Inverse problem of electron scattering on the potential of the multilayer semiconductor resonance-tunneling structure

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1th - 5th June 2026

This paper presents a theoretical investigation of the inverse problem of electron scattering in open double-barrier AlAs/GaAs nanostructures, which are fundamental components for resonant-tunneling devices and quantum cascade lasers. Focusing on the reconstruction of the spatial profile of the effective potential from complete time-dependent scattering data, the study employs the Gelfand-Levitan-Marchenko integral equation. The restored effective potential of the nanostructure, encompassing both stationary and time-dependent components, is analytically obtained using the scattering function. The proposed approach provides a robust mathematical framework for efficiently processing experimental spectral data and accurately modeling electron transport in complex semiconductor heterostructures.

Introduction

Electron tunneling in multilayer semiconductor quantum cascade lasers and detectors [1, 2] is physically equivalent to electron scattering by the effective potential of nanostructures in the presence of static and time-dependent fields. The geometric configuration of the potential profile in multilayer structures determines the spectral characteristics of electron quasi-stationary states and their scattering properties, such as lifetime and scattering cross section. Solving the forward problem of quantum scattering theory allows us to determine and analyze these spectral characteristics. However, in the presence of experimental or computational data on the electron wave function, a fundamentally different class of problems arises: reconstructing the spatial potential profile. This non-stationary inverse problem is critical for processing experimental data for subsequent modeling of electron transport.

1. Direct Problem: Theory and Analysis

In the general case, the direct problem of the theory of electron scattering in multilayer nanostructures consists of solving the full Schrödinger equation:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\frac{1}{m(x)}\frac{\partial}{\partial x}+U_{eff}(x)+H(x,t)\right]\Psi(x,t)$$

where $U_{eff}(x)$ is the effective potential of the nanostructure for an electron, H(x,t) is its time-dependent component, m(x) - is the time-dependent effective mass of an electron in a nanostructure., in particular:

$$m(x)=m_w\left\{\theta(-x)+\theta(z-d)+\sum_{i=1}^{2}\left[\theta(x-x_i)-\theta(x-x_{i+1})\right]\right\}+$$
$$+m_b\sum_{i=0}^{2}\left[\theta(x-x_i)-\theta(x-x_{i+1})\right].$$

$$H(x,t)=-e\xi\left[x\theta(-x)+(x-d)\theta(x-d)\right]$$
.

Solving the full Schrödinger equation makes it possible to determine the spectral parameters of electronic stationary states and to analyze their dependence on the geometric configuration of the structure.

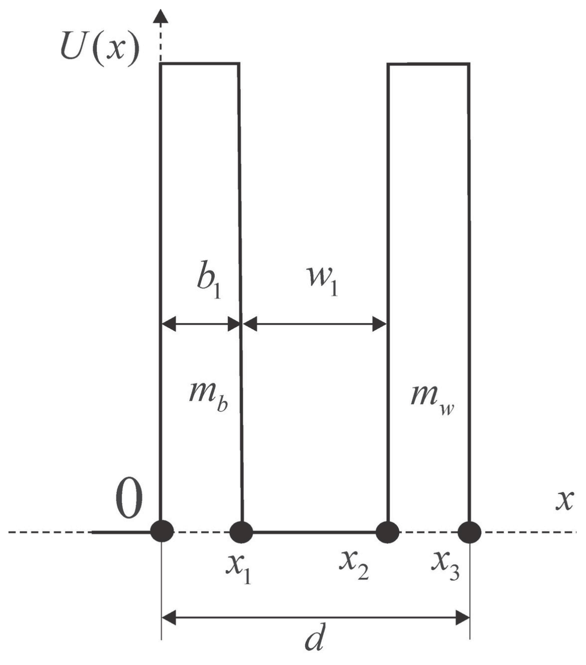

Fig. 1. Energy and geometric scheme of an open double-barrier AlAs/GaAs nanostructure.

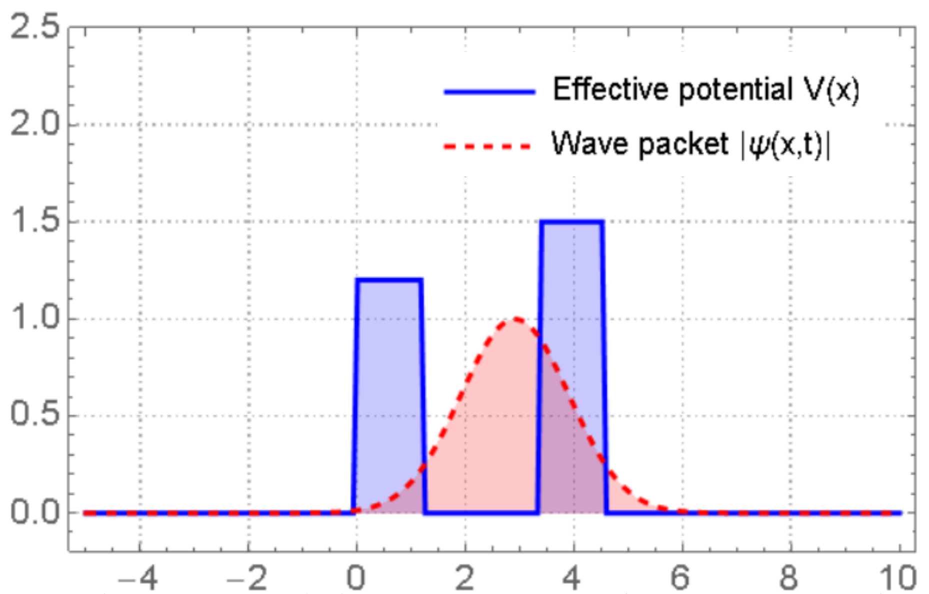

Fig. 2. The process of electron scattering by an open two-barrier nanostructure.

2. Inverse Problem: Potential Reconstruction. Mathematical Model of Inverse Scattering

The foundation of the inverse scattering problem lies in the asymptotic behavior of the electron wave function far from the nanostructure region (x→+∞, where Veff→0). For an electron incident from the left, the wave function takes the form:

$$\Psi(x,t)_{x\to+\infty}=\begin{cases}e^{ikx}+r(k,t)e^{-ikx}, & x\to-\infty\\ t(k,t)e^{ikx}, & x\to+\infty\end{cases}$$

Here, r(k,t) and t(k,t) are the time-dependent reflection and transmission coefficients, respectively. T

A completely different class of problems arises when experimental or computational data are available that provide information about the electronic wave function of a nanostructure and its behavior at the heterointerfaces. This represents a fundamentally different class of problems in quantum scattering theory, namely the reconstruction of the spatial profile of the potential in nanostructures from spectral and wave-function data.

For multilayer nanostructures, this class of problems is still in its early stages of development; however, its importance stems from the need to efficiently process experimental data in order to reconstruct potential profiles for subsequent theoretical calculations and modeling of electron transport.

In the present work, we solve the non-stationary inverse problem of quantum scattering theory, aimed at reconstructing the potential of a multilayer nanostructure from complete time-dependent scattering data.

The solution of the non-stationary inverse problem for multilayer nanostructures is based on the Gelfand-Levitan-Marchenko integral equation and consists of three key stages:

1. Input data generation (Scattering function): The function F(x,t) contains complete information about the scattering of a wave packet at heterointerfaces and is constructed on the basis of spectral data (reflection coefficient r(k,t) and energies of quasi-stationary states):

$$F(x,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}r(k,t)e^{ikx}dk+\sum_{n=1}^{N}c_n(t)e^{-\kappa_n x}$$

2. Marchenko equation (Data processing): The relationship between the scattering data and the unknown potential is established through a linear integral equation (for y>x):

$$K(x,y,t)+F(x+y,t)+\int_x^{\infty}K(x,z,t)F(z+y,t)dz=0$$

By solving this equation, we find the kernel of the transformation operator K(x,y,t), which takes into account the configuration of the nanostructure.

3. Recovery of the potential profile: The desired spatial profile of the effective potential $U_{eff}(x)$ (geometry of wells and barriers) and its time-dependent component U(x,t) are uniquely determined from the diagonal values of the kernel (y=x):

$$V_{eff}(x)+U(x,t)=-2\frac{d}{dx}K(x,x,t)$$

In our case the restored effective potential of the nanostructure as the sum of the stationary and time-dependent components is obtained in the form of Marchenko's functional equation with scattering function F(x,t):

$$U_{eff}(\xi,t)=H_0\left[x(\xi)\right]+H\left[x(\xi),t\right]+V_m(\xi);$$
$$V_m(\xi)=\left(\hbar^2/2m_0\right)\left[5(m')^2/16m^3-m''/4m^2\right]\Big|_{x=x(\xi)};$$
$$U_{eff}(\xi,t)=-2\frac{K(\xi,\xi,t)}{\partial\xi};$$
$$K(\xi,y,y)+F(\xi+y,t)+\int_{\xi}^{+\infty}K(\xi,s,t)F(s+y,t)ds=0,\ y\geq\xi.$$

3. Results and Analysis

To verify the efficiency and accuracy of the proposed method of the inverse scattering problem, numerical simulation was performed for a symmetric two-barrier resonant tunneling nanostructure AlAs/GaAs/AlAs. The following basic physical parameters were used for the calculations: quantum well material (GaAs): width w = 5.0 nm, effective electron mass m{GaAs} = 0.067 me. Barrier material (AlAs): width of each barrier b = 3.0 nm, effective electron mass m_AlAs} = 0.15 me. .Scattering input data: complex reflection coefficient r(k,t), obtained by solving the direct Schrödinger problem with Ben-Daniel-Duke boundary conditions.

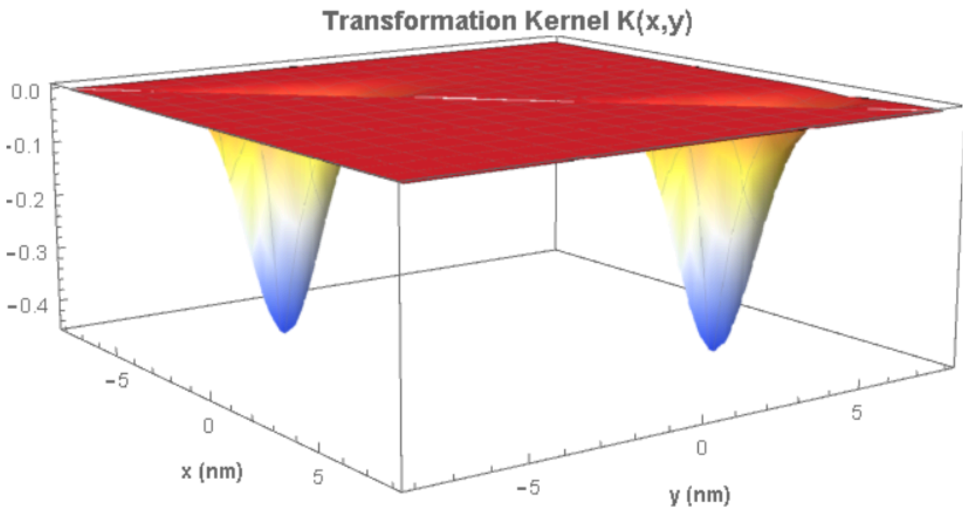

Fig. 3. Spatial dependence for the kernel of the operator K(x,y) of the Marchenko transformation

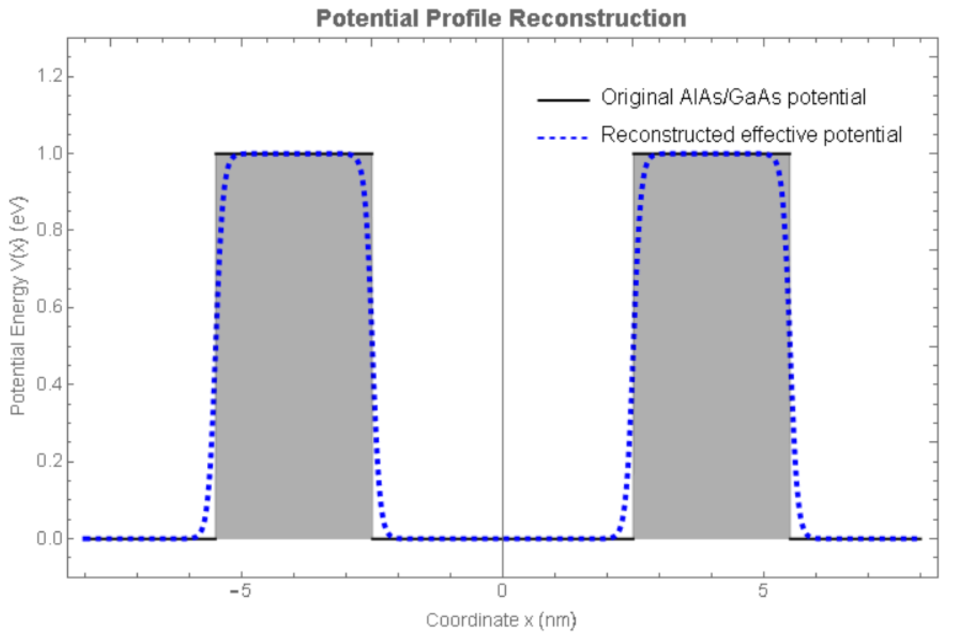

Fig. 4. Reconstructed potential profile of double-barrier nanosystem in the developed method.

Fig. 3 visualizes the 3D surface of the transformation kernel K(x,y), clearly illustrating its fundamental triangular property (K=0 for y<x) and highlighting the exact spatial locations of the heterojunctions along the diagonal.

Fig. 4 demonstrates the high accuracy of the proposed method, showing a near-perfect match between the original rectangular AlAs/GaAs barriers and the reconstructed effective potential.

Conclusions and Results

- This study solves a nonstationary inverse problem of quantum scattering theory aimed at reconstructing the potential of a multilayer nanostructure from complete time-dependent scattering data.
- It is shown that the reconstructed effective potential of the nanostructure can be obtained using the Marchenko functional equation.
- Solving the inverse problem for multilayer structures enables efficient processing of experimental data to accurately determine potential profiles.
- This approach provides a analytical basis for further theoretical calculations and accurate modeling of electron transport in resonant tunneling structures.

References

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