Design of semiconductor heterostructures with preset electron reflectance by inverse scattering techniques

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We present the application of the inverse scattering method to the design of semiconductor heterostructures having a preset dependence of the (conduction) electrons' reflectance on the energy. The electron dynamics are described by either the effective mass Schrödinger, or by the (variable mass) BenDaniel and Duke equations. The problem of phase (re)construction for the complex transmission and reflection coefficients is solved by a combination of Padé approximant techniques, obtaining reference solutions with simple analytic properties. Reflectance-preserving transformations allow bound state and reflection resonance management. The inverse scattering problem for the Schrödinger equation is solved using an algebraic approach due to Sabatier. This solution can be mapped unitarily onto a family of BenDaniel and Duke type equations. The boundary value problem for the nonlinear equation which determines the mapping is discussed in some detail. The chemical concentration profile of heterostructures whose self consistent potential yields the desired reflectance is solved completely in the case of Schrödinger dynamics and approximately for BenDaniel and Duke dynamics. The Appendix contains a brief digest of results from scattering and inverse scattering theory for the one-dimensional Schrödinger equation which are used in the paper.

Contents

I. INTRODUCTION

A semiconductor heterostructure can be modelled 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 (SCD). Essentially, these are the spatial dependence of the chemical composition (including dopant profiles), the applied external fields, etc. The system's behavior (response) is described by functional data (FD), such as the electric or thermal conductance, the energy dependence of the electron transmittance, the wavelength dependence of the optical absorption coefficient, etc. The FD can be computed using the solution of the equations, and are thus functionals of the SCD.

To design a heterostructure for a certain application is to find a set of SCD, which is physically (and technologically) achievable, such that the values of a chosen subset

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of FD will be within desirable ranges. The designer solves thus an inverse problem: inverting the functional dependence of the FD on the SCD. This problem is rather ill-posed. The desired ranges of FP may be unachievable. Generally speaking, even if a certain desired set of FD values is achievable, the set of SCD which achieves it is not unique. This absence of uniqueness is not bad in itself. If several solutions *can be obtained*, then one may further optimize the design in terms of other properties which were not included in the original specifications. The difficulty is mathematical. Inverting a one-to-one functional dependence can be a formidable task, which is further aggravated by the lack of uniqueness.

A brute-force approach to the problem is always possible: computing the FD for a set of achievable SCD (ideally all) and selecting the best. In practice, brute force optimization is restricted to rather small sets of parameters describing the FD. This is mostly due the fact that any conceivable penalty function will be non-convex. Its graph will have a rather complex multi-valley shape. The search algorithm is forced to do a thorough investigation of this landscape and will eventually fail through run time limitations. The intelligent designer will partially avoid such restrictions by noting trends, trying to break the design into combining manageable blocks and locally improving promising configurations.

Thus, cases when the solution of the inverse problem is realizable by methods which are less costly than the brute force approach can be rather useful. Even if one has to simplify somewhat the physical model, precious insights on new promising configurations can be obtained.

In this paper we will try to review the possible applications of inverse scattering techniques to some aspects of heterostructure design. Our physical model for the electron states in the heterostructure will be the (one band) effective mass approximation for the envelope function of the (conduction band) electrons.

The simplest approach is to assume a constant effective mass. Then, the envelopes of electron states satisfy an effective Schrödinger equation[1]. Choosing the z-axis along the growth direction,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m_e}\Delta\Psi(\boldsymbol{r},t) + U(z)\Psi(\boldsymbol{r},t). \quad (1.1)$$

Here, m_e is the (conduction band) electron's effective mass. The potential is

$$U(z) = \mathcal{E}(z) + U_{ext}(z) + \Phi_{sc}(z), \quad (1.2)$$

where $\mathcal{E}(z) = \mathcal{E}_{cond}[c(z)]$ is the (conduction) band offset (assumed to depend only on the local chemical composition, $c(z)$); $U_{ext}(z)$ is the (possibly equal to zero) external applied potential and we lumped in $\Phi_{sc}(z)$ the potential of the ionized (donor) impurities (dopants) and terms which will make the full potential $U(z)$ self-consistent. Various models can be considered for $\Phi_{sc}(z)$: a Hartree self consistent potential, exchange-correlation corrections can be incorporated. The only requirement is that $\Phi_{sc}(z)$ has to be an *explicitly defined* functional of the full potential $U(z)$.

The next step is to take into account the spatial dependence of the effective mass. The Schrödinger equation with constant effective mass (SE) for the envelope function, (1.1), is replaced by the BenDaniel and Duke[2] equation (BDD):

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = -\boldsymbol{\nabla}\frac{\hbar^2}{2m(z)}\boldsymbol{\nabla}\Psi(\boldsymbol{r},t) + U(z)\Psi(\boldsymbol{r},t). \quad (1.3)$$

Here the effective mass of the conduction band electrons $m(z) = m_{cond}[c(z)]$ is assumed to depend only on the local chemical composition $c(z)$. The self-consistent potential is given again by (1.2). The $\Phi_{sc}(z)$ term is now a functional of both $m(z)$ and $U(z)$.

In the following we will consider only stationary states of the equations (1.1) and (1.3). Furthermore, since the potential depends only on the coordinate along the growth direction, z, the motion in the perpendicular plane is free. Setting

$$\Psi(\boldsymbol{r},t) = \psi(z)\mathrm{e}^{\mathrm{i}(\boldsymbol{q}_\perp\boldsymbol{r}_\perp - Et/\hbar)}, \quad (1.4)$$

in the Schrödinger (1.1) and BenDaniel and Duke (1.3) equations, where E is the energy, $\boldsymbol{r}_\perp = (x,y,0)$ and $\boldsymbol{q}_\perp = (q_1,q_2,0)$ are, respectively, the coordinates and components of the quasi-momentum in the directions perpendicular to the growth axis, we obtain the one-dimensional Schrödinger,

$$\psi''(z) + \left[k^2 - \boldsymbol{q}_\perp^2 - V(z)\right]\psi(z) = 0, \quad (1.5)$$

and BDD

$$\left[\frac{m_\infty\psi'(z)}{m(z)}\right]' + \left[k^2 - \frac{m_\infty\boldsymbol{q}_\perp^2}{m(z)} - V(z)\right]\psi(z) = 0, \quad (1.6)$$

equations for $\psi(z)$. Here, and in the following, we use the notation m_∞ for the electron effective mass in the embedding material: $m_\infty = m_e$ for SE and $m_\infty = m(\pm\infty)$ for BDD. We introduce the notations

$$k = \frac{\sqrt{2m_\infty E}}{\hbar}; \quad V(z) = \frac{2m_\infty U(z)}{\hbar^2}. \quad (1.7)$$

Throughout this paper, the square root function is defined with non negative imaginary part: $\mathrm{Im}\left(\sqrt{E}\right) \geq 0$. For real positive E in (1.7), $k > 0$. The prime will often be used for derivatives.

The inverse spectral theory for the one-dimensional Schrödinger equation[3,4] has been successfully applied to some optimization problems for the bound states in semiconductor quantum wells[5–9]. Inverse scattering theory[10] for the one-dimensional Schrödinger equation, (1.5) with $\boldsymbol{q}_\perp = 0$, shows how one can recover the potential in (1.5) from the knowledge of the scattering data: the complex transmission and reflexion to the right/left coefficients $\{T(k),\, R_\pm(k)\}$ for all real values of the wave-number k.

Widely used in electric circuit modelling[10,11], it has been recently applied for designing heterostructure Bloch wave filters[12].

We want to solve the following problem: let the electron dynamics be given by either the SE, (1.5), or by the BDD equation, (1.6), with the self-consistent potential (1.2). Find chemical composition and dopant profiles, going to constant limits at infinity, such that the heterostructure defined by these data has a given energy dependence of the electron reflectance at $\boldsymbol{q}_\perp = 0$ and a given operating temperature:

$$\mathcal{R}(E) = |R_\pm(k)|^2 \,. \tag{1.8}$$

The zero of the energy scale is chosen at the conduction band minimum for the asymptotic composition at infinity.

In the SE case, the mini-bands are parabolic in $\boldsymbol{q}_\perp$ and (1.8) will hold for $\boldsymbol{q}_\perp \neq 0$ with E changed to $E + \hbar^2 \boldsymbol{q}_\perp^2 / 2m_e$. This is no longer true in the case of the BDD equation (1.6). For sufficiently small $|\boldsymbol{q}_\perp|$, the mini-bands will be approximately parabolic only as long as the $\frac{m_e \boldsymbol{q}_\perp^2}{m(z)}$ term in the effective potential in (1.6) can be treated as a first order perturbation. One could also select a nonzero value of $\boldsymbol{q}^2$ at which (1.8) is valid, such as the one corresponding to the transverse thermal energy at the desired operating temperature.

Since only the energy dependence of the reflectance is given, the first step in solving our problem is to find the sets of scattering data (SD) which are compatible with $\mathcal{R}(E)$, *i.e.* find the phases of the scattering data. In section II we show how to construct SD which correspond to real valued potentials $V(z)$ with exponential decay at infinity from $\mathcal{R}(E)$. Physically, one might expect that the potential is determined by the its bound state energies and its resonances. The reflectance $\mathcal{R}(E)$ embodies only information on the transmission resonances: sharp minima of the reflectance. There is another type of resonance, the reflection resonances, analogous to the resonances that occur in three-dimensional potential scattering on a spherically symmetric potential. These are sharp *phase* variations of the reflection coefficients. The information on reflection resonances and on the bound states is not apparent in the reflectance.

The transformations of the SD, which do not change the reflectance, will be discussed. Using these transformations, we will define reference solutions for the recovery of the SD from the reflectance. The reference solutions have no bound states and simpler analytic properties. Combinations of reflectance-preserving transformations can then be used to obtain the SD of other solutions to the phase reconstruction problem from the reference solutions, by dressing them up with bound states and reflection resonances.

We will use Padé approximation methods[13] to represent the scattering data and to find parameterizations for a large class of solutions, corresponding to potentials which tend exponentially to zero at infinity. We will find that on this type of input data, the (re)construction process amounts essentially to finding the roots of some polynomials and grouping them into subsets.

In section III we present a simple and efficient algorithm for solving the inverse scattering problem for scattering data in the form obtained in section II. We will use results due to Kay, Moses and Sabatier[14–18] for the inverse problem with rational coefficients[10].

In section IV we present the variable mass unitary mapping of the SE to the BDD equation[19,20,12]. We formulate the boundary value problem which must be solved for determining the coordinate transformation which defines the mapping, given the material relation between the effective mass and the band offset. This ill-conditioned problem can be solved by a a shooting method. In the case when the relation between the mass and the offset is linear, the solution takes a simpler form. We also give an efficient perturbative method for solving the mapping equation.

In section V we show that obtaining chemical composition profiles and self-consistent potentials for them in the SE in the inverse scattering approach is simpler than obtaining the self-consistent potential for a given chemical composition profile. We also discuss the functional equation which must be solved for obtaining the chemical (effective mass) profile corresponding to self-consistent potentials in the BenDaniel and Duke's equation.

For the reader's convenience, in Appendix A we give a brief outline of results from scattering and inverse scattering theory, which are needed and often referred to in the main body of the paper.

II. PHASE RECONSTRUCTION

Inverse scattering theory for the one-dimensional Schrödinger equation, (1.5) with $\boldsymbol{q}_\perp = 0$,

$$\psi''(z) + \left[k^2 - V(z)\right] \psi(z) = 0, \tag{2.1}$$

on which we give a primer in Appendix A, shows that one can recover a fast decaying and piecewise continuous potential in (2.1) from the knowledge of the scattering data (SD): the complex transmission and reflexion to the right/left coefficients $\{T(k),\, R_\pm(k)\}$ for all real values of the wave-number k *if there are no bound states.* If bound states are present, knowledge of the SD is not sufficient for unique recovery of the potential. If the number of bound states is exactly n, then a n-parameter family of potentials gives exactly the same scattering data.

The SD are completely determined by one of the reflexion coefficients and the values of the energies of the bound states. The phase of $T(k)$ can be obtained from a logarithmic dispersion relation. (see *e.g.* the book by Chadan and Sabatier[10], XVII.1.5). The other reflection coefficient can be obtained from (A11).

In this section we assume that the reflectance, $\mathcal{R}(E)$, is known on the positive energy half-axis, $E > 0$. We want to construct sets of SD which satisfy (1.8). Since the values of the SD for scattering by short-range and piecewise continuous potentials must satisfy the constraints[10,21] which are enumerated at the end of Appendix A 2, the function $\mathcal{R}(E)$ cannot be arbitrary. It must be non-negative and smaller than unity, with the exception of $\mathcal{R}(0)$, which is generically[22] equal to 1. If the potential is piecewise continuous, $\mathcal{R}(E)$ must go to zero no slower than E^{-2} for large values of E.

The transmittance $\mathcal{T}(E) = |T(k)|^2$, where $T(k)$ is the complex transmission coefficient, is readily recovered from $\mathcal{R}(E) + \mathcal{T}(E) = 1$. Thus, we know the absolute values of the scattering data and we need the phases.

A. Reflectance-preserving transformations

The problem of finding the phases of the scattering coefficients knowing only their absolute values on the real axis is underdetermined and has an infinite number of solutions. Before considering the phase (re)construction problem, we will introduce two types of transformations which modify the phases of the scattering data without changing the reflectance.

Let the set of scattering data

$$\{T(k),\, R_+(k)\, R_-(k)\}, \tag{2.2}$$

be a solution of the phase reconstruction problem, *i.e.* the scattering coefficients satisfy (1.8) and the conditions enumerated at the end of Appendix A 2. Then, as mentioned above, if the SD (2.2), has no bound states, there is an unique solution to the inverse scattering problem: a potential $V(z)$ in (2.1) such that the SD calculated for this equation coincide with (2.2). If $T(k)$ has n simple imaginary poles in the upper half plane, that is n bound states, then a n-parameter family of potentials can be constructed, such that the SD of each potential coincides with (2.2).

Let now $\lambda > 0$ be a positive number, such that $k = \mathrm{i}\lambda$ is not a pole of $T(k)$, *i.e.* that $E = -\hbar^2\lambda^2/2m_e$ is not a bound state of (2.2). Define a new set of SD by the transformation:

$$T(k) \to \frac{(k+\mathrm{i}\lambda)}{(k-\mathrm{i}\lambda)}T(k), \tag{2.3}$$

$$R_\pm(k) \to \frac{(\mathrm{i}\lambda+k)}{(\mathrm{i}\lambda-k)}R_\pm(k), \tag{2.4}$$

The new set of SD will also satisfy the conditions set out at the end of Appendix A 2, so that a $(n+1)$-parameter family of potentials can be constructed with each potential having the SD (2.3-2.4).

The transformation (2.3-2.4) can also remove bound states. If the initial SD, (2.2), have a bound state for $E = -\hbar^2\lambda^2/2m_e$, then the transformation (2.3-2.4) with λ changed into $-\lambda$ in the right-hand sides of the equations, transforms that bound state into an *anti-bound* state – an imaginary pole of $T(k)$ in $\mathrm{Im}(k) < 0$, leaving all the others in place.

Let ζ be an arbitrary complex number with nonzero real and imaginary parts. Then, we can define a second type of reflectance preserving transformation of the SD (2.2):

$$T(k) \to T(k), \tag{2.5}$$

$$R_-(k) \to \frac{(k-\zeta)(k+\zeta^*)}{(k-\zeta^*)(k+\zeta)}R_-(k), \tag{2.6}$$

$$R_+(k) \to \frac{(k-\zeta^*)(k+\zeta)}{(k-\zeta)(k+\zeta^*)}R_+(k). \tag{2.7}$$

Here and in the following, we use the notation * for complex conjugation. The transformed SD, (2.5-2.7), have the same reflectance and bound states as (2.2) and satisfy the conditions enumerated at the end of Appendix A 2. Using the inverse scattering method, one can construct from the SD, (2.5-2.7), a new n-parameter family of piecewise continuous potentials which goes to zero at infinity.

The transformation (2.5-2.7) has a simple interpretation. Assume that the imaginary part of ζ is much smaller than its real part, $|\mathrm{Im}(\zeta)| \ll |Re(\zeta)|$, and the initial reflection coefficients, $R_\pm(k)$, are slowly varying on the scale $|\mathrm{Im}(\zeta)|$ near $k = \pm\mathrm{Re}(\zeta)$. Then, the new scattering data (2.5-2.7) have a *reflection resonance* of width $|\mathrm{Im}(\zeta)|$ at $k = \pm\mathrm{Re}(\zeta)$. Indeed, the phases of the new reflexion coefficients vary by $\pm 2\pi$ in a small interval of width $2|\mathrm{Im}(\zeta)|$ centered on $k = \pm\mathrm{Re}(\zeta)$.

A third type of transformation adds purely imaginary resonances to the reflection coefficients leaving the transmission coefficient unchanged:

$$T(k) \to T(k), \tag{2.8}$$

$$R_+(k) \to \frac{(\mathrm{i}\lambda+k)}{(\mathrm{i}\lambda-k)}R_+(k), \tag{2.9}$$

$$R_-(k) \to \frac{(\mathrm{i}\lambda-k)}{(\mathrm{i}\lambda+k)}R_-(k), \tag{2.10}$$

where λ is an arbitrary real number. The new SD will also satisfy the conditions enumerated at the end of Appendix A 2. The reconstruction of the potential is done exactly as for the second type of transformation.

A sequence of transformations of the second and third type can be written as:

$$T(k) \to T(k), \tag{2.11}$$

$$R_-(k) \to \frac{S_N(k)}{S_N(-k)}R_-(k), \tag{2.12}$$

$$R_+(k) \to \frac{S_N(-k)}{S_N(k)}R_+(k), \tag{2.13}$$

where $S_N(k)$ is any polynomial whose zeros are invariant with respect to reflection through the imaginary axis, *i.e.* if ζ is a zero, then $-\zeta^*$ is also a zero of the polynomial. Such polynomials, normalized by the condition

$S_N(0) = 1$, satisfy $S_N(k) = [S_N(-k)]^*$ for real k. Let us recall that an arbitrary polynomial of degree n, $\Pi_n(x)$, with $\Pi_n(0) = 1$, can be expressed through its zeros:

$$\Pi_n(x) = \prod_{i=1}^{n} \left(1 - \frac{x}{x_i}\right). \tag{2.14}$$

Here x_i, $i = 1, \ldots, n$ are the zeros of $\Pi_n(x)$ (including multiple ones according to their algebraic multiplicity). Thus, $S_N(k)$ is completely determined.

B. The reference solutions

Let us assume that we have found a solution of the phase reconstruction problem. Generically, it will have some bound states and reflection resonances. Using suitably chosen transformations of type (2.3-2.4) one can obtain from it a solution for which the transmission coefficient has no poles in the upper complex half-plane (*i.e.* no bound states). Then, by a sequence of transformations of type (2.5-2.10) with suitably chosen parameters one can find a solution for which the reflection to the left coefficient has no poles or zeros in the upper half plane.

We will call this solution of the phase reconstruction problem *the left reference solution*. The left reference solution's transmission coefficient, $T^{(r-)}(k)$, and the reflection to the left coefficient, $R_-^{(r-)}(k)$, are analytic and have no zeros in $\mathrm{Im}(k) > 0$. In a similar way, we can define the right reference solution, for which $T^{(r+)}(k)$ and $R_+^{(r+)}(k)$, are analytic and have no zeros in $\mathrm{Im}(k) > 0$. The left and right reference solutions are connected by a transformation of type (2.11-2.13):

$$T^{(r+)}(k) = T^{(r-)}(k) = T^{(r)}(k), \tag{2.15}$$

$$R_-^{(r+)}(k) = \frac{S_{N+M}(k)}{S_{N+M}(-k)} R_-^{(r-)}(k), \tag{2.16}$$

$$R_+^{(r+)}(k) = \frac{S_{N+M}(-k)}{S_{N+M}(k)} R_+^{(r-)}(k). \tag{2.17}$$

Here, the polynomial

$$S_{N+M}(k) = A_N(k) B_M(-k), \tag{2.18}$$

where the zeros of the polynomial $A_N(k) \,/\, B_M(k)$ coincide (including multiplicities) with the poles/zeros of $R_-^{(r-)}(k)$ in $\mathrm{Im}(k) > 0$. Taking into account(2.14) the polynomials are completely determined.

The reference solutions are in a certain sense the maximally non-symmetric solutions. Indeed, as shown in the next section III, the potentials corresponding to the left/right reference solutions are identically zero for $x < 0$ / $x > 0$. Other solutions of the phase reconstruction problem can be obtained from the reference ones by adding bound states and reflection resonances with reflectance-preserving transformations of type (2.3-2.10).

The left reference solution's $R_-^{(r-)}(k)$ is analytic and has no zeros in $\mathrm{Im}(k) > 0$. Thus, the logarithm $\ln[R_-^{(r-)}(k)]$ is also analytic in $\mathrm{Im}(k) > 0$. The phase of the left reference solution (which is equal to the imaginary part of $\ln[R_-^{(r-)}(k)]$) can be obtained from the logarithm of its absolute value (which is equal to the real part of $\ln[R_-^{(r-)}(k)]$), using a (subtracted) logarithmic dispersion relation (See *e.g.*[23,24]).

We will proceed in a different manner, which is more adequate with the physical context.

The effective mass approximation is valid only for energies within an interval not exceeding several hundred millielectronvolts (meV) near the Γ point minimum in the $Al_xGa_{1-x}As$ system (or in the lattice matched $In_{1-x-y}Al_xGa_yAs$ systems). Thus, two sets of scattering data having the same (or close) low and intermediate-energy behavior, but whose exact high-energy behavior is different, can be considered equivalent. We need a good approximation of the SD in the physically relevant range of energies, which obeys the high-energy constraints set forward in the Appendix A. The Padé approximation method[13] is a good framework for that. An added bonus, which will be apparent in the following section III, is the simplification of the calculations needed for recovering the potential.

C. Padé phase reconstruction

We start with approximating the input design data for the reflectance by a type II [p,p+q+2] Padé approximant[13]:

$$\mathcal{R}(E) = \frac{\mathcal{P}_p(E)}{\mathcal{Q}_{p+q+2}(E)}, \tag{2.19}$$

where $\mathcal{P}_p(E)$ and $\mathcal{Q}_{p+q+2}(E)$ are polynomials of degrees p and, respectively, $p + q + 2$ with $p,\, q \geq 0$. Since the reflectance must be non-negative and less than 1 for all $E \geq 0$, the polynomials must satisfy

$$0 \leq \mathcal{P}_p(E) < \mathcal{Q}_{p+q+2}(E), \tag{2.20}$$

on the positive half-axis. The second inequality (2.20) is strict for all $E > 0$ and becomes an equality only for $E = 0$. This ensures that $\mathcal{R}(0) = 1$ as it should be in the generic case[22]. We can rewrite it in the form

$$\mathcal{Q}_{p+q+2}(E) = \mathcal{P}_p(E) + E\mathcal{K}_{p+q+1}(E), \tag{2.21}$$

where the polynomial $\mathcal{K}_{p+q+1}(E) > 0$ for $E \geq 0$. The polynomial $\mathcal{P}_p(E)$ is normalized by setting

$$\mathcal{P}_p(0) = 1. \tag{2.22}$$

Finally, the transmittance is approximated by the [p+q+2,p+q+2] Padé approximant:

$$\mathcal{T}(E) = 1 - \mathcal{R}(E) = \frac{E\mathcal{K}_{p+q+1}(E)}{\mathcal{P}_p(E) + E\mathcal{K}_{p+q+1}(E)}. \tag{2.23}$$

We can choose the coefficients of the polynomials in (2.19) as the parameters. These can be obtained from standard type II Padé fitting routines. Taking into account (2.20) with equality at $E = 0$ and (2.22), the fit is obtained by solving a system of $2p+q+2$ linear equations with $2p+q+2$ unknowns (the polynomials' coefficients), which make the fit exact at $2p+q+2$ chosen points. Thus, the [p,p+q+2] Padé (2.19) is fully determined. Eq. (2.23) does not introduce additional parameters.

As we will see further on, it is advantageous to reparameterize in terms of the zeros and poles of (2.19). Since the reflectance and the transmittance are real and nonnegative, the zeros and poles of (2.19) and (2.23) are either real negative or come in complex conjugate pairs. The only exception to this rule are eventual real positive zeros of $\mathcal{P}_p(E)$, which have an even order of degeneracy (generically =2). The heterostructure is transparent to Bloch waves (maximal transmission resonances) at the energies corresponding to these degenerate zeros.

Now, we want to find the left reference solution by solving eq. (1.8),

$$\left|R_-^{(r-)}(k)\right|^2 = \mathcal{R}(E), \tag{2.24}$$

with the reflectance given by (2.19). The reflection to the left coefficient, $R_-^{(r-)}(k)$, will be sought as a [p,p+q+2] Padé approximant in the variable k

$$R_-^{(r-)}(k) = -\frac{P_p(k)}{Q_{p+q+2}(k)}, \tag{2.25}$$

with the normalization

$$P_p(0) = Q_{p+q+2}(0) = 1, \tag{2.26}$$

which agrees with (2.22). As mentioned above, $R_-^{(r-)}(k)$ for the left reference solution of (2.24) is analytic in the upper half-plane and has no zeros there. Then, the zeros of both the denominator and numerator of (2.25) must lie in the lower complex half-plane. A further constraint on the roots follows from the relation (A13),

$$[R_-(k)]^* = R_-(-k). \tag{2.27}$$

This relation holds only if for each r, which is a zero/pole of (2.25), $-r^*$ is also a zero/pole.

Let us now use (2.14) to represent all the polynomials involved in the equation (2.24) as products:

$$\frac{\prod_{i=1}^{p}(1-k/p_i)(1+k/p_i)}{\prod_{j=1}^{p+q+2}(1-k/q_j)(1+k/q_j)} = \frac{\prod_{i=1}^{p}(1-E/\mathfrak{p}_i)}{\prod_{j=1}^{p+q+2}(1-E/\mathfrak{q}_j)}. \tag{2.28}$$

Here p_i and $\mathfrak{p}_i$, $i = 1, \ldots, p$ are the zeros of $P_p(k)$, respectively $\mathcal{P}_p(E)$, while q_j and $\mathfrak{q}_j$, $j = 1, \ldots, p+q+2$ are the zeros of $Q_{p+q+2}(k)$, respectively $\mathcal{Q}_{p+q+2}(E)$.

Taking into account the relation (1.7), $E = \hbar^2 k^2/m_e$, we find the following relations between the zeros of the polynomials:

$$\mathfrak{p}_i = \frac{\hbar^2 p_i^2}{2m_e}; \quad i = 1, \ldots, p; \tag{2.29}$$

$$\mathfrak{q}_j = \frac{\hbar^2 q_j^2}{2m_e}; \quad j = 1, \ldots, p+q+2. \tag{2.30}$$

These relations solve the problem up to the ambiguity of the signs of the square roots. Let us show that the reference solution is unique.

As mentioned in the Introduction, the square-root function as maps the complex plane cut along $[0, +\infty)$ onto the upper complex half-plane, *i.e.* if E is in the cut plane, then $\mathrm{Im}\left(\sqrt{E}\right) > 0$. Since the zeros and poles of the reference solution cannot lie in the upper half-plane the sign choices in (2.29-2.30) are unique[25]:

$$\hbar p_i = -\sqrt{2m_e\mathfrak{p}_i}; \quad i = 1, \ldots, p; \tag{2.31}$$

$$\hbar q_j = -\sqrt{2m_e\mathfrak{q}_j}; \quad j = 1, \ldots, p+q+2. \tag{2.32}$$

It remains to show that if r is one of the zeros, respectively poles, of (2.25), then $-r^*$ is also a zero, respectively pole. This is obvious if r is real[25] or imaginary. Otherwise, both the real and the imaginary parts of r^2 are nonzero. Then, r^{*2} is also a zero (pole) of (2.19), since as noted above these come in complex-conjugate pairs. But our definition of the square-root function leads to $\sqrt{r^{*2}} = -\left(\sqrt{r^2}\right)^*$.

Thus, (2.25) with the zeros and poles given by (2.31-2.32) is the unique left reference solution for the reflection to the left coefficient if the reflectance is given by the Padé approximant (2.19). We can readily recover the complex transmission coefficient of the reference solutions using the same approach.

The (complex) transmission coefficient of the reference solution is given by the [p+q+2,p+q+2] (diagonal) Padé approximant

$$T^{(r)}(k) = \frac{kK_{p+q+1}(k)}{Q_{p+q+2}(k)}, \tag{2.33}$$

normalized by setting the coefficient of k^{p+q+1} in the polynomial $K_{p+q+1}(k)$ equal to the coefficient of k^{p+q+2} in the already determined polynomial $Q_{p+q+2}(k)$, so that $\lim_{k\to\infty} T(k) = 1$. Let 0 and $\mathfrak{k}_j$, $j = 1, \ldots, p+q+1$ be the zeros of the transmittance, (2.23).

$$\mathcal{P}_p(\mathfrak{k}) = \mathcal{Q}_{p+q+2}(\mathfrak{k}). \tag{2.34}$$

Repeating the reasoning that led to (2.31), we recover the zeros κ_j of the polynomial $K_{p+q+1}(k)$

$$\hbar\kappa_j = -\sqrt{2m_e\mathfrak{k}_j}; \quad j = 1, \ldots, p+q+1, \tag{2.35}$$

and

$$K_{p+q+1}(k) = -\frac{\prod_{i=1}^{p+q+1}(\kappa_i - k)}{\prod_{j=1}^{p+q+2} q_j}. \tag{2.36}$$

Finally, using the relation (A16), we recover the left reference solution's $R_+^{(r-)}(k)$ as a [2p+q+1,2p+2q+3] Padé approximant:

$$R_+^{(r-)}(k) = -\frac{K_{p+q+1}(k)}{K_{p+q+1}(-k)}\frac{P_p(-k)}{Q_{p+q+2}(k)}. \tag{2.37}$$

The first fraction in the above expression is a phase factor.

Thus, if the reflectance is given in the Padé form (2.19), the left reference solution is uniquely determined. The right/left reflection coefficients of the right reference solution are given by right-hand side of (2.25)/(2.37). The potentials corresponding to the right/left reference solutions are mirror images: $V^{(r-)}(x) = V^{(r+)}(-x)$.

Other solutions can be obtained by using transformations of type (2.3 - 2.4) to introduce bound states into the reference solutions. Then, transformations of type (2.5 - 2.13) can be used for reflection resonance management. A distinguished class of solutions, having the same transmission coefficient as the reference ones and involving no additional parameters, can be obtained by redistributing reflection resonances between the reflection coefficients to the left/right. This is achieved by factorizing the polynomials P_p and K_{p+q+1}

$$P_p(k) = P_{p_+}(k)P_{p_-}(k); \quad K_{p+q+1}(k) = K_{n_+}(k)K_{n_-}(k), \tag{2.38}$$

into factors which satisfy the complex conjugation relation (2.27) for real k. Here, $p_+ + p_- = p$, $n_+ + n_- = p+q+1$ and all the factors are normalized by $P_{p_\pm}(0) = 1$. Applying the transformation (2.11-2.13) with $S(k) = K_{n_-}(k)P_{p_+}(-k)$ to the left reference solution, we obtain a solution having the same transmission coefficient $T^{(r)}(k)$, given by (2.33), and the reflection coefficients are given by the [n$_\pm$+p,n$_\pm$+p+q+2] Padé approximants

$$R_-(k) = -\frac{K_{n_-}(k)}{K_{n_-}(-k)}\frac{P_{p_+}(-k)P_{p_-}(k)}{Q_{p+q+2}(k)}, \tag{2.39}$$

$$R_+(k) = -\frac{K_{n_+}(k)}{K_{n_+}(-k)}\frac{P_{p_+}(k)P_{p_-}(-k)}{Q_{p+q+2}(k)}. \tag{2.40}$$

III. SOLUTION OF THE INVERSE SCATTERING PROBLEM FOR THE SCHRÖDINGER EQUATION WHEN THE SCATTERING DATA ARE RATIONAL FUNCTIONS

In this section we will present the solution of the inverse scattering problem for the one-dimensional Schrödinger equation in the case when the scattering data are given in the Padé approximant form we obtained in the preceding section II C. The inverse scattering problem in the case of rational coefficients has been first considered by Kay and Moses[14–17]. Significant results are due to Sabatier[18,10]. We will follow Sabatier's approach[18,10] quite closely.

As shown in the Appendix A 2, the potential in (2.1) can be recovered from the transformation kernels.

$$V(x) = \mp 2\frac{\mathrm{d}}{\mathrm{d}x}K_\pm(x; x \mp 0). \tag{3.1}$$

The transforming kernels $K_\pm(x;y)$ are the solutions of the Marchenko equations, (A33), (A35)

$$K_-(x;y) + M_-(x+y) = \int_{-\infty}^{x} \mathrm{d}s M_-(y+s)K_-(x;s) = 0, \tag{3.2}$$

$$K_+(x;y) + M_+(x+y) = \int_{x}^{\infty} \mathrm{d}s M_+(y+s)K_+(x;s) = 0. \tag{3.3}$$

The Marchenko kernels, $M_\pm(u)$, are given by (A34).

$$M_\pm(u) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\kappa \mathrm{e}^{\pm\mathrm{i}\kappa u}R_\pm(\kappa) + \sum_j \left(C_j^\pm\right)^{-2}\mathrm{e}^{\mp\lambda_j u}. \tag{3.4}$$

Here, $C_j^\pm$ are the normalization constants of the bound states, defined in (A14).

Inspection of (3.2) and (3.3) shows that the first variable, x, enters the equations only as a parameter. Also, for negative/positive x, the integral in (3.2)/(3.3) involves only negative/positive values of s. Since we need only the contact values of the transformation kernels in (3.1), it is natural to use the K_- version of (3.1), obtained by solving (3.2) for negative x, and the solution of (3.3) for positive x. Taking into account the definition of the Marchenko kernels, (3.4), we see that we can close the integration contour into $\mathrm{Im}(k) > 0$ in the expression of the relevant kernel (M_+/M_- for $x > 0/x < 0$). In particular, if one of the reflection coefficients is analytic there, its contribution to the corresponding Marchenko kernel is identically zero. In the absence of bound states, this implies that the corresponding $M_\pm = 0$ and, therefore, the potential will be zero on the corresponding half-axis.

If the reflection coefficients are rational functions, like the solutions of the phase reconstruction problem we obtained in section II C, they have at most a finite number of poles in $\mathrm{Im}(k) > 0$. The corresponding Marchenko kernels (3.4) will be given by finite sums of exponentials, which go to zero at the corresponding infinity. For simplicity's sake, we will assume that all the poles are simple. The multiple pole case can be dealt with as a limiting case of pole confluence. Then, the corresponding kernel, $M_+(u)/M_-(u)$ for $u > 0/u < 0$, is

$$M_\pm(u) = \mathrm{i}\sum_{j\in\Omega_\pm} \varrho_j^\pm \mathrm{e}^{\pm\mathrm{i}\nu_j^\pm u}. \tag{3.5}$$

Here the sets of (all distinct) complex numbers $\left\{\nu_j^\pm\right\}_{j\in\Omega_\pm}$ consist of the (simple) poles of $R_\pm(k)$ in $\mathrm{Im}(k) > 0$ and, if bound states with energies $-\hbar^2\lambda_j^2/2m_e$ are present, $\mathrm{i}\lambda_j$. The coefficients $\varrho_j^{\pm}$ are either the residues of the corresponding reflection coefficients or, if $\nu_j^{\pm}$ comes from a bound state, $-\mathrm{i}\left(C_j^{\pm}\right)^{-2}$.

Substituting the separable Marchenko kernels (3.5) into the Marchenko equation (3.2) for $x<0$, we obtain

$$K_-(x;y) = \mathrm{i}\sum_{j\in\Omega_-} \rho_j^- \mathrm{e}^{-\mathrm{i}\nu_j^- y} Y_j^-(x), \tag{3.6}$$

where

$$Y_j^-(x) = \mathrm{e}^{-\mathrm{i}\nu_j^- x} + \int_{-\infty}^{x} \mathrm{d}y K_-(x;y)\mathrm{e}^{-\mathrm{i}\nu_j^- y}. \tag{3.7}$$

Multiplying (3.6) by $\mathrm{e}^{-\mathrm{i}\nu_m^- x}$ and integrating with respect to y we obtain a system of $\#(\Omega_-)$ linear equations for the $\#(\Omega_-)$ unknowns $Y_j^-(x)$. Here we used the notation $\#(\Omega)$ for the number of elements in the set Ω. Substituting the solution into (3.6), we obtain after a little algebra

$$K_-(x;x-0) = -\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{Tr}\ln\left[1-\mathrm{e}^{-\mathrm{i}x\mathsf{N}^-}\mathsf{D}^-\mathrm{e}^{-\mathrm{i}x\mathsf{N}^-}\right]. \tag{3.8}$$

Here, N^- and D^- are $\#(\Omega_-)$ square matrices with

$$N_{mj}^- = \delta_{mj}\nu_j^-; \tag{3.9}$$

$$D_{mj}^- = \frac{\rho_j^-}{\nu_m^- + \nu_j^-}. \tag{3.10}$$

Solving in the same manner the equation for $K_+(x;y)$, we obtain

$$K_+(x;x+0) = \frac{\mathrm{d}}{\mathrm{d}x}\mathrm{Tr}\ln\left[1-\mathrm{e}^{-\mathrm{i}x\mathsf{N}^+}\mathsf{D}^+\mathrm{e}^{-\mathrm{i}x\mathsf{N}^+}\right]. \tag{3.11}$$

where the elements of the $\#(\Omega_+)$ square matrices N^+ and $\mathsf{D}^+(x)$ are

$$N_{mj}^+ = \delta_{mj}\nu_j^+; \tag{3.12}$$

$$D_{mj}^+ = \frac{\rho_j^+}{\nu_m^+ + \nu_j^+}. \tag{3.13}$$

We can substitute now (3.8) and (3.11) into (3.1) to obtain

$$V(x) = -8\mathrm{Tr}\left[\mathsf{N}^{\pm}\frac{1}{1-\mathsf{Q}^{\pm}(x)}\mathsf{N}^{\pm}\frac{\mathsf{Q}^{\pm}(x)}{1-\mathsf{Q}^{\pm}(x)}\right], \tag{3.14}$$

where the $\pm$ signs are for $x>0/x<0$ and

$$\mathsf{Q}^{\pm}(x) = \mathrm{e}^{2\mathrm{i}|x|\mathsf{N}^{\pm}}\mathsf{D}^{\pm}. \tag{3.15}$$

Thus, the potential is given by (3.14) in terms of a trace of the inverse of finite matrices.

IV. VARIABLE-MASS MAPPING: SCHRÖDINGER'S TO BENDANIEL AND DUKE'S EQUATION

In section III we have presented a simple algorithm for solving the inverse scattering problem for the one-dimensional Schrödinger equation in the case of rational SD.

If the conduction electron dynamics is described by the BDD equation, we will not start by posing the inverse scattering problem for that equation from scratch. Instead of that, we will use a family of unitary transformations[19,20,12]. The transformations map the one-dimensional Schrödinger equation, (1.5) with $\boldsymbol{q}_\perp = 0$, and potential $V_S(z)$,

$$\psi''(z) + \left[k^2 - V_S(z)\right]\psi(z) = 0, \tag{4.1}$$

into BenDaniel and Duke equations, (1.6), with $\boldsymbol{q}_\perp = 0$, and potential $V_{BDD}(z)$,

$$\left[\frac{m_\infty}{m(z)}\psi'(z)\right]' + \left[k^2 - V_{BDD}(z)\right]\psi(z) = 0, \tag{4.2}$$

with a variable effective mass $m(z)$ and a potential $V_{BDD}(z)$. The effective mass and the new potential are functionally related to the parameters defining the unitary transformation. Since the mapping is unitary, the SD for the equation (4.2) will be identical with the SD for (4.1). We start thus with a Schrödinger reference equation, (4.1), which is the solution of the inverse scattering problem. From it we obtain a family of BDD equations with the same scattering data. The problem is to choose among these transformations those which map the solution of the inverse problem for the SE onto acceptable BDD equations.

A. Unitary mapping

Let us introduce a (nonlinear) coordinate transformation

$$z = X(x), \tag{4.3}$$

which maps the interval $(-\infty,+\infty)$ into $(-\infty,+\infty)$. Here the function $X(x)$ is a smooth monotonically increasing function: $X'(x)>0$. The monotonicity ensures that a unique inverse transformation exists: $x = Z(z)$, with

$$Z[X(x)] = x \tag{4.4}$$

and $X[Z(z)] = z$. The inverse function $Z(z)$ is also smooth and monotonically increasing, with

$$Z'(z) = 1/X'[Z(z)]. \tag{4.5}$$

Let us associate with the coordinate transformation (4.3) a mapping $\hat{\mathsf{U}}_X$ of the space of square-integrable functions, L^2, which transforms each element of the space $f \in L^2$ into $\hat{\mathsf{U}}_X f$ with

$$(\hat{\mathsf{U}}_X f)(x) = \sqrt{X'(x)} f[X(x)]. \tag{4.6}$$

Making the change of variables (4.3) in the normalization integral

$$\begin{aligned}\langle f|f\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}z |f(z)|^2 = \int_{-\infty}^{+\infty} \mathrm{d}x X'(x) |f[X(x)]|^2 \\ &= \langle \hat{\mathsf{U}}_X f | \hat{\mathsf{U}}_X f\rangle = \langle f | \hat{\mathsf{U}}_X^* \hat{\mathsf{U}}_X | f\rangle, \end{aligned} \tag{4.7}$$

we see that the mapping $\hat{\mathsf{U}}_X$ maps the square integrable functions into square integrable functions conserving the norm, *i.e.* $\hat{\mathsf{U}}_X$ is isometric on L^2. Since the inverse transformation,

$$\left(\hat{\mathsf{U}}_X^{-1} f\right)(z) = \sqrt{Z'(z)} f[Z(z)]. \tag{4.8}$$

exists and is non-singular, the mapping $\hat{\mathsf{U}}_X$ is unitary:

$$\hat{\mathsf{U}}_X^* = \hat{\mathsf{U}}_X^{-1}. \tag{4.9}$$

We want to see the effect of the transformation $\hat{\mathsf{U}}_X$ on functions satisfying the Schrödinger equation (4.1). We will consider only the coordinate transformations for which the function $X(x)$ is twice differentiable with a piecewise continuous third derivative[26], X'''. Substituting (4.6) into (4.1), we obtain after some algebra,

$$\left[\frac{\chi'(x)}{[X'(x)]^2}\right]' + \left[k^2 - W_X(x)\right] \chi(x) = 0. \tag{4.10}$$

Here $\chi(x) = (\hat{\mathsf{U}}_X \psi)(x)$ and

$$W_X(x) = V_S[X(x)] + \frac{X'''(x)}{2[X'(x)]^3} - \frac{5[X''(x)]^2}{4[X'(x)]^4}. \tag{4.11}$$

The equation (4.10) satisfied by the transformed function $\chi(x)$ resembles the BDD equation (4.2) if we set

$$m(x) = m_\infty \left[X'(x)\right]^2 = m_{cond}[c(x)]. \tag{4.12}$$

The function $X(x)$ must satisfy

$$\lim_{x \to \pm\infty} X'(x) = 1. \tag{4.13}$$

This ensures that $m(x)$ tends at infinity to the constant limit m_∞. We will also require that $X'(x) - 1$ decays at infinity faster than $|x|^{-2-\delta}$ for some $\delta > 0$. In this case, the limits of $X(x) - x$ at $\pm\infty$ are finite. This ensures that the Jost solutions of the original Schrödinger equation are mapped into Jost-type solutions of the transformed one.

Let $f_\pm(x; k)$ be the Jost solutions of (4.1), which obey the boundary conditions (A3):

$$\lim_{x \to \pm\infty} \mathrm{e}^{\mp \mathrm{i} kx} f_\pm(x; k) = 1. \tag{4.14}$$

Then, applying to them the mapping (4.6), we obtain near the corresponding infinities

$$\lim_{x \to \pm\infty} \mathrm{e}^{\mp \mathrm{i} kx} (\hat{\mathsf{U}}_X f_\pm)(x; k) = \mathrm{e}^{\mathrm{i} k d_\pm}. \tag{4.15}$$

Here,

$$d_+ = \int_0^{+\infty} \mathrm{d}\xi \left[X'(\xi) - 1\right]; \quad d_- = \int_{-\infty}^0 \mathrm{d}\xi \left[X'(\xi) - 1\right]; \tag{4.16}$$

where we assumed $X(0) = 0$. Let $f_\pm^{(X)}(x; k)$ be the Jost-type solutions of the transformed equation (4.10), defined by the same boundary conditions (4.14). Taking into account the asymptotic behaviors of the Jost functions of the Schrödinger equation (4.1), we find the relation between the scattering data for the transformed equation and those of the original one:

$$T^{(X)}(k) = \mathrm{e}^{\mathrm{i} k (d_+ - d_-)} T(k), \tag{4.17}$$

$$R_\pm^{(X)}(k) = \mathrm{e}^{\pm 2 \mathrm{i} k d_\pm} R_\pm(k). \tag{4.18}$$

Thus, the reflectances of the original and the transformed equations are equal.

In the following subsection we will study the variable effective mass mapping nonlinear differential equation in the general case of an arbitrary dependence of the band offset on the concentration. We will show that the physically realizable concentration profiles for devices embedded in a material of homogeneous composition can be obtained by solving a (nonlinear) boundary value problem. A necessary condition for the existence of achievable solutions is that the dependence of the conduction band offset $\mathcal{E}_c$ on the effective mass be a *non-decreasing* one. If this condition is not satisfied, it may be still possible to embed the device in a *periodic* super lattice, a case which will not be discussed in this paper. In section IV D we consider in more detail the case when $\mathcal{E}_c(m)$ is a linear function, an approximation which seems quite reasonable in the *AlGaAs* system. In this case, the solution of the nonlinear boundary value problem can be then expressed through the canonical solutions of the Cauchy (initial value) problem for a third-order linear differential equation. We also discuss methods for obtaining stable approximate solutions.

B. Differential equation

Let us now compare the potentials W_X, (4.11), and V_{BDD}. The latter is given by (1.2) and (1.7):

$$V_{BDD}(x) = \frac{2m_\infty}{\hbar^2} \left[\mathcal{E}(x) - \mathcal{E}(\infty) + \Phi_{sc}(x)\right]. \tag{4.19}$$

Here, the band offset is

$$\mathcal{E}(x) = \mathcal{E}_{cond}[c(x)], \tag{4.20}$$

and we set $U_{ext}(x) = 0$. The zero of the energy scale is chosen at the value of the band offset for the embedding (asymptotic) composition.

The band offset, $\mathcal{E}(x)$ and the effective mass, $m(x)$ depend on the position only through their dependence on the local chemical composition $c(x)$, (4.12) and (4.20). We will consider only the case when the function $m(c)$ is invertible. Then, we can substitute the inverse function $c(m)$ into $\mathcal{E}_{cond}(c)$:

$$\mathcal{E}_{cond}(c) = \mathcal{E}_c(m). \tag{4.21}$$

In this section we consider only unbiased structures with negligible electron density. Then, in the square brackets in (4.19), $\Phi_{sc}(x)$ is equal to zero. Equating the two potentials (4.11) and (4.19) an using (4.12), we obtain a third-order nonlinear differential equation for $X(x)$:

$$\begin{aligned}\frac{X'''(x)}{2[X'(x)]^3} - \frac{5[X''(x)]^2}{4[X'(x)]^4} + V_S[X(x)] = \qquad\qquad \\ = \frac{2m_\infty}{\hbar^2}\left\{\mathcal{E}_c[m_\infty X'^2(x)] - \mathcal{E}_c(m_\infty)\right\}.\end{aligned} \tag{4.22}$$

The values of $X'(x)$ are restricted to the physically achievable interval

$$\sqrt{\frac{\underline{m}}{m_\infty}} \le \dot{X} \le \sqrt{\frac{\overline{m}}{m_\infty}}. \tag{4.23}$$

Here $\underline{m}$ and $\overline{m}$ are the minimal and, respectively, the maximal values of the effective mass, $m(c)$, in the physically achievable chemical composition range.

The equation (4.22) does not depend explicitly on x. Setting

$$X' = S\left[X(x)\right], \tag{4.24}$$

substituting this into (4.22) and replacing the derivatives with respect to x according to

$$\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}X}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}X} = S\frac{\mathrm{d}}{\mathrm{d}X}, \tag{4.25}$$

we obtain a second-order equation for S,

$$2\frac{S''}{S} - 3\frac{(S')^2}{S^2} = \frac{8m_\infty}{\hbar^2}\left[\mathcal{E}_c(m_\infty S^2) - \mathcal{E}_c(m_\infty) - U(X)\right]. \tag{4.26}$$

Here S' is the derivative of S with respect to X, $U(X) = \hbar^2 V_S(X)/2m_\infty$ is the potential in energy units. The asymptotic condition (4.13) reads now $S(\pm\infty) = 1$.

C. Boundary value problem

Let us consider potentials $V(X)$ which are identically equal to zero outside some interval $[X_-, X_+]$. For X outside this interval, the equation (4.26) does not depend explicitly on X so that its order may be further reduced. Setting

$$m(X) = m_\infty S^2 \tag{4.27}$$

and

$$S'(X) = Q(m(X)), \tag{4.28}$$

the equation (4.26) becomes

$$2\frac{\mathrm{d}Q^2}{\mathrm{d}m} - 3\frac{Q^2}{m} = \frac{10}{\hbar^2}\Big[\mathcal{E}_c(m) - \mathcal{E}_c(m_\infty)\Big]. \tag{4.29}$$

The solution of (4.29) is

$$Q^2(m) = \frac{4m^{\frac{3}{2}}}{\hbar^2}\int_{m_\infty}^{m}\left[\mathcal{E}_c(\mu) - \mathcal{E}_c(m_\infty)\right]\mu^{-\frac{3}{2}}\mathrm{d}\mu. \tag{4.30}$$

If m is close to m_∞, the right hand side of (4.30) goes to zero as $(m - m_\infty)^2$. Indeed, for small $|\mu - m_\infty|$, the term in square brackets in (4.30) is approximately equal to $\mathcal{E}_c'(m_\infty)\,(\mu - m_\infty)$ and

$$Q^2(m) \approx \frac{2\mathcal{E}_c'(m_\infty)}{\hbar^2}\,(m - m_\infty)^2 + \mathcal{O}\left[(m - m_\infty)^3\right]. \tag{4.31}$$

Since Q^2 is non-negative, inspection of (4.31) shows that the effective mass may tend to a constant limit at infinity *if and only if* the band offset dependence on the effective mass, $\mathcal{E}_c(m)$, is a *non-decreasing function*.

$$\frac{\mathrm{d}\mathcal{E}_c(m)}{\mathrm{d}m} \ge 0 \tag{4.32}$$

In plain words, if the effective mass does not follow the band offset, then the potential $V(X)$ cannot be embedded in an alloy of homogeneous composition. Noting that in this case the device may be embedded in a periodic superlattice, we will restrict ourselves here to the case (4.32).

Let us note that equation (4.26) may be solved in quadratures on the intervals $(-\infty, X_-)$ and $(X_+, +\infty)$. Indeed, substituting (4.30) into (4.28) and taking into account (4.27) we get

$$\frac{\mathrm{d}S}{\mathrm{d}X} = \pm\mathrm{sign}(1 - S)Q(m_\infty S^2), \tag{4.33}$$

where $Q(m)$ is the non-negative square root of the right hand side of (4.30) and the sign is positive on $(X_+, +\infty)$ and negative on $(-\infty, X_-)$.

The solution on $(X_+, +\infty)$ is given in parametric form by

$$X = X_+ + \mathrm{sign}\left[1 - S(X_+)\right]\int_{S_+(X_+)}^{s}\frac{\mathrm{d}\sigma}{Q(m_\infty\sigma^2)}, \tag{4.34}$$

$$x = x_+ + \mathrm{sign}\left[1 - S(X_+)\right]\int_{S_+(X_+)}^{s}\frac{\mathrm{d}\sigma}{\sigma Q(m_\infty\sigma^2)}, \tag{4.35}$$

where x_+ is the value of x which maps to X_+: $X_+ = X(x_+)$. A similar representation is valid for the interval $(-\infty, X_-)$.

Thus, we have obtained the solutions which are regular at infinity. There, $S(X) = 1 + \mathcal{O}\left[\mathrm{e}^{-\kappa|X|}\right]$ tends exponentially to the constant limit 1. The asymptotic rate of decay κ may be obtained from (4.31):

$$\kappa = \frac{2m_\infty}{\hbar}\sqrt{2\mathcal{E}_c'(m_\infty)}. \tag{4.36}$$

Let us now briefly discuss the asymptotic behavior at infinity for the regular solutions of (4.26) for potentials $V(X)$ which go to zero at infinity. One may readily see from (4.26) that $S(X)$ must still converge to 1 at infinity. As long as the potential $V(X)$ decays at infinity faster than $\mathrm{e}^{-\kappa|X|}$ the properties of the solutions discussed above remain asymptotically valid. For potentials with slower falloff at infinity, the regular solution tends asymptotically to the regular solution of the equation $S'' = 8m_\infty\mathcal{E}_c'(m_\infty)S/\hbar^2 + V(X)/2$.

It is important to note that any regular solution of (4.26) satisfies at all points $X_\pm$ outside the support of the potential the boundary conditions (4.33). To construct a solution of (4.26) which is regular on the whole axis X, we will chose a value for the embedding alloy effective mass, m_∞. The regular solutions on the interval $(-\infty, X_-)$ can be parameterized by the value $S(X_-) = \tau$. The value of the derivative at X_- is given by (4.33) with the minus sign:

$$S'(X_-;\tau) = -\mathrm{sign}\,[1-\tau]\,Q(m_\infty\tau^2), \tag{4.37}$$

where $Q(m)$ is the positive square root of the right-hand side of (4.30).

Then, we integrate the equation (4.26) numerically with the initial values defined above over the support of the potential up to X_+, obtaining $S(X_+;\tau)$ and $S'(X_+;\tau)$. If the solution is regular then it must satisfy (4.33) with the plus sign at X_+:

$$S'(X_+;\tau) = \mathrm{sign}\,[1-\tau]\,Q\left[m_\infty S^2(X_+;\tau)\right]. \tag{4.38}$$

If they exist, the solutions of equation (4.38) give the values of τ for which we can find regular solution of the differential equation (4.26) on the whole real axis. To be achievable these solutions must also satisfy the physical bounds (4.23).

Numerically, the shooting method outlined here is rather ill-conditioned. Since the general solution of (4.26) is singular, multiple-precision arithmetic has to be used for the integration of the differential equation if the support of the potential is not short enough. In the following section we will examine in more detail the important case when the dependence of the band offset on the effective mass is linear. We will show that in this case the solutions of the nonlinear equation (4.26) can be found among the solutions of a third-order *linear* equation.

D. Solution of the boundary value problem in the case of linear dependence of the band offset on the effective mass

For some alloys like $Al_cGa_{1-c}As$ in the concentration range $0 \leq c \leq .45$ the conduction band minimum is at the center of the Brillouin zone (Γ) and the dependence of $m_{cond}(c)$ and $\mathcal{E}_{cond}(c)$ on the concentration c approximately linear. In the $Al_cGa_{1-c}As$ system, for $0 \leq c \leq .45$, the offset from the position at $GaAs$ is

$$\mathcal{E}_c(m) = B(m - \underline{m}). \tag{4.39}$$

The constant B is

$$B = \frac{\Delta E}{\overline{m} - \underline{m}} = 9.41eV/m_0, \tag{4.40}$$

Here $\underline{m} = .067m_0$ is the conduction band effective mass for $GaAs$; $\overline{m} = .104m_0$ and ΔE are, respectively, the mass and band offset for $Al_{.45}Ga_{.55}As$. m_0 is the electron mass.

Substituting this into (4.26) we obtain

$$2S''S - 3(S')^2 = \kappa_\infty^2 S^2\left[S^2 - 1 - v(X)\right]. \tag{4.41}$$

Here,

$$\kappa_\infty^2 = 8Bm_\infty^2/\hbar^2, \tag{4.42}$$

$$v(X) = 4V(X)/\kappa_\infty^2 = U(X)/(Bm_\infty), \tag{4.43}$$

and $U(X) = \hbar^2 V(X)/2m_\infty$ is the potential measured in energy units.

Let us define a new unknown function

$$T(X) = 3 - 3/S(X). \tag{4.44}$$

Substituting (4.44) into (4.41) we obtain the equation satisfied by $T(X)$:

$$2TT'' - T'^2 + \kappa_\infty^2\left\{1 - [1+v]T^2\right\} = 0. \tag{4.45}$$

Here and whenever it does not lead to ambiguities we will omit the arguments of the functions. Taking the derivative of (4.45) we obtain a third-order linear equation for T:

$$T''' - \kappa_\infty^2(1+v)T' - \frac{1}{2}\kappa_\infty^2 v'T = 0. \tag{4.46}$$

An arbitrary solution of (4.46) will satisfy the second-order nonlinear equation (4.45) with the zero in the right hand side replaced by some constant $\mathcal{K}$:

$$2TT'' - T'^2 - \kappa_\infty^2[1+v]T^2 = \mathcal{K}. \tag{4.47}$$

If $\mathcal{K} = -\kappa_\infty^2$, the solution satisfies also (4.45).

Let $F_{\alpha\beta\gamma}(X;X_-)$ be the solution of the initial value (Cauchy) problem for the linear equation (4.46) satisfying the initial conditions

$$\begin{aligned} F_{\alpha\beta\gamma}(X_-;X_-) &= \alpha, \\ F'_{\alpha\beta\gamma}(X_-;X_-) &= \beta, \\ F''_{\alpha\beta\gamma}(X_-;X_-) &= \gamma, \end{aligned} \tag{4.48}$$

at the point X_-, which is a point of continuity of the potential $v(X)$. Since (4.46) is linear,

$$F_{\alpha\beta\gamma} = \alpha F_{100} + \beta F_{010} + \gamma F_{001}. \tag{4.49}$$

The function $F_{\alpha\beta\gamma}(X;X_-)$ also satisfies the second-order equation (4.47) with

$$\mathcal{K}_{\alpha\beta\gamma} = 2\alpha\gamma - \beta^2 - \kappa_\infty^2 \alpha^2 \left[1 + v(X_-)\right], \tag{4.50}$$

in the right hand side.

In IV C we outlined the shooting method for solving the boundary value problem which leads to the regular (acceptable) solutions of (4.26). It is well known that shooting methods are prone to numerical instabilities even for linear boundary value problems. Another unpleasant feature is the fact that we have to integrate the equation numerically over the support of the potential for each value of τ.

Let us state the boundary value problem for the function $T(X)$, assuming the potential $v(X)$ to be identically zero outside the interval (X_-, X_+). The solutions regular on $(-\infty, X_-)$ and $(X_+, +\infty)$ are

$$T_-(X) = 1 + \left[T(X_-) - 1\right] \mathrm{e}^{\kappa_\infty (X - X_-)}, \tag{4.51}$$
$$T_+(X) = 1 + \left[T(X_+) - 1\right] \mathrm{e}^{-\kappa_\infty (X - X_+)}. \tag{4.52}$$

Thus, the boundary conditions at $X_\pm$ which must be satisfied by the regular solution are

$$T'(X_-) = \kappa_\infty \left[T(X_-) - 1\right], \tag{4.53}$$
$$T'(X_+) = -\kappa_\infty \left[T(X_+) - 1\right]. \tag{4.54}$$

Thus, we can parameterize the regular solutions (4.51) by the value of $T(X_-) = \alpha$. Then, $T'(X_-)$ is given by (4.53). Then we integrate (4.45) up to X_+, where T and its derivative must satisfy (4.54), whence the acceptable values of α are determined.

Now, we can use the linear equation satisfied by T to express the solution of the initial value problem through the canonical solutions F_{100}, F_{010} and F_{001} of the initial value problem for (4.46). Using (4.45) with $v(X_-) = 0$ to find $T''(X_-)$, we find the solution satisfying (4.53)

$$\begin{aligned} T_\alpha(X) = {} & \alpha F_{100}(X;X_-) + \kappa_\infty(\alpha - 1) F_{010}(X;X_-) \\ & + \kappa_\infty^2 (\alpha - 1) F_{001}(X;X_-). \end{aligned} \tag{4.55}$$

At X_+, $T_\alpha(X)$ must satisfy the boundary condition (4.54). Whence we find α:

$$\alpha = 1 - \frac{F'_{100}(X_+;X_-) + \kappa_\infty \left[F_{100}(X_+;X_-) - 1\right]}{F'_{1\kappa_\infty\kappa_\infty^2}(X_+;X_-) + \kappa_\infty F_{1\kappa_\infty\kappa_\infty^2}(X_+;X_-)}, \tag{4.56}$$

where $F_{\alpha\beta\gamma}$ was defined in (4.48). Thus, the solution of the boundary value problem for the nonlinear equation (4.45) is expressed through the canonical solutions of the initial value problem at X_- for the linear equation (4.46).

The value of X_- can be chosen arbitrarily as long as the potential $v(X_-) = 0$. We may safely assume that $v(X) = 0$ in a neighborhood of X_-. The functions F_{100} and $F_{1\kappa_\infty\kappa_\infty^2}$ are also solutions of the second-order nonlinear equation (4.47) with $\mathcal{K}$ determined from (4.50). We have found the value of α, which determines the solution of the boundary value problem, through the solutions of two second order (albeit nonlinear) equations. Although the integration must be performed only once from X_- to X_+, it is still numerically unstable.

E. Approximate solutions

As mentioned above the numerical integration of the differential equation over typical device lengths 20-40nm, having the order of magnitude of the electron mean free path, is rather ill conditioned. Taking the values of the parameters for the *AlGaAs* system, above (4.40), and a value $m_\infty \approx .1 m_\infty$ for the effective mass of the embedding material, we obtain that the natural length scale for the differential equation (4.41) is $1/\kappa_\infty \approx .3nm$, which is comparable to the lattice period.

The equation (4.41) can be rewritten as

$$S^2 - 1 - v(X) = \frac{2S''S - 3(S')^2}{\kappa_\infty^2 S^2}. \tag{4.57}$$

Since the right-hand side of (4.57) has the small factor κ_∞^{-2}, one is tempted to proceed in a a *naïve* "quasi-classical" way and neglect the right-hand side entirely. Then,

$$S(X) \approx \sqrt{1 + v(X)}, \tag{4.58}$$

and finding the coordinate transformation $X(x)$ reduces to a simple quadrature. This gives surprisingly reasonable results.

Finding corrections to (4.58) seems a rather tedious task, especially for potentials which have discontinuities. We will note instead that from (4.43),

$$v(X) = \frac{U(X)}{Bm_\infty} \approx \frac{U(X)}{.94eV}, \tag{4.59}$$

for the *AlGaAs* system. Since typical potential values are $\pm$100-200meV, the potential $v(X)$ (measured in the natural units of the problem) is small compared to 1. A "small potential" perturbative approach to solving the boundary value problem is thus indicated.

Let us assume that $v \sim \alpha$ and seek S as a series

$$S(X) = S_{(0)}(X) + \alpha S_{(1)}(X) + \alpha^2 S_{(2)}(X) + \ldots, \tag{4.60}$$

substitute $v \to \alpha v$ and (4.41), rewritten as

$$S'' = 3S'^{\,2}/2S \,+\, \kappa_\infty^2 S\left[S^2 - 1 - v\right]/2\,, \qquad (4.61)$$

and expand into a power series in α. Then, after equating the terms with the same power of α and setting $\alpha = 1$, we obtain a hierarchy of linear differential equations for the functions $S_{(\ell)}(X)$, $\ell = 0, 1, \ldots$.

The first equation from (4.60) is $S''_{(0)}(X) = 0$. The solution must go to 1 when X goes to infinity so that $S_{(0)}(X) \to 1$, while all the other $S_{(\ell)}(X) \to 0$ as $X \to \pm\infty$. Then,

$$S_{(0)}(X) = 1. \qquad (4.62)$$

For $\ell \geq 1$, the hierarchy has the form

$$S''_{(1)} \,-\, \kappa_\infty^2 S_{(1)} = -\frac{1}{2}\kappa_\infty^2 v; \qquad (4.63)$$

$$S''_{(2)} \,-\, \kappa_\infty^2 S_{(2)} = \frac{3}{2}S'^{\,2}_{(1)} + \frac{1}{2}\kappa_\infty^2 S_{(1)}\left[3S_{(1)} - v\right]; \qquad (4.64)$$

$$\ldots$$

$$S''_{(\ell)} \,-\, \kappa_\infty^2 S_{(\ell)} = \mathcal{F}_\ell\left(X; S_{(1)}, \ldots, S_{(\ell-1)}, v\right); \qquad (4.65)$$

$$\ldots$$

Taking into account the boundary conditions for $X \to \pm\infty$, the solution of the ℓ-th equation in the hierarchy is

$$S_{(\ell)}(X) = -\frac{1}{2\kappa_\infty}\int_{-\infty}^{\infty} \mathrm{d}\xi \mathrm{e}^{-\kappa_\infty|X-\xi|} \mathcal{F}_\ell\left(\xi; S_{(1)}, \ldots, S_{(\ell-1)}, v\right), \qquad (4.66)$$

which can be verified by direct substitution.

The large κ_∞ limit of the first terms in the perturbative expansion (4.60) is

$$S_{(0)}(X) + S_{(1)}(X) \,=\, 1 + \frac{\kappa_\infty}{2}\int_{-\infty}^{\infty} \mathrm{d}\xi \mathrm{e}^{-\kappa_\infty|X-\xi|} v(\xi) \to 1 + \frac{1}{2}v(X), \qquad (4.67)$$

which coincides with the first terms in the perturbative expansion of the "quasi-classical solution" (4.58). Several terms we checked also have this property.

Having found $S(X)$, we can now find the coordinate transformation by a simple quadrature:

$$x = \int_0^X \frac{\mathrm{d}Y}{S(Y)}. \qquad (4.68)$$

In fact, this yields the inverse transformation, (4.5). Finally, the mass profile in the BDD equation is given in parametric form by (4.68) and

$$m(X) = m_\infty S(X). \qquad (4.69)$$

The concentration profile can now be readily recovered.

F. Example

We will illustrate the method by finding the specifications for a filter with two narrow transmission resonances, centered at $E_1 < E_2$, with the high-energy resonance significantly narrower than the low-energy one[12]. Apparently, this is difficult to achieve by the direct method[27].

We will start by constructing the Padé approximant for the reflectance. We will chose $q = 1$ in (2.19). This ensures that the potential in the Schrödinger equation (4.1) will be continuous. We will try to keep p, the degree of the denominator in (2.19), ass small as possible. Choosing the reflectance to be equal to zero at the energies E_1 and E_2, we find that we need at least $p = 4$. This means two double real zeros at E_1 and E_2. Thus, the denominator is

$$\mathcal{P}_4(E) = \mathcal{A}_2(E)\mathcal{B}_2(E) = (1 - E/E_1)^2(1 - E/E_2)^2. \qquad (4.70)$$

There is some freedom in choosing the numerator, $\mathcal{Q}_7(E)$. Baring other constraints, it is convenient to note that $\mathcal{Q}_7(E)$ has to have a pair of complex conjugate zeros in close vicinity to each of transmittance maxima E_1 and E_2. We will choose

$$\mathcal{Q}_7(E) = [\mathcal{A}_2(E) + E/F_1][\mathcal{B}_2(E) + E/F_2]\mathcal{Q}_3(E). \qquad (4.71)$$

Here F_1 (F_2) must be much larger than E_1 (E_2), to ensure that the zeros of the factors in the square brackets are close to the corresponding zeros of the denumerator. Indeed, in these conditions, the two poles near E_1 are given by

$$E \approx E_1\left(1 \pm \mathrm{i}\sqrt{E_1/F_1}\right), \qquad (4.72)$$

and a similar expression for the poles near E_2. It remains to determine the positive polynomial $\mathcal{Q}_3(E)$ in (4.71).

Since we want sharp transmittance maxima near E_1 and E_2, we want that the background reflectance,

$$\mathcal{R}_b(E) = 1/Q_3(E), \qquad (4.73)$$

will be close to 1 and relatively slowly varying in the range of energies $0, \overline{E}$, with $\overline{E} > E_2$. This can be achieved by choosing

$$\mathcal{Q}_3(E) = 1 + \frac{\delta}{2}\left[1 + \left(\frac{2E}{\overline{E}} - 1\right)^3\right]. \qquad (4.74)$$

Then, if $\delta \ll 1$, the background reflectance is monotonically decreasing with $\mathcal{R}_b(0) = 1$ and $\mathcal{R}_b(\overline{E}) \approx 1 - \delta$. It has a horizontal inflection point at $E = \overline{E}/2$ with $\mathcal{R}_b(\overline{E}) \approx 1 - \delta/2$.

Neglecting δ with respect to 1, the full widths at half maximum (FWHM) of the transmittance maxima are, respectively, $2\sqrt{E_1^3/F_1}$ and $2\sqrt{E_2^3/F_2}$. Thus, F_1 and F_2 can be obtained from the FWHM of the corresponding resonance.

We chose $E_1 = 40meV$ and $E_2 = 100meV$, with FWHMs equal to $9meV$ and, respectively, $3meV$ as initial data. Proceeding as explained in sections II, III, IV D we obtained an effective-mass profile which yielded the same reflectance as the input one. This continuous profile was digitized manually into 12 steps with lenghths which are integer numbers of lattice constants and heighths which are a combination of three concentrations, as described in Table 1. The Al concentration of the embedding alloy is 11.4%. In Fig. 1 we present the transmittance calculated for the resulting configuration. The digitization has introduced a few artefacts (the shoulder of the low energy line and a low amplitude broad maxima, one of which is visible in Fig. 1). The maxima were broadened and shifted a little from the design data. Nevertheless, the ratio of FWHM of the high/low energy maxima of transmittance is better than 2:1.

V. DETERMINATION OF CHEMICAL COMPOSITION AND DOPANT CONCENTRATION PROFILES OF HETEROSTRUCTURES WITH PRESET REFLECTANCE

In the section III we have shown how, given rational expressions for the scattering data (SD), one can construct the piecewise continuous potential $V(x)$, decaying exponentially at $+\infty$. The one-dimensional Schrödinger with $V(x)$ has the given SD. In section IV we mapped unitarily the one-dimensional Schrödinger equation onto a family of BenDaniel and Duke type equations depending on the function $X(x)$ which defines the transformation. We also discussed in some detail the solution of the nonlinear differential equation, which determines the effective mass profile in the case of an undoped heterostructure, with vanishing density of conduction electrons.

Now, we want to deal with the case when a nonzero density of conduction electrons is present and the potentials, (1.2) in the SE, (1.1), or in the BDD equation, (1.3), are self-consistent. Let the external potential $U_{ext}(z) = 0$ so that the potential in the BDD equation is

$$U(z) = \mathcal{E}_{cond}[c(z)] + \Phi_{sc}(z; m; U), \tag{5.1}$$

where we evidenced the functional dependence of $\Phi_{sc}(z; m; U)$ on the effective mass profile $m(z)$ and the full potential energy $U(z)$. In the SE case the effective mass is constant and Φ_{sc} depends only on $U(z)$. Inspection of (5.1) suggests the idea that for a given full potential $U(z)$, we can determine the chemical composition profile by moving the selfconsistent potential to the left hand side of (5.1). We will see that in the SE case this is relatively easy to do at a given operating temperature T_o. The situation is trickier in the case of BDD dynamics, where we will present a perturbative approach to solving the functional equation which replaces the nonlinear differential equation (4.22).

Let us start by considering the Hartree approximation for the self-consistent electrostatic potential. Then, $\Phi_{sc}(z; m; U)$ is the solution of Poisson's equation

$$[\varepsilon(z)\Phi'_{sc}(z)]' = 4\pi e \rho_{ch}(z). \tag{5.2}$$

Here $-e$ is the electron charge, $\varepsilon(z)$ is the dielectric constant, $\varepsilon(z) = \varepsilon[c(z)]$, and $\rho_{ch}(z)$ is the full charge density, the difference between the ionized donor charge density and the electron one.

$$\rho_{ch}(z) = e\left[n_d(z) - n_{el}(z)\right]. \tag{5.3}$$

The density of donor dopant ions is made of a uniform background density n_b and the local variation of the density of donors in the heterostructure $n_\ell(z)$, which goes to zero for large $|z|$:

$$n_d(z) = n_b + n_\ell(z). \tag{5.4}$$

We assume that the doping and temperature are such that all the donors are ionized and that the density of holes is negligible compared to the density of donors. Then, we can neglect the valence bands. Otherwise, a multi-band treatment is needed.

The electron dynamics is described either by the SE, (1.1), or by the BDD equation, (1.3). The equilibrium electron density, $n_{el}(z)$, can be calculated from the density of states for the corresponding equation, (1.1) or (1.3),

$$n_{el}(z) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}E\ \nu(z, E)}{1 + \mathrm{e}^{\beta(E-\mu)}}, \tag{5.5}$$

where β is the inverse temperature (in energy units) and μ is the chemical potential of the electrons.

A necessary condition for the stability of the system is that the full charge is equal to zero,

$$\int_{-\infty}^{+\infty} \mathrm{d}z \rho_{ch}(z) = 0. \tag{5.6}$$

In particular, the limiting value of electron density at infinity equals the background ion density, $n_{el}(\pm\infty) = n_b$. The limiting values of the potential at $\pm\infty$ will be equal only if dipolar moment of the charge density is zero,

$$\int_{-\infty}^{+\infty} \mathrm{d}z\, z\, \rho_{ch}(z) = 0. \tag{5.7}$$

Thus, $z^2\rho_{ch}(z)$ must go to zero at infinity and the solution of (5.2) is

$$\Phi_{sc}(z; m; U) = 2\pi e \int_{-\infty}^{+\infty} \mathrm{d}u \rho_{ch}(u) \left| \int_u^x \frac{\mathrm{d}v}{\varepsilon(v)} \right|. \tag{5.8}$$

For position-independent ε, which we will consider in the case of SE dynamics, (5.8) becomes the well-known

$$\Phi_{sc}(z; U) = \frac{2\pi e}{\varepsilon} \int_{-\infty}^{+\infty} \mathrm{d}u |z - u| \rho_{ch}(u). \tag{5.9}$$

We will consider separately the cases when the electron dynamics is described by the Schrödinger equation, (1.1), and by the BenDaniel and Duke equation, (1.3).

A. Schrödinger's equation

To compute $\Phi_{sc}(z;U)$ using (5.9), we need the electron density of states in (5.5). Since the transverse degrees of freedom separate, (1.4-1.5), we can integrate over the transverse quasimomenta and express the three dimensional density of states $\nu_S(z,E)$ through the density of states $\nu_0(z,E)$ of the one-dimensional SE (4.1):

$$\nu_S(z,E) = \frac{m_e}{\pi\hbar^2}\int_0^\infty \mathrm{d}\eta\nu_0(z,E-\eta). \qquad (5.10)$$

The one dimensional density of states $\nu_0(z,E)$ is proportional to the imaginary part of the Green function $G_0(z,z';E)$ of the one-dimensional SE (4.1)

$$\nu_0(z,E) = -\frac{1}{\pi}\lim_{\delta\downarrow 0}\mathrm{Im}\left[G_0(z,z;E+i\delta\right]. \qquad (5.11)$$

This allows a standardized treatment of the bound and continuum states.

For all E with $\mathrm{Im}(E)\neq 0$, the Green function is the solution of the equation

$$\left[E+\frac{\hbar^2}{2m_e}\frac{\mathrm{d}^2}{\mathrm{d}z^2}-U(z)\right]G_0(z,z';E) = \delta(z-z'), \qquad (5.12)$$

which is continuous at $z = z'$ and goes to zero for $z\to\pm\infty$. In terms of the Jost functions, defined in Appendix A 1, the solution is

$$\begin{aligned} G_0(z,z';E) &= \frac{m_e T(k)}{\mathrm{i}k\hbar^2} f_+(z;k)f_-(z';k); \quad z>z', \\ &= G(z',z;E); \quad z<z'. \end{aligned} \qquad (5.13)$$

Here $k=\sqrt{2m_eE}/\hbar$ and $T(k)$ is the transmission coefficient.

Substituting (5.10) and (5.11) into (5.5) we obtain the electron density

$$n_{el}(z) = \frac{m_e}{\pi\beta\hbar^2}\int_{-\infty}^\infty \mathrm{d}E\ln\left[1+\mathrm{e}^{\beta(\mu-E)}\right]\nu_0(z,E). \qquad (5.14)$$

Now, let us fix the *operating temperature* $T_o = 1/\beta_o$. The local dopant concentration profile, $n_\ell(z)$, will be chosen such that the conditions (5.6) and (5.7) hold at T_o. This can be done in many ways. For each $n_\ell(z)$, (5.1) yields a band offset profile

$$\mathcal{E}_{cond}[c(z)] = U(z) - \Phi_{sc}(z;U). \qquad (5.15)$$

If the values of the local doping profile $n_\ell(z)$ and the concentration profile, $c(z)$, which can be determined from (5.15) are physically achievable, a heterostructure with these specifications can be manufactured. Assuming Schrödinger dynamics for the conduction electrons, the selfconsistent potential at the operating temperature T_o will be $U(z)$. At T_o, the SD and the bound states of the electrons in the heterostructure will be those determined by $U(z)$.

Since the selfconsistent potential varies slowly with the temperature, at temperatures which not too far from T_o, the selfconsistent potential of the structure, which can be computed by standard means, will be close to $U(z)$. An important result of scattering theory, see *e.g.*[10], is that the SD and the bound states of the SE are continuous functionals of the potential. Thus, the SD and bound states in an interval of temperatures near T_o will be close to those at T_o.

Now, a big advantage of the inverse method becomes apparent. In the direct approach we give the composition profile $c(z)$ and the dopant profile $n_\ell(z)$, and have to compute the selfconsistent potential. This is a rather time-consumming iterative process, which has to be repeated after each modification of the chemical and dopant profiles. Only after this are we able to obtain the scattering data and check if they are desirable. In the inverse approach, we start from desirable SD and can obtain a whole class of specifications, parameterized by the local dopant profile n_ℓ, which yield the desired properties exactly at T_o and approximately in some neighborhood of T_o.

B. BenDaniel and Duke's equation

In section IV we have shown that to each monotonically increasing on $(-\infty,\infty)$ function $X(x)$, one can associate a unitary operator, $\hat{\mathsf{U}}_X$, which maps the SE onto a BDD type equation. There we considered only undoped heterostructures without occupied conduction electron states. Given the material relation between the band offset and the effective mass, we have shown how to solve the nonlinear differential equation which determines the transformation $X(x)$ and obtain the band offset (and effective mass) profile which has the same SD as the initial SE.

As in section IV B, we assume that the effective mass' dependence on the local chemical composition is invertible. Then, material relations exist in terms of the effective mass for the band offset, (4.39), and the *dielectric constant*,

$$\varepsilon(z) = \epsilon[m(z)]. \qquad (5.16)$$

The electrostatic part of the selfconsistent potential, $\Phi_{sc}(z;m;U)$, is given by (5.8) in terms of $\epsilon[m(z)]$ and the full charge density $\rho_{ch}(z;m;U)$. We can now repeat the calculation of the electron density of states like in section V A. The transverse degrees of freedom separate again and, after performing the angular integral over the transverse quasi-momenta

The electron density is given again by (5.5) where the density of states is the integral over the transverse momenta of the one dimensional density of states. S etting $q_\perp^2 = 2m_\infty\eta/\hbar^2$ and performing the angular integral over the transverse quasi-momenta we obtain

$$\nu(z,E)=\frac{m_\infty}{\pi\hbar^2}\int_0^\infty \mathrm{d}\eta\nu_\eta(z,E-\eta), \tag{5.17}$$

where $\nu_\eta(z,E)$ is the density of states of the one-dimensional BDD equation (4.2) with the potential V_{BDD} replaced by $V_\eta(z)=2m_\infty U_\eta(z)/\hbar^2$ where

$$U_\eta(z)=U_{BDD}(z)+\eta\left[1-\frac{m_\infty}{m(z)}\right] \tag{5.18}$$

The density of states for the one dimensional BDD equation can again be expressed in terms of its Green function,

$$\nu_\eta(z,E)=-\frac{1}{\pi}\lim_{\delta\downarrow 0}\mathrm{Im}\left[G_\eta(z,z;E+\mathrm{i}\delta)\right]. \tag{5.19}$$

For all E with $\mathrm{Im}(E)\neq 0$, the Green function $G_\eta(z,z';E)$ is the solution of the equation

$$\left[E+\frac{\mathrm{d}}{\mathrm{d}z}\frac{\hbar^2}{2m(z)}\frac{\mathrm{d}}{\mathrm{d}z}-U_\eta(z)\right]G_\eta(z,z';E)=\delta(z-z'), \tag{5.20}$$

which is continuous for $z=z'$ and goes to zero for $z\to\pm\infty$. Like in the case of the SE, the one dimensional BDD Green function can be expressed in terms of the Jost solutions, $f_\pm(z';k;\eta)$ of the BDD equation (4.2) with potential (5.18) which satisfy the boundary conditions (A3). Here, $k=\sqrt{2m_\infty E}/\hbar$. We will write here only the contact value needed in (5.19)

$$G_\eta(z,z;E)=\frac{m_\infty T(k)}{\mathrm{i}\hbar^2 k}f_+(z;k;\eta)f_-(z;k;\eta). \tag{5.21}$$

Substituting (5.17) into (5.5) and making the change of variable $E\to E+\eta$ in the double integral, we obtain

$$n_{el}(z)=\frac{m_\infty}{\pi\hbar^2}\int_{-\infty}^{+\infty}\mathrm{d}E\int_0^\infty \mathrm{d}\eta\frac{\nu_\eta(z,E)}{1+\mathrm{e}^{\beta(E+\eta-\mu)}}. \tag{5.22}$$

In the SE case, discussed above in subsection V A, $m(z)=m_\infty=m_e$ and $\nu_\eta(z,E)$ does not depend on η. This allowed us to perform explicitly the integration with respect to the energy of transverse motion, η, and obtain (5.14). Now, the mini-bands are not parabolic, and $\nu_\eta(z,E)$ depends on η. Nevertheless this dependence is weak for sufficiently small η. Let $T_o=1/\beta_o$ be the operating temperature.

In (5.22), with exponentially small error, the main contribution to the η integral comes from the interval $(0,\mu-\underline{E}+CT_o)$, where $\underline{E}$ is the bottom of the spectrum and the constant C is several units, Considering only band offsets which are linear in the effective mass, (4.39), the potential (5.1) is

$$U_{BDD}(x)=B[m(x)-m_\infty]+\Phi_{sc}(x;m;U). \tag{5.23}$$

so that

$$U_\eta(z)=B[m(z)-m_\infty][1-\eta/Bm(z)]+\Phi_{sc}(x;m;U). \tag{5.24}$$

We see the condition for neglecting the nonparabolicity contribution to the electron density is that $(0,\mu-\underline{E}+CT_o)$ is much smaller than the typical values of $Bm(z)$ [800-1000meV for $Al_xGa_{1-x}As$, see (4.59)].

After presenting the explicit recipe for computing the functional $\Phi_{sc}(z;m;U)$, let us apply the unitary transformation $\hat{\mathrm{U}}_X$, (4.6), associated with the coordinate transformation (4.3) to the one dimensional Schrödinger equation, (4.1) with potential $V_S(z)$. We obtain the BDD-type equation (4.10) with the potential (4.11) and effective mass (4.12).

The condition for the two equations to be identical is the coincidence of the potentials (5.23) and $U_X(x)=\hbar^2 W_X(x)/2m_\infty$, where $W_X(x)$ is given by (4.11).

$$U_X(x)=U_{BDD}(x). \tag{5.25}$$

This can be rewritten as

$$X'^2(x)-1-v[X(x)]-\kappa_\infty^{-2}\left\{\frac{2X'''(x)}{[X'(x)]^3}-\frac{5[X''(x)]^2}{[X'(x)]^4}\right\} = -\phi_{sc}(x;X';v). \tag{5.26}$$

Here, κ_∞ is defined by (4.42) and we introduced the potentials measured in units Bm_∞:

$$v(X)=\frac{U_S(X)}{Bm_\infty};\quad \phi_{sc}(x;X';v)=\frac{\Phi_{sc}(x;m;U)}{Bm_\infty}. \tag{5.27}$$

Taking into account (4.11), (4.12), (4.39) and (5.16), $m(x)$ and $W_X(x)$ are functionals of the coordinate transformation, X', and the potential, V_S, in the original Schrödinger equation, (4.1). We reparameterized the dependence of $\Phi_{sc}(x;m;U)$ in terms of these functions, as it appears in the second eq. (5.27).

Setting the self consistency term, $\phi_{sc}(x;X';v)$, equal to zero in (5.26), we recover the differential equation (4.22) in the linear case (4.39). The presence of $\phi_{sc}(x;X';v)$ makes (5.26) a functional equation.

We will attack this equation in a perturbative manner, as in section IV E. Indeed, as we have seen there, in some interesting cases $1/\kappa_\infty$ is of the order of the lattice spacing. A "quasiclassical" approach to this is to neglect the term within braces in the right hand side of (5.26), leading to

$$X'(x)\approx\sqrt{1+v(X)-\phi_{sc}(x;X';v)}. \tag{5.28}$$

Although this approximation seems reasonable, we will not pursue this further with the same motivation as in section IV E. Instead, we will develop again the "small potential" approach, using the same motivation as in section IV E. Since $\phi_{sc}(x;X';v)$ is generally smaller and slower varying than $v[X(x)]$, the estimate of type (4.59) will be better for ϕ.

Before proceeding further, let us write the selfconsistency term in the right hand side of (5.26) as a function of $X(x)$. As in section IV B, we can then reduce the order of the derivatives in the equation (5.26) using the fact that it will no longer depends explicitly on x, but only through $X(x)$ and its derivatives. Redefining the unknown function, the selfconsistency correction's ϕ dependence on x and the two densities which appear in the definition of ϕ as functions of $X(x)$,

$$S[X(x)] = X'(x); \tag{5.29}$$

$$\tilde{\phi}_{sc}[X(x);S;v] = \phi_{sc}(x;X';v); \tag{5.30}$$

$$\tilde{n}_{el}[X(x)] = n_{el}(x); \quad \tilde{n}_d[X(x)] = n_d(x). \tag{5.31}$$

and using (5.8) and (5.27), we obtain

$$\tilde{\phi}_{sc}(X;S;v) = \left[\int_{-\infty}^{X} \mathrm{d}z \int_{z}^{X} \mathrm{d}t + \int_{X}^{+\infty} \mathrm{d}z \int_{X}^{z} \mathrm{d}t\right] g(z,t), \tag{5.32}$$

where the we introduced the notation

$$g(z,t) = \frac{2\pi e^2 \left[\tilde{n}_d(z) - \tilde{n}_{el}(z)\right]}{B m_\infty S(z) S(t) \epsilon[m_\infty S^2(t)]}. \tag{5.33}$$

It remains to rewrite the density of states $\nu_\eta(x,E)$ as a function of $X(x)$. Let us apply the unitary transformation $\hat{\mathsf{U}}_X$ to the Schrödinger equation (4.1) with the potential $V_S(z)$ replaced by

$$V_{S\eta}(z) = V_S(z) + 2m_\infty \eta \left[1 - S^{-2}(z)\right]/\hbar^2. \tag{5.34}$$

The function $S(z)$ was defined in (5.29). The result of the transformation is the BDD equation (4.10) with the potential replaced by

$$W_{X\eta}(x) = W_X(x) + 2m_\infty \eta \left[1 - S^{-2}[X(x)]\right]/\hbar^2. \tag{5.35}$$

Here W_X is given by (4.11). By (5.25) and the definition of S, (5.29), we have that $W_{X\eta}[X(x)]$ coincides with the potential in the equation for the Green function (5.20), $U_\eta(x)$. Thus, the Green function $G_\eta(x,x',E)$ is the result of the unitary mapping with $\hat{\mathsf{U}}_X$ of the Green function of the Schrödinger equation (4.1) with potential V_S replaced by $V_{S\eta}$, (5.34). Finally, (5.19) can be rewritten as

$$\nu_\eta(x,E) = S[X(x)]\nu_{0\eta}(X(x),E). \tag{5.36}$$

Here, $\nu_{0\eta}(z,E)$ is given by (5.11) in terms of $G_{0\eta}(z,z;E)$. This is the Green function of the Schrödinger equation. It satisfies the equation (5.12) with $m_e = m_\infty$ and the potential $U(z)$ replaced by $\hbar^2 V_{S\eta}(z)/2m_\infty$. Thus, substituting (5.36) into (5.22), we obtain the electron density as a function of $X(x)$ and a functional of S and v.

We can now rewrite (5.26) in a form resembling (4.61):

$$S'' = 3S'^{\,2}/2S + \kappa_\infty^2 S\left[S^2 - 1 - v + \tilde{\phi}\right]/2, \tag{5.37}$$

where we omitted the arguments of the functions.

The small potential perturbative approach begins with introducing the formal small parameter α, setting

$$v \to \alpha v; \quad \tilde{\phi} \to \alpha\tilde{\phi} \tag{5.38}$$

Then we expand again S into the series (4.60) in powers of α. We substitute (4.60) and (5.38) into (5.37) and expand it into a power series in α. After equating the terms with the same power of α and setting $\alpha = 1$, we obtain the "small potential" expansion.

As in section IV E, the zero-th order coincides with a uniform structure. The equation $S''_{(0)}(X) = 0$, with the boundary condition $S_{(0)}(\pm\infty) \to 1$, leads to

$$S_{(0)}(X) = 1. \tag{5.39}$$

The problem with the rest of the series is that although the Green function G_0 can be expanded in terms of the potential:

$$G_0 = G^{(0)} + G^{(0)} U G^{(0)} + \ldots, \tag{5.40}$$

where $G^{(0)}(x,y;E) = \mathrm{e}^{\mathrm{i}k|x-y|}/2\mathrm{i}k$ is the free particle Green function, this expansion assumes that the potential is small compared to the kinetic energy. This is certainly wrong at the low energies we are interested in.

We will note instead that the nonparabolicity correction to V_S (the second term in (5.34)) is small. To first order in the expansion of S in powers of α, using the estimate (5.28), we obtain

$$U_{S\eta} \approx U_S + [U_S - \Phi_{sc}]\eta/Bm_\infty. \tag{5.41}$$

Here, $U_{S\eta} = \hbar^2 V_{S\eta}/2m_\infty$ and $U_S = \hbar^2 V_S/2m_\infty$ are, respectively, the potential (5.34) and the reconstructed potential in the Schrödinger equation measured in energy units. We omitted the arguments of the functions. If $\mu - \underline{E} + CT_o$ is much smaller than Bm_∞, then the term with square brackets in (5.41) is small compared to the first one.

Neglecting it, the self consistency term coincides in the first approximation with the one computed in section V A for the Schrödinger dynamics with mass m_∞ and dielectric constant $\epsilon(m_\infty)$:

$$\tilde{\phi}(X;1;v) = \Phi_{sc}(X;U_S)/Bm_\infty. \tag{5.42}$$

Now, we can solve for the first order correction $S_1(X)$:

$$S_1(X) = \frac{1}{4\kappa_\infty}\int_{-\infty}^{\infty} \mathrm{d}\xi \mathrm{e}^{-\kappa_\infty|X-\xi|}[v(\xi) - \tilde{\phi}(\xi)], \tag{5.43}$$

with $\tilde{\phi}$ given by (5.42). If the integrand is slowly varying on the scale $1/\kappa_\infty$, then we recover the perturbative expansion of "quasiclassical" formula (5.28).

$$2S_1(X) = v(X) - \tilde{\phi}(X;1;v). \tag{5.44}$$

Finally, we find the transformation as at the end of section IV E.

$$X(x) = x + \int_0^x \mathrm{d}y\, S_1(y), \qquad (5.45)$$

where we inverted the implicit relation (4.68) to first order. The mass (and concentration) profile can now be recovered. The result will be reasonable if the electron (and dopant) density is not too large. A more detailed account will be published elsewhere[28].

VI. CONCLUDING REMARKS

We have attained our stated purpose, constructing heterostructure chemical composition and dopant profiles such that the electron reflectance of the heterostructure is preset, by combining three inverse techniques:

1. Reconstruction of the phases of the scattering data from their absolute values. We did it by Padé discretization of the dispersion relations.

2. Reconstruction of the potential in the one dimensional Schrödinger equation from the scattering data. We used the Kay-Moses-Sabatier approach, since the reconstructed scattering data were rational functions of k.

3. Determination of the chemical concentration and dopant ion concentration profiles which yield a given self consistent potential for the Schrödinger equation or an effective mass profile and a self consistent potential for the BenDaniel and Duke equation. We simply reversed the definition of the self consistent potential in the Schrödinger case. In the case of BenDaniel and Duke dynamics we sketched a perturbative approach to solving the functional equation obtained by the variable mass mapping of the Schrödinger into the BenDaniel and Duke one – the method used for solving the non self consistent inverse problem for the BDD equation.

In section II we used Padé approximation for representing the reflectance and reconstructed the phases by discrete dispersion relations. The number of parameters is determined by two factors: the number of poles of the approximants for the transmittance and the reflectance $(p+q+2)$ and the degree of smoothness of the potential. The latter is determined by the rate of falloff at infinity of the reflection coefficients. If $R_\pm(k) \sim k^{-q-2}$, then the q-th derivative of the potential is piecewise continuous. The accuracy of representation of the scattering data increases with increasing p. So does the complexity of the calculations.

The reference solutions are in some sense maximally non-symmetric. This can be advantageous in optimizing non linear optical response functions, which vanish for symmetric potentials.

We have shown how to construct chemical profiles for compositionally graded heterostructures in lattice matched systems, like the systems $Ga_{1-x}Al_xAs$ or $In_{1-x-y}Ga_xAl_y$ matched on InP, such that in the effective mass approximation (with self-consistent potential) the conduction electron reflectance (at a preset operating temperature) is given by the designer. In the inverse approach, the construction of self-consistent potentials can be made at little extra cost. Indeed, in the brute-force direct approach one examines a number of possible configurations and, for each configuration, one has to construct iteratively the self-consistent potential and *only then* one can obtain the scattering data for the configuration.

In the inverse approach for the SE, once the reference potential is constructed from the synthesized scattering data, one can choose some doping profile and determine directly the compositional profile which yields the desired reflectance. The situation is somewhat more complicated in the case of the BDD equation. Here, we start again from the reference potential. Then, solving a nonlinear differential equation, we obtained the concentration (mass) profile corresponding to a non-selfconsistent potential. This is valid if the conduction electron density is negligible.

In the case of non negligible density of conduction electrons, a more complicated functional equation must be solved. The main difficulties are generated by the non-parabolic character of the minibands in the case of the BenDaniel and Duke's equation. Perturbative approaches were presented in section V B. A hybrid approach which looks promising is to search by brute force methods near the perturbative solution in the BDD case, looks promising.

We examined only Hartree self consistent potentials. It is obvious that the incorporation of exchange-correlation corrections which depend only on the local electronic density can be done at little extra cost.

We will mention without details another case in which the calculation of the selfconsistent solution is much simplified. When the electron plasma is thin and hot everywhere, $e^2\beta\,[n_{el}]^{1/3} \ll 1$ and $\hbar^2\beta\,[n_{el}]^{2/3}/m \ll 1$, we may use the (quasi)classical expression for the electron density:

$$n_{el}(z;m;U) = n_b\,[m(z)/m_\infty]^{3/2}\,\mathrm{e}^{-\beta U(z)}. \qquad (6.1)$$

Throughout this paper we have considered the heterostructure embedded in a homogeneous alloy and did not consider the biased case. The methods described here can be generalized to the case of different asymptotic compositions at $\pm\infty$ and/or presence of bias. This will be presented elsewhere[29].

We have examined throughout this paper only continuous potentials. If these are digitized using standard methods, the low energy dynamics and scattering will not be much affected.

If a more precise, multi-band description is needed, it should again be profitable to explore by brute-force standard methods the configurations which are close to the ones generated by our one-band approach. Perturbative calculations near this point could also be prove useful.

Finally, let us summarize the advantages of the inverse approach over the direct, brute force, one:

- In practice, the direct method is restricted to optimizing over small sets of parameters describing the structural data.
- The inverse approach allows the discovery of *new* promising configurations that can be subsequently optimized using perturbative and/or traditional (brute force) techniques.
- Obtaining chemical composition and dopant concentration profiles and corresponding to given self-consistent potentials for the Schrödinger dynamics is rather inexpensive. Although the effort is significantly larger in the case of BenDaniel and Duke dynamics, good starting configurations can be obtained perturbatively.

APPENDIX A: SCATTERING AND INVERSE SCATTERING FOR THE ONE DIMENSIONAL SCHRÖDINGER EQUATION

For the reader's convenience we will briefly review scattering and inverse scattering theory for the one-dimensional Schrödinger equation. We will use the Faddeev-Marchenko[30–32] approach. A detailed account may be found in the book by Chadan and Sabatier[10].

Setting the in-plane quasimomentum $\boldsymbol{q}_\perp = 0$ brings the one-dimensional Schrödinger equation (1.5) to the form

$$\psi''(z) + \left[k^2 - V(z)\right]\psi(z) = 0. \tag{A1}$$

We will consider only potentials which are piecewise continuous and fall sufficiently fast at infinity so that

$$\int_{-\infty}^{\infty} \mathrm{d}z(1+z^2)|V(z)| < \infty. \tag{A2}$$

Then, (A1) may have only a finite number of bound states with negative energy. For $E > 0$ the spectrum is absolutely continuous and doubly degenerate.

1. Jost functions, scattering data and their properties

The scattering is best described in terms of the Jost solutions of (A1), $f_\pm(z;k)$, which for $k = 0$ behave like outgoing waves near $\pm\infty$:

$$\lim_{z\to+\infty} f_+(z;k)\mathrm{e}^{-\mathrm{i}kz} = 1;$$
$$\lim_{z\to-\infty} f_-(z;k)\mathrm{e}^{\mathrm{i}kz} = 1. \tag{A3}$$

Let us summarize some properties of the Jost functions (JF) which are relevant for the scattering problem:

a. For real k the JF are continuous in z. $f_+(z;\pm k)$ are a pair of linearly independent solutions of (A1). The same holds for $f_-(z;\pm k)$.

b. The JF can be continued analytically from the positive half-axis ($k > 0$) to the upper complex half-plane $\mathrm{Im}(k) > 0$. Here, the JF are *analytic* in k with values which are continuous functions of z. They have no zeros in z for $\mathrm{Im}(k) > 0$.

c. For large complex $|k|$ in the upper half-plane, the JF behave like outgoing waves for all real z:

$$\mathrm{e}^{\mp\mathrm{i}kz} f_\pm(z;k) = 1 + \mathcal{O}(k^{-1}); \quad |k| \to \infty. \tag{A4}$$

The above propositions can be readily proved using the integral equation of Volterra type which is satisfied by the JF:

$$f_\pm(z;k) = \mathrm{e}^{\pm\mathrm{i}kz} + \int_z^{\pm\infty} \mathrm{d}y \frac{\sin k(y-z)}{k} V(y) f_\pm(y;k). \tag{A5}$$

Now, we have two pairs of linearly independent solutions of (A1), $f_\pm(z;\pm k)$. One of each pair behaves like an outgoing/ingoing near the corresponding infinity. Since (A1) can have only two linearly independent solutions, the outgoing wave JF can be expressed in terms of the ingoing wave ones:

$$T(k)f_+(z;k) = f_-(z;-k) + R_-(k)f_-(z;k); \tag{A6}$$
$$T(k)f_-(z;k) = f_+(z;-k) + R_+(k)f_+(z;k). \tag{A7}$$

Instead of seeking the asymptotic behaviors, the transmission, $T(k)$ and the reflection coefficients to the right/left, $R_\pm(k)$, can be expressed in terms of Wronskian determinants of the JF:

$$T(k) = \frac{2\mathrm{i}k}{W[f_+(z;k), f_-(z;k)]}; \tag{A8}$$
$$R_\pm(k) = \frac{W[f_-(z;\pm k), f_+(z;\mp k)]}{W[f_+(z;k), f_-(z;k)]}; \tag{A9}$$

where we use the notation:

$$W[f(z), g(z)] = f'(z)g(z) - f(z)g'(z), \tag{A10}$$

for the Wronskian of the functions $f(z)$ and $g(z)$. We remind the reader that the Wronskian of any two solutions of (A1) does not depend on z and is equal to zero if and only if the solutions are linearly dependent.

For real k the scattering coefficients $T(k)$ and $R_\pm(k)$ satisfy the following relations:

$$R_+(k)T(-k) + R_-(-k)T(k) = 0, \qquad \text{(A11)}$$
$$T(k)T(-k) + R_\pm(k)R_\pm(-k) = 1, \qquad \text{(A12)}$$

which express the unitarity of the S-matrix. Reality of the potential implies also that

$$T(k) = [T(-k)]^*; \quad R_\pm(k) = [R_\pm(-k)]^*. \qquad \text{(A13)}$$

Generically, $T(0) = 0$ and $R\pm(0) = -1$ (if there are no "zero energy bound states" — bounded, but not square integrable, solutions of the Schrödinger equation for $k = 0$). From (A8) and the remark *c.* above we see that $T^{-1}(k)$ can be continued analytically to the upper half-plane, $\mathrm{Im}(k) > 0$. Its zeros, if present, are the only possible (simple pole) singularities of $T(k)$ in the upper half plane. At such a zero, the two JF $f_\pm(z;k)$ are not linearly independent and decay exponentially for $z \to \pm\infty$. Thus, the poles of $T(k)$ in the upper half plane can occur only for $k = \mathrm{i}\lambda_j$, where $\hbar\lambda_j = \sqrt{-2m_e E_j} > 0$ and E_j are the energies of the bound states of (A1). The corresponding eigenfunctions $\psi_j(z)$ are real and are normalized by $\int_{-\infty}^{+\infty} \mathrm{d}x|\psi_j(x)|^2 = 1$. The two JF are proportional to the bound-state wave function:

$$f_\pm(z;\mathrm{i}\lambda_j) = C_j^\pm \psi_j(z), \qquad \text{(A14)}$$

where $C_j^\pm$ are real constants.

The asymptotic expansion of $T(k)$ near the bound-state pole $k = \mathrm{i}\lambda_j$ is

$$T(k) \approx \frac{\mathrm{i}}{C_j^+ C_j^-}\frac{1}{k - \lambda_j} + \mathcal{O}(1), \qquad \text{(A15)}$$

where $C_j^\pm$ are the constants in (A14). From here we can see that the bound-state poles of $T(k)$ must be simple. Otherwise, the product of the normalization constants is zero.

Generally speaking, the domains of analiticity of $R_\pm(k)$ will be smaller. If the potential $V(z)$ is zero on a half-axis and there are no bound states, then the corresponding reflection coefficient is analytic in the upper half-plane. Let us check this for the reflection to the left coefficient, $R_-(k)$, and potentials which vanish for $z < 0$. The denominator in (A9) is analytic and has no zeros since there are no bound states. In the numerator, $f_+(z;k)$ is always analytic and $f_-(z;-k) = \mathrm{e}^{\mathrm{i}kz}$ for $z < 0$. The other case can be dealt with in a similar manner.

From (A11 - A13) we obtain relations between the analytic continuations of the scattering data, which are valid whenever the arguments of the functions are within the domain of analiticity:

$$R_+(k)T(-k) + R_-(-k)T(k) = 0; \qquad \text{(A16)}$$
$$T(k)T(-k) + R_\pm(k)R_\pm(-k) = 1; \qquad \text{(A17)}$$
$$[T(k)]^* = T(-k^*); \quad [R_\pm(k)]^* = R_\pm(-k^*). \qquad \text{(A18)}$$

For positive energies, $E = \hbar^2k^2/2m_e$, (A12-A13) imply that the sum of the transmittance of the heterostructure and its reflectance,

$$\mathcal{T}(E) + \mathcal{R}(E) = |T(k)|^2 + |R_\pm(k)|^2 = 1 \qquad \text{(A19)}$$

equals unity.

2. Inverse scattering. The Marchenko equation.

If the potential in the Schrödinger equation (A1) is known, then, solving (A1) and using (A6-A7) one can obtain the scattering data (2.2). We want to explore the possibility of recovering the potential in the Schrödinger equation (A1) from the SD (2.2).

Let

$$F_\pm(z;k) = \mathrm{e}^{\mp\mathrm{i}kz} f_\pm(z;k). \qquad \text{(A20)}$$

The functions $F_\pm(z;k)$ are analytic in the upper half-plane. As a function of k, $F_\pm(z;k) - 1$ decays at infinity no slower than k^{-1}, (A4). This means that the Fourier transformation with respect to k will exist at least in the L^2 sense. We define the transformation kernels of the Schrödinger equation by the Fourier transforms

$$K_+(x;y) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k \mathrm{e}^{-\mathrm{i}k(y-x)}\left[F_+(x;k) - 1\right], \qquad \text{(A21)}$$
$$K_-(x;y) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k \mathrm{e}^{\mathrm{i}k(y-x)}\left[F_-(x;k) - 1\right]. \qquad \text{(A22)}$$

Closing the integration contour in the upper half-plane, we see that

$$K_+(x,y) = 0 \text{ for } x > y; \quad K_-(x,y) = 0 \text{ for } x < y. \qquad \text{(A23)}$$

The inverse Fourier transformations are:

$$F_+(x;k) = 1 + \int_x^{+\infty} \mathrm{d}u \mathrm{e}^{\mathrm{i}k(u-x)} K_+(x;u), \qquad \text{(A24)}$$
$$F_-(x;k) = 1 + \int_{-\infty}^{x} \mathrm{d}u \mathrm{e}^{\mathrm{i}k(x-u)} K_+(x;u). \qquad \text{(A25)}$$

Taking now the Fourier transformations of the Volterra equations, (A5), satisfied by the JF yields

$$K_+(x;y) = \frac{1}{2}\int_{\frac{x+y}{2}}^{+\infty} \mathrm{d}s\Big[V(s) + 2\int_0^{\frac{y-x}{2}} \mathrm{d}t V(s-t) K_+(s-t;s+t)\Big]. \qquad \text{(A26)}$$
$$K_-(x;y) = \frac{1}{2}\int_{-\infty}^{\frac{x+y}{2}} \mathrm{d}s\Big[V(s) + 2\int_{\frac{y-x}{2}}^{0} \mathrm{d}t V(s-t) K_-(s-t;s+t)\Big]. \qquad \text{(A27)}$$

Finally, taking the limit $y \to x \pm 0$ in (A26-A27) we obtain a simple relation between $K_\pm$ and the potential $V(x)$:

$$\lim_{y \downarrow x+0} K_+(x;y) = \frac{1}{2}\int_x^{+\infty} \mathrm{d}s V(s) \tag{A28}$$

$$\lim_{y \uparrow x-0} K_-(x;y) = \frac{1}{2}\int_{-\infty}^{x} \mathrm{d}s V(s). \tag{A29}$$

Thus, if we can construct K_+ (or K_-) from the scattering data, we may use one of the relations (A28-A29) to recover the potential by simple differentiation.

To make this connection, we will use the analytic properties of the scattering data. Applying Cauchy's formula to the analytic function $F_-(x;k) - 1$, which decays at infinity no slower than k^{-1}, we have

$$F_-(x;k) - 1 = \lim_{\delta \downarrow +0} \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{-\infty} \mathrm{d}\kappa \frac{F_-(x;\kappa) - 1}{\kappa - k - \mathrm{i}\delta}. \tag{A30}$$

Changing $\kappa \to -\kappa$ in (A30) and using (A7) yields

$$F_-(x;k) = 1 + \lim_{\delta \downarrow 0} \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{-\infty} \mathrm{d}\kappa \frac{1 - T(\kappa)F_+(x;\kappa)}{\kappa + k + \mathrm{i}\delta} + $$

$$+ \lim_{\delta \downarrow 0} \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{-\infty} \mathrm{d}\kappa \frac{R_-(\kappa)F_-(x;\kappa)\mathrm{e}^{-2\mathrm{i}\kappa x}}{\kappa + k + \mathrm{i}\delta}. \tag{A31}$$

In the first integral on the right hand side of (A31) we may close the contour in the upper half-plane. If there are no bound states, the integrand is analytic in the upper half-plane, and the integral is equal to zero. If bound states are present, the first integral in (A31) is equal to

$$I_1 = -\mathrm{i} \sum_j \frac{\left(C_j^-\right)^2 \mathrm{e}^{2\lambda_j x} F_-(x; \mathrm{i}\lambda_j)}{k + \mathrm{i}\lambda_j}, \tag{A32}$$

where we used (A14) to replace $F_+(x;\mathrm{i}\lambda_j)$ by $F_-(x;\mathrm{i}\lambda_j)$.

Taking the Fourier transform of (A31), using (A22) and the definition, (A25), of $K_-(x;y)$, yields the *Marchenko equation* for K_-:

$$K_-(x;y) + M_-(x+y) + \int_{-\infty}^{x} \mathrm{d}s M_-(y+s) K_-(x;s) = 0. \tag{A33}$$

Here, the Marchenko kernel, $M_-(u)$, is the sum of the Fourier transform of reflection to the left coefficient $R_-(k)$ and the contribution from the bound states, (A32):

$$M_-(u) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\kappa \mathrm{e}^{-\mathrm{i}\kappa u} R_-(\kappa) + \sum_j \left(C_j^-\right)^{-2} \mathrm{e}^{\lambda_j u}. \tag{A34}$$

A similar calculation yields the Marchenko equation for K_+:

$$K_+(x;y) + M_+(x+y) + \int_{x}^{+\infty} \mathrm{d}s M_+(y+s) K_+(x;s) = 0. \tag{A35}$$

The Marchenko kernel $M_+(u)$ is given by an expression similar to (A34), with all the $-$ signs changed into $+$ and λ_j replaced by $-\lambda_j$.

The Marchenko equation links *directly* the SD to the transformation kernels $K_\pm$ *bypassing the wave functions.* After solving (A33), the potential $V(x)$ is recovered from (A29)

$$V(x) = 2\frac{\mathrm{d}}{\mathrm{d}x} K_-(x; x-0). \tag{A36}$$

Let us remark that the first variable appears only as a parameter in (A33) and (A35).

Deift and Trubowitz[21] have given necessary and sufficient conditions for a one-to-one correspondence between a set of SD $\{T(k), R_\pm(k)\}$ which has no bound states, and a potential $V(z)$ satisfying (A2) obtained by solving Marchenko's equation, (A33).

1. $T(k)$ and $R_\pm(k)$ satisfy (A11-A13) on the real axis.

2. $T(k)$ is analytic in the upper half-plane and continuous up to the real axis.

3. $T(k) = 1 + \mathcal{O}(|k|^{-1})$, $\mathrm{Im}(k) \geq 0$, and $R_\pm(k) = \mathcal{O}(|k|^{-1})$, for real k as $|k| \to \infty$.

4. $T(k)$ has no zeros on the real axis, excepting possibly a simple one for $k = 0$. In the latter case,

$$1 + R_\pm(0) = 0. \tag{A37}$$

5. The Marchenko kernels $M_\pm(x)$ are absolutely continuous and for any given $a > 0$ there exists $c(a) > 0$ such that

$$\int_{-\infty}^{+\infty} \mathrm{d}x \theta[\pm(x-a)](1+x^2)|M'_\pm(x)| < c(a). \tag{A38}$$

The problem becomes a little trickier in the presence of bound states. Then, the Marchenko kernels $M_\pm(u)$, (A34), depend now not only on the energy of the bound state, which is given by the corresponding pole of $T(k)$, but also on the constants $C_j^\pm$, (A14). The scattering data contain information only on the product $C_j^- C_j^+$, which can be recovered from the residue of $T(k)$, (A15). For each bound state we can choose one of the parameters $C_j^\pm$ arbitrarily. The other is fixed by the (analytically continued) scattering data. Thus, assuming full knowledge of the scattering data, in the case when there are $n \geq 1$ bound states the solution of the inverse problem is not unique. There is a n-parameter family of potentials which correspond to the same scattering data.

From a physical point of view, one cannot recover the full information on the bound states in scattering experiments, which study only the behavior of the solutions at large distances, where the relevant information on the bound states is exponentially vanishing.

The numerical solution of the Marchenko equation for potential reconstruction is expensive from the computational point of view. To find a value for $V(x)$ one has to solve (A33) with high enough precision for the subsequent numerical differentiation. A lot of useless data is generated in the process, since we need only $\lim_{y\uparrow x} K_-(x;y)$ for using (A36) (or $\lim_{y\downarrow x} K_+(x;y)$). We will solve the Marchenko equation in the manner explained in section III, which is closer to the way we solve the phase reconstruction problem in section II. The resource management compares rather favorably to that of the codes[33,34] which have been written for the direct solution.

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TABLE I. 12 layer digitized $Al_cGa_{1-c}As$ filter. The Al concentrations are $c_1 = 0.05714$, $c_2 = 2c_1$, $c_3 = 4c_1$; the bulk Al concentration is $c_2 = 11.4\%$.

Layer #	Width (Atomic layers)	Width (nm)	Al concentration
1	6	1.696	$c_1 + c_2 + c_3$
2	9	2.543	0
3	18	5.088	c_3
4	5	1.413	c_2
5	10	2.827	$c_1 + c_2$
6	10	2.827	c_1
7	14	3.957	$c_1 + c_2$
8	14	3.957	c_1
9	13	3.675	$c_1 + c_2$
10	13	3.675	c_1
11	14	3.957	$c_1 + c_2$
12	11	3.109	$c1$

FIG. 1. Energy dependence of the transmittance of 12 layer digitized $Al_cGa_{1-c}As$ filter: continuous line — Eq.(4.2); dotted line — constant mass approximation Eq.(4.1) with $m_0 = m_\infty$. Insert: potential energy profile.