(z) = \frac{a_0}{\sqrt{q_\alpha}} e^{ik_\alpha z} \chi_\alpha$$ \hspace{0.5cm} and \hspace{0.5cm} $$\varphi^-_\alpha(z) = \frac{b_0}{\sqrt{q_\alpha}} e^{-ik_\alpha z} \chi_\alpha$$  \hspace{1cm} (218)

Figure 26. $I$–$V$ characteristics in Ga(Mn)As/GaAs spin injectors. a) The $I$–$V$ characteristics measured in ref.[250] for the spin injector $p^+Ga_{0.95}Mn_{0.05}As/n^+GaAs$ with stop layer. b) Magnetic field effects on the $I$–$V$ characteristic of the Ga(Mn)As/GaAs structure measured in ref. [251]. Reproduced with permission. [250] Copyright 2014, American Physical Society.

Figure 27. a) Schematic band structure of a biased Esaki potential barrier at the interface of the ferromagnetic/stop layer/nonmagnetic structure, with spin-split offset $\Delta_F$ in the valence band of the $p$ side and the nonequilibrium spin accumulation electrochemical potential $\mu_{IN}$ in the $n$ side. b) The spin-up and spin-down detection transmission coefficients, when $\Delta_F = 0.6$ eV and $E_{FP}$ is 0.112 eV below $E_F$. The vanishing of $T_{E\uparrow}$ at the threshold potentials $V_{t\uparrow}$ and $V_{t\downarrow}$, gives rise to the transmission spin polarization in the lower graph. Reproduced with permission. [184] Copyright 2014, American Physical Society.
Here \( k_{1,1} = \sqrt{\frac{2m}{\hbar^2}} (E_{fi} - U_{1,1}(x, V_b)) \) and \( q_{1,1} = \sqrt{\frac{2m}{\hbar^2}} (U_{1,1}(x, V_b) - E_{fi}) \), the corresponding wave numbers with \( E_{fi} = E_{Fp} \) and \( E_{Fp} \) the quasi-Fermi energies. Given the transfer matrices and the relations with the scattering amplitudes, \( T_i = (\delta^i)^{-1} \) and \( t_p = (\delta^p)^{-1} \), the transmission coefficients

\[
T_{\sigma,\sigma'} = \left| q_{\sigma,\sigma'} \right|^2 = \left| (\delta^i)^{-1} \right|^2
\]

(219)

and the transmission spin polarization for spin extraction, defined as

\[
P_{TE} = \frac{T_{fi} - T_{fi}}{T_{fi} + T_{fi}}
\]

(220)

were calculated. These quantities are plotted in the upper and lower panels of Figure 27, respectively. The current spin polarization, spin injection efficiency, and the spin accumulation defined as

\[
p_j \approx \frac{j_1 - j_1}{j_1 + j_1}, \quad p_{Q} \approx \frac{j_{Q} - j_{Q}}{j_{Q} + j_{Q}}, \quad \text{and} \quad \delta_{\mu} = -p_j
\]

(221)

where \( j_\sigma = j_{E\sigma} + j_{E\sigma} \) and \( Q = I, E \) (for injection and extraction), have similar behavior and, they are also very sensitive to exchange energy and the threshold potentials \( V_i \) and \( V_b \).

The currents were evaluated, as usual, from

\[
j_\sigma = \mathcal{G} \int \mathcal{D}_{\sigma}(E) \mathcal{D}_{\sigma}(E - eV_b) T^{\phi}_\sigma(E, V_b) f(E) g_{\Omega}(E) dE
\]

(222)

where \( \mathcal{G} \) is a geometrical factor, \( \mathcal{D}_{\sigma} \) and \( \mathcal{D}_{\sigma} \) the densities of states in the nonmagnetic and ferromagnetic sides, and \( f(E) \) and \( g(E) = 1 - f(E) \) the occupation probabilities. Since the experiment temperature is \( \approx 4 \text{K} \), the occupancy probabilities factor becomes \( \delta(E - E_{fi}) \). The currents shown in Figure 28 were calculated assuming that in the ferromagnetic side the DOS is \( \mathcal{D}_{\sigma} \propto e^{-\epsilon_\sigma} / (a_\sigma - \sigma_{\Delta_{fi}}/2 > 0) \) and \( \mathcal{D}_{\sigma} \propto (\epsilon_\sigma - q)^{2} \) with \( q = 1 \) for \( \epsilon_\sigma < -\Delta_{fi} \), \( q = p \) for \( -\Delta_{fi} < \epsilon_\sigma < 0 \), being \( a_\sigma \) and \( p \) parameters chosen to fit the DOS’s obtained numerically by Turek et al., and \( \mathcal{D}_{\sigma} = \mathcal{D}_{\sigma} \propto (E - \epsilon_\sigma)^{2 / 2} \) (for \( p = 1 \)). Here, \( \mathcal{D}_{\sigma} \) is the Kane’s \( \epsilon \) function.

\[
y(E) = \int_{-\infty}^{E} (E - eV_b - \xi)^{2 / 2} g(\xi) d\xi
\]

(223)

As can be seen in Figure 26, the calculated currents faithfully reproduce the experimental behavior. These results show also that in the presence of exchange, the spin splitting and the DOS are strongly correlated quantities, and define the shape and low-bias \( I-V \) characteristics of the F/N structures.

9.4. The Homogeneous Magnetic SLs

The transfer matrix method and TFPS approach to spintronics is a different approach than mainstream, mostly semi-classical, ones. We will briefly review the TFPS applied to study the transport and spin control in magnetic SLs.

The aim to control spin carriers transport through layered magnetic structures, has been of much interest. With this aim, in the presence of the phase coherence of a periodic magnetic field, Cardoso et al. carried out a research project that addressed different aspects of the interaction of spin 1/2 carriers with magnetic-field SLs, including issues such as Shubnikov–de Haas oscillations, the Landé factor, Fano resonances and the magnetic-field-tilting angle as a significant mechanism for the spin transitions in magnetic SLs. Taking advantage of these spin-transport phenomena, simple and efficient spin-filter and spin-inverter devices were proposed.

For practical reasons, a simple system was conceived, where only the external field changes periodically, that is, the same semiconductor under an external magnetic field whose amplitude varies periodically. We refer to this superlattice as the homogeneous magnetic superlattice (HMSL), and represent it as \((L_{fi} L_{fi} L_{fi})^n\), where \( L_{fi} \) stands for a stripe free of field and \( L_{fi} \) for a stripe under an external magnetic field. As shown in Figure 29, the HMSL is basically a quasi-2D semiconductor wave guide subject to an external magnetic field, which is blocked on stripes that alternate along the growing direction. As is well-known, the spin 1/2 electrons, moving in those regions subject to an external magnetic field, are described by

\[
\left[ \frac{1}{2m^2} \left( p - eA \right)^2 + (V(y, z) - E_f) \right] \Psi(r) + \left[ \frac{1}{2g^* \mu_0 \sigma \cdot B + V_r + V_D} \right] \Psi(r) = 0
\]

(224)

Figure 28. a) The effect of the parameter \( p \) on \( \mathcal{D}_{\sigma} \), in the neighborhood of the valence band edges. b) Total current through the Esaki barrier for the same parameters of Figure 27, and the densities of states explained in the text. Reproduced with permission. Copyright 2014, American Physical Society.
where $V(x, y)$ is a lateral confining potential, $V_R$ and $V_D$ are the Rashba and Dresselhaus spin-orbit interaction. If we have a tilted magnetic field, say $B = B_0 \sin \theta_B$, the spin precession and spin transitions induced by the Rashba and Dresselhaus interactions are negligible compared with those induced by the Zeeman interaction. Thus, for this review, we drop those terms. It was shown in ref. [108] that after some analytical calculation, one is left with the equation

$$\left( \frac{d^2}{dz^2} - \frac{z^2 \cos \theta_B}{l_B^2} + k_x^2 - \frac{g}{2l_B^2} \sigma \cdot \hat{B} \right) Z(z) = 0$$

whose solutions are the hypergeometric matrix functions $^3F_1$ and $^3F_2$

$$A_a(z) = _1F_1 \left( \frac{-1}{2}, \frac{1}{2}; \frac{1}{2}; \frac{z^2}{l_B^2} \right) e^{z^2 \cos \theta_B / 2l_B^2}$$

and

$$B_a(z) = _1F_1 \left( \frac{12 - b_a}{2}, \frac{3}{2}; \frac{1}{2}; \frac{z^2}{l_B^2} \right) e^{-z^2 \cos \theta_B / 2l_B^2}$$

In these functions, the matrix function $b_a$ is

$$b_a = \frac{l_B^2}{2 \cos \theta_B} \left( k_x^2 - \frac{g}{2l_B^2} \sigma \cdot \hat{B} - 1 \right)$$

with $l_B$ the magnetic length and $k_x$ the longitudinal wave number. We will show here examples of distinct spin-projection transmission coefficients. To better visualize the effect of the spin-dependent transmission coefficients, we will plot the space-time evolution of Gaussian pulses of spin 1/2 electrons. To this purpose, we need to calculate the WP

$$\Psi(z, t) = \int_{-\infty}^{\infty} dk e^{-\gamma (k-k_0)^2} \phi(z, k) e^{-iwt}$$

whose centroid at $t_0 = 0$ is located in the position $-z_0$. The sub-index $s$ refers to the spin projection. For the evaluation of this integral, one requires to know analytically the wave functions $\phi_s(z, k)$, inside and outside the SL, based on the solutions $A_s(z)$ and $B_s(z)$, and the transfer matrix method and the TFPS, to determine the transfer matrix $M(z, z_0)$ that connects the state vector at $z_0$ with the state vector at any point $z$ inside and outside the SL, one can evaluate the scattering amplitudes and the wave functions $\phi_s(z, k)$, $\phi_s(z, k)$ inside and outside the SL.

In this approach, schematically reviewed here, one can obtain different types of effects by varying the SL parameters and the magnetic field orientation. The behavior of the spin-up and spin-down transmission coefficients, $T_{uu}$ and $T_{dd}$, respectively, is an important guide to visualize in advance the outcome of desired effects for the WP through the HMSL. We will illustrate the HMSL acting as a spin filter, the tilting angle effect, and the HMSL acting as spin inverter.

### 9.4.1. The HMSL as Spin Filter

In Figure 30, we have the transmission coefficients $T_{uu}$ and $T_{dd}$, in the left, and the spin WPs in the right. The HMSL is a quasi-2D wave guide with widths $w_x = 50$ and $w_y = 3$ nm, under an external magnetic field with $B = 0.18T$ acting on stripes of width $L_{si} = 10$ nm, unit-cell width $l_c = 130$ nm, and $n = 6$ unit cells. We consider first that $\theta_B = 0$. In this case, no spin $|u$ to spin $|d$ transitions occur, i.e., $T_{ud} = T_{du} = 0$. This implies well defined band structures for the spin $|u$ and the spin $|d$ transmission coefficients, as shown in Figure 30a. In this example, an unpolarized electrons WP is prepared with centroid and WP components entirely in the gap of $T_d$ and in the resonant region of $T_u$. We expect that the HMSL will work as a spin filter for the spin $|u$ electrons. Indeed, the snapshots in Figure 30b, at $t = 0$ and at $t = 2\tau_u/\nu_u + \tau_d$, show the filter effect. At $t = 0$, the spin $|u$ and spin $|d$ Gaussian WPs with centroids located at $z_0 = -40l_c$, moving toward the HMSL. The centroids of these packets reach the left edge of the HMSL at $t_o = x_o/\nu_u$ with a group velocity $\nu_u$. In the lower frame, we plot the spin packets at $t = 2l_u + \tau_u$ and at $t = 2l_d + \tau_d$, when presumably they should be back at the starting point, having spent a time $\tau_u$ or $\tau_d$, respectively, in the HMSL. As expected, from the transmission coefficient behavior, the WP components are partially reflected and partially transmitted, while those of the spin $|u$ packet are completely reflected.

It is interesting to notice that, even though a shape distortion is seen for the spin-up WP, the transmitted Gaussian WPs are in the position that one would expect them, if the phase time prediction were correct and the same for most of the spin $|d$ Gaussian components. The tails of the Gaussian in Figure 30a transmit less and have also different tunneling times, while the spin $|d$ components, all have the same transmission coefficient and the same tunneling time (see lower panel in Figure 30a). For the centroid of the spin $|d$ electrons, the phase time predicts a tunneling time $\tau_d = 1.995 \times 10^{-12}$ s, while for spin $|u$ electrons, it predicts $\tau_u = 3.843 \times 10^{-13}$ s. These are quite different times and they are also rather different from the time $\tau_d \approx 1.625 \times 10^{-12}$ s that they would spend if they were to move (the same distance) in a region free of magnetic fields. This example shows clearly that the system behaves as a spin $|u$ filter and the phase time predictions are correct.
9.4.2. Spin Mixing and Space–Time Evolution when $\theta_B = 40^\circ$

We consider again the unpolarized WP of the previous example but now with the magnetic field in the HMSL tilted with $\theta_B = 40^\circ$. In Figure 31a, the transmission coefficients $T_{uu}$ and $T_{dd}$. Now, the reflection coefficient $R_{dd}$ (which was $\approx 1$) reduces to $\approx 0.7$ and the transmission coefficients are smaller than 1, as shown in Figure 31a. An important amount of flux passes from the spin↑ to the spin↓ packet, and vice versa. The spin↑ $\rightarrow$ spin↓ transitions are induced by the in-plane field component $B_y$. In addition, the band structures experience small red and blue shifts, respectively. The snapshots in Figure 31b show the WPs at $t = 2t_u + \tau_u$ and at $t = 2t_d + \tau_d$, when their centroids are back at $-z_o$ or transmitted at $nl_c + z_o$. It is worth noticing that the WP

![Figure 30. Spin-up and spin-down transmission coefficients and Gaussian WPs through a HMSL. a) The spin-up and spin-down transmission coefficients for $\theta_B = 0^\circ$ on a HMSL with $w_x = 50$ nm and $w_y = 3$ nm, $l_c = 130$ nm, $n = 6$, and $B = 0.18$T. The Gaussian curves in the gap of $T_{dd}$ and the allowed region of $T_{uu}$ show the position and shape of the unpolarized spin WP that will move through the HMSL. In the upper frame of (b), the spin↑ and spin↓ WPs at $t = 0$ and $-z_o = -40l_c$, moving toward the HMSL. In the lower frames, the spin↑ and spin↓ packets at $t = 2t_u + \tau_u$ and $t = 2t_d + \tau_d$, respectively, when presumably, both packets should be back at $-z_o$ (a distance $z_o$ from the HMSL). It is clear from these graphs, the filter effect manifest by the absence of transmitted spin-down WP components. The Gaussian curves centered at $-z_o$ and at $L + z_o$ are plotted as reference. Here, $L = nl_c = 0.78\mu$m is the HMSL length. Reproduced with permission.© 2008, Elsevier.]

![Figure 31. Transmitted and reflected spin↑ and spin↓ WPs when the magnetic field tilting angle is $\theta_B = 40^\circ$. The incoming packets are the same as in Figure 30. The spin↑ and spin↓ WPs are plotted for $t = 2t_u + \tau_u$ and $t = 2t_d + \tau_d$, respectively. Although the centroid phase time prediction describes well the transmitted spin-packet tunneling time, it does not represent the reflected spin-packet tunneling time because of the high WP distortion. The Gaussian curves centered at $-z_o$ and at $l_c + z_o$ are plotted for reference. Reproduced with permission.© 2008, Elsevier.]
9.4.3. Spin Inversion

In the previous examples, we had at \( t = 0 \) an unpolarized Gaussian WP defined in a spin\( \uparrow \) gap. The spin mixing made possible to have a small fraction of spin\( \downarrow \) electrons transmitted. We will see now that a spin inversion is also possible. In fact, if at \( t = 0 \) we have a polarized Gaussian WP, say a spin spin\( \downarrow \) WP in lower graph of 31a. Tilting the field, as we have just seen, and as shown in Figure 32 an important amount of electrons with spin\( \downarrow \) transmit the HMLS. This fraction grows with the tilting angle \( \theta \). Eventually the population of transmitted spin\( \downarrow \) electrons is equal and even larger than the population of spin\( \uparrow \) electrons. All one needs to complete the spin inversion is a second step of spin filter.

10. Highly Accurate Descriptions of High-Resolution Experiments: Tunneling and Blue-Emitting Lasers

We will outline here two examples where the theoretical predictions not only compare extremely well with high-resolution experimental results, they provide also the correct theoretical description. The first example is on the tunneling time through the photonic-band-gaps of (silica/titanium-oxide)\( n \) SLSs. This example implies calculations of scattering amplitudes and transmission coefficients, and was shown in ref. [232], that using the results of the TFPS, the experimental results of Steinberg et al. [74] and those of Spielmann et al. [75] are reproduced within the error bar of \( 10^{-16} \) s. The second example is on the optical response of \( (In_{x}Ga_{1-x}N/In_{x}Ga_{1-x}N) n \) SLSs. This example implies the calculation of SL energy eigenvalues and eigenfunctions. In the 1990s, Nakamura [258] using monochromators with a resolution of 0.016 nm, reported the optical response with new features in the spectra that could not be explained with the standard approach. It was shown recently, [165] that using the TFPS, it was possible to explain the experimental spectrum features within the accuracy of the experimental results.
Given the scattering amplitude $t_n = (t_{ni} + it_{ni})$ in Equation (106), and the definition of tunneling time

$$\tau_n = |t_n|^2(t_{ni} \partial t_{ni}/\partial \omega - t_{ni} \partial t_{ni}/\partial \omega)$$

(231)

the general and closed formula for the evaluation of this time is given by

$$\tau_n = \left(\frac{\hbar}{U_n - \alpha_i U_{n-1}}\right)^2 + \left(\alpha_n U_{n-1} \right)^2 \left(A_n \frac{d\alpha_n}{dE} + A_i \frac{d\alpha_i}{dE}\right)$$

(232)

with

$$A_n = \frac{\alpha_n}{1 - \alpha_n} \left((\alpha_n U_{n-1} + n U_{n-2}) U_n - (n + \alpha_n^2) U_{n-2}^2\right)$$

(233)

and

$$A_i = (U_n - \alpha_i U_{n-1}) U_{n-1}$$

(234)

was reported in ref.[232]. For the specific SL where the tunneling time was measured, the unit-cell transfer matrix elements are

$$\alpha = \frac{1}{4n_{12}^2 n_L} (n_{12}^2 n_{ZL}^2 e^{-i k_0 d_L} (n_{12}^2 n_{ZL}^2)^2 - e^{-i k_0 d_L} (n_{12}^2 n_{ZL}^2)^2)$$

(235)

$$\beta = \frac{n_{12}^2 - n_{11}^2}{2 n_{11} n_{L}} \sin k_0 d_L = i \beta_i$$

(236)

and adjusting the transfer matrix to include the extra layer $H$ or $L$ and the substrate of length $L_s$, it was possible to calculate the tunneling times shown in Figure 33. In Figure 33a, we show the tunneling time reported by Steinberg et al. through the SL (HL)$^n$H (substrate L) air, for $n = 5$, together with the calculated tunneling time $\tau_n$, and the transmission coefficient $T_n$. $\tau_f$ is the time that would be spent by moving with velocity $c$. In Figure 33b, the tunneling times (open circles) reported by Spielmann et al. through air (substrate L) (HL)$^n$air SLs made of titanium oxide (H) and silica (L) for different values of $n$ with error bar of $10^{-16}$ s. The black circles are the predictions of the TFPS. The open triangles are the calculated phase times by Spielmann et al.

10.2. Optical Response of the Blue-Emitting $(\text{In}_{0.05}\text{Ga}_{0.95}\text{N}/\text{In}_{0.10}\text{Ga}_{0.90}\text{N})^{10}$ SLs

An important development of the last years of the last century has been the production of blue light-emitting diodes, based on GaN/InGaN SLs. Following the discovery of the blue-emitting diodes, an overwhelming research activity began on the so-called wide-gap nitrides. At first, the attempts to produce the announced devices became a real challenge, afterwards, the explanation of the characteristics of the optical response spectra also became a challenge for the theorists. From a theoretical point of view, the continuous subbands predicted by the standard approaches were unable to explain and describe the main characteristics of the high-resolution optical spectra reported by Nakamura et al.[77,136,258] characterized by multiple and close resonances (see the upper right panel in Figure 34). Nakamura et al. suggested that the multiple resonances could be identified as longitudinal modes, but it was also argued that they could be fluctuations in the cavity field. Recently, using the TFPS and the ability to evaluate the eigenvalues and eigenfunctions of SLs, it has been possible to account for the optical response of SLs in the active zone of light-emitting devices, by evaluating the optical susceptibility in the approximation of the golden rule given by

$$\chi^{(2)} = \sum_{i,j^*,i^*,j} \int dz \left| \langle \Psi_{i j^*}^{\text{SC}}(z) | \Psi_{i^* j}^{\text{SC}}(z) \rangle \right|^2$$

(237)

Here, the eigenvalues and eigenfunctions from the conduction and valence bands are obtained from the explicit expressions outlined in the last sections. As can be seen in the lower panel of Figure 34, the optical susceptibility is faithfully reproduced.[165,202]

An important characteristic of the subband spectra to understand the structure of the optical response is the detachment of the surface energy levels. The surface states in the subband of the structure of the optical response is the detachment of the surface energy levels, the surface states in the subband of the conduction band, with energies $E_{1,10} = 0.119074$ eV and $E_{1,11} = 0.119082$ eV, measured from the band edge, are detached 3.2 meV from the subband energy levels, grouped in an energy interval of 13.9 meV. The transitions to the first subband of the
valence band are forbidden by the new selection rules. The transitions responsible of the spectrum around 420 nm, are those to the second subband of the valence band. In this subband, the surface energy levels around $-0.1001244$ eV are detached from the other levels that are grouped between $-0.092$ and $-0.0954$ eV. The detachment of the surface states is an important feature that allows one to identify the transitions responsible for the isolated high energy peaks (as transition from surface to surface energy levels) and the groups of peaks in the optical spectra, see the sketch in the left panel of Figure 34. This calculations show that the multiple resonances correspond to optical transitions between truly quantum states within subbands of the conduction and valence bands. Lately, we have also shown that the 1 nm difference between the observed and predicted spectrum width, is due to the piezoelectric effect with a local field of $0.0055$ eV nm$^{-1}$.

11. Conclusion

We reviewed the TFPS from basic properties to general results for quasi-1D periodic systems. The transfer matrix method was introduced as a tool for dealing with dynamic equations of systems with an arbitrary number $N$ of propagation modes, where we define the transfer matrices $M_N$ and $W_N$ of dimension $2N \times 2N$. We illustrated matrices of dimension $2 \times 2$ for specific examples of one propagating mode, and introduced the transfer matrix in the WKB approximation. We have then reviewed the general relations of transfer matrices $M_N$ and $W_N$ with the scattering amplitudes, the representations of the transfer matrix in the orthogonal, unitary, and symplectic universality classes, and their group structures. Based on the transfer matrix properties, particularly on the transfer-matrix combination rule, we outlined the derivation of the matrix recurrence relation, whose solutions make it possible to determine analytically the transfer matrix $M_{NN}$ of a periodic system with $n$ unit cells and $N$ propagating modes, provided that the unit-cell transfer matrix $M_N$ is known. Since most of the applications of this theory deal with the one propagating mode limit, we only presented the final results for the matrix polynomials $p_{NN}$, and showed that in the one propagating mode limit, one has the recurrence relation of the Chebyshev polynomials of the second kind, which were first found by Jones and Abeles. The transfer matrix $M_{NN}$ and the matrix polynomials $p_{NN}$, which carry all the information of the periodic system, the complex processes, and the multiple reflections that particles or wave functions experience along the periodic structure, are rigorously determined for any number of propagation modes $N$, arbitrary potential profile, and any number of unit cells $n$. We have then shown that given the polynomials $p_{NN}$ and $p_{1n} = U_n$, the matrix elements and all physical quantities, such as the scattering amplitudes, the resonant energies, and the Landauer conductance, are expressed in a simple way in terms of these polynomials. In the second part of this review, we presented the more recent results related to the calculation of the energy eigenvalues and eigenfunctions for confined SLs in the 1D limit. These quantities resolve the fine structure in the bands and at the same time give the possibility of determining the true discrete dispersion relation, as opposed to the continuous dispersion relation obtained when the transfer matrix method is combined with the Floquet theorem. We dedicate a brief section to comment on this approach. We end up the TFPS review with a summary of the analysis of parity symmetries of eigenfunctions and resonant functions.

The TFPS was applied to a broad variety of physical systems, and we have presented here the application of this theory to a number of physical systems. We addressed first the calculation

Figure 34. SL spectra and optical response. a) The energy levels in subbands of the conduction and valence bands. The continuous subbands (light blue) are from the Kronig–Penney model. The discrete lines are the predictions of the TFPS. The set of transitions responsible of the group structure in the optical spectrum are also shown. b) Upper panel is the optical response of the blue-emitting $(\text{In}_{0.05} \text{Ga}_{0.95} \text{N})/(\text{In}_{0.2} \text{Ga}_{0.8} \text{N})^N$ SLs, and in the lower panel are the predictions of the TFPS. The experimental resolution was of 0.016 nm. Reproduced with permission. Copyright 2018, Elsevier.
of the conductance of a biased DB, and show that an unexplained and frequently observed feature in negative-resistance region can be explained using the multichannel transfer matrix method. We have then discussed the transmission in ballistic transistors and the conductance in a channel-coupling SL with layers of \(\delta\)-scatter potentials. We devoted a section to review the application of the TFPS to study the transmission and space–time evolution of electromagnetic and electron WPs through optical, left-handed and magnetic SLs. Furthermore, it was demonstrated that the TFPS can be used to investigate superluminal, optical antimatter, spin filter and spin inversion effects. To conclude, we have chosen two examples were high-resolution experiments have been performed, and the theoretical predictions are extremely good. The tunneling time through SLs, with error bars of \(\approx 10^{-15}\) s, and the optical response of blue-emitting InGaN SLs, where new features in the optical spectra, with a resolution of \(\approx 0.038\) meV, and a discrete structure of the subband energy levels are revealed. The aim of this review has been to show that solid-state physics continues evolving towards a truly quantum approach, which was somehow obscured by infinite systems, where the energy spectrum becomes continuous. The discrete spectrum, surface states, and other new properties that emerge in the TFPS are important advances, relevant to theoretical physics, experimental physics, and applications.

**Acknowledgements**

I acknowledge my mentors Pier A. Mello and Thomas Brody, authors of relevant contributions to physics, from whom I learned the value of scientific honesty and conceptual rigor; that the north of the theoretical physics is the physical reality.

The author is grateful to Herbert P. Simanjuntak and Arturo Robledo for the careful reading of the manuscript and the valuable suggestions.

**Conflict of Interest**

The author declares no conflict of interest.

**Keywords**

eigenvalues and eigenfunctions of superlattices, electronic transport, optical response of superlattices, theory of finite periodic systems, transfer matrix method, transmission coefficients, tunneling time

Received: August 10, 2021
Revised: November 3, 2021
Published online: December 24, 2021

[1] G. Bastard, Phys. Rev. B 1981, 24, 5693.
[2] S. R. White, L. J. Sham, Phys. Rev. Lett. 1981, 47, 879.
[3] G. Bastard, Phys. Rev. B 1982, 25, 7584.
[4] M. Altarelli, F. Bassani, in Handbook on Semiconductors, Vol I: Band Theory and Transport Properties (Ed: W. Paul), Amsterdam, North-Holland 1982.
[5] R. E. Borland, Proc. R. Soc. London, Ser. A 1961, 84, 926.
[6] A. Y. Cho, Appl. Phys. Lett. 1971, 19, 467.
[7] H. Kroemer, Proc. Rad. Rad. Eng. 1957, 45, 1535.
[8] L. V. Keldysh, Fiz. Tverd. Tela 1962, 4, 2265 [English translation: Sov. Phys. - Solid State 1963, 4, 1658].
[9] L. Esaki, R. Tsu, IBM J. Res. Dev. 1970, 14, 61.
[10] R. D. Dupuis, P. D. Dapkus, N. Holonyak, E. A. Rezek, R. Chin, Appl. Phys. Lett. 1978, 32, 295.
[11] H. Kroemer, Proc. IEEE 1963, 51, 1782.
[12] Zh. I. Alfërov, V. M. Andreëv, V. I. Korol’kov, D. N. Trav’jakov, V. M. Tuchkevich, Fiz. Tekh. Poluprovodn. 1967, 1, 1579 [English translation: Sov. Phys. Semicond. 1968, 1, 1131].
[13] H. Rupprecht, J. M. Woodall, C. D. Pettit, Appl. Phys. Lett. 1967, 11, 81.
[14] Zh. I. Alfërov, V. M. Andreëv, D. Z. Garbuzov, Yu. V. Zhilyaev, E. P. Morozov, E. L. Portnoi, V. G. Trofim, Fiz. Tekh. Poluprovodn. 1970, 4, 1826 [English translation: Sov. Phys. Semicond. 1971, 5, 174].
[15] I. Hayashi, M. B. Panish, P. W. Foy, S. Sumski, Appl. Phys. Lett. 1970, 17, 109.
[16] H. J. Seemann, E. Vogt, Ann. Phys. (Leipzig) 1929, 394, 976.
[17] A. J. Bradley, A. H. Jay, Proc. Roy. Soc. London, Ser. A-Math Phys. Sci. 1938, 136, 210.
[18] R. Peierls, Proc. Roy. Soc. London, Ser. A-Math Phys. Sci. 1936, 154, 2027.
[19] A. H. Wilson, Proc. Camb. Philos. Soc. 1938, 34, 81.
[20] R. Hultgren, C. A. Zapfe, Z. Kristallogr. 1938, 99, 509.
[21] J. S. Wang, Phys. Rev. 1945, 67, 98.
[22] J. C. Slater, Phys. Rev. 1949, 76, 452.
[23] J. F. Nicholas, Proc. Phys. Soc. A 1953, 66, 201.
[24] P. A. Flinn, C. M. McManus, J. A. Rayne, J. Phys. Chem. Solids 1960, 15, 189.
[25] M. J. Marcinkowski, L. Zwell, Acta Metal. 1963, 11, 373.
[26] I. Y. Ledvik, V. N. Nikitin, C. A. Petropavlovskii, G. S. Vasil’eva, J. Appl. Spectrosc. 1965, 3, 269.
[27] B. Movaghart, J. Leo, A. MacKinnon, Semicond. Sci. Technol. 1988, 3, 397.
[28] Z. Y. Xu, V. G. Kreismanis, C. L. Tang, Appl. Phys. Lett. 1983, 43, 415.
[29] M. J. Ludowise, W. T. Dietze, C. R. Lewis, Appl. Phys. Lett. 1983, 42, 487.
[30] H. Sakaki, J. Yoshino, Y. Sekiguchi, Electron. Lett. 1984, 20, 320.
[31] Y. H. Wu, M. Werner, S. Wang, Appl. Phys. Lett. 1984, 45, 606.
[32] I. Hayashi, IEEE Trans. Electron. Devices 1984, 31, 1630.
[33] D. Kirillov, J. L. Merz, P. D. Dapkus, J. C. Coleman, J. Appl. Phys. 1984, 55, 1105.
[34] B. Cai, A. J. Seeds, J. S. Roberts, IEEE Photon. Tech. Lett. 1994, 6, 496.
[35] Zh. I. Alfërov, A. I. Vasil’ev, S. V. Ivanov, P. S. Kopev, N. N. Ledentsov, M. E. Lutsenko, B. Ya. Melter, V. M. Ustinov, Pis’ma Zh. Tekh. Fiz. 1988, 14, 1803 [English translation: Sov. Tech. Phys. Lett. 1988, 14, 782].
[36] G. Ji, D. Huang, U. K. Reddy, T. S. Henderson, R. Houdre, H. Morkoe, J. Appl. Phys. 1987, 62, 3366.
[37] Y. Narukawa, Y. Kawakami, S. Fujita, S. Fujita, S. Nakamura, Phys. Rev. B 1997, 55, R1938.
[38] W. T. Tsang, C. Weisbuch, R. C. Miller, R. Dingel Appl. Phys. Lett. 1979, 35, 673.
[39] M. Zuniga, J. A. Kong, L. Tsang, J. Appl. Phys. 1980, 51, 2315.
[40] R. D. Dupuis, P. D. Dapkus, Appl. Phys. Lett. 1977, 31, 466.
[41] N. Holonyak Jr., R. M. Kolbas, E. A. Rezek, R. Chin, R. D. Dupuis, P. D. Dapkus, J. Appl. Phys. 1978, 49, 5392.
[42] R. Dingel, H. L. Störmér, A. C. Gossard, W. Wiegmann, Appl. Phys. Lett. 1978, 33, 665.
[43] R. F. Kazarinov, R. A. Suris, Sov. Phys.—Semicond. 1972, 6, 120.
[44] B. A. Vojak, N. Holonyak Jr., R. Chin, E. A. Rezek, R. D. Dupuis, P. D. Dapkus, J. Appl. Phys. 1979, 50, 5835.
[45] R. M. Kolbas, N. Holonyak Jr., B. A. Vojak, K. K. Hess, M. Altarelli, R. D. Dupuis, P. D. Dapkus, Solid State Commun. 1979, 31, 1033.
J. J. Wierer, M. R. Krames, J. E. Epler, N. F. Gardner, M. G. Craford, T. Baba, K. Inoshita, H. Tanak, J. Yonekura, M. Ariga, A. Matsutani, E. Yablonovitch, O. J. Glembocki, B. V. Shanabrook, N. Bottka, W. T. Beard, J. Comas. Phys. Rev. Lett. 1985, 46, 970.

S. H. Pan, H. Shen, Z. Hang, F. H. Pollak, W. Zhuang, Q. Xu, A. P. Roth, R. A. Masut, C. Lacelle, D. Morris, Phys. Rev. B 1988, 38, 3375.

E. Yablonovitch, Phys. Rev. Lett. 1987, 58, 2059.

J. B. Pendry, J. Mod. Opt. 1994, 41, 209.

T. Baba, K. Inoshita, H. Tanak, J. Yonekura, M. Ariga, A. Matsutani, T. Miyamoto, F. Koyama, K. Iga, J. Lightwave Technol. 1999, 17, 2113.

J. J. Wiener, M. R. Krames, J. E. Eppler, N. F. Gardner, M. G. Craford, J. R. Wends, J. A. Simmons, M. M. Sigalas, Appl. Phys. Lett. 2004, 84, 3885.

L. C. Botten, N. A. P. Nicolovici, A. A. Asatryan, R. C. McPhedran, C. M. de Sterke, P. A. Robinson, J. Opt. Soc. Am. B 2000, 17, 2165.

L. C. Botten, N. A. P. Nicolovici, A. A. Asatryan, R. C. McPhedran, C. M. de Sterke, P. A. Robinson, J. Opt. Soc. Am. B 2000, 17, 2177.

J. D. Joannopoulos, R. D. Meade, S. C. Johnson, J. N. Winn, in Photonic Crystals: Molding the Flow of Light, Princeton University Press, Princeton, UK 1995

K. Okamoto, K. Inoue, Y. Kawakami, S. Fujita, M. Terazima, A. Tsujimura, I. Kidoguchi, Rev. Sci. Instrum. 2003, 74, 575.

H. Jia, K. Yasumoto, Microw. Opt. Technol. Lett. 2005, 47, 256.

P. Pereyra, Photonicas 2020, 7, 29.

P. Pereyra, Photonics 2021, 8, 86.

R. E. Camley, D. L. Mills, Phys. Rev. B 1984, 29, 1695.

P. Lambin, J. P. Vigneron, A. A. Lucas, Phys. Rev. B 1985, 32, 8203.

D. Xue, C.-H. Tsai, Solid State Commun. 1985, 56, 651.

R. F. Wallis, R. Szenics, J. J. Quinn, G. F. Giuliani, Phys. Rev. B 1987, 36, 1218.

V. U. Nazarov, Phys. Rev. B 1994, 49, 17342.

J. J. Quinn, Nucl. Instrum. Methods Phys. Res. B 1995, 96, 460.

D. Bria, B. DiJafari-Rouhani, A. Akjoju, L. Brdzynski, J. P. Vigneron, E. H. El Boudouti, A. Nougauoi, Phys. Rev. E 2004, 69, 066613.

R. de L Kronig, W. G. Penney, Proc. Roy. Soc. 1911, 130, 499.

A. M. Steinberg, P. G. Kwiat, R. Chiao, Phys. Rev. Lett. 1993, 71, 708.

C. Spielmann, R. Szipoecs, A. Stingl, F. Krausz, Phys. Rev. Lett. 1994, 73, 2308.

S. Nakamura, S. Peartond, G. Fasol, in The Blue Laser Diode. The Complete History, Springer-Verlag, Berlin 1997, p. 247.

S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, H. Kiyoku, Y. Sugimoto, Appl. Phys. Lett. 1996, 68, 3269.

Y. Nawakami, S. Fujita, S. Fujita, S. Nakamura, Phys. Rev. B 1997, 55, R1938.

S. Datta, B. Das, Appl. Phys. Lett. 1990, 56, 665.

M. N. Baibich, J. M. Broto, A. Fert, F. N. Van Dau, F. Petroff, P. Ettene, G. Creuzet, A. Fiederich, J. Chazelas, Phys. Rev. Lett. 1988, 61, 2472.

A. Van Esch, L. Van Bockstal, J. De Boeck, G. Verbanck, A. S. van Steenbergen, P. J. Wellmann, B. Grietens, R. Bogaerts, F. Herlach, G. Borghs, Phys. Rev. B 1997, 56, 103.
[210] M. Morales, A. Robledo-Martinez, P. Pereyra, Microelectron. J. 2008, 39, 394.
[211] A. Robledo-Martinez, J. C. Sandoval, P. Pereyra, Microelectron. J. 2009, 40, 788.
[212] T. C. L. G. Sollner, P. E. Tannenwald, D. D. Peck, W. D. Goodhue, J. Appl. Phys. 1984, 45, 1319.
[213] A. R. Bonnefоri, R. T. Collins, T. C. McGill, R. D. Burnham, F. A. Ponce, Appl. Phys. Lett. 1985, 246, 285.
[214] H. Morkoç, J. Chen, U. K. Reddy, T. Henderson, S. Luryi, Appl. Phys. Lett. 1986, 49, 70.
[215] S. Ray, P. Ruden, V. Sokolov, R. Kolbas, T. Boonstra, J. Williams, Appl. Phys. Lett. 1986, 48, 1666.
[216] E. R. Brown, T. C. L. G. Sollner, W. D. Goodhue, C. D. Parker, Appl. Phys. Lett. 1987, 50, 83.
[217] C. I. Huang, M. J. Paulus, C. A. Bozada, S. C. Dudley, K. R. Evans, C. E. Stutz, R. L. Jones, M. E. Cheney, Appl. Phys. Lett. 1987, 51, 121.
[218] T. K. Woodward, T. C. McGill, R. D. Burnham, Appl. Phys. Lett. 1987, 50, 451; b) T. K. Woodward, T. C. McGill, H. F. Chung, R. D. Burnham, Appl. Phys. Lett. 1987, 51, 1542.
[219] B. Su, V. J. Goldman, M. Santos, M. Shayegan, Appl. Phys. Lett. 1991, 58, 747.
[220] Z. H. Dai, J. Ni, Y. M. Sun, W. T. Wang, Eur. Phys. J. B 2007, 60, 439.
[221] M. Feiginov, C. Sydlo, O. Cojocari, P. Meissner, Europhys. Lett. 2011, 94, 48007.
[222] Y. Zeng, Ch. I. Kuo, R. Kapadia, Ch-Y. Hsu, A. Javey, C. Hu, J. Appl. Phys. 2013, 114, 024502.
[223] D. Y. K. Ko, J. C. Inkson, Semicond. Sci. Technol. Rev. 1988, 3, 791.
[224] F. Capasso, R. A. Kiehl, J. Appl. Phys. 1985, 58, 1366.
[225] M. S. Shur, L. F. Eastman, IEEE Trans. Electron Devices 1979, 26, 1677.
[226] M. Heiblum, M. I. Nathan, D. C. Thomas, C. M. Knoedler, Phys. Rev. Lett. 1985, 55, 2200.
[227] A. F. J. Levi, R. H. Hayes, P. M. Platzman, W. Wiegmann, Phys. Rev. Lett. 1985, 55, 2071.
[228] F. Capasso, K. Mohammed, A. Y. Cho IEEE J. Quantum Elect. 1986, 22, 1853.
[229] S.-Y. Cheng, P.-H. Lin, W.-C. Wang, J.-Y. Chen, W.-C. Liu, W. Lin, Electron. Lett. 1997, 33.
[230] S. E. Ullaro, E. Castaño, G. Kirzchenow, Phys. Rev. B 1990, 41, R12350.
[231] P. Pereyra, An Anzaldo-Meneses, Microelectron. J. 2005, 36, 419.
[232] P. Pereyra, Phys. Rev. Lett. 2000, 84, 1772.
[233] D. Bohm, in Quantum Theory, Prentice-Hall, New York 1951.
[234] E. P. Wigner, Phys. Rev. 1955, 98, 145.
[235] M. Büttiker, R. Landauer, Phys. Rev. Lett. 1982, 49, 1739.
[236] M. Büttiker, Phys. Rev. B 1983, 27, 6178.
[237] E. H. Hauge, J. A. Støvring, Rev. Mod. Phys. 1989, 61, 917.
[238] V. G. Veselago, Sov. Phys. Usp. 1968, 10, 509.
[239] D. R. Smith, N. Kroll Phys. Rev. Lett. 2000, 14, 2933.
[240] J. B. Pendry, Phys. Rev. Lett. 2000, 85, 1966.
[241] S. D. Gupta, R. Arun, C. S. Agarwal, Phys. Rev. B 2004, 68, 111304.
[242] Y. Zhang, A. Mascarenhas, Mod. Phys. Lett. B 2005, 19, 21.
[243] M. Perrin, S. Fasquel, Th. Decocopan, X. Mélique, O. Vanbésien, E. Lheuret, D. Lippens, J. Opt. A: Pure Appl. Opt. 2005, 7, 53.
[244] T. M. Grzegorczyk, J. A. Kong, J. Electromagn. Waves Appl. 2006, 20, 2053.
[245] A. P. Vinogradov, A. V. Dorofeeenko, S. Zouhdi, Phys. Uspekhi 2008, 51, 485.
[246] H. O. Moser, C. Rockstuhl, Laser Photonics Rev. 2012, 6, 219.
[247] a) A. Fert, H. Jaffres, Phys. Rev. B 2001, 64, 184420; b) A. Fert, H. Jaffres, J. Appl. Phys. 2002, 91, 811.
[248] D. L. Smith, R. N. Silver, Phys. Rev. B 2001, 64, 045323.
[249] S. Takahashi, S. Maekawa, Phys. Rev. B 2003, 67, 052409.
[250] J. Shiogai, M. Ciorga, M. Utz, D. Schuh, M. Kohda, D. Bougeard, T. Nojima, J. Nitta, D. Weiss, Phys. Rev. B 2014, 89, R081307.
[251] H. Holmberg, N. Lebedeva, S. Novikov, J. Ikonen, P. Kuivalainen, M. Malfait, V. V. Moshchalkov, Europhys. Lett. 2005, 71, 811.
[252] P. Pereyra, D. Weiss, Proc. SPIE 2014, 9931, 993124.
[253] M. Turek, J. Siewert, J. Fabian, Phys. Rev. B 2008, 78, 085211.
[254] E. O. Kane, Phys. Rev. 1963, 131, 79.
[255] S. Seikin, M. Shen, M.-C. Cheng, Y. Primvra, J. Appl. Phys. 2003, 94, 1769.
[256] P. K. Young, J. A. Gupta, E. Johnston-Halperin, R. Epstein, Y. Kato, D. D. Awschalom, Semicond. Sci. Technol. 2002, 17, 275.
[257] M. Oestreich, M. Bender, J. Hübner, D. Hägele, W. W. Rühle, T. Hartmann, P. J. Klar, W. Heimbродt, M. Lampalzer, K. Volz, W. Stolz, Semicond. Sci. Technol. 2002, 17, 285.
[258] S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsuohita, H. Kyok, Y. Sugimoto, Jpn. J. Appl. Phys. 1996, 35, L217.
[259] A. Ranañi, D. Mugnai, P. Fabeni, G. P. Pazzi, Appl. Phys. Lett. 1991, 58, 774.
[260] A. Enders, G. Nimtz, J. Phys. 1 1992, 2, 1693.
[261] R. Landauer, Th. Martin, Rev. Mod. Phys. 1994, 66, 217.
[262] L. A. MacColl, Phys. Rev. 1932, 40, 621.
[263] It is worth emphasizing that in order to establish the relation between $S$ and $M$ we have to use the same basis of wave functions.
[264] Most of the content in this section was published in Refs. [154,158,190].