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Darboux transformations for reconstruction of quantum well potentials

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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 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.

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1. Introduction

In the last few years the rapid progress has been achieved in *nanoelectronics*. This 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, is able 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 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 equation with the position-dependent effective mass. As is known, the method of intertwining relations is equivalent to the Darboux transformations and is closely related to the supersymmetry method in

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quantum mechanics. Some investigations should be noted in this direction. Among them are Darboux transformations in the (λ^2, E) plane [11]-[13], supersymmetry and phase-equivalent potentials for equations with linear energy-dependent potentials [14]. However, no successional study of the potential reconstruction problem for the Schrödinger equation with a nonconstant mass has not been made yet. In particular, the interrelations between the differential and integral transformation operators have not been established, the chain of Darboux transformations have not been constructed. In this work we try to fill in the gaps in this field.

2. Reconstruction of quantum well potentials using intertwining operator technique

2.1. Reconstruction of QW potentials in part of the spectrum

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 $\epsilon_1, \epsilon_2, ...\epsilon_N$ of the levels within the QW ;
(ii) $\lim_{x\to\infty} V_N = E_0$. The last value can be considered as the depth of QW.

Arranging the binding energies $k^2 = E_0 - \epsilon_n$ in descending order so that $k_1 > k_2 > ... > k_N$, 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:

$$V_N(x, E_0) = E_0 - 2\frac{d^2}{dx^2}\ln D(x), \tag{1}$$

where

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

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

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

We shall 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 ISP-method in order to reconstruct the potential $V_N(x, E_0)$, but we can suppose that the changes of a 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 "improved" one $\widetilde{V}(x)$, in order to have the spectrum needed.

2.2. First-order Darboux transformation and supersymmetry

Now we consider a *generalized* Schrödinger equation with the the position-dependent effective mass $m^*(x)$

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

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 Refs. 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 some special case of 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

$$\left(-\frac{1}{m_A^*}\frac{d^2}{dx^2} + E_c^A\right)\phi(x) = \mathcal{E}\chi(x)),$$
$$\left(-\frac{1}{m_B^*}\frac{d^2}{dx^2} + E_c^B\right)\phi(x) = \mathcal{E}\chi(x)),$$

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 $\Delta E_c = E_c^B - E_c^A$. 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

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

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 current. A correct set of matching conditions is

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

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 (2). In this section however, we apply the intertwining relation technique to construct a chain of exactly solvable Hamiltonians whose kinetic energy operators are not Hermitian, if $m^*(x)$ is space dependent.

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 $V(x)$ is supposed to be equal to $V_N(x, E_0)$. This equation is reduced to the generalized Schrödinger equation of the form:

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

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 the 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 $m^*(x)$ 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 (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

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

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

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

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

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:

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

and finally, to the 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

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

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

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

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 equation

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

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:

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

This one can be rewritten as

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

which means that

$$(1/m^*)\left(-K' + K^2 - v\right) = \mu,$$

where μ 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 $\mu = -\lambda$, one arrives at the equation

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

Here $\mathcal{U}(x)$ is supposed to be invertible at all x. The last equation then 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

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

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:

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

$$\widetilde{V} = V + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K\right)\right] \tag{16}$$

$$= V + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} - 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}(\ln\mathcal{U})'\right)\right],$$

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

It follows immediately from (17) that $\mathcal{L}\mathcal{U} = 0$. In order to obtain the 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 $\phi(x=0) = 0, \quad \phi'(x)|_{x=0} = 1$, 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

$$\begin{aligned}\hat{\eta}(x) &= \eta(x)\int^x dx'|\eta^2|^{-1} \qquad (19)\\ &= \frac{1}{\sqrt{m^*(x)}\mathcal{U}(x)}\int^x dx'\mathcal{U}(x')m^*(x')\mathcal{U}(x').\end{aligned}$$

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 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 (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 any new singularity, exept the singularities due to $V(x)$ (of course, we asumme $m^*(x) \neq 0$ 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 bounded state with respect to the initial Hamiltonian by using factorization of Hamiltonians and supersymmetry.

2.3. 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

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

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

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

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

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

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

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 also the transformation operator 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

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

Evidently, the function η is also a transformation function. 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 (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 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 equations. 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 (4) to the solutions of (3). So, if within the first procedure (15)–(17) we constructed the potential $\widetilde{V}$ with one bounded state removed , now we can construct the potential V with an addional bounded state.

2.4. 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)

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

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

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

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

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

It is clear that 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

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

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

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

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

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

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

and $K_m = -\chi'_{m-1}\chi^{-1}_{m-1}$.
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 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:

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

after some manipulations the new potential can be expressed as:

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

By using (34) 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 $W_{1,\mathcal{E}}(x) = \mathcal{U}_1(x)\phi'(\mathcal{E}, x) - \mathcal{U}'_1(x)\phi(\mathcal{E}, x)$:

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

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 (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 $\mathcal{V}_3$:

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

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

2.5. 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:

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

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

$$\phi_2(x) = (\lambda_1 - \mathcal{E})\phi(x) - \tag{50}$$

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

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:

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

Now let us consider the 2-nd order Darboux transformation at $\lambda_1=\lambda_2\equiv\lambda$. Earlier within the first-order procedure, we 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 $\hat\eta$

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

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

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

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

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

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 $\frac{d}{dx}\ln W_{1,2}(x)$ 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 (54) and (55) can be rewritten as

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

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

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 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 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 (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 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 bounded 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 bounded 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 bounded 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.

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 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 the possible strategy of the QW potential reconstruction, if the spectrum of QW is predetermined.

The proposed approach is based on the combination of *Inverse Scattering Problem Method* and *Darboux* 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.

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