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КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

RECONSTRUCTION OF QUANTUM WELL POTENTIALS

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The intertwining operator technique is applied to the generalized Schrödinger equation with a position-dependent effective mass. It is shown on concrete examples how to construct the quantum well potential with a desired spectrum for the Schrödinger equation with a non-Hermitian kinetic energy operator.

Техника операторов сплетения применяется к обобщенному уравнению Шредингера с эффективной массой, зависящей от пространственной переменной. На конкретных примерах показано, как конструировать потенциальные ямы для уравнения Шредингера с неэрмитовым оператором кинетической энергии.

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INTRODUCTION

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 quantum wells and superlattices to multilevel computer logic [1, 2]. The progress in this field became possible due to the development of technologies and techniques, such as crystal-growth techniques (e.g., molecular-beam-epitaxy) for the production of a nonuniform semiconductors. The Schrödinger equation with a space-variable-dependent effective mass is extensively used for investigation of the electronic properties of semiconductor heterostructures [3–5].

DARBOUX TRANSFORMATIONS FOR SCHRÖDINGER EQUATION WITH A POSITION-DEPENDENT MASS

Quantum well potentials determine the main properties of these structures. Therefore, the problem of reconstruction of quantum well potentials with predetermined energy spectrum is

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very important. In [6] an intertwining operator technique has been developed for quantum systems described by the generalized Schrödinger equation in the form

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

where $m^*(x)$ is a position-dependent «effective mass» and $\hbar^2/2 = 1$.

The aim of this paper is to construct concrete exactly solvable potentials $V(x)$ with given position-dependent «masses» on the base of the Darboux transformation and Liouville transformation technique for the Schrödinger equation with the Hamiltonian in the form (1). Suppose that the solution of the eigenvalue problem to Eq. (1) with the given potential $V(x)$ and position-dependent $m^*(x)$ is known and we would like to solve a similar problem for another Hamiltonian $\widetilde{\mathcal{H}}$ containing a new potential $\widetilde{V}(x)$ and a spectrum which 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

$$\mathcal{L}\mathcal{H} = \widetilde{\mathcal{H}}\mathcal{L}, \quad \widetilde{\phi}(x) = \mathcal{L}\phi(x), \tag{3}$$

where the operator $\mathcal{L}$ intertwines the Hamiltonians $\mathcal{H}$ and $\widetilde{\mathcal{H}}$.

As was shown in [6], the intertwining operator $\mathcal{L}$, the transformed potential $\widetilde{V}$ and the solutions $\widetilde{\phi}$ are given by

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

$$\widetilde{V} = V + \frac{1}{\sqrt{m^*}}\left[\frac{d^2}{dx^2}\frac{1}{\sqrt{m^*}} + 2\frac{d}{dx}\left(\frac{1}{\sqrt{m^*}}K\right)\right], \tag{5}$$

$$\widetilde{\phi} = \mathcal{L}\phi = \frac{1}{\sqrt{m^*}}\left[\frac{d}{dx} - (\ln U)'\right]\phi. \tag{6}$$

Here $\mathcal{U}(x)$ is some fixed solution of (1) with $\mathcal{E} = -\kappa^2$. As in the case of the Schrödinger equation, the potentials V and $\widetilde{V}$, the corresponding functions $\phi(k,x)$ and $\widetilde{\phi}(k,x)$, $k^2 = \mathcal{E}$, are related through the transformation operator $\mathcal{L}$. The difference is that in our case $\mathcal{L}$ includes a position-dependent mass (4). As a consequence, the new potential $\widetilde{V}$ and solutions $\widetilde{\phi}$ depend on the effective mass $m^*(x)$ (see (5), (6)). In order to reconstruct the quantum well potential with the predetermined spectrum by using these formula, it is necessary to know the exact solutions of Eq. (1) with the given $m^*(x)$ and $V(x)$. To obtain these solutions, we will use the Liouville transformation. Let us start with the Sturm–Liouville equation (1) in a more simple form with the potential $V = 0$ given on the interval $[0, X]$

$$-\frac{1}{m^*(x)}\frac{d^2}{dx^2}\phi(x) = \mathcal{E}\phi(x). \tag{7}$$

Introducing a new variable $\xi = \xi(x)$ and a new function $\psi(\xi)$

$$m^* = p^2, \quad p = \frac{d\xi}{dx}, \quad \xi = \frac{1}{C}\int^{x} p(x')\,dx',$$
$$C = \frac{1}{\pi}\int^{X} p(x')\,dx', \quad \phi(x) = |p|^{-1/2}(\xi)\psi(\xi), \tag{8}$$

Eq. (7) can be reduced to the standard Schrödinger equation:

$$-\psi''(\xi) + V(\xi)\psi(\xi) = \mathcal{E}\psi(\xi), \tag{9}$$

where the potential $V(\xi)$ has the form:

$$V(\xi) = \frac{1}{2}\left[\frac{p_\xi''}{p} - \frac{1}{2}\left(\frac{p_\xi'}{p}\right)^2\right]. \tag{10}$$

The potential $V(\xi)$ can be also represented as

$$V(\xi) = \frac{N''(\xi)}{N(\xi)}, \quad N(\xi) = p^{1/2}(\xi).$$

To construct exactly solvable models for the generalized Schrödinger equation (1), we can do the following: first, we solve the Schrödinger equation with the given potential; second, by using the inverse Liouville transformation, we find solutions to Eq. (7); at last, by using the Darboux transformations (5), (6), we construct new potentials $\widetilde{V}(x)$ and solutions $\widetilde{\phi}(x)$ on the base of the obtained solutions to Eq. (7). In a particular case, when an effective mass does not depend on a space variable, $m^*(x) = m \equiv \text{const}$, the derived generalized Darboux transformations turn into the corresponding Darboux transformations for potentials and solutions for the standard Schrödinger equation with a position-independent mass.

As an example, we choose the effective mass in the form

$$m^*(x) = \frac{\alpha^2}{(\alpha x + \beta)^4}. \tag{11}$$

By using (8) and (10), we immediately find

$$p(x) = \frac{\alpha}{(\alpha x + \beta)^2}, \quad \xi(x) = \frac{1}{(\alpha x + \beta)C}, \quad V(\xi) = 0. \tag{12}$$

In the ξ variable, therefore, we have the case of free moving $V(\xi) = 0$. The solutions with zero boundary conditions at $x = 0$, $\psi(\xi = 0) = 0$, are $\psi(\xi) = \dfrac{\sin k\xi}{k}$, where $k^2 = \mathcal{E}$. In accordance with (8), we get the solution to Eq. (7)

$$\phi(k, x) = \frac{C(\alpha x + \beta)}{k\sqrt{\alpha}}\sin\left(\frac{k}{\alpha x + \beta}\right). \tag{13}$$

Having found the exact solutions to Eq. (7), we can generate new potentials $\widetilde{V}$ with corresponding solutions to the generalized Schrödinger equation (2) on the base of Darboux transformations (4)–(6).

Let us take the energy of transformation $k^2 = -\kappa^2$. It means $k = i\kappa$ and κ is real and positive. The corresponding solution is

$$\mathcal{U}(x) = \frac{C(\alpha x + \beta)}{\kappa\sqrt{\alpha}} \sinh\left(\frac{\kappa}{\alpha x + \beta}\right). \tag{14}$$

According to (5) and (6) the transformed potential and solutions are determined as

$$\widetilde{V}(x) = \frac{2\kappa^2}{\cosh^2(\kappa/(\alpha x + \beta)) - 1}\ , \tag{15}$$

$$\widetilde{\phi}(k, x) = \\ = \frac{C(\alpha x + \beta)\left[-k\cos\left(\frac{k}{\alpha x + \beta}\right)\sinh\left(\frac{\kappa}{\alpha x + \beta}\right) + \kappa\sin\left(\frac{k}{\alpha x + \beta}\right)\cosh\left(\frac{\kappa}{\alpha x + \beta}\right)\right]}{k\sqrt{\alpha}\sinh\left(\frac{\kappa}{\alpha x + \beta}\right)}. \tag{16}$$

The built potential $\widetilde{V}(x)$ has a singularity at the point x in which $\cosh(\kappa/(\alpha x + \beta)) = 1$, i.e., at $\kappa/(\alpha x + \beta) = 0$. To avoid the singularity at $x \geqslant 0$, one can take $\alpha > 0$ and $\beta > 0$. The solution to Eq. (2) at the energy of transformation can be obtained by using second linear independent solution $\bar{\mathcal{U}}$ to (7) (for details see [6])

$$\eta(x) = \mathcal{L}\hat{\mathcal{U}}(x) = \frac{1}{\sqrt{m^*(x)}}\frac{1}{\mathcal{U}(x)}. \tag{17}$$

Substitution of (14) and (11) into (17) gives us

$$\eta(x) = \frac{\kappa(\alpha x + \beta)}{C\sqrt{\alpha}\sinh\left(\frac{\kappa}{\alpha x + \beta}\right)}. \tag{18}$$

One can get also second solution of (2) at the energy of transformation λ. By using Liouville's formula, one gets

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

We can consider the Schrödinger equation on a finite interval $\xi \in [0, d]$ with Dirichlet boundary conditions at both ends $\psi(\xi = 0) = 0$ and $\psi(\xi = d) = 0$. In this case, we have the same coupling between variables x and ξ as in (12) and $d = 1/(\alpha X + \beta)$, $C = d/\pi$. The solution of the Schrödinger equation (9) with $V(x) = 0$ is

$$\psi(\xi) = \frac{\sin k_n\xi}{k_n}, \quad k_n = \frac{n\pi}{d}, \quad n = 1, 2, \ldots$$

All given formulae for the solution to the generalized Schrödinger equation are valid with the evident changing $k \to k_n$. The above procedure can be repeated as many times as it is needed to construct a new potential and corresponding exact solutions.

Now let us consider a second-order Darboux transformation. The potential and corresponding solutions can be presented as

$$V_2(x) = V(x) + \frac{2}{\sqrt{m^*(x)}}\frac{d}{dx}[\sqrt{m^*(x)}\,\eta_2(x)\,\mathcal{U}(x)], \tag{20}$$

$$\phi_2(x) = \phi(x) + \eta_2(x)\int^x dx'\,\mathcal{U}(x')\,m^*(x')\,\phi(x'), \tag{21}$$

where $\eta_2(x)$ is the solution at the energy of transformation $k^2 = -\kappa^2$

$$\eta_2(x) = -\frac{C_1\mathcal{U}(x)}{1 + C_1\int^x dx'\,m^*(x')\,\mathcal{U}^2(x')}. \tag{22}$$

Substitution of (14) into (22) gives us

$$\eta_2(x) = \frac{C_1\kappa^2(\alpha x+\beta)\sinh\left(\dfrac{\kappa}{\alpha x+\beta}\right)}{\sqrt{\alpha}\left(\kappa^3 + C_1\left(\dfrac{1}{4}\sinh\left(\dfrac{2\kappa}{\alpha x+\beta}\right) - \dfrac{\kappa}{2(\alpha x+\beta)}\right) + C_2\right)}, \tag{23}$$

where $C_2 = \frac{1}{4}\sinh\left(\frac{2\kappa}{\beta}\right) - \frac{\kappa}{2\beta}$ and C_1 can play the role of a normalization constant of the bound state at $\mathcal{E} = -\kappa^2$. Clearly, using these $\eta_2(x)$, $m^*(x)$ and $\mathcal{U}(x)$ in (20) and (21) we construct new potential and pertinent solutions in a closed analytical form. For the potential we get

$$V_2(x) = \frac{2(\alpha x+\beta)^2}{\alpha}\frac{d}{dx}\left[\frac{C_1\sinh^2\left(\dfrac{\kappa}{\alpha x+\beta}\right)}{\left(\kappa^3 + C_1\left(\dfrac{1}{4}\sinh\left(\dfrac{2\kappa}{\alpha x+\beta}\right) - \dfrac{\kappa}{2(\alpha x+\beta)}\right) + C_2\right)}\right]. \tag{24}$$

The expression for the solution is more cumbersome, but it is evident how it is expressed in terms of the effective mass $m^*(x)$ and the obtained solutions $\mathcal{U}(x)$, $\phi(x)$ and $\eta_2(x)$.

One can take $\mathcal{U}$ in the form

$$\mathcal{U}(x) = \frac{\alpha x+\beta}{\kappa}\cosh\left(\frac{\kappa}{\alpha x+\beta}\right). \tag{25}$$

It corresponds to $\phi(\xi) = \cosh(\kappa\xi)/\kappa$ that is the solution of the free Schrödinger equation. With using (5) and (6) we obtain a transformed potential and corresponding solutions in the form

$$\widetilde{V}(x) = -\frac{2\kappa^2}{\cosh^2(\kappa/(\alpha x+\beta))}, \tag{26}$$

$$\widetilde{\phi}(k,x) = \\ = \frac{C(\alpha x+\beta)\left[-k\cos\left(\dfrac{k}{\alpha x+\beta}\right)\cosh\left(\dfrac{\kappa}{\alpha x+\beta}\right)+\kappa\sin\left(\dfrac{k}{\alpha x+\beta}\right)\sinh\left(\dfrac{\kappa}{\alpha x+\beta}\right)\right]}{k\sqrt{\alpha}\cosh\left(\dfrac{\kappa}{\alpha x+\beta}\right)}. \tag{27}$$

The solution to the transformed equation (2) can be obtained from (17) with $\mathcal{U}(x)$ from (25)

$$\eta(x) = \frac{\kappa(\alpha x+\beta)}{C\sqrt{\alpha}\cosh\left(\dfrac{\kappa}{\alpha x+\beta}\right)}. \tag{28}$$

It is clear how one gets the potential and solutions within the second-order Darboux transformations.

CONCLUSION

In this paper we have focused one's attention on concrete examples how to apply the Darboux transformation technique for quantum systems with a position-dependent effective mass, in order to generate potentials whose wave functions can be determined algebraically.

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