Nanoscale physics

A numerical solution of the stationary Schrödinger equation for multilayer quantum structure in a frequency domain

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It is well known that quantum cascade lasers are produced on a base of the multilayer quantum structures [1]. Potential energy of such a quantum structure is a set of potential wells and barriers of certain width and height. There is a need to know the discrete energy levels and the appropriate wave functions of a multilayer quantum structure for design of these lasers [1].

Determination of energy levels (wave functions) of quantum multilayer structures by traditional method is reduced to a solution of transcendental equation, and it is rather complicated. Moreover, complexity of solution increases (nonlinearly) when number of potential wells and barriers increases. Analysis of such structures is significantly simplified in a frequency domain [2].

In this work we present method where wave equation is transformed into integral equation by Fourier transform and it can be solved by numerical method. Finally, the solution is reduced to the eigenvalue/eigenvector problem. Obtained eigenvalues are discrete energy levels, and eigenvectors are corresponding Fourier transforms of the wave functions. The method is characterized by high accuracy and numerical stability.

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2. *Fitio V.M., Yaremchuk I.Y., Romakh V.V., Bobitski Y.V.* A solution of one-dimensional stationary Schrödinger equation by the Fourier transform // ACES Journal. – 2015. – **30**, N 5. – P. 534–539.