Journal of Computational Physics 231 (2012) 6173–6180

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Solution of the 1D Schrödinger equation in semiconductor heterostructures using the immersed interface method

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ARTICLE INFO

Article history:
Received 12 January 2011
Received in revised form 9 September 2011
Accepted 13 May 2012
Available online 26 May 2012

Keywords:
Schrödinger equation
Immersed interface method
Finite difference method
Semiconductors
Potential profiles

ABSTRACT

Due to the enormous progress in computer technology and numerical methods that has been achieved over the past several decades, the use of numerical simulation methods in all scientific disciplines gain more and more importance. In the physics field, these methods have provided remarkable numerical solutions to problems considered analytically intractable. The solution of the Schrödinger equation in semiconductor heterostructures is a good example. However, many of these numerical schemes are cumbersome to implement for nonexperts in numerical computing. With this reason as motivation, a novel method simple enough to implement yet powerful enough to solve Schrödinger equation in semiconductor devices with high accuracy is presented herein.

1. Introduction

In a large number of problems encountered in physics, and specifically in the modelling of semiconductor heterostructures, a fast and accurate solution of the one-dimensional time-independent Schrödinger equation has to be found in order to better understand the physical properties of such devices and to simulate their expected performance. The abovementioned is an effect of the characteristic dimensions of up-to-date devices that have progressed further than the submicron regime where quantum effects play a paramount role. However, analytic solutions to these types of problems are rarely encountered or even nonexistent. For this reason, several methods have been devoted to the numerical solution of such issues, including the transmission line method [1], spectral methods [2–4], the so called shooting method [5–8], matrix transfer method [9–11], finite element method [12–14], and of more immediate interest, the finite difference method [11,15,16]. Many of these techniques are cumbersome to implement thus knowledge in numerical computing might be required which constitutes an obstacle for nonexperts. As demonstrated in the forthcoming sections, the presented method has been readily and successfully implemented for the solution of eigenvalue problems in arbitrary potential profiles originated in semiconductor devices. The foundation of the herein presented algorithm is the immersed interface method (IIM) that has been developed in recent years predominantly designed for interface problems and which modifies the numerical schemes in the neighbourhood of or on the interfaces [17]. Its application in solving the Schrödinger equation in semiconductor heterostructures is described in Section 2 whereas some numerical examples appear in Section 3 to exemplify the generality and ease for computing the eigenstates of such profiles when using this novel numerical approach.

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http://dx.doi.org/10.1016/j.jcp.2012.05.017

2. Derivations

For the analysis, we consider a quantum well (QW) of arbitrary potential profile. Under the effective mass approximation, the envelope function of an electron or a hole in the QW, is given by the one-dimensional time independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m_e(z)}\frac{d}{dz}+U(z)\right)\Psi(z)=E\Psi(z), \tag{1}$$

where E is the energy of the particle, $U(z)$ is the potential, $m_e(z)$ is the effective mass of the particle and $2\pi\hbar$ is Planck's constant. We will use normalized parameters to facilitate the derivation of the following equations. Hence, the energy E, the potential $U(z)$, and the coordinate z, are normalized as $\varepsilon = E/E_0$, $u(\zeta) = U(z)/E_0$, $\zeta = z/d$, respectively, where $E_0 = \hbar^2\ \pi^2/2m_e(0)d^2$, $m_e(0)$ is the effective mass of the particle at $z = 0$, and d the width of the potential $U(z)$. With this notation, the Schrödinger equation, Eq. (1), can be written in the following form

$$\left(-\frac{1}{\pi^2}\frac{d}{d\zeta}\frac{1}{m^*(\zeta)}\frac{d}{d\zeta}+u(\zeta)\right)\Psi(\zeta)=\varepsilon\Psi(\zeta), \tag{2}$$

where $m^*(\zeta) = m_e(z)/m_e(0)$. If we consider the effective mass of the particle to be a piecewise constant, then it can be taken outside the derivative. Therefore, Eq. (2) has the form

$$\left(-\frac{1}{\pi^2 m^*(\zeta)}\frac{d^2}{d\zeta^2}+u(\zeta)\right)\Psi(\zeta)\ =\ \varepsilon\Psi(\zeta) \tag{2a}$$

to further simplify Eq. (2a), we can define $M = M(\zeta) = \frac{1}{\pi^2 m^*(\zeta)}$ so that Eq. (2a) can be rewritten as

$$-M\Psi_{\zeta\zeta}+u(\zeta)\Psi=\varepsilon\Psi, \tag{3}$$

where the subscripts denote differentiation. In the finite difference method (FDM), the range of integration (a,b) is divided into $N-1$ equal subintervals, grid points, of length h represented as $\zeta_i = a + (i-1)h$, $i = 1,2,3,\ldots,N$ and $h = (b-a)/(N-1)$. On the other hand, the piecewise constant function M is allowed to have discontinuities at some grid points. For the analysis, we can consider one of these discontinuities, i.e. $\zeta = \zeta^*$ where the potential $u(\zeta)$ may also have an abrupt change at such a point. The point ζ^* might be an element of the set of grid points or will have two of them as its neighbours, i.e., $\zeta_j \leqslant \zeta^* < \zeta_{j+1}$, as shown in Fig. 1. In order to solve Eq. (3) under the FDM, it is convenient to replace the second order derivative by a finite difference approximation such as the central divided difference scheme. This scheme will result in an eigenvalue problem with a large tridiagonal matrix which can then be solved with the use of conventional numerical libraries such as ARPACK [18]. A similar procedure is found in [16]. However, the direct use of the final equations reported in [16] leads to far-reaching numerical difficulties. The correct form of such equations is of paramount importance for its numerical implementation. By the same token, we derive here their correct final form.

If the definition of the second order central finite difference approximation is substituted in Eq. (3), we have

$$-M(\zeta_i)\left\{\frac{1}{h^2}[\psi(\zeta_{i+1})-2\psi(\zeta_i)+\psi(\zeta_{i-1})]\right\}+u(\zeta_i)\psi(\zeta_i)=\varepsilon\psi(\zeta_i), \tag{4}$$

rearranging terms in Eq. (4) we get

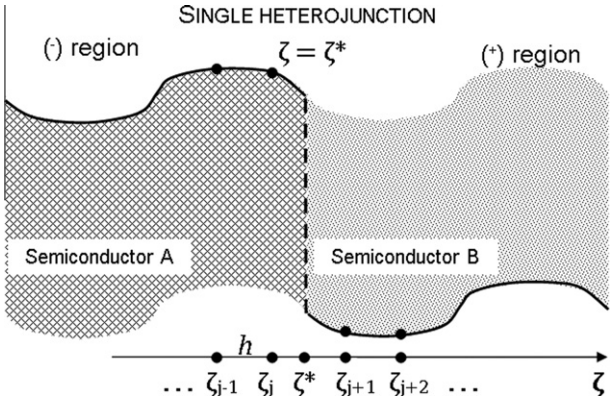

Fig. 1. Arbitrary potential profile, continuous line, originated in a single heterojunction and grid points close to the interface or discontinuity.