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MATHEMATICAL MODELING OF QUANTUM WELL POTENTIALS VIA GENERALIZED DARBOUX TRANSFORMATIONS

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The Darboux transformation operator technique is applied to the generalized Schrödinger equation with a position-dependent effective mass and with linearly energy-dependent potentials. It is shown how to construct the quantum well potentials in nanoelectronics with a given spectrum. The method is illustrated by several examples.

Техника преобразований Дарбу применяется к обобщенному уравнению Шредингера с эффективной массой, зависящей от пространственной переменной, и с потенциалами, зависящими от энергии. Показано, как конструировать квантовые потенциальные ямы с заданным спектром, необходимые в наноэлектронике. Метод проиллюстрирован на нескольких примерах.

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INTRODUCTION

The problem of generating exactly solvable models in quantum mechanics has been considered for more than 50 years starting from the Schrödinger paper [1]. Many advances have been made in the area of their different applications and in the field of classifying quantum mechanical potentials according to their symmetry properties. Recently the research efforts on this topic have been considerably intensified due to the rapid development of nanoelectronics, the basic elements of which are low-dimensional structures such as quantum wells, wires, dots and superlattices [2,3]. For investigation of nonuniform semiconductors, in which carrier effective mass depends on position, the generalized Schrödinger equation with position-dependent effective mass is used [5–12].

One of the most important problems of quantum engineering is the construction of multiquantum well structures possessing desirable spectral properties. The technique of Darboux transformations [9–14] allows one to model quantum well potentials with the given spectrum. The method of Darboux transformations allows one to eliminate or add bound states (see, e.g., [9,10]) or construct phase-equivalent potentials whose scattering data coincide and differ only by normalization factors (e.g., [13, 15, 16]). The paper is devoted to an application of the Darboux transformations (or an intertwining operator technique) to the generalized Schrödinger equation. We use concrete examples to demonstrate how to generate potentials with required spectrum.

1. CHAIN OF DARBOUX TRANSFORMATIONS

Here we apply the intertwining operator technique to the equation with a position-dependent mass and weighted energy

$$-\left[\frac{d}{dx}\left(\frac{1}{m(x)}\right)\frac{d}{dx}\right]\phi(x)+v(x)\phi(x)=h(x)\,\mathcal{E}\phi(x), \tag{1}$$

in order to construct the potential which supports the desirable spectrum. Here $m(x)$ stands for the particle's effective mass; $h(x)$ and $v(x)$ denote the potentials; $\phi(x)$ is the wave function and $\mathcal{E}$ denotes the real-valued energy. In fact, (1) is the effective mass Schrödinger equation with linearly energy-dependent potential. This equation can be rewritten as

$$\mathcal{H}\phi(x)=\mathcal{E}\phi(x),\quad \mathcal{H}=-\frac{1}{hm}\frac{d^2}{dx^2}-\frac{1}{h}\left(\frac{1}{m}\right)'\frac{d}{dx}+\frac{v}{h}, \tag{2}$$

where the prime denotes differentiation with respect to x and arguments have been omitted. For the purpose of simplification of the description, below let us introduce the first-order Darboux transformations obtained in [10]. By using the technique of intertwining relations

$$\mathcal{L}\mathcal{H}=\mathcal{H}_1\mathcal{L}, \tag{3}$$

we have obtained the intertwining operator $\mathcal{L}$, the transformed potential $v_1(x)$, and the corresponding solutions $\phi_1(x)$ in the form

$$\mathcal{L}=\frac{1}{\sqrt{h\,m}}\left(\frac{d}{dx}+K\right),\quad K=-\frac{\mathcal{U}_1'}{\mathcal{U}_1}, \tag{4}$$

$$v_1=v+\frac{2\sqrt{h}}{\sqrt{m}}\frac{d}{dx}\frac{K}{\sqrt{mh}}-\frac{\sqrt{h}}{\sqrt{m}}\frac{d}{dx}\left[\frac{1}{h}\frac{d}{dx}\left(\frac{\sqrt{h}}{\sqrt{m}}\right)\right], \tag{5}$$

$$\phi_1=\mathcal{L}\phi=\frac{1}{\sqrt{hm}}\left[\frac{d}{dx}-(\ln\mathcal{U}_1)'\right]\phi. \tag{6}$$

Note that the transformation function $\mathcal{U}_1$ defines the transformation operator $\mathcal{L}$ and the new potential v_1 and corresponding solutions ϕ_1. The new potential depends not only on the potential v and on the additional potentials m and h. Evidently, employing the Darboux transformation once again to the obtained model, one can construct new exactly solvable models for the generalized Schrödinger equation.

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

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

In this way one gets

$$v_n=v_{n-1}+2\sqrt{\frac{h}{m}}\frac{d}{dx}\frac{K_n}{\sqrt{mh}}-\sqrt{\frac{h}{m}}\frac{d}{dx}\left[\frac{1}{h}\frac{d}{dx}\left(\sqrt{\frac{h}{m}}\right)\right], \tag{7}$$

$$\phi_n=\mathcal{L}\phi=\mathcal{L}_n\phi_{n-1}=\mathcal{L}_n\mathcal{L}_{n-1}\cdots\mathcal{L}_1\phi, \tag{8}$$

where $\mathcal{L}$ is the nth order differential operator:

$$\mathcal{L} = \mathcal{L}_n \mathcal{L}_{n-1} \cdots \mathcal{L}_1, \quad \mathcal{L}_n = \frac{1}{\sqrt{mh}} \left(\frac{d}{dx} + K_n \right), \\ K_n = -\chi'_{n-1} \chi_{n-1}^{-1}, \quad K_1 = -\frac{\mathcal{U}'_1}{\mathcal{U}_1} \tag{9}$$

and $\chi_{n-1} \equiv \chi_{n-1}(x, \lambda_n)$ is obtained by means of the «n»-order transformation, applied to the solution $\mathcal{U}_n$ of Eq. (1) or (2) with the eigenvalue λ_n

$$\chi_{n-1} = \mathcal{L}_{n-1} \mathcal{U}_n = \frac{1}{\sqrt{mh}} \left(\frac{d}{dx} + K_{n-1} \right) \mathcal{U}_n. \tag{10}$$

It is clear that χ_{n-1} is the solution of Eq. (2) with the potential v_{n-1}, and χ_{n-1} can be taken as a new transformation function for the Hamiltonian $\mathcal{H}_{n-1}$ to generate a new potential. It should be noted that the chain of n first-order Darboux transformations results in a chain of exactly solvable Hamiltonians $\mathcal{H} \to \mathcal{H}_1 \to \ldots \to \mathcal{H}_n$.

Consider as an example the 2nd order transformation in detail. Using the explicit expressions (7)–(9), we get a formula for the potential v_2:

$$v_2 = v_1 + \frac{2\sqrt{h}}{\sqrt{m}} \frac{d}{dx} \frac{K_2}{\sqrt{mh}} - \frac{\sqrt{h}}{\sqrt{m}} \frac{d}{dx} \left[\frac{1}{h} \frac{d}{dx} \left(\frac{\sqrt{h}}{\sqrt{m}} \right) \right] \tag{11}$$

and corresponding solutions

$$\phi_2 = \mathcal{L}\phi \ = \mathcal{L}_2 \phi_1. \tag{12}$$

Here $\mathcal{L} = \mathcal{L}_2 \mathcal{L}_1$, where $\mathcal{L}_1$ is actually $\mathcal{L}$ defined in (4), whereas $\mathcal{L}_2$ is determined as follows:

$$\mathcal{L}_2 = \frac{1}{\sqrt{m\ h}} \left(\frac{d}{dx} + K_2 \right), \quad K_2 = -\frac{\chi'_1}{\chi_1}, \tag{13}$$

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 Eq. (1) or (2) with the eigenvalue λ_2

$$\chi_1 = \mathcal{L}_1 \mathcal{U}_2 = \frac{1}{\sqrt{m\ h}} \left(\frac{d}{dx} - \frac{\mathcal{U}'_1}{\mathcal{U}_1} \right) \mathcal{U}_2. \tag{14}$$

Let us represent χ_1 as follows:

$$\chi_1 = \frac{1}{\sqrt{mh}} \frac{W_{1,2}}{\mathcal{U}_1}, \tag{15}$$

where $W_{1,2} = \mathcal{U}_1 \mathcal{U}'_2 - \mathcal{U}'_1 \mathcal{U}_2$ is the Wronskian of the functions $\mathcal{U}_1$ and $\mathcal{U}_2$. With this and taking into account v_1, after some transformations the new potential can be expressed as

$$v_2 = v - 2\sqrt{\frac{h}{m}} \frac{d}{dx} \left[\sqrt{\frac{m}{h}} \frac{\frac{d}{dx}(W_{1,2}/m)}{W_{1,2}} \right]. \tag{16}$$

By using (12) find now the corresponding functions ϕ_2, $\phi_2 = \left(\dfrac{d}{dx} + K_2\right)\phi_1$. By analogy with χ_1, the function ϕ_1 can be written in terms of the Wronskian $W_{1,\mathcal{E}} = \mathcal{U}_1\phi' - \mathcal{U}'_1\phi$:

$$\phi_1 = \frac{1}{\sqrt{mh}}\frac{W_{1,\mathcal{E}}}{\mathcal{U}_1}. \tag{17}$$

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

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

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

$$\phi_2 = \frac{1}{mh}\left(\phi'' - \frac{\mathcal{U}''_1}{\mathcal{U}_1}\phi\right) - \frac{d}{dx}\Big(\ln W_{1,2}\Big)\frac{1}{mh}\frac{W_{1,\mathcal{E}}}{\mathcal{U}_1} = \frac{1}{mh}\frac{W_{1,2,\mathcal{E}}}{W_{1,2}}. \tag{18}$$

It is easily seen from (16) and (18) that due to the 2nd order Darboux transformation, the potential and solutions obtained in this way are completely expressed in terms of the known effective mass function m and energy-dependent potential h and the solutions $\mathcal{U}_1, \mathcal{U}_2, \phi$ to the initial equation, with no use of the solutions to the intermediate one with the potential v_1.

Clearly, for the next transformation step to be made, one should take a new transformation function χ_2, which 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. Then it can be used to produce a new transformed operator $\mathcal{L}_3 = d/dx + K_3,\ K_3 = -\chi'_2\chi_2^{-1}$ for generating new potential v_3 and solutions ϕ_3 and so on, according to (7)–(9).

By using the second-order Darboux transformation, one can construct the phase-equivalent potentials without changing spectrum of the initial potential. For this let us present the 2nd order transformation at the energy $\lambda_2 = \lambda_1 = \lambda$ and rewrite them in the integral form

$$v_2 = v - 2\sqrt{\frac{h}{m}}\frac{d}{dx}\left(\frac{1}{\sqrt{mh}}\frac{h\,\Gamma\mathcal{U}^2}{1 + \Gamma\int\limits_{x_0}^{x} dx'\ h(x')\mathcal{U}^2(x')}\right), \tag{19}$$

$$\phi_2 = \phi - \frac{\Gamma\mathcal{U}}{1 + \Gamma\int\limits_{x_0}^{x} h(x')\mathcal{U}^2(x')\ dx'}\left[C + \int\limits_{x_0}^{x} h(x')\mathcal{U}(x')\phi(x')\ dx'\right], \tag{20}$$

where the limits of integration depend on the boundary conditions. For example, for regular solutions satisfying the boundary conditions $\phi(x = 0) = 0,\ \phi'|_{x=0} = 1$, the integration limits are $[0, x]$. Here Γ plays a role of a normalization constant or a difference between the normalization constants of the bound state λ for the potentials v_2 and v, respectively. For the first case two Hamiltonians $\mathcal{H}$ and $\mathcal{H}_2$ differ by one bound state. For the second case $\mathcal{H}$ and $\mathcal{H}_2$ are phase-equivalent Hamiltonians.

2. APPLICATION

As an illustrative example we present the transformed potential and solutions corresponding to the second- and third-order Darboux transformations. We start with the generalized Schrödinger equation (1) taken in the form

$$-\left[\frac{d}{dx}\,(x)\,\frac{d}{dx}\right]\phi(x)+\frac{1}{4x}\phi(x)=x\mathcal{E}\phi(x). \tag{21}$$

The general solution of this equation is

$$\phi(x)=\frac{C_1\sin(kx)}{k\sqrt{x}}+\frac{C_2\ \cos(kx)}{k\sqrt{x}}. \tag{22}$$

By using the Darboux transformation technique, one can generate potentials with one bound state and obtain corresponding solutions on the base of exact solutions for the effective mass Schrödinger equation [10]. Here we construct the potentials for the generalized equation (1) with two and three bound states and also construct the family of phase equivalent potentials. By a first-order supersymmetry transformation applied to a special case $\mathcal{U}_1$ of the general solution (22) $\mathcal{U}_1=\dfrac{C\ \cosh(\kappa_1 x)}{\kappa_1\sqrt{x}}$, we obtain the potential v_1 and corresponding solutions ϕ_1 as

$$v_1(x)=\frac{1}{4x}-2x\kappa^2\left(1-\tanh^2(\kappa_1 x)\right),$$

$$\phi_1(x)=\frac{C_1\cos(kx)}{\sqrt{x}}-\frac{C_1\kappa_1\sin(kx)\tanh(\kappa_1 x)}{k\sqrt{x}}.$$

The solution at the energy of transformation $\mathcal{E}_1=-\kappa_1^2$ reads

$$\eta=\sqrt{\frac{m}{h}}\ \frac{1}{\mathcal{U}}=\frac{\kappa_1}{C\ \sqrt{x}\cosh(\kappa_1 x)} \tag{23}$$

and corresponds to the bound state $\mathcal{E}_1=\lambda_1$. The transformed potential having two bound states at energies $\lambda_1=-\kappa_1^2$ and $\lambda_2=-\kappa_2^2$ can be written as

$$v_2=\frac{9}{4x}-2x\frac{d^2}{dx^2}\ln W_{1,2}, \tag{24}$$

where $W_{1,2}=\dfrac{C^2}{\kappa_2\kappa_1 x}\Big(\kappa_2\cosh(\kappa_1 x)\cosh(\kappa_2 x)-\kappa_1\sinh(\kappa_2 x)\sinh(\kappa_1 x)\Big)$ and the corresponding solutions are

$$\phi_2=\frac{\kappa_1\sqrt{x}}{C\ \cosh(\kappa_1 x)}\left(\frac{d}{dx}W_{1,\mathcal{E}}-\frac{d\Big(\ln W_{1,2}\Big)}{dx}W_{1,\mathcal{E}}\right),$$

where $W_{1,\mathcal{E}}=\dfrac{C_1 C}{k\kappa_1 x}\Big(k\ \cosh(\kappa_1 x)\cos(kx)-\kappa_1\sinh(\kappa_1 x)\sin(kx)\Big)$.

By using (7) one can construct the potential v_3 for the generalized Schrödinger equation (1) having three bound states

$$v_3 = v_2 - 2x\frac{d}{dx}\ln\chi_2 + \frac{1}{x}, \tag{25}$$

where v_2 is determined in (24) and χ_2 is determined as

$$\chi_2 = \frac{1}{mh}\frac{W_{1,2,3}}{W_{1,2}}. \tag{26}$$

For our case $W_{1,2,3}$ is given by

$$\begin{aligned} W_{1,2,3} = \frac{C^3}{x^{3/2}\kappa_1\kappa_2\kappa_3}\Big[&\cosh(\kappa_1 x)\cosh(\kappa_2 x)\kappa_2\sinh(\kappa_3 x)\kappa_3^2 - \\ &- \cosh(\kappa_1 x)\sinh(\kappa_2 x)\kappa_2^2\cosh(\kappa_3 x)\kappa_3 - \sinh(\kappa_1 x)\kappa_1\ \sinh(\kappa_2 x)\sinh(\kappa_3 x)\kappa_3^2 + \\ &+ \sinh(\kappa_1 x)\kappa_1\ \sinh(\kappa_3 x)\sinh(\kappa_2 x)\kappa_2^2 + \cosh(\kappa_1 x)\sinh(\kappa_2 x)\kappa_1^2\cosh(\kappa_3 x)\kappa_3 - \\ &- \cosh(\kappa_1 x)\kappa_1^2\cosh(\kappa_2 x)\kappa_2\sinh(\kappa_3 x)\Big]. \end{aligned} \tag{27}$$

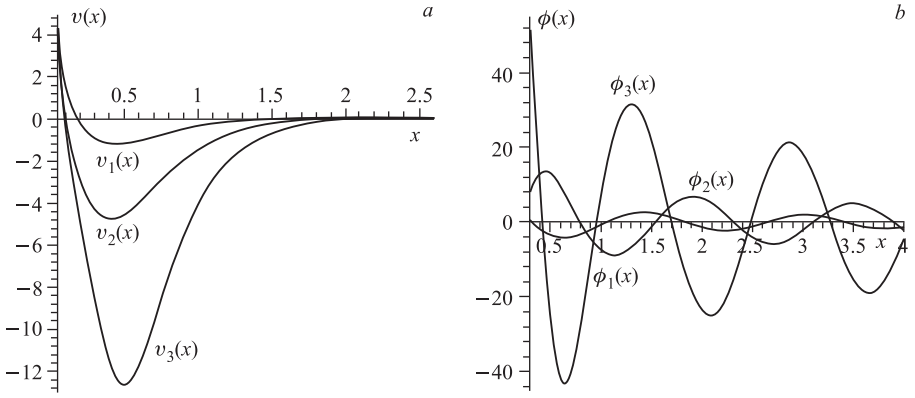

Fig. 1. *a*) Potentials $v_n, n = 1, 2, 3$, having one, two and three bound states, respectively; *b*) the corresponding solutions ϕ_n taken at $k = 6$

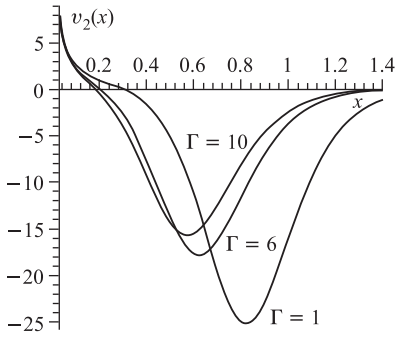

Fig. 2. Phase-equivalent potentials $v_2(x)$ with the bound state $\lambda = -16$ at a different choice of the normalization Γ

As an illustrative example we present the potentials v_1, obtained at the energy of transformation $\mathcal{E}_1 = 4$, v_2 obtained at the energies of transformation $\mathcal{E}_1 = 4,\ \mathcal{E}_2 = 16$ and v_3 at the energies of transformation $\mathcal{E}_1 = 4,\ \mathcal{E}_2 = 16,\ \mathcal{E}_3 = 25$. They are depicted in Fig. 1 with their corresponding solutions, calculated at $k = 6$. Phase-equivalent potentials v_2, calculated in correspondence with (19) at a different choice of the normalization Γ, are presented in Fig. 2.

CONCLUSION

We have constructed a chain of Darboux transformations for a generalized Schrödinger equation with position-dependent mass and with energy-dependent potentials. Using concrete examples, we have shown how to apply the Darboux transformation technique for modeling quantum well potentials with the given spectrum for investigation of low-dimensional structures in nanoelectronics.

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