We discuss the construction of optimized electronic filters using inverse scattering methods. We study a wide range of densities and temperatures, room temperature included. Discretization methods of the potential (including the self-consistent potential of the conduction electrons) are worked out that retain all its properties.

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I. INTRODUCTION

A semiconductor heterostructure can be modeled by a system of equations describing (with a certain degree of completeness and precision) the state of the system. The equations depend on a set of structural and compositional data: the spatial dependence of the chemical composition (including dopant profiles), the applied external fields, etc. The system behavior (response) is described by functional data, such as the electric or thermal conductance, the energy dependence of the electron transmittance, the wavelength dependence of the optical absorption coefficient, etc. The functional data can be computed using the solution of the equations, and are thus functionals of the structural and compositional data.

To design a heterostructure for a certain application it is to find a set of structural and compositional data, which is physically (and technologically) achievable, such that the values of a chosen subset of functional data will be within a desirable range. The designer, in principle, solves an inverse problem: inverting the dependence of the functional data on the structural and compositional data.

In the usual approach, the starting point is a proposed configuration of the structural and compositional data which is then varied to optimize the component’s performance; at each iteration the spectral-scattering data describing the performance have to be re-calculated. In this method, much depends on the initial choice of parameters as in general several non equivalent local extrema of the response are present in the parameter space.

Inverse methods, when available, are not subject to this drawback. Contrary to the previous situation, the designer starts from data describing the system’s performance, such as current spectral response curves and determines the optimal structural and compositional data. He automatically gets an optimized set of parameters. Even if the model used to make the optimization calculation feasible lacks all the details of the full physical situation, one has still the possibility to use the traditional approach to fine tune the results from such a new starting point.

The inverse method we use requires three different steps [1,2]:

1. The reconstruction of the phase of the transmittivity of a quantum device using Finite Dispersion Relations under the very convenient form of the Padé approximations.

2. The Standard Inverse Scattering method, making use of the results of Kay and Sabatier [3,4] for the inverse problem with rational coefficients (Padé approximations). This allows to build an efficient algorithm for solving the inverse problem and obtaining the potential.

3. A unitary transformation that maps the place dependent mass problem of a BenDaniel equation onto the usual constant mass Schrödinger problem keeping the potential in the equation local [2].

By applying the previous procedure, it becomes possible to design new realistic quantum wells [5,6] submitted to optimization constraints. In particular, one can use inverse methods to design and fabricate novel color sensitive QWIPs in the medium- and long-wave IR. Moreover, one of the most unexpected and astonishing results of the inverse method is that inclusion of the self-consistent potential of the conduction electrons is far much simpler than in the usual direct approach [2].

As a first application, we will use the versatility of the inverse scattering methods for the Schroedinger/BenDaniel-Poisson model [1,2], for designing and building prototypes of improved electronic filters.

An aspect that has not yet been dealt with in depth is how to discretize the potential profiles obtained by inverse scattering methods so as to make their production viable while maintaining at the same time their properties, their electron wave reflectance in particular. An added complication is the necessary presence in the devices of substantial densities of conduction electrons: the electric potentials they generate do not, if suitably compensated by doping the devices [2], significantly alter the reflectance of the “smooth” potentials obtained by inverse scattering; but what about the discretized potentials? The aim of the present paper is to deal with the problems stemming from this necessity to both discretize the potentials and have substantial densities of conduction electrons. To avoid unnecessary complica-
tions, we shall skip the last step of the procedure described in Ref. [2], namely the mapping of the (constant mass) Schrödinger equation into the (variable mass) BenDaniel and Duke equation, as it has no direct bearing on the present discussion.

Throughout the present paper we shall make use of the “natural” units thus defined: energy (e.u.): 0.1 eV; mass: 0.1 m_e; length: 1 nm; time: 2.3845 fs; in these units \( \hbar = 2.7604 \).

II. INVERSE SCATTERING PROBLEM

The procedure to build a potential having a given reflectance profile for electron waves and no bound state is described in detail in Ref. [2]; here we wish to stress that while standard type II Padé [7] fitting routines can be a useful first step in building a Padé approximant, it is often the case that the parameters thus found must be adjusted, as care must be taken to avoid obtaining a potential either impossible to build because exceeding in height the available potential difference (for Al,GaAs, where \( c \) is the Aluminum concentration, this value is about 3 e.u.) or impractical to grow because having a support too wide and/or too many peaks. The reconstruction of the potential makes use of the poles and residues of the reflection coefficient \( R_+ (k) \) for plane waves incoming from \(+\infty\) where \( k = \sqrt{mE/\hbar^2} \) is the electron momentum. The frequencies of oscillation relate to the real part \((a_j)\) of the poles (where \( j = 1,n, n \) being the number of poles), the decay factors to the imaginary part \((b_j)\), and the amplitudes to the residues \((\rho_j)\). Large values of the \( a_j \)'s give fast oscillations of the potential; small values of the \( b_j \)'s result in slow decays of the oscillations and therefore in a wide support for the potential; finally, large \( \rho_j \)'s -that are often the case when poles are very close to each other- result in large oscillations of the potential; all three must therefore be avoided. Sometimes these conditions can be satisfied with no problems, sometimes instead they force us to some kind of compromise. An example of the latter case is a bandpass filter: since the more the poles are close to the real axis and close to each other the more the transmission plateau is flat and close to unity, some extra care must be taken when choosing the Padé approximant parameters.

III. DISCRETIZATION OF THE POTENTIAL

A continuous potential as the one obtained by inverse scattering [2] is impractical to build; we must therefore discretize it by a sequence as small as possible of flat steps. Several options are possible, the choice depending on the characteristics of the heterostructure we wish to build:

a) placing the steps at the inflection points of the original potential and choosing their height to be equal to that of the original potential gives us an (almost) zero transmittance in the forbidden zones and an almost satisfactory plateau in Fig. 2 without significant shifts. A desirable characteristic of this method is the unexpected reduced width of the two peaks in Fig. 1. A second scheme can be used to enhance this characteristic:

b) If we move the position of the steps to the zeroes of the original potential, both peaks are now shifted, but we have succeeded to reduce the width of both of them by a factor of 4!

As a rule, both methods should be tested and the one that gives the result nearest to the desired one retained.

IV. DOPING FOR NON-ZERO DENSITY OF CONDUCTION ELECTRONS

The (selfconsistent) electric field generated by the conduction electrons can seriously modify the effective potential and thus alter the transmission profile. It must therefore be compensated. We achieve this in two steps: first, from the potential obtained by inverse scattering we subtract the selfconsistent field of the electrons themselves and of some suitable doping charge such that the total charge and dipole moment in the device are zero (see Ref. [2]); then, after obtaining the “chemical composition potential” by discretization of the resulting potential, we calculate the selfconsistent field for this new potential itself, adjusting the position and value of the doping charge, so that again the total charge and dipole in the device are zero and the effective potential is as close as possible to the “chemical composition potential” itself.

An iterative selfconsistent calculation starting from the doping charge and dipole moment obtained for the potential before discretization converges in the worst case we considered in less than ten steps to a precision of five digits. Note that, once the correct doping has been added, the changes to the potential are usually very small; on the other hand a wrong doping is bound to seriously deteriorate the transmittance profile. In both of the following examples we assumed the doping to be in the form of a sheet charge; this approximation is valid as long as the doping can be kept in a region more narrow than the steps of the potential; should this not be the case, a suitable charge width should be considered and taken into account, requiring only minor changes to the codes.

V. TWO EXAMPLES

To illustrate the above procedure, we now give two examples. The starting point for both is a Padé approximant to the reflectance of the form:

\[
R(E) = \frac{A_{2N}(E)}{(A_{2N}(E) + EK_{2(N+2)}(E))} \quad (1)
\]

\[
K_{2(N+2)}(E) = \Pi_{j=1,N+2} \left( (E - F_j)^2 + \delta_j^2 \right) \quad (2)
\]
\[ A_{2N}(E) = g \cdot \Pi_{i=1,N} (E - E_i)^2 \quad E_i, F_j, \delta_j \in \mathbb{R}^+ \quad (3) \]

Eq. (1) guarantees that \( R(0) = 1 \); it was already given in Ref. [2] but there higher degrees for \( K_{2(N+2)}(E) \) were allowed. We choose to use the lowest possible degree ensuring the absence of \( \delta \)-function terms in the potential [8]. Eq. (2) guarantees that, excepted the zero at the origin, the transmittance has complex conjugate zeroes; Eq. (3) instead guarantees that the reflectance has real double zeroes. The three equations together guarantee that \( 0 \leq R(E) < 1 \) for \( E > 0 \).

We assume the devices to be grown from \( Al_xGa_{1-x}As \); we therefore use as parameters those for the substrate \( GaAs \): effective electron mass \( m_\infty = 0.67 \) in natural units, and electrical permeability \( \varepsilon = 13 \).

### A. A Filter with Two Narrow Transmission Resonances

Our construction of a filter with two narrow peaks, the one at higher energy being the narrower [9], starts from a Padé approximant having the same number of poles and zeroes as the one given in Refs. [2,1] but in the form (1) given above with: \( N = 2 \), \( g = 1.5 \), \( E_1 = 0.4 e.u., E_2 = 1.1 e.u., F_1 = 0.2 e.u., \delta_1 = 0.05 e.u., F_2 = 0.8 e.u., \delta_2 = 0.01 e.u., F_3 = 1.2 e.u., \delta_3 = 0.10 e.u., F_4 = 1.5 e.u., \) and \( \delta_4 = 0.20 e.u. \). \( E_1 \) and \( E_2 \) give the positions of the transmittance peaks; the four \( F_j \) frame them and determine the peaks’ width.

The final transmittance using procedure \( b) \) to discretize the potential, is shown in Fig. 1 for three temperatures (\( T = 70, 233, \) and \( 300 K \)) and two background electron densities (\( 10^{13}, 10^{15} \)); the six curves are indistinguishable. The compensating doping charges and their positions are given in table 1. We have also studied other temperatures and densities that are not reported for lack of space. Only at the highest density studied (\( 10^{17} \) \textit{el/cm}\(^3\)) the reflectance is strongly affected by the electron density, especially at low temperatures. The reason is that since at low temperatures the deviation from the background value of the electron density is less spread out, it has sharper peaks which are reflected in analogous sharp peaks in the selfconsistent electrical field; the plateaus of the discretized potential are therefore more strongly deformed than at higher temperatures.

### B. A Bandpass Filter

For this case some preliminary remarks are in order: the reflectance of an ideal bandpass filter should be zero inside the band and one everywhere else. On the other hand for a (piecewise) continuous potential that decays at infinity we have:

\( a) \ R(E) \to 0 \) for \( E \to \infty \).

As a consequence, the forbidden region will have to be finite; it will be our aim to make it as wide as possible on both sides of the transmission band.

\( b) \ R(E) \to 1 \) only for \( E = 0 \); otherwise \( R(E) < 1 \).

Therefore, there will be a residual transmittance in the forbidden region; it will be our aim to make it as small as possible.

\( c) \ R(E) \) can be zero only on a set of points which is at most countable.

Because of this, the desired transmission band will have to be built by a superposition of peaks, close enough that the transmission plateau is almost flat and sharp enough that the transition from forbidden region to allowed band is narrow compared to the band width.

We found convenient to choose the following parameters in eq. (1): \( N = 3, \ g = 20, \ E_1 = 0.9 e.u., E_2 = 1.1 e.u., E_3 = 1.3 e.u., F_1 = F_2 = 0.3 e.u., \delta_1 = 0.08 e.u., \delta_2 = 0.22 e.u., \delta_3 = 0.48 e.u., \delta_4 = 0.30 e.u., \) and \( \delta_5 = 0.16 e.u. \). The transmittance plateau is given by the three reflectance zeroes in \( E_i \), \( i = 1, 2, 3; \) the five \( F_j \) frame them and determine the two forbidden zones at each side of the allowed band.

The final transmittance using procedure \( a) \) to discretize the potential, shown in Fig. 2 for the same three temperatures and two background electron densities used in the previous example, is again equal in all cases; the compensating doping charges and their positions are given in table 2. Again we found that only at the highest density studied (\( 10^{17} \) \textit{el/cm}\(^3\)) the reflectance is strongly affected by the electron density.

### VI. CONCLUSIONS AND ACKNOWLEDGEMENTS

We have shown that both discretization of the potential and substantial densities of conduction electrons can be dealt with in ways that preserve the essential characteristics of the desired reflectance. We should note that in both the examples given the background electron distribution is repelled from the potential and therefore the required compensating doping is of the N-type; this can sometimes be impractical. A way to circumvent the problem is to add a (monodimensional) bound state via a Darboux transformation [8]: the high electron density in it ensures that the doping be of the P-type.

Finally, we would be glad to receive feedback from readers. We are ready to analyze and design electronic filters that are difficult or impossible to deal with by the ordinary method.

We wish to acknowledge the participation to the first phases of the present research of the late G.A. Mezincescu, who has been for a long time a driving force in our group.
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FIG. 1. The reflectance of our double peak filter at $T = 70, 233, 300$ $K$ for two different densities of conduction electrons ($10^{13}$ el/cm$^3$ and at $10^{15}$ el/cm$^3$): all six curves are indistinguishable on this scale from the "optimal" reflectance obtained using procedure a) described in the text and truncating the support at 50 nm. The width ratio of the two peaks is approximately 3.

FIG. 2. The reflectance of our bandpass filter at $T = 70, 233, 300$ $K$ for two different densities of conduction electrons ($10^{13}$ el/cm$^3$ and at $10^{15}$ el/cm$^3$): all six curves are indistinguishable on this scale from the "optimal" reflectance obtained using procedure b) described in the text and truncating the support at 100 nm.

| $T(K)$ | el.density(el/cm$^3$) | charge(cm$^{-2}$) | position(nm) |
|-------|------------------------|-------------------|--------------|
| 70    | $10^{13}$              | $-3.1729 \times 10^7$ | 12.8         |
| 70    | $10^{15}$              | $-3.1455 \times 10^9$ | 12.9         |
| 233   | $10^{13}$              | $-1.8134 \times 10^7$ | 10.4         |
| 233   | $10^{15}$              | $-1.8113 \times 10^9$ | 10.3         |
| 300   | $10^{13}$              | $-1.6038 \times 10^7$ | 10.1         |
| 300   | $10^{15}$              | $-1.6061 \times 10^9$ | 10.1         |

TABLE I. Doping charge and position at different temperatures and background electron densities for the filter with two narrow transmission peaks described in the text.

| $T(K)$ | el.density(el/cm$^3$) | charge(cm$^{-2}$) | position(nm) |
|-------|------------------------|-------------------|--------------|
| 70    | $10^{13}$              | $-2.3239 \times 10^7$ | 9.0          |
| 70    | $10^{15}$              | $-2.3008 \times 10^9$ | 9.0          |
| 233   | $10^{13}$              | $-1.8134 \times 10^7$ | 6.8          |
| 233   | $10^{15}$              | $-1.8113 \times 10^9$ | 6.8          |
| 300   | $10^{13}$              | $-1.6038 \times 10^7$ | 6.5          |
| 300   | $10^{15}$              | $-1.6061 \times 10^9$ | 6.6          |

TABLE II. Doping charge and position at different temperatures and background electron densities for the bandpass filter described in the text.
