An Adaptive Basis Function for Meshless Simulation of Quantum Wave Packets at Optical Frequencies

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Abstract — In this work, an adaptive and efficient basis function is presented by which the Schrodinger equation can be solved using meshless method in an accurate and fast approach. The base of this achievement is the quantum wave packet. The proposed basis function reduces time consumption of the meshless method, approximately to half. Also, it inherits the fundamental properties of wave packets. Therefore, an accuracy and precision in simulation of wave function is obtained which is higher than some other numerical methods such as conventional meshless method or finite element method (FEM). This precision will be shown in practice by simulating a quantum well laser.

Index Terms — Meshless method, basis function, Schrodinger's equation, Gaussian wave packets, Kronecker delta property.

I. Introduction

The nano-scale quantum theory is a more fundamental theory than classical electromagnetics. It provides a more accurate description of many phenomena which are never observed in the macroscopic world. This theory forms a framework for understanding and development of semiconductor materials at THz and optical frequencies such as transistors or lasers. In order to test such theory on devices and applications, it has become more popular from business point of view to construct efficient computational models before any physical experimentation takes place.

In the past, some computational techniques as drift-diffusion would use to simulate the optical quantum devices. However, such techniques were not adequate to model the new breed of devices in which the quantum effect of a single electron can play a significant part in a device's operation. On the other hand, such numerical methods would analyze the entire problem domain under a quantum point of view. But, in many optical frequency devices as quantum well lasers, the quantum effects occur only in a localized region, whereas the rest of device's domain can be described by classical models [1].

For this purpose, many numerical methods were proposed that the weak form techniques, due to their treatment with lower differentiability orders and simpler imposition of boundary conditions, are more powerful than other methods. The FEM and meshless method are of this kind [2].

In this work, an efficient meshless method is proposed for which the basis function, in contradiction with existing basis functions [3]-[5], is adaptive and inherits the properties of the wave packets as initial condition for Schrodinger's equation. This smart basis function possesses a special property, i.e., the Kronecker delta property, that makes the method faster than conventional meshless methods.

Due to practical importance of quantum well lasers, the proposed technique is used to analyze this device and the comparison between results of different weak form methods, confirms the validity of new technique.

The rest of the paper has been organized as follows. In section II, the existing meshless methods will be overviewed. Afterwards in section III, the smart basis function is proposed to improve the meshless method. Finally, by simulating a quantum well laser in section IV, the validity of the smart basis function will be proved, practically.

II. The Meshless Method

Consider the following partial differential equation (PDE)

$$Lu = w \tag{1}$$

in which L is the differential operator, u is the unknown function and w is the excitation function.

The weak form technique, replaces a PDE by its corresponding integral equation known as functional. This replacement is based on Ritz's or Galerkin's method. Using Ritz's method, the functional of (1) is

$$F(u) = \frac{1}{2}[< Lu, u > - < u, w > - < w, u >] \tag{2}$$

where $F(u)$ is the functional of PDE and

$$< a, b > = \int_{\Omega} a\bar{b} d\Omega \tag{3}$$

in which $\bar{b}$ is the complex conjugate of b and Ω is the problem domain. The meshless method proposes the following approximation function $\tilde{u}$ to be used in (2)

$$\tilde{u}(x) = \sum_{i=1}^{n} R_i(x) a_i = R^T(x) A \tag{4}$$

where $R_i(x)$ is the basis function for ith node, a_i is the corresponding coefficient and $R^T(x)A$ is the matrix representation of (4). Usually, there are three common basis functions known as multiquadric (MQ), Gaussian (EXP) and thin plate spline (TPS) for radial point interpolation meshless method (RPIM) [2].

Since every computational technique is based on the calculation of solution function in some scattered nodes, say u_i, (4) can be rewritten as

$$\tilde{u}(x)=\sum_{i=1}^{n} N_i(x)u_i = N^T(x)U \quad (5)$$

in which, N_i is the shape function derived as

$$N^T(x)=R^T(x)R_0^{-1} \quad (6)$$

And

$$R_0=\begin{pmatrix} R_1(x_1) & \dots & R_n(x_1) \\ \vdots & \ddots & \vdots \\ R_1(x_n) & \cdots & R_n(x_n) \end{pmatrix} \quad (7)$$

Substituting (5) into (2) and finding the stationary (extremum) points of F with respect to u_i, the matrix U is obtained as the solution function.

Even though the meshless method, due to its approximation spaces that are not necessarily of polynomials, is more accurate than FEM, but there are two major problems with this method. First of all, it contains a middle matrix inversion step, i.e., (6), that takes noticeable computational time. Secondly, the existing basis functions do not inherit any property related to wave function (as the solution of Schrodinger's equation) to help them model the wave function with higher precision.

The next section proposes an adaptive and smart basis function that eliminates two existing problems in conventional meshless methods.

III. Adaptive Shape Function

According to Heisenberg's uncertainty principle, there is a special function as the initial condition for Schrodinger's equation where determines the momentum and position of an electron with highest precision. This function is Gaussian wave packet as

$$\psi(x)=(\frac{1}{2\pi\sigma^2})^{\frac{1}{4}}\exp(-\frac{x^2}{4\sigma^2})\exp(jk_0x) \quad (8)$$

where σ is the uncertainty and $\hbar k_0$ is the electron's mean of momentum [1]. The property of highest precision leads us toward considering above function as a possible basis function that is smart with respect to quantum computations. Imposing some modifications sounds necessary before any consideration. Every basis function is real-valued. Hence, $|\psi|$ and $real(\psi)$ can be possible candidates. Due to two shape parameters of $real(\psi)$, i.e., σ and k_0, in contrast with the only shape parameter of $|\psi|$, i.e., σ, the $real(\psi)$ contains more degree of freedom and seems more suitable.

This selection brings an important property that is the smartness of basis function with respect to wave (state) function; because it inherits the behavior of quantum wave function. So, the smart basis function is proposed as

$$B(x)=(\frac{1}{2\pi\sigma^2})^{\frac{1}{4}}\exp(-\frac{x^2}{4\sigma^2})\cos(k_0x) \quad (9)$$

From now on, the main controversy is to determine the two shape parameters, i.e., σ and k_0. With comparison with the Gaussian basis function, it is found that the maximum amplitude of smart basis function must be unit. Therefore,

$$\sigma=\frac{1}{\sqrt{2\pi}} \quad (10)$$

and the first property of basis function is imposed into *B(x)* as

$$B(x)=\exp(-\frac{\pi}{2}x^2)\cos(k_0x) \quad (11)$$

About k_0, let offer an intelligently choice such that $k_0=\frac{\pi}{2}$. This selection yields

$$B(x)=\exp(-\frac{\pi}{2}x^2)\cos(\frac{\pi}{2}x) \quad (12)$$

This choice, beside the decay effect of smart basis function, brings a significant property for *B(x),* i.e., the Kronecker delta property [2]. The effect of this property can be seen as below

$$R_0=\begin{pmatrix} B_1(x_1)=1 & \dots & B_n(x_1)=0 \\ \vdots & \ddots & \vdots \\ B_1(x_n)=0 & \cdots & B_n(x_n)=1 \end{pmatrix} \quad (13)$$

where shows that R_0 has been changed to identity matrix. So, the inversion step (7) is canceled and the computational time consumption improves.

For summing up, the two existing issues of meshless methods in area of quantum device simulation are eliminated using the smart basis function (13). The next section shows the validity of the proposed basis function used in meshless method in simulation of quantum well laser.

IV. Simulation of Wave propagation in Quantum Well Laser

The main structure of quantum well laser is shown in Fig. 1 in which two infinite potential wells guide the wave packet through a specific channel and a potential barrier in between, changes the direction of ray in some regions.

For simulating, the time dependent Schrodinger's equation is discretized [3] on time axis using finite difference forward scheme and the spatial part will be discretized using smart meshless method as

$$j\hbar BU^{m+1}=(\Delta tK-i\hbar B)U^m \quad (14)$$

where Δt is time increment, superscript m shows the finite deference time iteration process and matrices K and B are defined as

$$K_{ij}=\int_\Omega(\nabla N_i.\nabla N_j+2VN_iN_j)d\Omega$$
$$B_{ij}=\int_\Omega 2N_iN_jd\Omega \quad (15)$$

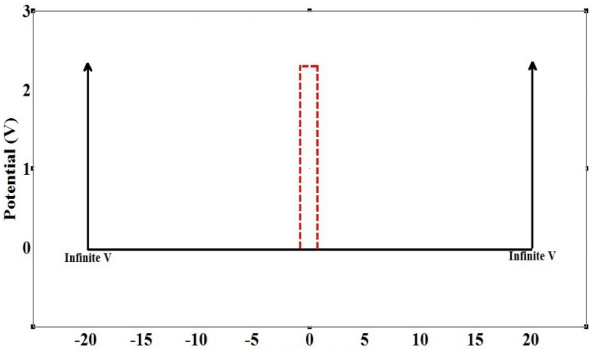

Fig. 1: Quantum well laser structure with potential barrier

V is potential of barrier at the center of quantum well laser structure and in this problem is set as 2.5 V and N_i is the smart proposed basis (shape) function.

The initial condition for eigen value problem (15) is a Gaussian wave packet for which $\sigma = 2$ and $k_0 = 3$. The snapshots of wave packet, propagating through the laser structure at different times, i.e., $t=7\Delta t$ and $15\Delta t$ are shown in Figs. 2(a) and 2(b). As seen, due to the greater value of momentum ($k_0 = 3$) than the potential barrier (V=2.5 V), most of the wave packets is transmitted through the barrier which confirms the accuracy of smart meshless method.

Comparing the results of different numerical methods, i.e., the proposed (Smart), QRPIM (Previous) meshless methods and FEM, based on the following error definition

$$error = \frac{1}{n} \frac{\sum_{i=1}^{n} | u_i^{exact} - u_i^{numerical} |}{\sum_{i=1}^{n} | u_i^{exact} |} \tag{16}$$

are shown in Fig. 3. As seen, the smart basis function has helped the meshless method solve the problem with more precision and less time consumption rate.

V. Conclusion

In this work, an adaptive and smart basis function for meshless method aimed to simulate the optical frequency devices was proposed. This function inherits the properties of wave packets in quantum problems and increases the accuracy of simulation. Also, this new method reduces the time consumption. Testing this method in simulation of quantum well laser structure, the results were in higher precision than some other numerical methods.

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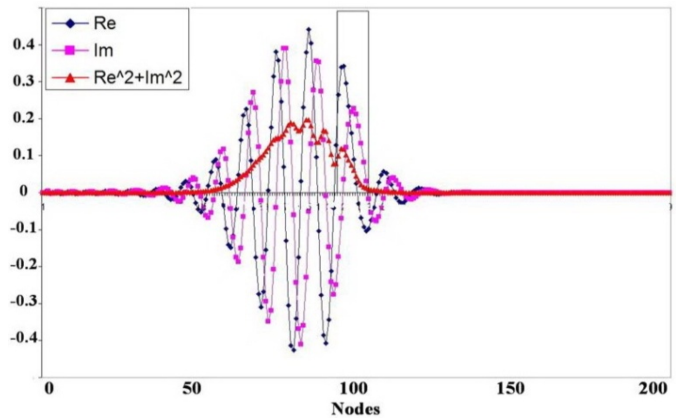
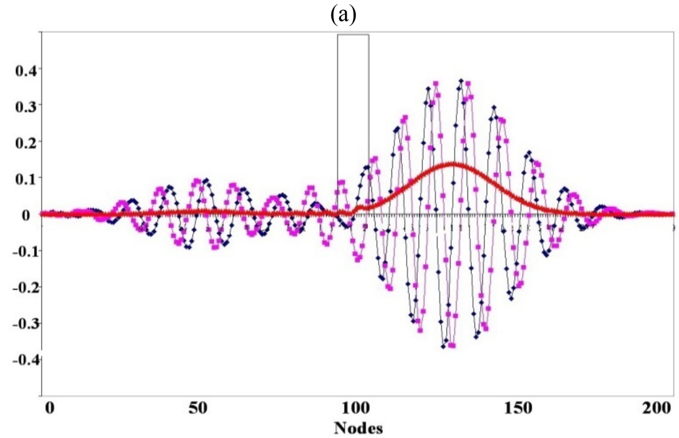


(a)



(b)

Fig. 2: The wave packet propagating through the quantum well laser structure at different times. (a) Wave packet at $t=7\Delta t$. (b) Wave packet at $t=15\Delta t$.

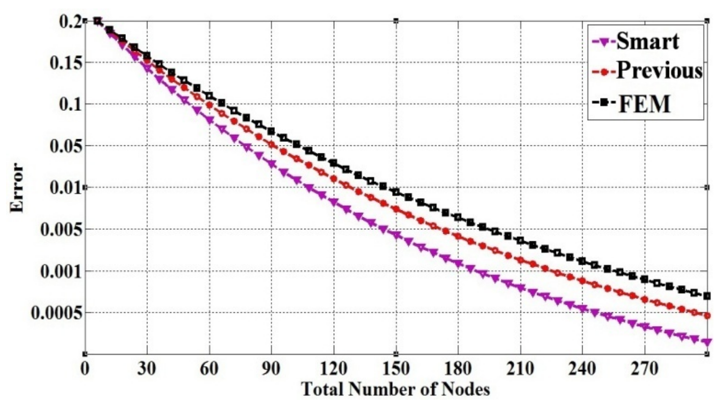


Fig. 3: Error Comparision between different methods.