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RECONSTRUCTION OF QUANTUM WELL POTENTIALS VIA THE INTERTWINING OPERATOR TECHNIQUE

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One of the most important issues of *quantum engineering* is the construction of low-dimensional structures possessing desirable properties. For example, in different areas of possible applications of the structures containing quantum wells (QW), one often needs a predetermined QW energy spectrum. Then the following question arises: can one reconstruct the shape of QW which supports this spectrum? In this paper we outline a possible strategy of the QW potential shape reconstruction, if the QW spectrum is given in advance. The proposed approach is based on the combination of different techniques such as *Inverse Scattering Problem Method*, *Darboux* and *Liouville* transformation. It enables to take into account the space-variable dependent effective mass of charge carriers and allows the kinetic energy operator to be of non-Hermitian as well as Hermitian form. The proposed technique allows one to construct phase-equivalent potentials, to add the new bounded states to (or remove some of them from) the spectrum supported by an initial potential and provides a systematic procedure for generating new exactly solvable models.

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1. Introduction

In recent years we have been witnesses of the rapid progress in *nanoelectronics* which is already on the way to continuing the outstanding success of microelectronics. This became possible among others, due to the development of technologies and techniques, such as *Molecular Beam Epitaxy*

(MBE) for instance, which enables to deposit thin layers of different materials one on top of the other, with almost an atomic precision. The last one, in its turn, is able to produce a variety of *low-dimensional structures*, ranging from a heterojunction formed at a single interface, through quantum wells to superlattices. It would not be an overstatement to say that a new paradigm of electronics emerged, for which even the name has been already coined, *Quantum Technology* or *Quantum Engineering*. It seems, however, that quantum engineering in its present stage, in spite of all its successes and maturity, is still *passive* in the sense that it makes use of, figuratively speaking, less "degrees of freedom" than it possibly could. It means that the "palette" of QW-potential shapes is still limited to a few most popular ones: rectangular, parabolic or semi-parabolic and this circumstance obviously restricts the possibility to choose and control the energy spectrum of QW produced by means of MBE. Meantime, in different areas of possible applications of the low-dimensional structures mentioned above, one often needs a specific kind of spectrum known beforehand and a question arises: how to produce the QW with a predetermined spectrum? At least from the theorist's point of view, this question can be reformulated as follows: suppose the spectrum of QW is known; that is, one knows the number of quantum levels and the distances between them (remember, the spectrum is not necessarily equidistant as in case of a parabolic well or similar to the spectrum of a square well); can one reconstruct the QW-potential which supports this spectrum? An affirmative answer to the question would make quantum engineering more flexible and *active*, providing the opportunity to develop multitude of novel quantum devices.

The aim of this paper is to develop an approach to the QW-potential reconstruction which combines different techniques, such as *Inverse Scattering Problem Method*, *Darboux* (or intertwining operator technique) and *Liouville* transformations in reference to the generalized (it means, with space-variable dependent mass) Schrödinger equation.

2. Necessary preliminaries

As we already mentioned, one often needs to know, how to reconstruct the potential provided that the spectrum supported by this potential is known beforehand. One can look at the problem also as follows: suppose we have a set of "scattering data", whatever it means; we do not define them precisely right now. Can we find a potential which produces this set of data? An affirmative answer to this question was obtained for the first time by mathematicians Gel'fand, Levitan [1,2] and Marchenko [3] (see also references therein). They elaborated a method of potential reconstruction by means of spectral or scattering data which is now known under the name of *Inverse Scattering Problem Method* (ISP). We shall term their method or approach also as a GLM-method (approach). In a particular case of QW, the question is reduced to the following: suppose we have a number of quantum levels with the given distances between them; what the potential shape (or which the form of) QW should be in this case; or in other words, can we find the potential of QW, if the spectrum and the depth of QW are given? In Ref. [4] the provisional positive answer to this question was obtained by means of the ISP-method. In Ref. [4] the reader also can find the details concerning the motivation for such an inquiry. Here, for the sake of consistency and reader's convenience, we outline the main ideas of GLM-approach only very briefly.

Consider the eigenvalue problem of the Schrödinger equation with the potential $V(x)$ in one space dimension

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\phi(x,k) = k^2\phi(x,k)\,, \tag{1}$$

(here we assume $\hbar^2/2m = 1$). The GLM-method may be viewed as a dispersion theory for the Schrödinger wave function of (1). From the solution to (1) with k complex, one can define Jost functions $f_1^\pm$ and $f_2^\pm$ which are analytic in the upper-half k-plane with the following asymptotic behavior

$$f_1^\pm(x,k) \sim \exp(\pm ikx)\,, \qquad \text{as } x \to +\infty\,,$$
$$f_2^\pm(x,k) \sim \exp(\mp ikx)\,, \qquad \text{as } x \to -\infty\,,$$

and construct a meromorphic function $\Phi(x,k)$ as

$$\begin{aligned}\Phi(x,k) &= a^{-1}(k) f_2^+(x,k)\exp(ikx)\,, \qquad \operatorname{Im} k > 0\,,\\ &= f_1^-(x,k^*)\exp(ikx)\,, \qquad \operatorname{Im} k < 0\,,\end{aligned}$$

where $a^{-1}(k)$ is a conventional transmission coefficient.

Thus, $\Phi(x,k)$ is completely determined by its singularity structure which consists of a cut along the real k-axis and some number, say, N of bound-state poles on the positive imaginary axis. The spectral weight of the cut is essentially a scattering-state wave function multiplied by the reflection coefficient, both evaluated at real k. Similarly, the pole residues are essentially constants times bound-state wave functions. Upon Fourier transformation the dispersion relation for Φ becomes the Marchenko integral equation [3] (see also [5] for details) which determines the wave functions. The inverse problem of the potential reconstruction by means of scattering data can be reduced, generally speaking, to solving an integral equation

$$K(x,x') + Q(x,x') + \int_x^\infty K(x,x'')Q(x'',x')dx'' = 0$$

and thereupon, to a simple differentiation of its kernel

$$V(x) = -2\frac{d}{dx}K(x,x)$$

which is given entirely in terms of the reflection coefficient and $2N$ bound-state parameters. Here

$$Q(x,x') = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}[1 - S(k)]\exp(ik(x+x'))dk + \sum_{n}^{N} M_n^2 \exp(-\kappa_n(x+x'))\,,$$

where $S(k)$, E_n and M_n^2 are scattering data: $S(k)$ is a scattering matrix, $E_n = (i\kappa_n)^2$ are bound-state energies and M_n^2 are its normalization constants.

If the reflection coefficient can be represented by rational functions of k, the Marchenko equation can be solved exactly by algebraic technique. The most simple case corresponds to a reflection coefficient vanishing for all real k ($S(k) = 1$); then the expression for $Q(x,x')$ contains only the sum over the bound states, and the integral equation reduces to a system of N linear algebraic equations with respect to the kernel $K(x,x')$. The potential $V(x)$ also can be reconstructed by means of $2N$ parameters. A half of the parameters makes N bound-state energies E_n, $n = 1, 2, \ldots\ N$, while the others are the normalizing constants M_n^2 which in *Nuclear Physics* are assumed to be obtained from scattering data as $M_n^2 = i\mathrm{Res}S(k)|k = i\kappa_n$. It corresponds to the transparent and symmetric potentials. These $2N$ numbers supply a complete set of the parameters for solving the inverse problem to exist and be unique. Obviously, in case of QWs a second half of the scattering data (the normalizing constants) is inaccessible. It turns out however, that the way out actually exists. The possibility to reconstruct the infinitely deep and symmetric potentials solely by means of bounded states was established for the first time by Levitan and Gasymov who proved the *The Theorem about Two-spectrum* [6,2]. The meaning of this theorem in brief is the following: to reconstruct symmetric potentials $V(x) = V(-x)$, it suffices to know only the positions of energy levels without knowing the normalizing constants. Later on, this fact was re-discovered by Thacker, Quigg and Rosner [7] who modeled the confining potentials binding massive quarks and antiquarks in meson systems. They were able even to fit approximately the lower parts of infinitely deep wells (parabolic, harmonic oscillator, linear and rectangular wells) by means of a limited number of levels whose positions are known, using some additional technical trick which is termed a *stabilizing parameter*. This observation was used in Ref. [4] in order to reconstruct the shape of QW provided that its energy spectrum and depth are known in advance. The problem however is, that in the approach developed there, the electron effective mass was supposed to be constant and independent of the space variable, while in reality it is space-dependent. It is because in practice the quantum wells of different shapes are produced by means of MBE technique, when the semiconductor layers are grown subsequently one by one and these layers are characterized by different electron effective masses. The subsequent semiconductor layers stuck together make a quantum well and, as a result, one can consider such structure as having an effective mass which depends on the space variable. Proceed now to the thorough treatment of this problem.

3. Reconstruction of quantum well potentials using the intertwining operator technique

3.1. ISP and reconstruction of quantum well potentials

The above discussion suggests the following strategy of the QW potential reconstruction. At first, one has to search for the solution of our problem among the potentials of a special class of reflectionless and symmetric potential $V(x) = V(-x)$, using the ISP-method as it was done in [4]. Then one can amend the potential reconstructed in this way, using the intertwining operator technique and taking into account the dependence of the electron effective mass on the space variable. Now we are able to describe this recipe in more details. Suppose that one-dimensional potential $V(x)$ can be represented by the function $V_N(x, m^*, E_0)$ which obeys the following conditions:

- *(i)* V_N supports precisely N bounded states of the quantum system with the effective mass m^*. The bound-state energies coincide with the energies $\epsilon_1, \epsilon_2, \ldots \epsilon_N$ of the levels within the QW;
- *(ii)* $\lim_{x\to\infty} V_N = E_0$. The last value can be considered as a depth of QW.

Arranging the binding energies $k^2 = E_0 - \epsilon_n$ in a descending order so that $k_1 > k_2 > \ldots > k_N$, and $\epsilon_1 = E_0 - k_1^2$ refers to the ground-state energy, one can use for QW potential reconstruction the technique developed by Schonefeld *et al.,* [8] for studying the convergence of the reflectionless approximation to the confining potentials. Omitting the intermediate calculations, we give here only the final results:

$$V_N(x, E_0) = E_0 - 2\frac{d^2}{dx^2}\ln D(x)\,, \tag{2}$$

where

$$D(x) = \sum_S \exp\Big(-2x\sum_{p\in S} k_p\Big)\prod(S,\tilde{S})\,,$$

$$\prod(S,\tilde{S}) = \prod_{m\in S, n\in\tilde{S}} \frac{k_m + k_n}{k_m - k_n}\,.$$

Here the sum ranges over all subsets S of $\{1,2,\,\ldots\,,N\}$ including the null set and the full set, while $\tilde{S}$ denotes the complement of the set S.

Now we consider a *generalized* Schrödinger equation, that is with the potential $V_N(x,E_0)$ and the position-dependent effective mass. Obviously, the new spectrum obtained in this way might differ from that which was used in the ISP-method in order to reconstruct the potential $V_N(x,E_0)$. However, we can suppose that the changes of the spectrum are not dramatic, because in practice the space variable dependence of the effective mass is weak. Further on, we shall show that it is possible to amend this potential and obtain an "improved" one, $\widetilde{V}(x)$, in order to have the spectrum needed.

3.2. First-order Darboux transformation and supersymmetry

The problem of the space-variable dependent effective mass attracts now persistent attention because it is not obvious whether the effective mass approximation is applicable to heterostructures, or not (see [9,10] and the references therein). Before we start our discussion, let us make some general remarks. Remember, the QW of the shape other than rectangular, is produced by stacking up a number (some times even a considerable number) of layers of different materials, each of which is characterized by its own effective mass. This stack of layers can be considered as a special case of the heterostructure. Then if one tries to solve the Sturm–Liouville problem for a corresponding Schrödinger equation (we refer to this problem also as a *direct* one), treating the heterostructure as a whole and applying the effective-mass theory, one encounters some difficulties, whose nature is the following. First, the total electron wave function is a product of the slowly varying *envelope* function and the Bloch function of the local extremum in the host's band structure. The Bloch functions in the two materials on either side of a heterojunction must be similar for the effective-mass approximation to be valid. An obvious condition is that they must belong to the same point in Brillouin zone, and this can fail for some materials. The second point concerns the matching of the envelope functions at the interface. Consider a junction at $x = 0$ between two regions of materials, say, A and B. The Schrödinger equations for the envelope function in the two subsequent regions (we consider only one-dimensional model) are

$$\left(-\frac{1}{m_A^*}\frac{d^2}{dx^2} + E_{\mathrm{c}}^A\right)\phi(x) = \mathcal{E}\phi(x)\,,$$

$$\left(-\frac{1}{m_B^*}\frac{d^2}{dx^2} + E_{\mathrm{c}}^B\right)\phi(x) = \mathcal{E}\phi(x)\,,$$

where m_A^* and m_B^* are the electron effective masses for the materials A and B, respectively, $\hbar^2/2 = 1$, and the difference in the bottoms of the conduction bands is $\Delta E_{\rm c} = E_{\rm c}^B - E_{\rm c}^A$. If the materials were the same, one can match the value and the derivative of the wave function at the interface by means of usual conditions

$$\phi^A(0_-) = \phi^B(0_+)\,, \qquad \frac{d\phi^A(x)}{dx}|_{x=0_-} = \frac{d\phi^B(x)}{dx}|_{x=0_+}\,,$$

where 0_- means the side of the interface in material A and so on. This simple condition is not correct for the heterostructure where the two effective masses are different, because it does not conserve the current. A correct set of matching conditions is

$$\phi^A(0_-) = \phi^B(0_+)\,, \qquad \frac{1}{m_A^*}\frac{d\phi^A(x)}{dx}|_{x=0_-} = \frac{1}{m_B^*}\frac{d\phi^B(x)}{dx}|_{x=0_+}\,.$$

The condition for matching the derivative now includes the effective mass. A more mathematical argument is that the matching condition which does not include effective masses assumes that the Schrödinger equation takes the form

$$-\frac{1}{m^*(x)}\frac{d^2\phi}{dx^2} + V(x)\phi(x) = \mathcal{E}\phi(x)\,.$$

Note that the kinetic energy operator is not Hermitian, if $m^*(x)$ is space dependent. In this section we are dealing with the intertwining relation technique, which is universal, and applying this technique to construct a chain of exactly solvable Hamiltonians whose kinetic energy operators are not Hermitian. In the next section (Sec. 4), we also develop an approach which gives a possibility to treat the cases both with the Hermitian and with non Hermitian kinetic energy operators on the same footing.

Let us start with the equation

$$\mathcal{H}\phi(x) = \mathcal{E}\phi(x)\,, \qquad \mathcal{H} = -\frac{1}{m^*(x)}\frac{d^2}{dx^2} + V(x)\,, \tag{3}$$

where $m^*(x)$ is a position dependent "effective mass" and $V(x)$ is supposed to be equal to $V_N(x, E_0)$. This equation is reduced to the generalized Schrödinger equation of the form:

$$\mathcal{H}_0\phi_0(x) = \mathcal{E}m^*(x)\phi_0(x)\,, \qquad \mathcal{H}_0 = -\frac{d^2}{dx^2} + v(x)\,,$$

where $v(x) = V(x)m^*(x)$. In fact, it is the Schrödinger equation with linearly energy-dependent potentials. The Darboux transformations for the

Schrödinger equations with variable values of energy and angular momentum were suggested in [11] and in a more general form in [12]. Then in Refs. [13,14] algebraic transformations have been elaborated for a Sturm–Liouville problem for studying phase-equivalent linearly energy-dependent potentials and for constructing exactly solvable three-body models with two-central potentials. On the other hand, the intertwining operator method provides a universal approach to creating new exactly solvable models and can be applied to the operators of a very general form (see for example [15–17]). In this paper, we apply the intertwining operator technique to the equation (3) with a position-dependent mass in order to construct the potential which supports the desirable spectrum.

Suppose that the solution of the eigenvalue problem to the equation (3) with the given potential $V(x)$ and position dependent mass $m^*(x)$ are known and we would like to solve a similar problem for another Hamiltonian $\widetilde{\mathcal{H}}$, the spectrum of which probably differs from the spectrum of the Hamiltonian (3) by a single quantum state:

$$\widetilde{\mathcal{H}}\widetilde{\phi}(x) = \mathcal{E}\widetilde{\phi}(x)\,, \qquad \widetilde{\mathcal{H}} = -\frac{1}{m^*(x)}\frac{d^2}{dx^2} + \widetilde{V}(x)\,. \tag{4}$$

We start with standard intertwining relations (see, for instance [15,16]):

$$\mathcal{L}\mathcal{H} \;=\; \widetilde{\mathcal{H}}\mathcal{L}\,, \tag{5}$$

$$\widetilde{\phi}(x) \;=\; \mathcal{L}\phi(x)\,, \tag{6}$$

where the operator $\mathcal{L}$ intertwines the Hamiltonians $\mathcal{H}$ and $\widetilde{\mathcal{H}}$. We search for the intertwining operator $\mathcal{L}$ in a general form

$$\mathcal{L} = B(x)\frac{d}{dx} + A(x)\,, \tag{7}$$

where $A(x)$ and $B(x)$ are to be determined. Once the operator $\mathcal{L}$ is known, the solutions $\widetilde{\phi}$ can be obtained from (6) by applying $\mathcal{L}$ to the known solutions ϕ. To find the explicit form of $\mathcal{L}$, we use the equations (3), (4) and the intertwining relations (5), (6):

$$\Big[-\frac{1}{m^*(x)}\frac{d^2}{dx^2} + \widetilde{V}(x)\Big]\mathcal{L}\phi(x) = \mathcal{L}\Big[-\frac{1}{m^*(x)}\frac{d^2}{dx^2} + V(x)\Big]\phi(x)\,.$$

After some algebra we arrive at:

$$-\frac{1}{m^*}(A''\phi + 2A'\phi' + A\phi'') - \frac{1}{m^*}(B''\phi' + 2B'\phi'' + B\phi''') + \widetilde{V}(A\phi + B\phi')$$
$$= A\Big(-\frac{1}{m^*}\phi'' + V\phi\Big) + B\Big(-\frac{1}{m^*}\phi''' - \Big(\frac{1}{m^*}\Big)'\phi'' + V'\phi + V\phi'\Big)\,,$$

and finally, to a next system of equations:

$$\frac{1}{m^*}A + 2\frac{1}{m^*}B' = B\Big(\frac{1}{m^*}\Big)' + A\frac{1}{m^*}\,, \tag{8}$$

$$\frac{1}{m^*}2A' + \frac{1}{m^*}B'' - \widetilde{V}B = -BV, \tag{9}$$

$$-\frac{1}{m^*}A'' + \widetilde{V}A = AV + BV'\,. \tag{10}$$

From (8) it immediately follows that

$$\frac{2B'}{B} = \frac{-m^{*'}}{m^*}\,, \qquad B = \frac{C}{\sqrt{m^*}}\,, \tag{11}$$

where C is an arbitrary constant. From (9), (10) one gets

$$\widetilde{V} = V + \frac{1}{m^*}\frac{B''}{B} + \frac{1}{m^*}\frac{2A'}{B} \tag{12}$$

and

$$-\frac{1}{m^*}A'' + \left(\frac{1}{m^*}2A' + B''\right)B^{-1}A = BV'\,.$$

In order to integrate the last equation, let us introduce a new auxiliary function $K(x)$ defined as $A(x) = B(x)K(x)$. Then we arrive at a nonlinear differential equation

$$\Big(-K'' + 2K'K - V'm^*\Big) + \frac{2B'}{B}\Big(K^2 - K'\Big) = 0\,.$$

Taking into account the relation $V = v/m^*$ and the first of the relations (11), the last equation can be easily transformed into another one, in a single unknown K only:

$$\Big(-K'' + 2K'K - v'\Big) - \frac{m^{*'}}{m^*}\Big(-K' + K^2 - v\Big) = 0\,.$$

This one can be rewritten as

$$\frac{d}{dx}\left(\frac{1}{m^*}\Big(-K' + K^2 - v\Big)\right) = 0\,,$$

which means that

$$\left(\frac{1}{m^*}\right)\Big(-K' + K^2 - v\Big) = \nu\,,$$

where ν is an integration constant. The last equation is analogous to Riccati equation. Introducing a new function $\mathcal{U}(x)$ as $K = -\mathcal{U}'\mathcal{U}^{-1}$ and changing $\nu = -\lambda$, one arrives at the equation

$$-\frac{1}{m^*(x)}\mathcal{U}''(x) + V(x)\mathcal{U}(x) = \lambda\mathcal{U}(x)\,. \tag{13}$$

Here $\mathcal{U}(x)$ is supposed to be invertible at all x. The last equation is nothing else but the initial equation (3) which is supposed to be solved, and $\mathcal{E} = \lambda$ is a point of spectrum of $\mathcal{H}$. Therefore, we assume that the solutions of (13) are known for the given values of λ. Having found the explicit form of B (see (11)), using the formula for K mentioned above, from the relation $A = BK$ one gets $A(x) = -C\left(\ln\mathcal{U}(x)\right)'\sqrt{1/m^*(x)}$. Once $\mathcal{U}$ is known, the transformation operator $\mathcal{L}$, the new potential $\widetilde{V}(x)$ and the corresponding solutions of the transformed equation (4) are defined up to an arbitrary constant C. Without loss of generality, we can put it safely equal to unity. After this we have

$$B(x) = 1/\sqrt{m^*(x)}\,, \quad A(x) = K/\sqrt{m^*(x)}\,, \quad K = -\left(\ln\mathcal{U}(x)\right)'\,. \tag{14}$$

To make further transformations, let us calculate $B''/B = \sqrt{m^*}(1/\sqrt{m^*})''$. Using this and (14) in (7), (12) and (6) we construct the intertwining operator $\mathcal{L}$, the transformed potential $\widetilde{V}(x)$ and the solutions $\widetilde{\phi}$ in the form:

$$\mathcal{L} = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K\right) = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} - (\ln\mathcal{U})'\right)\,, \tag{15}$$

$$\begin{aligned}\widetilde{V} &= V + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K\right)\right] \\ &= V + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} - 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}(\ln\mathcal{U})'\right)\right]\,,\end{aligned} \tag{16}$$

$$\widetilde{\phi} = \mathcal{L}\phi = \frac{1}{\sqrt{m^*}}\left[\frac{d}{dx} - (\ln U)'\right]\phi\,. \tag{17}$$

It follows immediately from (17) that $\mathcal{L}\mathcal{U} = 0$. In order to obtain a solution of the equation (4) at the energy of transformation λ, we shall use the second linear independent solution to (3), namely $\hat{\mathcal{U}}(x) = \mathcal{U}(x)\int^x dx'|\mathcal{U}(x')|^{-2}$ where the integration limits depend on the boundary conditions. In particular, for regular solutions satisfying the boundary conditions $\phi(x=0) = 0$, $\phi'(x)|_{x=0} = 1$, the lower integration limit is 0 and the upper one is x, while for the Jost solutions the integration limits are $-\infty$ and x, respectively. As a result we get

$$\eta(x) = \mathcal{L}\hat{\mathcal{U}}(x) = \frac{1}{\sqrt{m^*(x)}}\frac{1}{\mathcal{U}(x)}\,. \tag{18}$$

Once η is found, one can get a second solution of (4) at the energy of transformation λ. By using the Liouville's formula once more, one gets

$$\hat{\eta}(x) = \eta(x) \int^{x} dx' |\eta^2|^{-1} = \frac{1}{\sqrt{m^*(x)}\mathcal{U}(x)} \int^{x} dx' \mathcal{U}(x') m^*(x') \mathcal{U}(x') \,. \tag{19}$$

Hence, the information about all solutions of the initial equations (3) provides the knowledge of all solutions of the transformed equations (4). As in the case of Schrödinger equation, the functions $\phi(x, \mathcal{E})$ and $\widetilde{\phi}(x, \mathcal{E})$ correspond to Hamiltonians $\mathcal{H}$ and $\widetilde{\mathcal{H}}$, respectively, are related through the transformation operator $\mathcal{L}$ (see (17)). The difference is that in our case $\mathcal{L}$ includes a position-dependent mass. As a consequence, the new potential $\widetilde{V}$ and solutions $\widetilde{\phi}$ depend on the effective mass $m^*(x)$. The function $\eta(x)$ defined by (18) at the energy of transformation $\mathcal{E} = \lambda$ cannot be normalized and this is the reason why λ does not belong to the discrete spectrum of $\widetilde{\mathcal{H}}$. Therefore, Hamiltonians $\mathcal{H}$ and $\widetilde{\mathcal{H}}$ are isospectral with one exception of the bound state with the energy $\mathcal{E} = \lambda$, which is removed from the initial spectrum of $\mathcal{H}$. Note that if the transformation function $\mathcal{U}(x)$ corresponds to the ground state, *i.e.*, $\mathcal{U}(x)$ is nodeless, then the transformed potential $\widetilde{V}(x)$ has no new singularity, except the singularities due to $V(x)$ (of course, we assume $m^*(x) \neq 0$ at all x). However, if we apply this transformation to an arbitrary state other than a ground state, the transformed potential $\widetilde{V}(x)$ might contain extra singularities, which are not present in the initial potential $V(x)$ and hence, the Hamiltonian $\widetilde{H}$ becomes physically meaningless. As we shall see later, the difficulties with singularities can be circumvented by means of second-order Darboux transformations. Now we show how one can construct a Hamiltonian with an additional bounded state with respect to the initial Hamiltonian by using factorization of Hamiltonians and supersymmetry.

The supersymmetry is based on factorization properties of Darboux transformation operators $\mathcal{L}$ and $\mathcal{L}^{+}$. The definition of formally conjugate operators is $D^\dagger = (CQ)^\dagger = Q^\dagger C^\dagger$ and $(d/dx)^\dagger = -d/dx$. In our case, the scalar product of functions is defined by not standard way (f, g) but with the weight of $m^*(x)$: $(f, g)_m = \int m^*(x) f(x) g(x)$. In this case instead of operator $D^\dagger$ it is necessary to consider the operator $m^{*-1} D^\dagger m^*$. Therefore, the operator $\mathcal{L}^\dagger$ adjoint to $\mathcal{L}^\dagger = (1/\sqrt{m(x)})(d/dx + K)$ is determined as

$$\mathcal{L}^\dagger = \frac{1}{\sqrt{m^*}} \left(-\frac{d}{dx} - \frac{m^{*\prime}}{2m^*} + K \right) . \tag{20}$$

Now let us consider the superposition $\mathcal{L}^\dagger\mathcal{L}$ and $\mathcal{L}\mathcal{L}^\dagger$:

$$\mathcal{L}^\dagger\mathcal{L} = -\frac{1}{m^*}\frac{d^2}{dx^2} + \frac{1}{m^*}(-K' + K^2)\,, \tag{21}$$

$$\mathcal{L}\mathcal{L}^\dagger = -\frac{1}{m^*}\frac{d^2}{dx^2} + \frac{1}{m^*}(K' + K^2) - \frac{1}{2}\frac{m^{*''}}{m^{*2}} + \frac{3}{4}\frac{m^{*'}m^{*'}}{m^{*3}} - \frac{m^{*'}}{m^{*2}}K\,. \tag{22}$$

Express the potential V from equation (13) in the form $V = \mathcal{U}''/(m^*\mathcal{U}) + \lambda$. Using $K' = -[\mathcal{U}'/\mathcal{U}]' = -\mathcal{U}''/\mathcal{U} + (\mathcal{U}'/\mathcal{U})^2$ we represent V as

$$V = \frac{1}{m^*}\left(-K' + K^2\right) + \lambda\,. \tag{23}$$

Substitution of (23) into (16) leads to the following representation of the transformed potential:

$$\widetilde{V} = \frac{1}{m^*}(K' + K^2) + \frac{1}{\sqrt{m^*}}\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} - \frac{m^{*'}}{m^{*2}}K + \lambda\,. \tag{24}$$

Using (23) and (24), after some transformations the formulae (21) and (22) can be rewritten as

$$\mathcal{L}^\dagger\mathcal{L} = -\frac{1}{m^*}\frac{d^2}{dx^2} + V - \lambda = \mathcal{H} - \lambda\,, \tag{25}$$

$$\mathcal{L}\mathcal{L}^\dagger = -\frac{1}{m^*}\frac{d^2}{dx^2} + \widetilde{V} - \lambda = \widetilde{\mathcal{H}} - \lambda\,. \tag{26}$$

From (26) one can obtain the intertwining relation

$$\mathcal{H}\mathcal{L}^\dagger = \mathcal{L}^\dagger\widetilde{\mathcal{H}}\,, \tag{27}$$

which means that the operator $\mathcal{L}^\dagger$ is a transformation operator too and realizes the transformation of the solutions of equation (4) to solutions of (3), $\phi \propto \mathcal{L}^\dagger\widetilde{\phi}$. As one can see from the comparison of the relations (15) and (20), the operator $\mathcal{L}^\dagger$ is not an inverse of $\mathcal{L}$. One can show that the operators $\mathcal{L}$ and $\mathcal{L}^\dagger$ can be expressed in terms of η, which are solutions of transformed equations (4) at the energy λ with the potential $\widetilde{V}$ determined by (16). For this aim let us express K in terms of η, by means of (18).

$$K = -\frac{\mathcal{U}'}{\mathcal{U}} = \frac{m^{*'}}{2m^*} + \frac{\eta'}{\eta}\,.$$

Using this in (15) and (20), we obtain

$$\mathcal{L} = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + \frac{m^{*'}}{2m^*} + \frac{\eta'}{\eta}\right)\,, \qquad \mathcal{L}^\dagger = \frac{1}{\sqrt{m^*}}\left(-\frac{d}{dx} + \frac{\eta'}{\eta}\right)\,. \tag{28}$$

Evidently, the function η is also a transformation function. Clearly, $\mathcal{L}^\dagger\eta = 0$, *i.e.*, η belongs to the kernel of the operator $\mathcal{L}^\dagger$. As one can see from (28) and (19), the application of the operator $\mathcal{L}^\dagger$ to the second linearly independent solution $\hat{\eta}$ to equation (4) gives back the solutions $\mathcal{U}$ of the initial problem at the energy of transformation. Indeed,

$$\mathcal{L}^\dagger\hat{\eta} = \frac{1}{\sqrt{m^*}}\left(-\frac{d}{dx} + \frac{\eta'}{\eta}\right)\eta(x)\int^{x} dx'|\eta^2|^{-1} = \mathcal{U}\,.$$

Hence, a one-to-one correspondence between the spaces of solutions of equations (3) and (4) is established, and the operators $\mathcal{L}$ and $\mathcal{L}^\dagger$ realize the correspondence.

Note, one can interchange the role of the initial and final equations. The function η becomes a transformation function for the intertwining operator $\mathcal{L}^\dagger$, which will make the transformation in the opposite direction: from the potential $\widetilde{V}$ to the potential V and from the solutions of (4) to the solutions of (3). So, if within the first procedure (15)–(17) we constructed the potential $\widetilde{V}$ with one bound state removed, now we can construct the potential V with an additional bound state.

3.3. Second-order and the chain of Darboux transformations

Let us define the second-order Darboux transformation as a sequence of two Darboux transformations performed in a row

$$\mathcal{L} = \mathcal{L}_2\mathcal{L}_1\,, \tag{29}$$

where $\mathcal{L}_1$ is actually $\mathcal{L}$ defined in (14)

$$\mathcal{L}_1 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_1\right), \qquad K_1 = -\frac{\mathcal{U}_1'}{\mathcal{U}_1}\,, \tag{30}$$

whereas $\mathcal{L}_2$ is determined as follows:

$$\mathcal{L}_2 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_2\right), \qquad K_2 = -\frac{\chi_1'}{\chi_1}\,, \tag{31}$$

and $\chi_1 \equiv \chi_1(x, \lambda_2)$ is obtained by means of the first-order transformation, applied to the solution $\mathcal{U}_2$ of the equation (13) or (3) with the eigenvalue λ_2

$$\chi_1 = \mathcal{L}_1\mathcal{U}_2 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} - \frac{\mathcal{U}_1'}{\mathcal{U}_1}\right)\mathcal{U}_2\,. \tag{32}$$

Clearly, χ_1 is the solution of equation (13) with the potential $V_1 = V + 2K_1'$, defined as in (16), and χ_1 can be taken as a new transformation function for the Hamiltonian $\mathcal{H}_1$ to generate a new potential

$$V_2 = V_1 + \frac{1}{\sqrt{m^*(x)}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*(x)}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*(x)}}K_2\right)\right], \tag{33}$$

and corresponding solutions

$$\phi_2 = \mathcal{L}_2\phi_1 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_2\right)\phi_1\,, \qquad \phi_1 = \mathcal{L}_1\phi\,. \tag{34}$$

Here the function ϕ_1, denoted earlier as $\tilde{\phi}$, is an eigenfunction of the Hamiltonian $\mathcal{H}_1$

$$\phi_1 = \frac{1}{\sqrt{m^*}}\left[\frac{d}{dx} - (\ln U)_1'\right]\phi\,. \tag{35}$$

In other words, the action of the second-order operator (29) on the solutions ϕ leads to the solutions of $\mathcal{H}_2$

$$\phi_2 = \mathcal{L}\phi = \mathcal{L}_2\mathcal{L}_1\phi\,. \tag{36}$$

Iterating this procedure m times in regard to given operator $\mathcal{H}$, one arrives at the operator $\mathcal{H}_m$, which satisfies the intertwining relation

$$\mathcal{L}\mathcal{H} = \mathcal{H}_m\mathcal{L}\ .$$

In this way one gets

$$V_m \ = \ V_{m-1} + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K_{m-1}\right)\right], \tag{37}$$

$$\phi_m \ = \ \mathcal{L}\phi = \mathcal{L}_m\phi_{m-1} = \mathcal{L}_m\mathcal{L}_{m-1}\,\ldots\,\mathcal{L}_1\phi\,, \tag{38}$$

where $\mathcal{L}$ is the m-th order differential operator:

$$\mathcal{L} = \mathcal{L}_m\mathcal{L}_{m-1}\,\ldots\,\mathcal{L}_1\,, \quad \mathcal{L}_m = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_m\right), \quad K_m = -\chi_{m-1}'\chi_{m-1}^{-1}\,. \tag{39}$$

It should be noted that the chain of m first-order Darboux transformations results in a chain of exactly solvable Hamiltonians $\mathcal{H} \to \mathcal{H}_1 \to\ \ldots\ \to \mathcal{H}_m$.

Consider now the 2-nd order transformation in detail. Using the explicit expression for V_1 which appears in the first-order Darboux transformation, we get a formula for the potential V_2:

$$V_2 = V + \frac{2}{\sqrt{m^*}}\left(\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}}\right) + \frac{2}{\sqrt{m^*}}\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K\right), \tag{40}$$

where $K = K_1 + K_2$. Let us represent χ_1 as

$$\chi_1(x) = \frac{1}{\sqrt{m^*(x)}}\,\frac{W_{1,2}(x)}{\mathcal{U}_1(x)}\,, \tag{41}$$

where $W_{1,2}(x) = \mathcal{U}_1(x)\mathcal{U}_2'(x) - \mathcal{U}_1'(x)\mathcal{U}_2(x)$ is the Wronskian of the functions $\mathcal{U}_1(x)$ and $\mathcal{U}_2(x)$. Plugging (41) into the formula (31) for K_2, after some transformations we obtain

$$K_2(x) = -\frac{d}{dx}\left[\ln \frac{W_{1,2}(x)}{\sqrt{m^*(x)}\mathcal{U}_1(x)}\right]. \tag{42}$$

After this $K = K_1 + K_2$ can be represented as

$$K = -\frac{\mathcal{U}_1'}{\mathcal{U}_1} + \frac{m^{*'}}{2m^*} + \frac{\mathcal{U}_1'}{\mathcal{U}_1} - \frac{W_{1,2}'}{W_{1,2}} = \frac{m^{*'}}{2m^*} - \frac{W_{1,2}'}{W_{1,2}}\,.$$

With this taking into account, making in (40) the next substitution:

$$\frac{1}{2}\,\frac{d}{dx}\frac{m'}{m^{*3/2}} = -\frac{d^2}{dx^2}\frac{1}{m^{*1/2}}\,,$$

after some manipulations the new potential can be expressed as:

$$V_2(x) = V(x) - \frac{2}{\sqrt{m^*}}\frac{d}{dx}\left[\frac{1}{\sqrt{m^*}}\frac{d}{dx}\ln W_{1,2}(x)\right]. \tag{43}$$

By using (34) find now the corresponding functions $\phi_2(x)$, $\phi_2 = (1/\sqrt{m^*})$ $(d/dx + K_2)\phi_1$. By analogy with χ_1 the function $\phi_1(x)$ can be written in terms of the Wronskian $W_{1,\mathcal{E}}(x) = \mathcal{U}_1(x)\phi'(\mathcal{E},x) - \mathcal{U}_1'(x)\phi(\mathcal{E},x)$:

$$\phi_1(x) = \frac{1}{\sqrt{m^*(x)}}\,\frac{W_{1,\mathcal{E}}(x)}{\mathcal{U}_1(x)}\,. \tag{44}$$

Let us now calculate the derivative of $\phi_1 = \mathcal{L}_1\phi$, that is

$$(\mathcal{L}_1\phi)' = \left(\frac{1}{\sqrt{m^*}\mathcal{U}_1}\right)' W_{1,\mathcal{E}}(x) + \frac{1}{\sqrt{m^*}}\phi'' - \frac{1}{\sqrt{m^*}}\frac{\mathcal{U}_1''}{\mathcal{U}_1}\phi\,.$$

Making use of the last expression and the relation (42) for K_2, we obtain, after some simplification, the formula

$$\phi_2(x) = \frac{1}{m^*(x)}\left(\phi''(x) - \frac{\mathcal{U}_1''(x)\phi(x)}{\mathcal{U}_1(x)}\right) - \frac{d}{dx}\Big(\ln W_{1,2}(x)\Big)\frac{W_{1,\mathcal{E}}(x)}{m^*(x)\mathcal{U}_1(x)}\,. \tag{45}$$

It is easily seen from (43) and (45) that due to the 2-nd order Darboux transformation, the potential and solutions obtained in this way are completely expressed in terms of the known effective mass function $m^*(x)$ and the solutions $\mathcal{U}_1(x), \mathcal{U}_2(x), \phi(\mathcal{E}, x)$ to the initial equation, with no use of the solutions to the intermediate one with the potential $V_1(x)$.

Clearly, for the next transformation step to be made, one should take a new transformation function χ_2, that corresponds to the potential V_2. It can be obtained by applying the operator $\mathcal{L} = \mathcal{L}_2\mathcal{L}_1$ to the solutions $\mathcal{U}_3$ corresponding to the eigenvalue λ_3:

$$\chi_2 = \frac{1}{m^*(x)}\left(\mathcal{U}_3'' - \frac{\mathcal{U}_1''}{\mathcal{U}_1}\mathcal{U}_3\right) - \frac{d}{dx}\left(\ln W_{1,2}(x)\right)\frac{W_{1,3}(x)}{m^*(x)\mathcal{U}_1(x)}\,.$$

Then it can be used to produce a new transformed operator $\mathcal{L}_3 = (1/\sqrt{m^*})$ $(d/dx + K_3)$, $K_3 = -\chi_2'\chi_2^{-1}$ for generating new potential V_3 and solutions ϕ_3 and so on, according to (37)–(39).

3.4. The integral form of Darboux transformations

The transformed solutions (44) and (45) can be represented in the integral form. Let us consider to this end the generalized Schrödinger equation written down as

$$-\phi''(x) + m^*(x)V(x) = \mathcal{E}m^*(x)\phi(x)\,. \tag{46}$$

Multiplying both sides of the equation (46) for the function $\phi(\mathcal{E}, x)$ by $\mathcal{U}_1(x)$ at the energy of transformation λ_1 and subtracting from the obtained expression the equation similar to (46) but written down for $\mathcal{U}_1(x)$ and multiplied by $\phi(\mathcal{E}, x)$, we arrive at

$$\frac{d}{dx}W_{1,\mathcal{E}}(x) = (\lambda_1 - \mathcal{E})m^*(x)\mathcal{U}_1(x)\phi(\mathcal{E}, x)\,. \tag{47}$$

The last expression can be easily integrated:

$$W_{1,\mathcal{E}}(x) = (\lambda_1 - \mathcal{E})\int\limits_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx' + C\,. \tag{48}$$

Inserting the last expression into the formula for ϕ_1 (44), we arrive at the integral form of the 1st order transformed solutions:

$$\phi_1(x) = \frac{\left[C + (\lambda_1 - \mathcal{E})\int_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx'\right]}{m^*(x)\mathcal{U}_1(x)}\,. \tag{49}$$

Here C and a are some arbitrary constants. By analogy, applying this technique to the equation (3) for ϕ and $\mathcal{U}_1$, using (48) in (45), we get the integral form for the 2-nd order transformed solutions

$$\phi_2 = (\lambda_1 - \mathcal{E})\phi(x) - \frac{d}{dx}\Big(\ln W_{1,2}(x)\Big)\frac{C + (\lambda_1 - \mathcal{E})\int_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx'}{m^*(x)\,\mathcal{U}_1(x)}\,. \tag{50}$$

Here the integration limits depend on the boundary conditions. In particular, for regular solutions satisfying the boundary conditions $\phi(x = 0) = 0$, $\phi'(x)|_{x=0} = 1$, the lower integration limit is 0 and the upper one is x, while for the Jost solutions the integration limits are x and ∞, respectively. The constant C is determined by the values of the Wronskian at zero or at infinity, depending on the way the problem is posed. Notice that the functions $\mathcal{U}$ and ϕ can be chosen in such a way that the constant C becomes zero. Analogously to (47), one has $W'_{1,2}(x)/(\lambda_1 - \lambda_2) = m^*(x)\mathcal{U}_1(x)\mathcal{U}_2(x)$ and

$$\frac{W'_{1,2}(x)}{W_{1,2}(x)} = \frac{m^*(x)\mathcal{U}_1(x)\mathcal{U}_2(x)}{c_1 + \int^x dx' m^*(x')\mathcal{U}_1(x')\mathcal{U}_2(x')}\,. \tag{51}$$

Using the last formula and assuming $C = 0$, after some transformations one can represent ϕ_2 as follows:

$$\phi_2 = (\lambda_1 - \mathcal{E})\phi(x) - \frac{(\lambda_1 - \mathcal{E})\,\mathcal{U}_2(x)\int_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx'}{c_1 + \int^x dx' m^*(x')\mathcal{U}_1(x')\mathcal{U}_2(x')}\,. \tag{52}$$

Now let us consider the 2-nd order Darboux transformation at $\lambda_1 = \lambda_2 \equiv \lambda$. Earlier within the first-order procedure, we have already obtained two linear independent solutions (18) and (19) at $\lambda_1 = \lambda_2$. The second transformation can be made by means of a linear combination of the solutions η and $\hat{\eta}$

$$\chi_1(x) = c_1\eta(x) + \widehat{\eta}(x) = \frac{1}{\sqrt{m^*(x)}\mathcal{U}(x)}\left(c_1 + \int^x dx'\mathcal{U}^2(x')m^*(x')\right)\,. \tag{53}$$

In order to find the transformed potential and solutions, calculate $K_2 = -\chi_1'/\chi_1$ and $K = K_1 + K_2$

$$K(x) = \frac{m^{*'}(x)}{2m^*(x)} - \frac{m^*(x)\mathcal{U}_1^2(x)}{\left(c_1 + \int^x dx'\mathcal{U}^2(x')m^*(x')\right)}\,.$$

Plugging the last expression into the formula (40) which defines the potential, we arrive at

$$V_2(x) = V(x) - \frac{2}{\sqrt{m^*(x)}}\frac{d}{dx}\left(\frac{1}{\sqrt{m^*(x)}}\frac{\mathcal{U}^2(x)m^*(x)}{(c_1 + \int^x dx'\mathcal{U}^2(x')m^*(x')}\right)\,. \tag{54}$$

The operator $\mathcal{L}_2$ (31) with χ_1 defined by (53), acts on the function ϕ_1 represented by its integral form (49) so that it leads to

$$\phi_2 = (\lambda - \mathcal{E})\phi(x) - \frac{\mathcal{U}(x)(\lambda - \mathcal{E}) \int^x dx' \mathcal{U}(x') m^*(x') \phi(x')}{c_1 + \int^x dx' \mathcal{U}^2(x') m^*(x')} \,. \tag{55}$$

It is worth mentioning, that the formulae for the new potential V_2 and the solution ϕ_2 can be obtained directly from the relations (43) and (45), if one takes into account that at $\lambda_1 = \lambda_2 \equiv \lambda$, the expression (51) for $(d/dx)\ln W_{1,2}(x)$ should be changed by

$$\frac{d}{dx} \ln P(x) = \frac{m^*(x)\mathcal{U}^2(x)}{c_1 + \int^x dx' \mathcal{U}^2(x') m^*(x')} \,,$$

with $P(x) = c_1 + \int^x dx' \mathcal{U}^2(x') m^*(x')$.

Without loss of generality one can take a linear combination of the functions η and $\hat{\eta}$ as $\chi_1(x) = \eta(x) + C\widehat{\eta}(x)$, and change $(\lambda - \mathcal{E})\phi(x) \to \phi(x)$ for simplification. Then formulae (54) and (55) can be rewritten as

$$V_2(x) \; = \; V(x) - \frac{2}{\sqrt{m^*(x)}} \frac{d}{dx} \left(\frac{1}{\sqrt{m^*(x)}} \frac{C\mathcal{U}^2(x) m^*(x)}{(1 + C \int^x dx' \mathcal{U}^2(x') m^*(x')} \right), \tag{56}$$

$$\phi_2 \; = \; \phi(x) - \frac{\mathcal{U}(x) C \int^x dx' \mathcal{U}(x') m^*(x') \phi(x')}{1 + C \int_{x_0}^x dx' \mathcal{U}^2(x') m^*(x')} \,. \tag{57}$$

The constant C plays a role of a normalization constant or a difference between the normalization constants of the bound state λ for the potentials $V_2(x)$ and $V(x)$, respectively. Notice, the choice of arbitrary constants x_0 and C allows one to avoid the problems with zero-equal denominators, or in other words, it means that one can make transformations on an arbitrary bounded state and construct the potential without singularities. Notice also, that $m^*(x)$ itself does not lead to the singularities, because the effective mass $m^*(x) \neq 0$ and assumed to be smooth and at least twice differentiable function with respect to space-variable.

The solution of the equation (3) with the potential (56) at the energy of transformation λ can be achieved by means of operator $\mathcal{L}_2$ acting on the solution η from (18), obtained within the first transformation step

$$\eta_2(x) = \mathcal{L}_2 \eta = \frac{1}{\sqrt{m^*(x)}} \left(\frac{d}{dx} - \frac{\chi'(x)}{\chi(x)} \right) \frac{1}{\sqrt{m^*(x)}} \frac{1}{\mathcal{U}(x)} \,,$$

where χ' is assumed to be of the form (53). Finally we get

$$\eta_2(x) = - \frac{C\mathcal{U}(x)}{1 + C \int^x dx' m^*(x') \mathcal{U}^2(x')} \,. \tag{58}$$

One can rewrite the potential (56) and the solutions (57) in terms of $\eta_2(x)$ as

$$V_2(x) = V(x) + \frac{2}{\sqrt{m^*(x)}}\frac{d}{dx}[\sqrt{m^*(x)}\eta_2(x)\mathcal{U}(x)]\,, \tag{59}$$

$$\phi_2(x) = \phi(x) + \eta_2(x)C\int^x dx'\mathcal{U}(x')m^*(x')\phi(x')\,. \tag{60}$$

The relations (56)–(60) are the results of performing two subsequent transformations with the same energy. Therefore, it allows one to construct phase-equivalent potentials. Indeed, if $C = N_2^2 - N^2$ is the difference in normalization constants of the bound state λ for the potentials $V_2(x)$ and $V(x)$ respectively, then the formulae (56), (57) and (58) correspond to phase-equivalent potentials whose scattering data coincide and differ only by a normalization factor. Note, the phase-equivalent potentials have a different shape. They can be deeper and narrower or more shallow and wider and possess the same spectral data, except for normalization constants.

If we assume the transformation function $\mathcal{U}(x)$ to be taken at the energy of the bound state, which we would like to add to the initial spectrum, and $C = N^2$ is the corresponding normalization constant, then the formulae (56), (57) and (58) give the possibility to construct a potential with a new bound state λ provided the other spectral characteristics of the spectra produced by the potentials $V_2(x)$ and $V(x)$, coincide. Notice, that the function $\mathcal{U}(x)$, which is the solution of the initial equation with the potential V, has to be taken at the energy of transformation λ. To sum up, it can be said that by means of the technique described above, it is possible to remove some bound states or to add new ones and to construct the phase-equivalent potentials. The procedure can be repeated as many times as it is needed to construct a new potential with a desirable spectrum. Note, the generalized Darboux transformations under consideration turn into the ordinary expressions for potentials and solutions for the standard Schrödinger equation in a particular case of position-independent mass $m^*(x) = m \equiv \text{const}$.

Finally, it should be noted that using the technique presented in [12,13], it is not difficult to generalize these results to include a case when the second order transformation is applied simultaneously to N bound states. This, however, is beyond the scope of this paper and will be a subject of another publication.

4. Liouville transformation and QW potential reconstruction

In this section we propose an approach different from that developed in the previous section to the reconstruction of QWs potentials, which is based on the following observations. First, in most cases the number of bound states in QW is limited from above by some reasonable value of about 6–10 which, in its turn, is determined by the technological limitations. Secondly, in most cases one can safely suppose that effective mass $m^*(x)$ is a smooth and, at least, twice differentiable weakly position-dependent function. Therefore, we can use the *Liouville transformation* together with algebraic Darboux transformations in order to reconstruct the QW potentials with a predetermined spectrum. This approach is applicable to the case of the straightforward reconstruction of QW potential discussed previously, as well as to the case when the Hermitian kinetic energy operator enters explicitly the generalized Schrödinger equation.

Let us start from the equation of the form

$$-\frac{d^2}{dq^2}\Phi(q) = m^*(q)\lambda\Phi(q)\,, \tag{61}$$

where q stands for space variable. Thus, one can interpret this equation as a generalized Schrödinger equation with the potential $V \equiv 0$. Introduce now new variables and a new function as follows (this is one of the special cases of Liouville transformation):

$$m^* = p^2\,, \qquad \sqrt{m^*} = \frac{dx}{dq}\,, \qquad \Phi(q) = p^{-1/2}\Psi(x)\,. \tag{62}$$

Then, taking into account (62), the equation (61) can be reduced to the following:

$$-p^{3/2}\left[\Psi^{''}(x) + \frac{1}{2}\left\{\frac{1}{2}\left(\frac{p_x^{'}}{p}\right)^2 - \frac{p_x^{''}}{p}\right\}\Psi(x)\right] = p^2\lambda p^{-1/2}\Psi(x)\,,$$

which can be written down as a standard Schrödinger equation

$$-\Psi^{''}(x) + V(x)\Psi(x) = \lambda\Psi(x)\,,$$

where the potential $V(x)$ is of the form:

$$V(x) = \frac{1}{2}\left[\frac{p_x^{''}}{p} - \frac{1}{2}\left(\frac{p_x^{'}}{p}\right)^2\right]\,.$$

Since

$$\frac{p^{''}}{p} = \frac{d}{dx}\left(\frac{p^{'}}{p}\right) + \left(\frac{p^{'}}{p}\right)^2\,,$$

the potential $V(x)$ can also be represented as

$$V(x) = \frac{1}{2}\left[\frac{d^2}{dx^2}\ln p + \frac{1}{2}\left(\frac{d}{dx}\ln p\right)^2\right], \tag{63}$$

or returning back to the variable m^*,

$$V(x) = \frac{1}{4}\left[\frac{m^{*''}}{m^*} - \frac{3}{4}\left(\frac{m^{*'}}{m^*}\right)^2\right].$$

Now assuming the solution of the eigenvalue problem to the Schrödinger equation with this potential is known, one can add or subtract one by one as many bound states as needed, using the algebraic Darboux transformations described in the previous section.

As for the effective mass theory with the Hermitian kinetic energy operator is considered, it seems that a consensus among the specialists has been already achieved, since in the majority of corresponding studies the following form of the Hamiltonian is used (see, for example, [10]):

$$H = \left[\hat{P}\frac{1}{m^*(q)}\hat{P}\right] + V(q),$$

where $\hat{P}$ is a momentum operator. Then, in order to use the Liouville transformation approach, one should start with the equation

$$-\frac{d}{dq}\left\{\frac{1}{m^*(q)}\frac{d}{dq}\Phi\right\} = \lambda\Phi.$$

Making the next substitutions

$$p = \frac{1}{\sqrt{m^*(q)}} = \frac{dq}{dx}, \qquad \Phi = p^{-1/2}\Psi,$$

after some manipulations similar to that which were previously done, one get the standard Schrödinger equation

$$-\Psi''(x) + V(x)\Psi(x) = \lambda\Psi(x),$$

with the potential defined as in (63) but with $p(q) = 1/(\sqrt{m^*(q)})$. Finally we obtain

$$V(x) = \frac{1}{4}\left[-\frac{m^{*''}}{m^*} + \frac{5}{4}\left(\frac{m^{*'}}{m^*}\right)^2\right].$$

5. Conclusion

The basic elements of contemporary micro- and nanoelectronics are low-dimensional structures which are the structures composed of QWs, quantum wires and quantum dots and produced by means of various techniques including the most impressive one, molecular beam epitaxy. The entirety of such methods and techniques are sometimes termed as *Quantum Engineering* or *Quantum Technology.* One of the most important issues of quantum engineering is the construction of multi-quantum well structures possessing desirable properties. This problem appears in different contexts, ranging from the construction of multi-level computer logic to photovoltaics of third generation [18,19]. From the theorist's point of view, the problem can be formulated as follows: assume one requires a definite spectrum of QW, because it is determined by some specific needs and circumstances. Can one reconstruct the QW potential which supports this very spectrum? In this paper we answer this question in affirmative and outline a possible strategy of the QW potential reconstruction, if the spectrum of QW is predetermined.

The proposed approach is based on the combination of various techniques such as *Inverse Scattering Problem Method*, *Darboux* and *Liouville* transformation. Bearing in mind that the effective masses of charge carriers in the subsequent layers of different materials which make QW, are different, we match the intertwining operator technique, in order to take into account the position-dependent mass in Eq. (3). The first- and second-order of Darboux transformations, as well as the chain of Darboux transformations are considered, and interrelation between the differential and integral transformations is established. The developed approach allows one to construct phase-equivalent potentials and to add (or if necessary, to remove) some states to (or from) the spectrum supported by the initial potential, whose form can be established for instance, by means of ISP-method.

The another possible way to take into account the position-dependent masses of charge carriers is to use the Liouville transformation. It also allows one to incorporate and treat on the same footing the proper form of Hermitian kinetic energy operator. This operator appears in the context of applicability to heterostructures the effective mass approximation, the subject of today's research activities.

In this paper we have formulated the basic concepts and developed the necessary mathematical tools. The next step of this work will be to find families of exactly solvable models, *e.g.* a class of shape invariant potentials. Note, the presented Darboux transformations in a particular case of a position-independent mass turn into the ordinary expressions for potentials and solutions for the standard Schrödinger equation. More thorough numerical examinations of specific cases are required and it will be done elsewhere.

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