Reconstruction of Quantum Well Potentials via the Intertwining Operator Technique

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Abstract

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? We outline the possible strategy of the QW potential shape reconstruction, if the spectrum of QW is given in advance.

By using the intertwining operator technique we show how to construct the quantum well potential with a desired spectrum for the Schrödinger equation with a position-dependent effective mass. The first- and second-order Darboux transformations, supersymmetry, chain of Darboux transformations are considered for the Schrödinger equation with a nonconstant mass. An interrelation is established between the differential and integral transformation operators. The method allows one to generate potentials with additional and with removal bound states in comparison with the spectrum of an initial potential as well as to construct phase-equivalent potentials and provides a systematic procedure for generating new exactly solvable models.

1 Introduction

The study of quantum systems with position-dependent effective mass has attracted recently considerable attention due to its possible applications in different areas of research. In particular, the Schrödinger Eq. with space-variable-dependent effective mass is widely used for the description of electronic properties of semiconductor heterostructures [1] - [3]. The concept of effective mass is connected to an energy-dependent potentials [4]– [8] and to the energy density functional approach, which are used in nuclear physics [11], helium clusters and metal clusters [12]–[15].

As for the semiconductor heterostructures is concerned, the progress in this area became possible, 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 atomic precision. The last one, in its turn, provides the opportunity to produce a variety of *low-dimensional structures*, ranging from a heterojunction formed at a single interface, through quantum wells (QW) 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, there is often need to have a specific kind of spectrum known beforehand. The problem is: how to produce the QW with a predetermined 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 on the base of the intertwining operator technique for generalized Schrödinger Eq. with the position-dependent effective mass. As is known, the method of intertwining operators is closely related

to the Darboux transformations and the supersymmetry method in quantum mechanics. Some important works which were done already, should be mentioned in this connection. Among them are [6]-[8], devoted to the Darboux transformations in the (λ^2, E) plane and Ref. [4, 5, 9] in which the supersymmetry and phase-equivalent potentials for the Eqs. with the linear energy-dependent potentials were discussed. Some exactly solvable models with the smooth potential and mass steps have been presented in [16]–[18] and for the reconstruction of energy-dependent potentials in [4]–[10]. However, no substantial study of the potential reconstruction problem for the Schrödinger Eq. with a space-variable dependent mass has been reported yet. In particular, the intertwining technique for generalized Schrödinger Eq. has not been elaborated, the chain of Darboux transformations have not been considered and the interrelations between the differential and integral transformation operators have not been established for the Darboux transformations of different order. In this work we try to fill in these gaps.

2 The generalized Darboux transformations

2.1 First-order Darboux transformation

Let us start with the equation with a position-dependent effective mass:

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

where $m^*(x)$ is a position-dependent mass, $V(x)$ denotes the potential and $\hbar^2/2 = 1$. This equation is reduced to the generalized Schrödinger Eq. of the form:

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

where $v(x) = V(x)m^*(x)$. In fact, it is the Schrödinger Eq. with linearly energy-dependent potentials. The Darboux transformations for the Schrödinger Eq. with variable values of energy and angular momentum were proposed in [6] and in a more general form in [7]. Then in Refs. [4, 5, 8] 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 the universal approach to creating new exactly solvable models and can be applied to the operators of a very general form (see for example [19]-[22]). In this paper, we apply the intertwining operator technique to the equation (1) 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 Eq. (1) with the given potential $V(x)$ and position dependent $m^*(x)$ are known and we would like to solve a similar problem for another Hamiltonian $\widetilde{\mathcal{H}}$ containing a new potential $\widetilde{V}(x)$ and the spectrum which probably differs from the spectrum of the Hamiltonian (1) by a single quantum state:

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

We start with standard intertwining relations

$$\mathcal{L}\mathcal{H} = \widetilde{\mathcal{H}}\mathcal{L}, \tag{3}$$

$$\widetilde{\phi}(x) = \mathcal{L}\phi(x), \tag{4}$$

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

$$\mathcal{L} = B(x)d/dx + A(x), \tag{5}$$

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 (4) by applying $\mathcal{L}$ to the known solutions ϕ. To find the explicit form of $\mathcal{L}$,

we use the Eqs. (1), (2) and the intertwining relations ((3), (4):

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

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 the next system of Eqs.:

$$\frac{1}{m^*}A+2\frac{1}{m^*}B^{'}=B\Big(\frac{1}{m^*}\Big)^{'}+A\frac{1}{m^*}, \tag{6}$$
$$\frac{1}{m^*}2A^{'}+\frac{1}{m^*}B^{''}-\widetilde{V}B=-BV, \tag{7}$$
$$-\frac{1}{m^*}A^{''}+\widetilde{V}A=AV+BV^{'}. \tag{8}$$

From (6) it immediately follows that

$$2B^{'}/B=-m^{*'}/m^*, B=C/\sqrt{m^*}, \tag{9}$$

where C is an arbitrary constant. From (7), (8) one gets

$$\widetilde{V}=V+\frac{1}{m^*}\frac{B^{''}}{B}+\frac{1}{m^*}\frac{2A^{'}}{B} \tag{10}$$

and

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

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 Eq.

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

Taking into account the relation $V=v/m^*$ and the first of the relations (9), 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

$$(1/m^*)\Big(-K^{'}+K^2-v\Big)=\mu,$$

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

$$-\frac{1}{m^*(x)}\mathcal{U}^{''}(x)+V(x)\mathcal{U}(x)=\lambda\mathcal{U}(x). \tag{11}$$

Here $\mathcal{U}(x)$ is supposed to be invertible at all x. The last equation then is nothing else but the initial Eq. (1) 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 (11) are known for the given values of λ. Having found the explicit form of B (see (9), 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 Eq. (2) are defined up to an arbitrary constant C. Without loss of generality, we can put it safely equal to unity. After this we have

$$B(x)=\frac{1}{\sqrt{m^*(x)}},\ A(x)=\frac{K(x)}{\sqrt{m^*(x)}},\ K=-\left(\ln\mathcal{U}(x)\right)'. \tag{12}$$

To make further transformations, let us calculate $B''/B=\sqrt{m^*}(1/\sqrt{m^*})''$. Using this and (12) in (5), (10) and (4) we construct the intertwining operator $\mathcal{L}$, the transformed potential $\widetilde{V}(x)$ and the solutions $\widetilde{\phi}$ in the form:

$$\mathcal{L}=\frac{1}{\sqrt{m^*}}\left(\frac{d}{dx}+K\right)=\frac{1}{\sqrt{m^*}}\left(\frac{d}{dx}-\left(\ln\mathcal{U}\right)'\right), \tag{13}$$

$$\begin{aligned}\widetilde{V}&=V+\frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}}+2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K\right)\right] \qquad (14)\\ &=V+\frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}}-2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}(\ln\mathcal{U})'\right)\right],\end{aligned}$$

$$\widetilde{\phi}=\mathcal{L}\phi=\frac{1}{\sqrt{m^*}}\left[\frac{d}{dx}-\left(\ln U\right)'\right]\phi. \tag{15}$$

It follows immediately from (15) that $\mathcal{L}\mathcal{U}=0$. In order to obtain the solution of Eq. (2) at the energy of transformation λ, we shall use the second linear independent solution to (1), 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

$$\eta(x)=\mathcal{L}\hat{\mathcal{U}}(x)=\frac{1}{\sqrt{m^*(x)}}\frac{1}{\mathcal{U}(x)}. \tag{16}$$

Once η is found, one can get a second solution of (2) at the energy of transformation λ. By using the Liouville's formula once more, one gets

$$\hat{\eta}(x)=\eta(x)\int^x dx'|\eta^2|^{-1}=\frac{1}{\sqrt{m^*(x)}\mathcal{U}(x)}\int^x dx'\mathcal{U}(x')m^*(x')\mathcal{U}(x'). \tag{17}$$

Hence, the information about all solutions of the initial Eqs. (1) provides the knowledge of all solutions of the transformed Eqs. (2). As in the case of Schrödinger Eq., 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 (15)). The difference is that in our case $\mathcal{L}$ includes the 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 (16) 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 any 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 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 bound state with respect to the initial Hamiltonian by using factorization of Hamiltonians and supersymmetry.

2.2 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 $(\frac{d}{dx})^\dagger = -\frac{d}{dx}$. In our case, the scalar product of functions is defined by not the 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 $\mathcal{L} = \frac{1}{\sqrt{m^*}}(\frac{d}{dx} + K)$ is determined as

$$\mathcal{L}^\dagger = \frac{1}{\sqrt{m^*}} \left(-\frac{d}{dx} - \frac{m^{*\prime}}{2m^*} + K \right). \tag{18}$$

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

$$\mathcal{L}^\dagger \mathcal{L} = -\frac{1}{m^*}\frac{d^2}{dx^2} + \frac{1}{m^*}(-K' + K^2), \tag{19}$$

$$\mathcal{L}\mathcal{L}^\dagger = -\frac{1}{m^*}\frac{d^2}{dx^2} + \frac{1}{m^*}(K' + K^2) - \frac{1}{2}\frac{m^{*\prime\prime}}{m^{*2}} + \frac{3}{4}\frac{m^{*\prime} m^{*\prime}}{m^{*3}} - \frac{m^{*\prime}}{m^{*2}} K. \tag{20}$$

Express the potential V from Eq. (11) 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

$$V = \frac{1}{m^*}(-K' + K^2) + \lambda \ . \tag{21}$$

Substitution of (21) into (14) leads to the following representation of the transformed potential:

$$\widetilde{V} = \frac{1}{m^*}(K' + K^2) + \frac{1}{\sqrt{m^*}}\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} - \frac{m^{*\prime}}{m^{*2}} K + \lambda \ . \tag{22}$$

Using (21) and (22), after some transformations the formulae (19 and (20) can be rewritten as

$$\mathcal{L}^\dagger \mathcal{L} = -\frac{1}{m^*}\frac{d^2}{dx^2} + V - \lambda = \mathcal{H} - \lambda; \tag{23}$$

$$\mathcal{L}\mathcal{L}^\dagger = -\frac{1}{m^*}\frac{d^2}{dx^2} + \widetilde{V} - \lambda = \widetilde{\mathcal{H}} - \lambda. \tag{24}$$

From (24) one can obtain the intertwining relation

$$\mathcal{H}\mathcal{L}^\dagger = \mathcal{L}^\dagger \widetilde{\mathcal{H}}\,, \tag{25}$$

which means that the operator $\mathcal{L}^\dagger$ is also the transformation operator and realizes the transformation of the solutions of Eq. (2) to solutions of (1), $\phi \propto \mathcal{L}^\dagger \widetilde{\phi}$. As one can see from the comparison of the relations (13) and (18), 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

Eqs. (2) at the energy λ with the potential $\widetilde{V}$ determined by (14). For this aim let us express K in terms of η, by means of (16).

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

Using this in (13) and (18), we obtain

$$\mathcal{L} = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + \frac{m^{*'}}{2m^*} + \frac{\eta'}{\eta}\right), \quad \mathcal{L}^\dagger = \frac{1}{\sqrt{m^*}}\left(-\frac{d}{dx} + \frac{\eta'}{\eta}\right) \tag{26}$$

Evidently, the function η is also a transformation function. It is clear that $\mathcal{L}^\dagger\eta = 0$, i.e., η belongs to the kernel of the operator $\mathcal{L}^\dagger$. As one can see from (26) and (17), the application of the operator $\mathcal{L}^\dagger$ to the second linearly independent solution $\hat{\eta}$ to Eq. (2) 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 Eqs. (1) and (2) is established, and these are the operators $\mathcal{L}$ and $\mathcal{L}^\dagger$, which produce the correspondence.

Note, one can interchange the role of the initial and final Eqs. The function η becomes 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 (2) to the solutions of (1). So, if within the first procedure (13)–(15) we constructed the potential $\widetilde{V}$ with one bound state removed, now we can construct the potential V with an additional bound state.

2.3 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

$$\mathcal{L} = \mathcal{L}_2\mathcal{L}_1, \tag{27}$$

where $\mathcal{L}_1$ is actually $\mathcal{L}$ defined in (13)

$$\mathcal{L}_1 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_1\right), \quad K_1 = -\frac{\mathcal{U}_1'}{\mathcal{U}_1}, \tag{28}$$

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

$$\mathcal{L}_2 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_2\right), \quad K_2 = -\frac{\chi_1'}{\chi_1}, \tag{29}$$

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 Eq. (11) or (1) with the eigenvalue λ_2

$$\chi_1 = \mathcal{L}_1\mathcal{U}_2 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} - \frac{\mathcal{U}_1'}{\mathcal{U}_1}\right)\mathcal{U}_2. \tag{30}$$

Clearly, χ_1 is the solution of Eq. (11) with the potential V_1, defined as in (14), and χ_1 can be taken as a new transformation function for the Hamiltonian $\mathcal{H}_1$ to generate a new potential

$$V_2 = V_1 + \frac{1}{\sqrt{m^*(x)}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*(x)}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*(x)}}K_2\right)\right] \tag{31}$$

and corresponding solutions

$$\phi_2 = \mathcal{L}_2\phi_1 = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_2\right)\phi_1, \quad \phi_1 = \mathcal{L}_1\phi. \tag{32}$$

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

$$\phi_1 = \frac{1}{\sqrt{m^*}}\left[\frac{d}{dx} - (\ln U)_1^{'}\right]\phi. \tag{33}$$

In other words, the action of the second-order operator (27) on the solutions ϕ leads to the solutions of $\mathcal{H}_2$

$$\phi_2 = \mathcal{L}\phi = \mathcal{L}_2\mathcal{L}_1\phi. \tag{34}$$

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

$$V_m = V_{m-1} + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K_{m-1}\right)\right], \tag{35}$$

$$\phi_m = \mathcal{L}\phi = \mathcal{L}_m\phi_{m-1} = \mathcal{L}_m\mathcal{L}_{m-1}...\mathcal{L}_1\phi, \tag{36}$$

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

$$\mathcal{L} = \mathcal{L}_m\mathcal{L}_{m-1}...\mathcal{L}_1, \quad \mathcal{L}_m = \frac{1}{\sqrt{m^*}}\left(\frac{d}{dx} + K_m\right), \quad K_m = -\chi'_{m-1}\chi_{m-1}^{-1}. \tag{37}$$

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

Consider now the 2-nd order transformation in detail. Using the explicit expression for V_1 which appears in the 1-st order transformation, we get for the potential V_2:

$$V_2 = V + \frac{2}{\sqrt{m^*}}\left(\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}}\right) + \frac{2}{\sqrt{m^*}}\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K\right), \tag{38}$$

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

$$\chi_1(x) = \frac{1}{\sqrt{m^*(x)}}\frac{W_{1,2}(x)}{\mathcal{U}_1(x)}, \tag{39}$$

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 (39) into the formula (29) for K_2, after some transformations we obtain

$$K_2(x) = -\frac{d}{dx}\left[\ln\frac{W_{1,2}(x)}{\sqrt{m^*(x)}\mathcal{U}_1(x)}\right]. \tag{40}$$

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 (38) the next substitution:

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

after some manipulations the new potential can be expressed as:

$$V_2(x) = V(x) - \frac{2}{\sqrt{m^*}}\frac{d}{dx}\left[\frac{1}{\sqrt{m^*}}\frac{d}{dx}\ln W_{1,2}(x)\right]. \tag{41}$$

By using (32) find now the corresponding functions $\phi_2(x)$. By analogy with χ_1 the function $\phi_1(x)$ can be written in terms of the Wronskian $W_{1,\mathcal{E}}(x) = \mathcal{U}_1(x)\phi'(\mathcal{E},x) - \mathcal{U}_1'(x)\phi(\mathcal{E},x)$:

$$\phi_1(x) = \frac{1}{\sqrt{m^*(x)}} \frac{W_{1,\mathcal{E}}(x)}{\mathcal{U}_1(x)}. \tag{42}$$

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

$$(\mathcal{L}_1\phi)' = \frac{1}{\sqrt{m^*}\mathcal{U}_1'} + \frac{1}{\sqrt{m^*}}\phi'' - \frac{1}{\sqrt{m^*}}\frac{\mathcal{U}_1''}{\mathcal{U}_1}\phi.$$

Making use of the last expression and the relation (40) for K_2, we obtain, after some simplification, the formula

$$\phi_2(x) = \frac{1}{m^*(x)}\left(\phi''(x) - \frac{\mathcal{U}_1''(x)\phi(x)}{\mathcal{U}_1(x)}\right) - \frac{d}{dx}\Big(\ln W_{1,2}(x)\Big)\frac{W_{1,\mathcal{E}}(x)}{m^*(x)\mathcal{U}_1(x)}. \tag{43}$$

It is easily seen from (41) and (43) 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 $\mathcal{V}_3$:

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

Then it can be used to produce a new transformed operator $\mathcal{L}_3 = \frac{1}{\sqrt{m^*}}\left(d/dx + K_3\right), \quad K_3 = -\chi_2'\chi_2^{-1}$ for generating new potential V_3 and solutions ϕ_3 and so on, according to (35)–(37).

2.4 The integral form of Darboux transformations

The transformed solutions (42) and (43) can be represented in the integral form. Let us consider to this end the generalized Schrödinger equation written down as

$$-\phi''(x) + m^*(x)V(x)\phi(x) = \mathcal{E}m^*(x)\phi(x). \tag{44}$$

Multiplying both sides of the equation (44) 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 (44) but written down for $\mathcal{U}_1(x)$ and multiplied by $\phi(\mathcal{E},x)$, we arrive at

$$\frac{d}{dx}W_{1,\mathcal{E}}(x) = (\lambda_1 - \mathcal{E})m^*(x)\mathcal{U}_1(x)\phi(\mathcal{E},x). \tag{45}$$

The last expression can be easily integrated:

$$W_{1,\mathcal{E}}(x) = (\lambda_1 - \mathcal{E})\int_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx' + C. \tag{46}$$

Inserting the last expression into the formula for ϕ_1 (42), we arrive at the integral form of the 1st order transformed solutions:

$$\phi_1(x) = \frac{\left[C + (\lambda_1 - \mathcal{E})\int_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx'\right]}{m^*(x)\mathcal{U}_1(x)}. \tag{47}$$

Here C and a are some arbitrary constants. By analogy, applying this technique to the equation (1) for ϕ and $\mathcal{U}_1$, using (46) in (43), we get the integral form for the 2-nd order transformed solutions

$$\phi_2(x) = (\lambda_1 - \mathcal{E})\phi(x) - \frac{d}{dx}\Big(\ln W_{1,2}(x)\Big)\frac{(C + (\lambda_1 - \mathcal{E})\int_a^x m^*(x')\mathcal{U}_1(x')\phi(x')dx')}{m^*(x)\mathcal{U}_1(x)}. \tag{48}$$

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 (45), one has $W'_{1,2}(x)/(\lambda_1 - \lambda_2) = m^*(x)\mathcal{U}_1(x)\mathcal{U}_2(x)$ and

$$\frac{W'_{1,2}(x)}{W_{1,2}(x)} = \frac{m^*(x)\mathcal{U}_1(x)\mathcal{U}_2(x)}{c_1 + \int^x dx' m^*(x')\mathcal{U}_1(x')\mathcal{U}_2(x')}. \tag{49}$$

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

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

Now let us consider the 2-nd order Darboux transformation at $\lambda_1 = \lambda_2 \equiv \lambda$. Earlier within the first-order procedure, we already obtained two linear independent solutions (16) and (17) at $\lambda_1 = \lambda_2$. The second transformation can be made by means of a linear combination of the solutions η and $\hat{\eta}$

$$\chi_1(x) = c_1\eta(x) + \widehat{\eta}(x) = \frac{1}{\sqrt{m^*(x)}\mathcal{U}(x)}\left(c_1 + \int^x dx'\mathcal{U}^2(x')m^*(x')\right). \tag{50}$$

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

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

Plugging the last expression into the formula (38) which defines the potential, we arrive at

$$V_2(x) = V(x) - \frac{2}{\sqrt{m^*(x)}}\frac{d}{dx}\left(\frac{1}{\sqrt{m^*(x)}}\frac{\mathcal{U}^2(x)m^*(x)}{(c_1 + \int^x dx'\mathcal{U}^2(x')m^*(x')}\right). \tag{51}$$

The operator $\mathcal{L}_2$ (29) with χ_1 defined by (50), acts on the function ϕ_1 represented by its integral form (47) so that it leads to

$$\phi_2(x) = (\lambda - \mathcal{E})\phi(x) - \frac{\mathcal{U}(x)(\lambda - \mathcal{E})\int^x dx'\mathcal{U}(x')m^*(x')\phi(x')}{c_1 + \int^x dx'\mathcal{U}^2(x')m^*(x')}. \tag{52}$$

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 (41) and (43), if one takes into account that at $\lambda_1 = \lambda_2 \equiv \lambda$, the expression (49) for $\frac{d}{dx}\ln W_{1,2}(x)$ 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 the 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 (51) and (52) can be rewritten as

$$V_2(x) = V(x) - \frac{2}{\sqrt{m^*(x)}}\frac{d}{dx}\left(\frac{1}{\sqrt{m^*(x)}}\frac{C\mathcal{U}^2(x)m^*(x)}{(1 + C\int^x dx'\mathcal{U}^2(x')m^*(x')}\right). \tag{53}$$

$$\phi_2 = \phi(x) - \frac{\mathcal{U}(x)C\int^x dx'\mathcal{U}(x')m^*(x')\phi(x')}{1 + C\int_{x_o}^x dx'\mathcal{U}^2(x')m^*(x')}. \tag{54}$$

The constant C plays the role of a normalization constant or the 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_o 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 bound 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 (1) with the potential (53) at the energy of transformation λ can be achieved by means of operator $\mathcal{L}_2$ acting on the solution η from (16), 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 (50). Finally we get

$$\eta_2(x) = -\frac{C\mathcal{U}(x)}{1 + C\int^x dx'm^*(x')\mathcal{U}^2(x')}. \tag{55}$$

One can rewrite the potential (53) and the solutions (54) in terms of $\eta_2(x)$ as

$$V_2(x) = V(x) + \frac{2}{\sqrt{m^*(x)}}\frac{d}{dx}[\sqrt{m^*(x)}\eta_2(x)\mathcal{U}(x)], \tag{56}$$

$$\phi_2(x) = \phi(x) + \eta_2(x)C\int^x dx'\mathcal{U}(x')m^*(x')\phi(x'). \tag{57}$$

The relations (53) – (57) are the results of performing two subsequent transformations with the same energy. Therefore, it allows one to construct the 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 (53), (54) and (55) 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 more deeper and narrow 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 (53), (54) and (55) 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, one can remove some bound states from the spectrum or to add new ones to it 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.

3 Conclusion

The basic elements of contemporary micro- and nanoelectronics are the 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 then the QW-potential which supports this very spectrum? In this paper we answer this question in affirmative and outline the possible strategy of the QW-potential reconstruction, if the spectrum of QW is predetermined.

The proposed approach is based on the generalized Darboux transformation technique. 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. (1). 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 inverse scattering problem method.

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