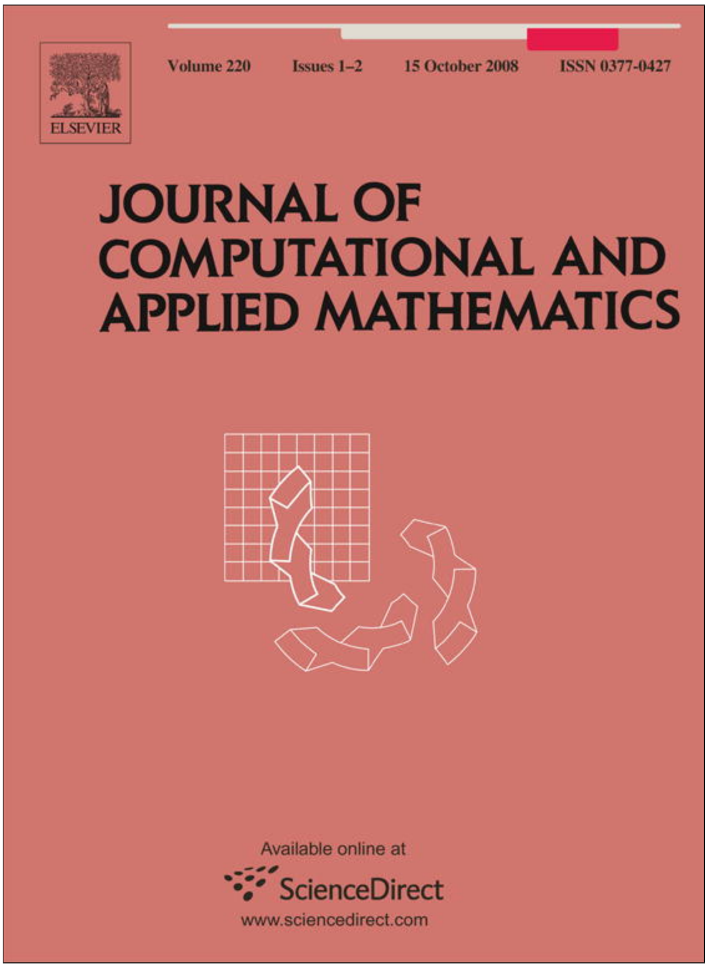
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A Fourier spectral-discontinuous Galerkin method for time-dependent 3-D Schrödinger–Poisson equations with discontinuous potentials

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Abstract

In this paper, we propose a high order Fourier spectral-discontinuous Galerkin method for time-dependent Schrödinger–Poisson equations in 3-D spaces. The Fourier spectral Galerkin method is used for the two periodic transverse directions and a high order discontinuous Galerkin method for the longitudinal propagation direction. Such a combination results in a diagonal form for the differential operators along the transverse directions and a flexible method to handle the discontinuous potentials present in quantum heterojunction and supperlattice structures. As the derivative matrices are required for various time integration schemes such as the exponential time differencing and Crank Nicholson methods, explicit derivative matrices of the discontinuous Galerkin method of various orders are derived. Numerical results, using the proposed method with various time integration schemes, are provided to validate the method.

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Keywords: Discontinuous Galerkin method; Spectral method; Derivative matrix; Schrödinger Poisson equations; Schrödinger Newton equations; Total-scattering wave formula; PML; Discontinuous potentials

1. Schrödinger–Poisson equations and discontinuous potentials

A self-consistent system of nonlinear Schrödinger–Poisson equations for a complex wave function $\Psi(\mathbf{x}, t)$ and potential $V_{\mathrm{ch}}(\mathbf{x}, t)$, $\mathbf{x} = (x, y, z)$ is defined as

$$\mathrm{i}\frac{\partial \Psi}{\partial t} = -\frac{1}{2}\nabla^2 \Psi + (V_{\mathrm{in}} + V_{\mathrm{ch}})\Psi, \tag{1.1}$$

$$\nabla^2 V_{\mathrm{ch}} = -|\Psi|^2, \tag{1.2}$$

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where $V_{\text{in}}(\mathbf{x}, t)$ is some given external potential or intrinsic potential due to the band structures of the materials used for quantum confinement in heterojunctions and quantum supperlattices [10].

This simple looking nonlinear system has important applications in quantum systems and requires subtle physical interpretations and much computational efforts for self-consistent solutions. To motivate the research in this paper, we will first give some background of several physical problems which can be modelled by the nonlinear Schrödinger–Poisson equations (1.1) and (1.2).

Quantum many body system: A system of N electrons and N_v nuclei interacting via the Coulomb potential is described by the linear Schrödinger equation for the wave function $\psi = \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)$

$$\begin{aligned} &\mathrm{i}\hbar\partial_t\psi = -\sum_{j=1}^{N}\frac{\hbar^2}{2m_j}\triangle_j\psi + \sum_{1\leqslant j<k\leqslant N}\frac{q^2}{|\mathbf{r}_j-\mathbf{r}_k|}\psi + V_{\text{ext}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t)\psi, \\ &\psi(t=0) = \psi_I(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N), \end{aligned} \tag{1.3}$$

where m is the mass of electron, q is the charge of one electron and $\hbar$ is the reduced Planck constant. $V_{\text{ext}}(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)$ is a generic, time-dependent external potential from the interaction between electrons and nuclei and time-dependent electric and magnetic fields. The solutions of the many-particle Schrödinger equation poses great computational challenges, which has been only solved for very small number of particles. Due to the prohibitive high cost of solving many-particle Schrödinger equations, it is of practical importance to derive one particle equation models in the form of (1.1) and (1.2) to approximate the many body system. The rigorous mathematical justification of one particle equation for time-dependent quantum system is still an active research topic. Recently, the one particle Schrödinger–Poisson equations for time-dependent many Boson system is derived in [3] in the weak coupling limit. The Poisson equation for $V_{\text{ch}}(\mathbf{x}, t)$ in this case models the "mean field potential" from other particles on the one particle of interest.

Quantum-gravity system: The Schrödinger–Newton equations for a quantum-mechanical particle of mass m moving in its own gravitational potential are the pair of coupled nonlinear partial differential [15]

$$\mathrm{i}\hbar\frac{\partial\Psi\mathbf{x}t}{\partial t} = -\frac{\hbar^2}{2m}\triangle_{\mathbf{x}}\Psi(\mathbf{x}, t) + mV(\mathbf{x}, t)\Psi(\mathbf{x}, t), \quad \mathbf{x}\in\mathbf{R}^3, \tag{1.4}$$

$$\triangle_x V(\mathbf{x}, t) = 4\pi Gm|\Psi(\mathbf{x}, t)|^2, \tag{1.5}$$

where $V(\mathbf{x}, t)$ is the gravitational potential and G the Newton's gravitational constant. And we can see that the Schrödinger–Newton equations are of the same form of the Schrödinger–Poisson equations (1.1) and (1.2).

TDDFT for many body quantum system: In quantum chemistry, time-dependent density functional theory (TDDFT) generalizes the classical Hartree–Fock approximation of many electron system by addressing the exchange and correlation effects. It has become an important tool to find excited electronic state energies [25]. The time-dependent Kohn–Sham (TDKS) equations for N particle systems involve N-wave functions $\Psi_j(x, t)$ and are given as

$$\mathrm{i}\hbar\frac{\partial\Psi_j(\mathbf{x}, t)}{\partial t} = \left(-\frac{\triangle}{2m} + \upsilon_s[n](\mathbf{x}, t)\right)\Psi_j(\mathbf{x}, t), \quad \mathbf{x}\in\mathbf{R}, \quad j = 1, 2, \ldots, N, \tag{1.6}$$

$$\upsilon_s[n](\mathbf{x}, t) = V_{\text{ext}}(\mathbf{x}, t) + \int\frac{n(\mathbf{x}', t)}{|\mathbf{x}-\mathbf{x}'|}\,\mathrm{d}\mathbf{x}' + V_{\text{XC}}[n](\mathbf{x}, \mathbf{t}), \tag{1.7}$$

$$n(\mathbf{x}, t) = q\sum_{j=1}^{N}|\Psi_j(\mathbf{x}, t)|^2,$$

where the second term of the potential $\upsilon_s[n](\mathbf{x}, t)$ can be solved with a Poisson equation and $V_{\text{XC}}(\mathbf{x}, \mathbf{t})$ is the exchange-correlation potential. Therefore, TDKS equations are similar to the time-dependent Schrödinger–Poisson equations. The only difference is the exchange-correlation potential term takes a more complex form

$$V_{\text{XC}}[n](\mathbf{x}, \mathbf{t}) = \frac{\delta E_{\text{XC}}[n]}{\delta n},$$

where $E_{\text{XC}}[n]$ denotes the exchange-correlation energy for which approximations like the local density approximation (LDA) can be used [12].

Discontinuous potentials: In many applications, especially with localized potential structures of heterojunction and quantum supperlattice structures formed by an array of quantum dots [10], the intrinsic potential $V_{\text{in}}(\mathbf{x})$ will be discontinuous, thus producing discontinuities in the wave functions in the cases of different electron masses across the discontinuities. It is important to have a numerical method to handle such discontinuities in the wave functions with high accuracy and ease. For this reason, we propose to use the discontinuous Galerkin (DG) method [26] to handle this discontinuity in wave functions along the propagation z-direction. Meanwhile, in many quantum supperlattices, such as arrays of quantum dots, the potential is or can be modelled by periodic functions over the transverse (x, y) plane, where a Fourier spectral method is a natural candidate [11]. For these two reasons, we adopt a hybrid spectral-discontinuous Galerkin method for coupled nonlinear time-dependent Schrödinger–Poisson equations with discontinuous potentials.

In addition, we will investigate various time integration schemes with the hybrid method. To achieve larger time steps, exponential time differencing (ETD) scheme has attracted much attention [8], recently. The ETD method uses a time integrating factor associated with the linear part of the semi-discretized system, namely, the derivative matrices resulting from the numerical discretization of the differential operator. In our Fourier spectral-DG method, the derivative operators along the transverse (x, y) directions are diagonal matrices. As a matter of fact, the Schrödinger–Poisson equations become a series of differential in equations in (z, t), to which the ETD could be applied. In order to find the time integrating factor for these $(z-t)$ differential equations, we will need the explicit form of the z-derivative matrices from the DG methods. The explicit form of the derivative matrices will also be needed for implicit time discretizations such as the Crank Nicholson scheme. Derivative matrices will be derived for DG methods with two types of numerical flux definitions.

Self-consistent solutions of Schrödinger–Poisson equation are important in the simulation of carrier transport in nanoelectronics such as the resonant tunnelling diode (RTD) [19,6,17] and MOSFET [22,18]. In most situations, time independent Schrödinger–Poissons are solved for the eigenstates of the quantum system [4,7]. However, in some situations a time-dependent solution will be needed due to the transient nature of the external potentials such as in a laser excited process. Previous work on time-dependent Schrödinger–Poisson includes the work of [9] which considers spherically symmetric Schrödinger–Poisson equations with finite difference method in space discretization and Crank–Nicholson type predicator–corrector scheme for time integration. The authors of [14] present a numerical study of the time-dependent Schrödinger–Newton equations in three dimensions with three kinds of symmetry: spherically symmetric, axially symmetric and translational symmetric. The numerical discretization methods again include Crank–Nicholson method for time integration and finite difference for space discretization method and spectral method for the Poisson equation. A finite difference method is also used in [21] to solve spherically symmetric Schrödinger–Poisson equations. Recently, a time-splitting spectral method is proposed in [2] to solve the Schrödinger–Poisson problems with periodic boundary conditions in all three spatial directions.

The rest of the paper is organized as follows. In Section 2, we will reduce 3-D equations into a set of 1-D equations with the Fourier Galerkin method in the (x, y) directions. In Section 3, we give DG methods for second-order z-derivative in the Poisson equations, and the explicit forms of derivative matrices will be given for two types of numerical fluxes (central and upwinding) used in the DG methods. In Section 4, the Fourier spectral-DG methods and various time integration schemes will be investigated. In Section 5, after addressing the boundary condition issues including PML layers and total-scattering wave formulations for the Schrödinger equation, we present numerical results to validate the proposed method. The following numerical tests are provided: the accuracy of the derivative matrices; the accuracy of various time integrations for the time-dependent Schrödinger equation; finally, the computation of a 3-D time-dependent nonlinear Schrödinger–Poisson equations with discontinuous potentials, which models quantum supperlattices formed by an array of periodic quantum dots. In Section 6, a conclusion will be given.

2. High order Fourier spectral-DG methods

The Schrödinger–Poisson system in three dimensions can be written as

$$\mathrm{i}\frac{\partial \Psi}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V_{\text{tot}}\right]\Psi(x, y, z, t), (x, y, z) \in [0, 2\pi]^2 \times [0, L], \quad t \geqslant 0, \tag{2.1}$$

$$\nabla^2 V_{\text{ch}} = -|\Psi(x, y, z, t)|^2, \tag{2.2}$$

where $\mathrm{i}=\sqrt{-1}$ and the external/intrinsic potential $V_{\mathrm{in}}(x, y, z, t)$ and the total potential $V_{\mathrm{tot}}(x, y, z, t)$ are assumed to be periodic in (x, y) plane with a period 2π. Also, $\Psi(x, y, z, t)$, the particle wave function, is assumed to be a periodic functions in (x, y) variables. We have set the Planck constant $\hbar=1$ and the mass $m=1$, the electron charge in (2.2) $q=1$. The total potential function $V_{\mathrm{tot}}(x, y, z, t)$ is the sum of the external/intrinsic potential V_{in} and the self-consistent potential due to the charge V_{ch}, i.e.,

$$V_{\mathrm{tot}}(x, y, z, t)=V_{\mathrm{in}}(x, y, z, t)+V_{\mathrm{ch}}(x, y, z, t). \tag{2.3}$$

Due to the periodicity of the problem in the (x, y) directions, we will use a Fourier spectral method in the transverse (x, y) directions while a DG method will be applied to the z-direction to treat the possible derivative discontinuities of the wave functions from the jumps of the potentials at material interfaces. The wave function is then written as

$$\Psi(x, y, z, t)=\sum_{m,n} \exp(\mathrm{i}(mx+ny)) u_{m,n}(z, t), \tag{2.4}$$

where m, n are integers. Similarly, we can assume that the charge potential energy V_{ch} can be written as

$$V_{\mathrm{ch}}(x, y, z, t)=\sum_{m,n} \exp(\mathrm{i}(mx+ny)) v_{m,n}(z, t), \tag{2.5}$$

where $v_{m,n}(z, t)$ are complex-valued functions and $v_{-n,-m}$ and $v_{m,n}$ are conjugate to each other for a real-valued $V_{\mathrm{ch}}(x, y, z, t)$. Substituting (2.4) and (2.5) into the Schrödinger–Poisson system yields

$$\begin{aligned}\mathrm{i}\frac{\partial}{\partial t}\sum_{m,n} \exp(\mathrm{i}(mx+ny)) u_{m,n}(z, t)= & -\nabla^2\left(\sum_{m,n} \exp(\mathrm{i}(mx+ny)) u_{m,n}(z, t)\right) \\ & +(V_{\mathrm{in}}+V_{\mathrm{ch}})\left(\sum_{m,n} \exp(\mathrm{i}(mx+ny)) u_{m,n}(z, t)\right),\end{aligned} \tag{2.6}$$

$$\nabla^2\left(\sum_{m,n} \exp(\mathrm{i}(mx+ny)) v_{m,n}(z, t)\right)=-\left|\sum_{m,n} \exp(\mathrm{i}(mx+ny)) u_{m,n}(z, t)\right|^2. \tag{2.7}$$

The Galerkin projection of (2.6) and (2.7) into the orthogonal Fourier basis yields a set of 1-D differential equations

$$\begin{aligned}\mathrm{i}\frac{\partial}{\partial t} u_{m,n}(z, t)= & -\frac{\partial^2}{\partial z^2} u_{m,n}(z, t)+(m^2+n^2) u_{m,n}(z, t)+V_{\mathrm{in}} u_{m,n}(z, t) \\ & +\sum_{n_1+n_2=n, m_1+m_2=m} v_{m_1,n_1}(z, t) u_{m_2,n_2}(z, t),\end{aligned} \tag{2.8}$$

$$\frac{\partial^2}{\partial z^2} v_{m,n}(z, t)=-\sum_{m_2-m_1=m, n_2-n_1=n} \bar{u}_{m_1,n_1}(z, t) u_{m_2,n_2}(z, t)+(m^2+n^2) v_{m,n}(z, t). \tag{2.9}$$

Eqs. (2.8) and (2.9) form a system of 1-D ordinary differential equations for (z, t)-variables, for which the spatial z-derivative will be discretized by the DG method while the time derivative will be approximated by various time integration schemes.

3. DG discretization for Poisson equation

We will illustrate the DG method for a Poisson equation in the 1-D case. The equation is written into 1-D form

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\frac{\mathrm{d}}{\mathrm{d}z} u(z)\right)=f(z) \quad \text{in } [0, L] \tag{3.1}$$

with the following typical boundary conditions:

$$u(0)=\beta, \quad \frac{\partial}{\partial z}u(L)=\gamma. \tag{3.2}$$

Following [26,16], we introduce a new variable

$$q=u'(z), \tag{3.3}$$

and obtain a first-order system

$$\frac{\mathrm{d}}{\mathrm{d}z}(\varepsilon(z)q(z))-f(z)=0, \tag{3.4}$$

$$u'(z)-q(z)=0. \tag{3.5}$$

Assuming the computational domain [0, L] is discretized into N elements, we let $I_j=[z_{j-1/2}, z_{j+1/2}]$ denote the jth element where $0=z_{1/2}<z_{3/2}<\cdots<z_{N+1/2}=L$. The finite element space is

$$V_h=\{v\in L^1[0,L]: v|_{I_j}\in P^k(I_j),\ j=1,\ldots,N\}, \tag{3.6}$$

where $P^k(I)$ denotes the space of polynomials in I of degree at most k. The approximate solution (u_h, q_h) by the DG method is defined with the following weak form:

$$\forall v_{h,u}\in P^k(I_j):$$

$$-\int_{I_j}\varepsilon(z)q_h(z)\frac{\mathrm{d}v_{h,u}(z)}{\mathrm{d}z}\,\mathrm{d}z+h_{q,j+1/2}(t)v_{h,u}(z^-_{j+1/2})-h_{q,j-1/2}(t)v_{h,u}(z^+_{j-1/2})=\int_{I_j}f(z)v_h\,\mathrm{d}z, \tag{3.7}$$

$$\forall v_{h,q}\in P^k(I_j):$$

$$-\int_{I_j}u_h(z,t)\frac{\mathrm{d}v_{h,q}(z)}{\mathrm{d}z}\,\mathrm{d}z-h_{u,j+1/2}(t)v_{h,q}(z^-_{j+1/2})+h_{u,j-1/2}(t)v_{h,q}(z^+_{j-1/2})$$
$$=\int_{I_j}q_h(z,t)v_{h,q}(z)\,\mathrm{d}z, \tag{3.8}$$

where $(h_{q,j+1/2}, h_{u,j+1/2})$ is the numerical flux which approximates $(\varepsilon q, u)$ at $z_{j+1/2}$, respectively.

For $z\in I_j$

$$u_h(z,t)=\sum_{k=1}^{s}u_k^j\phi_k^j(z), \tag{3.9}$$

$$q_h(z,t)=\sum_{m=1}^{s}q_m^j\phi_m^j(z), \tag{3.10}$$

where s is the number of basis functions, ϕ_k^j is the basis functions and u_k^j and q_m^j are the time-dependent coefficients.

After replacing u_h and q_h with the expressions (3.9) and (3.10) and setting the test function $v_h=\phi_n^j$ in (3.7) and (3.8), we can get the following linear system for the coefficients u_k^j and q_m^j for $j=1,\ldots,N$ and $n=1,\ldots,s$:

$$-\varepsilon_j\sum_{m=1}^{s}M_{nm}^{z,j}q_m^j+h_{q,j+1/2}\phi_n^j(z_{j+1/2})-h_{q,j-1/2}\phi_n^j(z_{j-1/2})=\int_{I_j}f(z)\phi_n^j(z)\,\mathrm{d}z, \tag{3.11}$$

$$-\sum_{k=1}^{s}M_{mk}^{z,j}u_k^j+h_{u,j+1/2}\phi_m^j(z_{j+1/2})-h_{u,j-1/2}\phi_m^j(z_{j+1/2})=\int_{I_j}\sum_{k=1}^{s}q_k^j\phi_k^j\phi_m^j\,\mathrm{d}z, \tag{3.12}$$

where the stiff matrix is

$$M_{nm}^{z,j} = \int_{I_j} \phi_m^j(z) \frac{\mathrm{d}\phi_n^j}{\mathrm{d}z}\,\mathrm{d}z. \tag{3.13}$$

Also we assume that $\varepsilon(z)$ is piecewise constant,

$$\varepsilon(z) = \varepsilon_j \quad \text{for } z \in I_j.$$

In the following, we will present the resulting finite difference formula with appropriate derivative matrices for the physical variable u with the auxiliary variable q eliminated. We first express q_k^j using u_k^j by solving (3.12) (note that, this operation need not solve a linear system of size sN, and only a small size linear system of $\mathrm{O}(s)$ for each element), and then replace q_l^j in (3.11), then we will get a linear system of size sN for u_k^j only.

Assuming that the local mass matrix is diagonal, which can be achieved by using Legendre polynomials as the basis functions for $P^k(I_j)$

$$\int_{I_j} \phi_k^j(z)\phi_m^j(z)\,\mathrm{d}z = \begin{cases} 0 & \text{if } k \neq m, \\ c_{j,m} & \text{if } k = m. \end{cases} \tag{3.14}$$

we obtain q_m^j in terms of u_k^j

$$q_m^j = \frac{1}{c_{j,m}} \left[-\sum_{k=1}^{s} M_{mk}^{z,j} u_k^j + h_{u,j+1/2}\phi_m^j(z_{j+1/2}) - h_{u,j-1/2}\phi_m^j(z_{j-1/2}) \right]. \tag{3.15}$$

Substituting (3.15) and (3.11) results in

$$\begin{aligned} &-\varepsilon_j \sum_{m=1}^{s} M_{nm}^{z,j} \frac{1}{c_{j,m}} \left[-\sum_{k=1}^{s} M_{mk}^{z,j} u_k^j + h_{u,j+1/2}\phi_m^j(z_{j+1/2}) - h_{u,j-1/2}\phi_m^j(z_{j-1/2}) \right] \\ &\quad + h_{q,j+1/2}\phi_n^j(z_{j+1/2}) - h_{q,j-1/2}\phi_n^j(z_{j-1/2}) = \int_{I_j} f(z)\phi_n^j(z)\,\mathrm{d}z. \end{aligned} \tag{3.16}$$

3.1. Derivative matrix D_{sN} for a central flux

First, we will derive the derivative matrix for unknowns u_k^j using the central numerical flux proposed in [16]

$$h_{u,j+1/2} = \tfrac{1}{2}(u(z_{j+1/2}^-) + u(z_{j+1/2}^+)), \tag{3.17}$$

$$h_{q,j+1/2} = \tfrac{1}{2}(\varepsilon_j q(z_{j+1/2}^-) + \varepsilon_{j+1} q(z_{j+1/2}^+)). \tag{3.18}$$

The above fluxes at the boundaries $z_{1/2} = 0$, $z_{N+1/2} = L$ will be modified using the boundary condition (3.2) as follows:

$$h_{u,1/2} = \tfrac{1}{2}(\beta + u(z_{1/2}^+)), \quad h_{q,1/2} = \varepsilon_1 q(z_{1/2}^+), \tag{3.19}$$

$$h_{u,N+1/2} = u(z_{N+1/2}^-), \quad h_{q,N+1/2} = \tfrac{1}{2}\varepsilon_N (q(z_{N+1/2}^-) + \gamma). \tag{3.20}$$

We have assumed that the material constant is continuous across both boundaries, i.e., $\varepsilon_0 = \varepsilon_1$ and $\varepsilon_N = \varepsilon_{N+1}$. At the left boundary $z_{1/2}$, as the function value is known, we set $u(z_{1/2}^-) = \beta$ and $q(z_{1/2}^-) = q(z_{1/2}^+)$. At the right boundary, the derivative boundary value is given, we set $q(z_{N+1/2}^+) = \gamma$ and $u(z_{N+1/2}^+) = u(z_{N+1/2}^-)$.

Now (3.16) is rewritten as

$$\varepsilon_j \sum_{k=1}^{s}\sum_{m=1}^{s}\frac{1}{c_{j,m}}M_{nm}^{z,j}M_{mk}^{z,j}u_k^j$$
$$\times \underbrace{-\varepsilon_j \sum_{m=1}^{s}\frac{1}{c_{j,m}}M_{nm}^{z,j}\phi_m^j(z_{j+1/2})h_{u,j+1/2}}_{\text{A}} + \underbrace{\varepsilon_j \sum_{m=1}^{s}\frac{1}{c_{j,m}}M_{nm}^{z,j}\phi_m^j(z_{j-1/2})h_{u,j-1/2}}_{\text{B}}$$
$$+ \underbrace{h_{q,j+1/2}\phi_n^j(z_{j+1/2})}_{\text{C}}\underbrace{-h_{q,j-1/2}\phi_n^j(z_{j-1/2})}_{\text{D}} = \int_{I_j} f(z)\phi_n^j(z)\,\mathrm{d}z. \tag{3.21}$$

For $j=1,2,N-1,N$, the flux defined in Eqs. (3.19) and (3.20) will be used. For $3\leqslant j\leqslant N-2$, using the flux of Eqs. (3.17) and (3.18), we have

$$2\text{A} = -\varepsilon_j \sum_{m=1}^{s}\frac{1}{c_{j,m}}M_{nm}^{z,j}\phi_m^j(z_{j+1/2})\sum_{k=1}^{s}(\phi_k^j(z_{j+1/2})u_k^j + \phi_k^{j+1}(z_{j+1/2})u_k^{j+1}), \tag{3.22}$$

$$2\text{B} = \varepsilon_j \sum_{m=1}^{s}\frac{1}{c_{j,m}}M_{nm}^{z,j}\phi_m^j(z_{j-1/2})\sum_{k=1}^{s}(\phi_k^{j-1}(z_{j-1/2})u_k^{j-1} + \phi_k^j(z_{j-1/2})u_k^j), \tag{3.23}$$

$$2\text{C}/\phi_n^j(z_{j+1/2}) = \varepsilon_j q^j(z_{j+1/2}) + \varepsilon_{j+1}q^{j+1}(z_{j+1/2}). \tag{3.24}$$

Replacing q_m^j in (3.24) with (3.15), (3.24) reads

$$\begin{aligned}
&2\text{C}/\phi_n^j(z_{j+1/2})\\
&\quad= (\varepsilon_j q_m^j\phi_m^j(z_{j+1/2}) + \varepsilon_{j+1}q_m^{j+1}\phi_m^{j+1}(z_{j+1/2}))\\
&\quad= \varepsilon_j\left[\frac{1}{c_{j,m}}(-M_{mk}^{z,j}u_k^j + h_{u,j+1/2}\phi_m^j(z_{j+1/2}) - h_{u,j-1/2}\phi_m^j(z_{j-1/2}))\phi_m^j(z_{j+1/2})\right]\\
&\qquad+ \varepsilon_{j+1}\left[\frac{1}{c_{j+1,m}}(-M_{mk}^{z,j+1}u_k^{j+1} + h_{u,j+3/2}\phi_m^{j+1}(z_{j+3/2}) - h_{u,j+1/2}\phi_m^{j+1}(z_{j+1/2}))\phi_m^{j+1}(z_{j+1/2})\right]\\
&\quad= \varepsilon_j\left(-\frac{1}{c_{j,m}}M_{mk}^{z,j}\phi_m^j(z_{j+1/2})u_k^j\right) + \varepsilon_{j+1}\left(-\frac{1}{c_{j+1,m}}M_{mk}^{z,j+1}\phi_m^{j+1}(z_{j+1/2})u_k^{j+1}\right)\\
&\qquad+ \varepsilon_j\frac{1}{c_{j,m}}\phi_m^j(z_{j+1/2})\phi_m^j(z_{j+1/2})h_{u,j+1/2} - \varepsilon_j\frac{1}{c_{j,m}}\phi_m^j(z_{j-1/2})\phi_m^j(z_{j+1/2})h_{u,j-1/2}\\
&\qquad+ \varepsilon_{j+1}\frac{1}{c_{j+1,m}}\phi_m^{j+1}(z_{j+3/2})\phi_m^{j+1}(z_{j+1/2})h_{u,j+3/2}\\
&\qquad- \varepsilon_{j+1}\frac{1}{c_{j+1,m}}\phi_m^{j+1}(z_{j+1/2})\phi_m^{j+1}(z_{j+1/2})h_{u,j+1/2}.
\end{aligned} \tag{3.25}$$

In (3.25) and the rest of this subsection, double index k or m implies summation over $1\leqslant k\leqslant s$, $1\leqslant m\leqslant s$, respectively. No summation is assumed over the element j index.

Substituting the numerical flux (3.17) into (3.25) yields

$$\begin{aligned}
&2\mathrm{C}/\phi_n^j(z_{j+1/2})\\
&=\varepsilon_j\left(-\frac{1}{c_{j,m}}M_{mk}^{z,j}\phi_m^j(z_{j+1/2})u_k^j\right)+\varepsilon_{j+1}\left(-\frac{1}{c_{j+1,m}}M_{mk}^{z,j+1}\phi_m^{j+1}(z_{j+1/2})u_k^{j+1}\right)\\
&+\varepsilon_j\frac{1}{c_{j,m}}\phi_m^j(z_{j+1/2})\phi_m^j(z_{j+1/2})\frac{1}{2}(u_k^j\phi_k^j(z_{j+1/2})+u_k^{j+1}\phi_k^{j+1}(z_{j+1/2}))\\
&-\varepsilon_j\frac{1}{c_{j,m}}\phi_m^j(z_{j-1/2})\phi_m^j(z_{j+1/2})\frac{1}{2}(u_k^{j-1}\phi_k^{j-1}(z_{j-1/2})+u_k^j\phi_k^j(z_{j-1/2}))\\
&+\varepsilon_{j+1}\frac{1}{c_{j+1,m}}\phi_m^{j+1}(z_{j+3/2})\phi_m^{j+1}(z_{j+1/2})\frac{1}{2}(u_k^{j+1}\phi_k^{j+1}(z_{j+3/2})+u_k^{j+2}\phi_k^{j+2}(z_{j+3/2}))\\
&-\varepsilon_{j+1}\frac{1}{c_{j+1,m}}\phi_m^{j+1}(z_{j+1/2})\phi_m^{j+1}(z_{j+1/2})\frac{1}{2}(u_k^j\phi_k^j(z_{j+1/2})+u_k^{j+1}\phi_k^{j+1}(z_{j+1/2})).
\end{aligned}\tag{3.26}$$

Similarly, we have

$$\begin{aligned}
&-2\mathrm{D}/\phi_n^j(z_{j-1/2})\\
&=\varepsilon_{j-1}\left(-\frac{1}{c_{j-1,m}}M_{mk}^{z,j-1}\phi_m^{j-1}(z_{j-1/2})u_k^{j-1}\right)+\varepsilon_j\left(-\frac{1}{c_{j,m}}M_{mk}^{z,j}\phi_m^j(z_{j-1/2})u_k^j\right)\\
&+\varepsilon_{j-1}\frac{1}{c_{j-1,m}}\phi_m^{j-1}(z_{j-1/2})\phi_m^{j-1}(z_{j-1/2})\frac{1}{2}(u_k^{j-1}\phi_k^{j-1}(z_{j-1/2})+u_k^j\phi_k^j(z_{j-1/2}))\\
&-\varepsilon_{j-1}\frac{1}{c_{j-1,m}}\phi_m^{j-1}(z_{j-3/2})\phi_m^{j-1}(z_{j-1/2})\frac{1}{2}(u_k^{j-2}\phi_k^{j-2}(z_{j-3/2})+u_k^{j-1}\phi_k^{j-1}(z_{j-3/2}))\\
&+\varepsilon_j\frac{1}{c_{j,m}}\phi_m^j(z_{j+1/2})\phi_m^j(z_{j-1/2})\frac{1}{2}(u_k^j\phi_k^j(z_{j+1/2})+u_k^{j+1}\phi_k^{j+1}(z_{j+1/2}))\\
&-\varepsilon_j\frac{1}{c_{j,m}}\phi_m^j(z_{j-1/2})\phi_m^j(z_{j-1/2})\frac{1}{2}(u_k^{j-1}\phi_k^{j-1}(z_{j-1/2})+u_k^j\phi_k^j(z_{j-1/2})).
\end{aligned}\tag{3.27}$$

• Difference equations for variable u: From (3.21)–(3.23), (3.26) and (3.27), we have the difference equations for u for $j=3,4,\ldots,N-2$,

$$\sum_{k=1}^{s}a_{n,k}^{j,j-2}u_k^{j-2}+\sum_{k=1}^{s}a_{n,k}^{j,j-1}u_k^{j-1}+\sum_{k=1}^{s}a_{n,k}^{j,j}u_k^j+\sum_{k=1}^{s}a_{n,k}^{j,j+1}u_k^{j+1}+\sum_{k=1}^{s}a_{n,k}^{j,j+2}u_k^{j+2}=f_n^j,\tag{3.28a}$$

where $1\leqslant n\leqslant s$, and for $j=1,2,N-1,N$ the equations are

$$\sum_{k=1}^{s}a_{n,k}^{j,j}u_k^j+\sum_{k=1}^{s}a_{n,k}^{j,j+1}u_k^{j+1}+\sum_{k=1}^{s}a_{n,k}^{j,j+2}u_k^{j+2}+b_n^j=f_n^j,\quad j=1,\tag{3.28b}$$

$$\sum_{k=1}^{s}a_{n,k}^{j,j-1}u_k^{j-1}+\sum_{k=1}^{s}a_{n,k}^{j,j}u_k^j+\sum_{k=1}^{s}a_{n,k}^{j,j+1}u_k^{j+1}+\sum_{k=1}^{s}a_{n,k}^{j,j+2}u_k^{j+2}+b_n^j=f_n^j,\quad j=2,\tag{3.28c}$$

$$\sum_{k=1}^{s}a_{n,k}^{j,j-2}u_k^{j-2}+\sum_{k=1}^{s}a_{n,k}^{j,j-1}u_k^{j-1}+\sum_{k=1}^{s}a_{n,k}^{j,j}u_k^j+b_n^j=f_n^j,\quad j=N,\tag{3.28d}$$

$$\sum_{k=1}^{s}a_{n,k}^{j,j-2}u_k^{j-2}+\sum_{k=1}^{s}a_{n,k}^{j,j-1}u_k^{j-1}+\sum_{k=1}^{s}a_{n,k}^{j,j}u_k^j+\sum_{k=1}^{s}a_{n,k}^{j,j+1}u_k^{j+1}+b_n^j=f_n^j,\quad j=N-1,\tag{3.28e}$$

where

$$f_n^j = \int_{I_j} f(z)\phi_n^j(z)\,\mathrm{d}z, \quad 1 \leqslant j \leqslant N \tag{3.29}$$

and $a_{n,k}^{j,l}$ is the nonzero element $((N-1)j+n, (N-1)l+k)$ of the matrix of the linear system. The formulas for $a_{n,k}^{j,l}$ b_n^j are given in Appendix A.

Finally, the matrix form of Eq. (3.44a)–(3.44e) is

$$D_{sN}\begin{pmatrix} \mathbf{u}^1 \\ \mathbf{u}^2 \\ \mathbf{u}^3 \\ \mathbf{u}^4 \\ \vdots \\ \mathbf{u}^{N-1} \\ \mathbf{u}^N \end{pmatrix} + \begin{pmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \\ \mathbf{0} \\ \mathbf{0} \\ \vdots \\ \mathbf{b}^{N-1} \\ \mathbf{b}^N \end{pmatrix} = \begin{pmatrix} \mathbf{f}^1 \\ \mathbf{f}^2 \\ \mathbf{f}^3 \\ \mathbf{f}^4 \\ \vdots \\ \mathbf{f}^{N-1} \\ \mathbf{f}^N \end{pmatrix}, \tag{3.30}$$

where $\mathbf{u}^j = (u_1^j, u_2^j, \ldots, u_s^j)$ denotes the vector with components u_k^j appearing in (3.9), and $\mathbf{f}^j = (f_1^j, f_2^j, \ldots, f_s^j)$ denotes the vector with elements f_n^j given by (3.29) and the block pentadiagonal derivative matrix

$$D_{sN} = \begin{pmatrix} A^{(1,1)} & A^{(1,2)} & A^{(1,3)} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ A^{(2,1)} & A^{(2,2)} & A^{(2,3)} & A^{(2,4)} & 0 & 0 & \cdots & 0 & 0 & 0 \\ A^{(3,1)} & A^{(3,2)} & A^{(3,3)} & A^{(3,4)} & A^{(3,5)} & 0 & \cdots & 0 & 0 & 0 \\ 0 & A^{(4,2)} & A^{(4,3)} & A^{(4,4)} & A^{(4,5)} & A^{(4,6)} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & A^{(N,N-2)} & A^{(N,N-1)} & A^{(N,N)} \end{pmatrix}, \tag{3.31}$$

while $A^{(j,l)} = (a_{n,k}^{j,l})$ is a matrix of dimension $s \times s$. $\mathbf{b}^j = (b_1^j, b_2^j, \ldots b_s^j)$, $j = 1, 2, N-1, N$ denotes the vector which comes from the boundary conditions.

If we take the basis function as

$$\phi_k^j(z) = L_k(\xi^j(z)), \quad k = 1, 2, \ldots, s, \;\; z \in I_j,$$
$$\xi^j(z) = \frac{2(z - z_j)}{h_j}, \tag{3.32}$$

where h_j is the length of the jth element and L_k is the Legendre polynomial of degree $k-1$, e.g.,

$$L_1(\xi) = 1, \quad L_2(\xi) = z, \quad L_3(\xi) = \tfrac{1}{2}(3\xi^2 - 1),$$
$$L_4(\xi) = \tfrac{1}{2}(5\xi^3 - 3\xi), \quad L_5(\xi) = \tfrac{1}{8}(35\xi^4 - 30\xi^2 + 3).$$

These basis functions make the mass matrix diagonal with diagonal elements

$$c_{j,1} = h_j, \quad c_{j,2} = \frac{h_j}{3}, \quad c_{j,3} = \frac{h_j}{5}, \quad c_{j,4} = \frac{h_j}{7}, \quad c_{j,5} = \frac{h_j}{9} \tag{3.33}$$

and, the nonzero elements of the corresponding stiff matrix are

$$M_{2,1}^{z,j} = 2, \quad M_{3,2}^{z,j} = 2, \quad M_{4,1}^{z,j} = 2, \quad M_{4,3}^{z,j} = 2, \quad M_{5,2}^{z,j} = 2, \quad M_{5,4}^{z,j} = 2.$$

For simplicity, we assume that $\varepsilon_j = 1$, for all j, and all the elements are of the same length h. The block matrices in D_{sN} can be explicitly found for the basis functions of order $1 \leqslant s \leqslant 5$. The matrices $A^{(j,l)}$, $A^{(j,l-1)}$, $A^{(j,l+1)}$ for $3 \leqslant j \leqslant N-2$ are given as follows. For $j = 1,\ 2,\ N-1,\ N$, some matrices are a little different from the above one because of the influence of the boundary condition. We also list them and the responding vectors out.

• *Case* 1: $s = 5$

$$A^{(j,j)} = \begin{pmatrix} -\frac{45}{2h} & 0 & -\frac{33}{2h} & 0 & -\frac{5}{2h} \\ 0 & -\frac{55}{2h} & 0 & -\frac{35}{2h} & 0 \\ -\frac{33}{2h} & 0 & -\frac{45}{2h} & 0 & -\frac{17}{2h} \\ 0 & -\frac{35}{2h} & 0 & -\frac{55}{2h} & 0 \\ -\frac{5}{2h} & 0 & -\frac{17}{2h} & 0 & -\frac{45}{2h} \end{pmatrix},$$

$$A^{(j,j-1)} = (A^{(j,j+1)})^{\mathrm{T}} = \begin{pmatrix} \frac{10}{h} & \frac{23}{2h} & \frac{7}{h} & \frac{13}{2h} & 0 \\ -\frac{23}{2h} & -\frac{13}{h} & -\frac{17}{2h} & -\frac{8}{h} & -\frac{3}{2h} \\ \frac{7}{h} & \frac{17}{2h} & \frac{4}{h} & \frac{7}{2h} & -\frac{3}{h} \\ -\frac{13}{2h} & -\frac{8}{h} & -\frac{7}{2h} & -\frac{3}{h} & \frac{7}{2h} \\ 0 & \frac{3}{2h} & -\frac{3}{h} & -\frac{7}{2h} & -\frac{10}{h} \end{pmatrix},$$

$$A^{(j,j-2)} = (A^{(j,j+2)})^{\mathrm{T}} = \begin{pmatrix} \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} \\ -\frac{5}{4h} & -\frac{5}{4h} & -\frac{5}{4h} & -\frac{5}{4h} & -\frac{5}{4h} \\ \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} \\ -\frac{5}{4h} & -\frac{5}{4h} & -\frac{5}{4h} & -\frac{5}{4h} & -\frac{5}{4h} \\ \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} & \frac{5}{4h} \end{pmatrix},$$

$$A^{(1,1)} = \begin{pmatrix} -\frac{85}{4h} & -\frac{1}{4h} & -\frac{49}{4h} & -\frac{19}{4h} & \frac{35}{4h} \\ -\frac{5}{4h} & -\frac{111}{4h} & -\frac{17}{4h} & -\frac{51}{4h} & -\frac{45}{4h} \\ -\frac{61}{4h} & \frac{1}{4h} & -\frac{73}{4h} & -\frac{19}{4h} & \frac{11}{4h} \\ -\frac{5}{4h} & -\frac{71}{4h} & -\frac{17}{4h} & -\frac{91}{4h} & -\frac{45}{4h} \\ -\frac{5}{4h} & \frac{1}{4h} & -\frac{17}{4h} & -\frac{19}{4h} & -\frac{45}{4h} \end{pmatrix},$$

$$A^{(1,2)} = \begin{pmatrix} \frac{35}{4h} & -\frac{41}{4h} & \frac{23}{4h} & \frac{21}{4h} & -\frac{5}{4h} \\ \frac{51}{4h} & -\frac{57}{4h} & \frac{39}{4h} & -\frac{37}{4h} & -\frac{11}{4h} \\ \frac{23}{4h} & -\frac{29}{4h} & \frac{11}{4h} & -\frac{9}{4h} & -\frac{17}{4h} \\ \frac{31}{4h} & -\frac{37}{4h} & -\frac{19}{4h} & -\frac{17}{4h} & -\frac{9}{4h} \\ -\frac{5}{4h} & -\frac{1}{4h} & -\frac{17}{4h} & \frac{19}{4h} & -\frac{45}{4h} \end{pmatrix}, \quad \mathbf{b}^1 = \begin{pmatrix} \frac{85}{4h} \\ -\frac{91}{4h} \\ \frac{73}{4h} \\ -\frac{71}{4h} \\ \frac{45}{4h} \end{pmatrix}\beta, \quad \mathbf{b}^2 = \begin{pmatrix} \frac{5}{4h} \\ -\frac{5}{4h} \\ \frac{5}{4h} \\ -\frac{5}{4h} \\ \frac{5}{4h} \end{pmatrix}\beta,$$

$$A^{(N,N)} = \begin{pmatrix} -\frac{45}{4h} & \frac{45}{4h} & -\frac{21}{4h} & \frac{45}{4h} & \frac{35}{4h} \\ \frac{51}{4h} & -\frac{59}{4h} & \frac{51}{4h} & -\frac{19}{4h} & \frac{51}{4h} \\ -\frac{33}{4h} & \frac{33}{4h} & -\frac{57}{4h} & \frac{33}{4h} & -\frac{1}{4h} \\ \frac{31}{4h} & -\frac{39}{4h} & \frac{31}{4h} & -\frac{79}{4h} & \frac{31}{4h} \\ -\frac{5}{4h} & \frac{5}{4h} & -\frac{29}{4h} & \frac{5}{4h} & -\frac{85}{4h} \end{pmatrix}, \quad \mathbf{b}^N = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}\gamma,$$

$$A^{(N-1,N)} = \begin{pmatrix} \frac{45}{4h} & -\frac{41}{4h} & \frac{33}{4h} & -\frac{21}{4h} & \frac{5}{4h} \\ \frac{51}{4h} & -\frac{47}{4h} & \frac{39}{4h} & -\frac{27}{4h} & \frac{11}{4h} \\ \frac{33}{4h} & -\frac{29}{4h} & \frac{21}{4h} & -\frac{9}{4h} & -\frac{7}{4h} \\ \frac{31}{4h} & -\frac{27}{4h} & \frac{19}{4h} & -\frac{7}{4h} & -\frac{9}{4h} \\ \frac{5}{4h} & -\frac{1}{4h} & -\frac{7}{4h} & \frac{19}{4h} & -\frac{35}{4h} \end{pmatrix}, \quad \mathbf{b}^{N-1} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

- *Case* 2: $s = 4$

$$A^{(j,j)} = \begin{pmatrix} -\frac{18}{h} & 0 & -\frac{12}{h} & 0 \\ 0 & -\frac{14}{h} & 0 & -\frac{4}{h} \\ -\frac{12}{h} & 0 & -\frac{18}{h} & 0 \\ 0 & -\frac{4}{h} & 0 & -\frac{14}{h} \end{pmatrix},$$

$$A^{(j,j-1)} = (A^{(j,j+1)})^{\mathrm{T}} = \begin{pmatrix} \frac{10}{h} & \frac{7}{h} & \frac{7}{h} & \frac{2}{h} \\ -\frac{7}{h} & -\frac{4}{h} & -\frac{4}{h} & \frac{1}{h} \\ \frac{7}{h} & \frac{4}{h} & \frac{4}{h} & -\frac{1}{h} \\ -\frac{2}{h} & \frac{1}{h} & \frac{1}{h} & \frac{6}{h} \end{pmatrix},$$

$$A^{(j,j-2)} = (A^{(j,j+2)})^{\mathrm{T}} = \begin{pmatrix} -\frac{1}{h} & -\frac{1}{h} & -\frac{1}{h} & -\frac{1}{h} \\ \frac{1}{h} & \frac{1}{h} & \frac{1}{h} & \frac{1}{h} \\ -\frac{1}{h} & -\frac{1}{h} & -\frac{1}{h} & -\frac{1}{h} \\ \frac{1}{h} & \frac{1}{h} & \frac{1}{h} & \frac{1}{h} \end{pmatrix},$$

$$A^{(1,1)} = \begin{pmatrix} -\frac{19}{h} & -\frac{2}{h} & -\frac{10}{h} & -\frac{7}{h} \\ -\frac{1}{h} & -\frac{12}{h} & -\frac{2}{h} & \frac{3}{h} \\ -\frac{13}{h} & -\frac{2}{h} & -\frac{16}{h} & -\frac{7}{h} \\ \frac{1}{h} & -\frac{2}{h} & -\frac{2}{h} & -\frac{7}{h} \end{pmatrix},$$

$$A^{(1,2)} = \begin{pmatrix} \frac{11}{h} & -\frac{8}{h} & \frac{8}{h} & -\frac{3}{h} \\ \frac{6}{h} & -\frac{3}{h} & \frac{3}{h} & \frac{2}{h} \\ \frac{8}{h} & -\frac{5}{h} & \frac{5}{h} & 0 \\ \frac{1}{h} & \frac{2}{h} & -\frac{2}{h} & \frac{7}{h} \end{pmatrix}, \quad \mathbf{b}^1 = \begin{pmatrix} \frac{19}{h} \\ -\frac{16}{h} \\ \frac{16}{h} \\ -\frac{11}{h} \end{pmatrix}\beta, \quad \mathbf{b}^2 = \begin{pmatrix} -\frac{1}{h} \\ \frac{1}{h} \\ -\frac{1}{h} \\ \frac{1}{h} \end{pmatrix}\beta,$$

$$A^{(N,N)} = \begin{pmatrix} -\frac{9}{h} & \frac{9}{h} & -\frac{3}{h} & -\frac{9}{h} \\ \frac{6}{h} & -\frac{8}{h} & \frac{6}{h} & \frac{2}{h} \\ -\frac{6}{h} & \frac{6}{h} & -\frac{12}{h} & \frac{6}{h} \\ \frac{1}{h} & -\frac{3}{h} & \frac{1}{h} & -\frac{13}{h} \end{pmatrix}, \quad \mathbf{b}^N = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}\gamma,$$

$$A^{(N-1,N)} = \begin{pmatrix} \frac{9}{h} & -\frac{8}{h} & \frac{6}{h} & -\frac{3}{h} \\ \frac{6}{h} & -\frac{5}{h} & \frac{3}{h} & 0 \\ \frac{6}{h} & -\frac{5}{h} & \frac{3}{h} & 0 \\ \frac{1}{h} & 0 & -\frac{2}{h} & \frac{5}{h} \end{pmatrix}, \quad \mathbf{b}^{N-1} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

- *Case* 2: $s = 3$

$$A^{(j,j)} = \begin{pmatrix} -\frac{15}{2h} & 0 & -\frac{3}{2h} \\ 0 & -\frac{21}{2h} & 0 \\ -\frac{3}{2h} & 0 & -\frac{15}{2h} \end{pmatrix},$$

$$A^{(j,j-1)} = (A^{(j,j+1)})^{\mathrm{T}} = \begin{pmatrix} \frac{3}{h} & \frac{7}{2h} & 0 \\ -\frac{7}{2h} & -\frac{4}{h} & -\frac{1}{2h} \\ 0 & \frac{1}{2h} & -\frac{3}{h} \end{pmatrix},$$

$$A^{(j,j-2)} = (A^{(j,j+2)})^{\mathrm{T}} = \begin{pmatrix} \frac{3}{4h} & \frac{3}{4h} & \frac{3}{4h} \\ -\frac{3}{4h} & -\frac{3}{4h} & -\frac{3}{4h} \\ \frac{3}{4h} & \frac{3}{4h} & \frac{3}{4h} \end{pmatrix},$$

$$A^{(1,1)} = \begin{pmatrix} -\frac{27}{4h} & -\frac{1}{4h} & \frac{9}{4h} \\ -\frac{3}{4h} & -\frac{41}{4h} & -\frac{15}{4h} \\ -\frac{3}{4h} & -\frac{1}{4h} & -\frac{15}{4h} \end{pmatrix},$$

$$A^{(1,2)} = \begin{pmatrix} \frac{9}{4h} & -\frac{11}{4h} & -\frac{3}{4h} \\ \frac{17}{4h} & -\frac{19}{4h} & \frac{5}{4h} \\ -\frac{3}{4h} & \frac{1}{4h} & -\frac{15}{4h} \end{pmatrix} \quad \mathbf{b}^1 = \begin{pmatrix} \frac{27}{4h} \\ -\frac{29}{4h} \\ \frac{15}{4h} \end{pmatrix}\beta, \quad \mathbf{b}^2 = \begin{pmatrix} \frac{3}{4h} \\ -\frac{3}{4h} \\ \frac{3}{4h} \end{pmatrix}\beta,$$

$$A^{(N,N)} = \begin{pmatrix} -\frac{15}{4h} & \frac{15}{4h} & \frac{9}{4h} \\ \frac{17}{4h} & -\frac{25}{4h} & \frac{17}{4h} \\ -\frac{3}{4h} & \frac{3}{4h} & -\frac{27}{4h} \end{pmatrix}, \quad \mathbf{b}^N = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}\gamma,$$

$$A^{(N-1,N)} = \begin{pmatrix} \frac{15}{4h} & -\frac{11}{4h} & \frac{3}{4h} \\ \frac{17}{4h} & -\frac{13}{4h} & \frac{5}{4h} \\ \frac{3}{4h} & \frac{1}{4h} & -\frac{9}{4h} \end{pmatrix}, \quad \mathbf{b}^{N-1} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

- *Case* 3: $s = 2$

$$A^{(j,j)} = \begin{pmatrix} -\frac{5}{h} & 0 \\ 0 & -\frac{3}{h} \end{pmatrix},$$

$$A^{(j,j-1)} = (A^{(j,j+1)})^{\mathrm{T}} = \begin{pmatrix} \frac{3}{h} & \frac{1}{h} \\ -\frac{1}{h} & \frac{1}{h} \end{pmatrix},$$

$$A^{(j,j-2)} = (A^{(j,j+2)})^{\mathrm{T}} = \begin{pmatrix} -\frac{1}{2h} & -\frac{1}{2h} \\ \frac{1}{2h} & \frac{1}{2h} \end{pmatrix},$$

$$A^{(1,1)} = \begin{pmatrix} -\frac{11}{2h} & -\frac{3}{2h} \\ \frac{1}{2h} & -\frac{3}{2h} \end{pmatrix},$$

$$A^{(1,2)} = \begin{pmatrix} \frac{7}{2h} & -\frac{3}{2h} \\ \frac{1}{2h} & \frac{3}{2h} \end{pmatrix}, \quad \mathbf{b}^1 = \begin{pmatrix} \frac{11}{2h} \\ -\frac{7}{2h} \end{pmatrix}\beta, \quad \mathbf{b}^2 = \begin{pmatrix} -\frac{1}{2h} \\ \frac{1}{2h} \end{pmatrix}\beta,$$

$$A^{(N,N)} = \begin{pmatrix} -\frac{5}{2h} & \frac{5}{2h} \\ \frac{1}{2h} & -\frac{5}{2h} \end{pmatrix}, \quad \mathbf{b}^N = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}\gamma,$$

$$A^{(N-1,N)} = \begin{pmatrix} \frac{5}{2h} & -\frac{3}{2h} \\ \frac{1}{2h} & \frac{1}{2h} \end{pmatrix}, \quad \mathbf{b}^{N-1} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

- *Case* 4: $s = 1$, the block pentadiagonal matrices reduce into five scalar numbers,

$$A^{(j,j)} = -\frac{1}{2h}, \quad A^{(j,j+1)} = A^{(j,j-1)} = 0, \quad A^{(j,j+2)} = A^{(j,j-2)} = \frac{1}{4h},$$

$$A^{(1,1)} = -\frac{1}{4h},$$

$$A^{(1,2)} = -\frac{1}{4h}, \quad \mathbf{b}^1 = \frac{1}{4h}\beta, \quad \mathbf{b}^2 = \frac{1}{4h}\beta,$$

$$A^{(N,N)} = -\frac{1}{4h}, \quad \mathbf{b}^N = \frac{1}{2}\beta,$$

$$A^{(N-1,N)} = \frac{1}{4h}, \quad \mathbf{b}^{N-1} = 0.$$

3.2. Derivative matrix D_{sN} for a upwinding flux

In [26] a different numerical flux with upwinding approaches is proposed

$$h_{u,j+1/2} = u(z^-_{j+1/2}), \tag{3.34}$$

$$h_{q,j+1/2} = \varepsilon_{j+1} q(z^+_{j+1/2}), \tag{3.35}$$

For $j = 1$ or N, using the boundary condition (3.2), the numerical flux (3.34) and (3.35) will be changed into

$$h_{u,1/2} = \beta, \quad h_{q,1/2} = \varepsilon_1 q(z^+_{1/2}), \tag{3.36}$$

$$h_{u,N+1/2} = u(z^-_{N+1/2}), \quad h_{q,N+1/2} = \varepsilon_N \gamma. \tag{3.37}$$

In this case, the derivative matrix D_{sN} is found to be a block tridiagonal matrix instead of the block pentadiagonal matrix in (3.31) and only $\mathbf{b}^1$, $\mathbf{b}^N$ are nonzero in (3.30)

$$D_{sN} = \begin{pmatrix} A^{(1,1)} & A^{(1,2)} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ A^{(2,1)} & A^{(2,2)} & A^{(2,3)} & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & A^{(3,2)} & A^{(3,3)} & A^{(3,4)} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & A^{(N-1,N-2)} & A^{(N-1,N-1)} & A^{(N-1,N)} \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & A^{(N,N-1)} & A^{(N,N)} \end{pmatrix}, \tag{3.38}$$

where $A^{(j,l)} = (a^{j,l}_{n,k})$ is a matrix of dimension $s \times s$ and for $2 \leqslant j \leqslant N-1$,

$$\begin{aligned} a^{j,j}_{n,k} &= \varepsilon_j \frac{1}{c_{j,m}} M^{z,j}_{nm} M^{z,j}_{mk} - \varepsilon_j \frac{1}{c_{j,m}} M^{z,j}_{nm} \phi^j_m(z_{j+1/2}) \phi^j_k(z_{j+1/2}) \\ &\quad + \phi^j_n(z_{j+1/2})(-\varepsilon_{j+1}) \frac{1}{c_{j+1,m}} \phi^j_k(z_{j+1/2}) \phi^{j+1}_m(z_{j+1/2}) \phi^{j+1}_m(z_{j+1/2}) \\ &\quad - \phi^j_n(z_{j-1/2}) \left[-\varepsilon_j \frac{1}{c_{j,m}} M^{z,j}_{mk} \phi^j_m(z_{j-1/2}) + \varepsilon_j \frac{1}{c_{j,m}} \phi^j_k(z_{j+1/2}) \phi^j_m(z_{j+1/2}) \phi^j_m(z_{j-1/2}) \right], \end{aligned} \tag{3.39}$$

$$\begin{aligned} a^{j,j+1}_{n,k} &= \phi^j_n(z_{j+1/2}) \left[-\varepsilon_{j+1} \frac{1}{c_{j+1,m}} M^{z,j+1}_{mk} \phi^{j+1}_m(z_{j+1/2}) \right. \\ &\quad \left. + \varepsilon_{j+1} \frac{1}{c_{j+1,m}} \phi^{j+1}_m(z_{j+3/2}) \phi^{j+1}_m(z_{j+1/2}) \phi^{j+1}_k(z_{j+3/2}) \right], \end{aligned} \tag{3.40}$$

$$\begin{aligned} a^{j,j-1}_{n,k} &= \varepsilon_j \frac{1}{c_{j,m}} M^{z,j}_{nm} \phi^j_m(z_{j-1/2}) \phi^{j-1}_k(z_{j-1/2}) \\ &\quad + \phi^j_n(z_{j-1/2}) \varepsilon_j \frac{1}{c_{j,m}} \phi^j_m(z_{j-1/2}) \phi^j_m(z_{j-1/2}) \phi^{j-1}_k(z_{j-1/2}). \end{aligned} \tag{3.41}$$

Using the flux Eq. (3.36) and $j = 1$, we have

$$b_n^j = \varepsilon_j \frac{1}{c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j-1/2})\beta - \phi_n^j(z_{j-1/2}) \left[-\varepsilon_j \frac{1}{c_{j,m}} \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j-1/2})\beta \right].$$

The expressions of $a_{n,k}^{j,j}$ and $a_{n,k}^{j,j+1}$ are the same as that of (3.39) and (3.40), respectively. Using the flux Eq. (3.37) and $j = N$, we have

$$\begin{aligned} a_{n,k}^{j,j} &= \varepsilon_j \frac{1}{c_{j,m}} M_{nm}^{z,j} M_{mk}^{z,j} - \varepsilon_j \frac{1}{c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j+1/2}) \phi_k^j(z_{j+1/2}) \\ &\quad - \phi_n^j(z_{j-1/2}) \left[-\varepsilon_j \frac{1}{c_{j,m}} M_{mk}^{z,j} \phi_m^j(z_{j-1/2}) + \varepsilon_j \frac{1}{c_{j,m}} \phi_k^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j-1/2}) \right]. \end{aligned} \tag{3.42}$$

The expression of $a_{n,k}^{j,j-1}$ is the same as that of (3.41), and

$$b_n^j = \phi_n^j(z_{j+1/2})\varepsilon_j \gamma.$$

The matrices $A^{(j,l)}$, $A^{(j,l-1)}$, $A^{(j,l+1)}$ for $2 \leqslant j \leqslant N-1$ are given for the basis functions of order $1 \leqslant s \leqslant 5$. The different matrix blocks and vectors at boundary elements are also given.

Case 1: $s = 5$

$$A^{(j,j)} = \begin{pmatrix} -\frac{50}{h} & -\frac{2}{h} & -\frac{44}{h} & -\frac{12}{h} & -\frac{30}{h} \\ -\frac{2}{h} & -\frac{50}{h} & -\frac{8}{h} & -\frac{40}{h} & -\frac{22}{h} \\ -\frac{44}{h} & -\frac{8}{h} & -\frac{50}{h} & -\frac{18}{h} & -\frac{36}{h} \\ -\frac{12}{h} & -\frac{40}{h} & -\frac{18}{h} & -\frac{50}{h} & -\frac{32}{h} \\ -\frac{30}{h} & -\frac{22}{h} & -\frac{36}{h} & -\frac{32}{h} & -\frac{50}{h} \end{pmatrix},$$

$$A^{(j,j-1)} = (A^{(j,j+1)})^{\mathrm{T}} = \begin{pmatrix} \frac{25}{h} & \frac{25}{h} & \frac{25}{h} & \frac{25}{h} & \frac{25}{h} \\ -\frac{23}{h} & -\frac{23}{h} & -\frac{23}{h} & -\frac{23}{h} & -\frac{23}{h} \\ \frac{19}{h} & \frac{19}{h} & \frac{19}{h} & \frac{19}{h} & \frac{19}{h} \\ -\frac{13}{h} & -\frac{13}{h} & -\frac{13}{h} & -\frac{13}{h} & -\frac{13}{h} \\ \frac{5}{h} & \frac{5}{h} & \frac{5}{h} & \frac{5}{h} & \frac{5}{h} \end{pmatrix},$$

$$A^{(N,N)} = \begin{pmatrix} -\frac{25}{h} & -\frac{23}{h} & -\frac{19}{h} & \frac{13}{h} & -\frac{5}{h} \\ \frac{23}{h} & -\frac{25}{h} & \frac{17}{h} & -\frac{15}{h} & \frac{3}{h} \\ -\frac{19}{h} & \frac{17}{h} & -\frac{25}{h} & \frac{7}{h} & -\frac{11}{h} \\ \frac{13}{h} & -\frac{15}{h} & \frac{7}{h} & -\frac{25}{h} & -\frac{7}{h} \\ -\frac{5}{h} & \frac{3}{h} & -\frac{11}{h} & -\frac{7}{h} & -\frac{25}{h} \end{pmatrix}, \quad \mathbf{b}^1 = \begin{pmatrix} \frac{25}{h} \\ -\frac{23}{h} \\ \frac{19}{h} \\ -\frac{13}{h} \\ \frac{5}{h} \end{pmatrix}\beta, \quad \mathbf{b}^N = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}\gamma.$$

• *Case* 2: $s=4$

$$A^{(j,j)}=\begin{pmatrix}-\frac{32}{h} & -\frac{2}{h} & -\frac{26}{h} & -\frac{12}{h}\\ -\frac{2}{h} & -\frac{32}{h} & -\frac{8}{h} & -\frac{22}{h}\\ -\frac{26}{h} & -\frac{8}{h} & -\frac{32}{h} & -\frac{18}{h}\\ -\frac{12}{h} & -\frac{22}{h} & -\frac{18}{h} & -\frac{32}{h}\end{pmatrix},$$

$$A^{(j,j-1)}=(A^{(j,j+1)})^{\mathrm{T}}=\begin{pmatrix}\frac{16}{h} & \frac{16}{h} & \frac{16}{h} & \frac{16}{h}\\ -\frac{14}{h} & -\frac{14}{h} & -\frac{14}{h} & -\frac{14}{h}\\ \frac{10}{h} & \frac{10}{h} & \frac{10}{h} & \frac{10}{h}\\ -\frac{4}{h} & -\frac{4}{h} & -\frac{4}{h} & -\frac{4}{h}\end{pmatrix},$$

$$A^{(N,N)}=\begin{pmatrix}-\frac{16}{h} & \frac{14}{h} & -\frac{10}{h} & \frac{4}{h}\\ \frac{14}{h} & -\frac{16}{h} & \frac{8}{h} & -\frac{6}{h}\\ -\frac{10}{h} & \frac{8}{h} & -\frac{16}{h} & -\frac{2}{h}\\ \frac{4}{h} & -\frac{6}{h} & -\frac{2}{h} & -\frac{16}{h}\end{pmatrix},\quad \mathbf{b}^1=\begin{pmatrix}\frac{16}{h}\\ -\frac{14}{h}\\ \frac{10}{h}\\ -\frac{4}{h}\end{pmatrix}\beta,\quad \mathbf{b}^N=\begin{pmatrix}1\\1\\1\\1\end{pmatrix}\gamma.$$

• *Case* 2: $s=3$

$$A^{(j,j)}=\begin{pmatrix}-\frac{18}{h} & -\frac{2}{h} & -\frac{12}{h}\\ -\frac{2}{h} & -\frac{18}{h} & -\frac{8}{h}\\ -\frac{12}{h} & -\frac{8}{h} & -\frac{18}{h}\end{pmatrix},$$

$$A^{(j,j-1)}=(A^{(j,j+1)})^{\mathrm{T}}=\begin{pmatrix}\frac{9}{h} & \frac{9}{h} & \frac{9}{h}\\ -\frac{7}{h} & -\frac{7}{h} & -\frac{7}{h}\\ \frac{3}{h} & \frac{3}{h} & \frac{3}{h}\end{pmatrix},$$

$$A^{(N,N)}=\begin{pmatrix}-\frac{9}{h} & \frac{7}{h} & -\frac{3}{h}\\ \frac{7}{h} & -\frac{9}{h} & \frac{1}{h}\\ -\frac{3}{h} & \frac{1}{h} & -\frac{9}{h}\end{pmatrix},\quad \mathbf{b}^1=\begin{pmatrix}\frac{9}{h}\\ -\frac{7}{h}\\ \frac{3}{h}\end{pmatrix}\beta,\quad \mathbf{b}^N=\begin{pmatrix}1\\1\\1\end{pmatrix}\gamma.$$

Case 3: $s=2$

$$A^{(j,j)}=\begin{pmatrix}-\frac{8}{h} & -\frac{2}{h}\\ -\frac{2}{h} & -\frac{8}{h}\end{pmatrix},$$

$$A^{(j,j-1)} = (A^{(j,j+1)})^{\mathrm{T}} = \begin{pmatrix} \frac{4}{h} & \frac{4}{h} \\ -\frac{2}{h} & -\frac{2}{h} \end{pmatrix},$$

$$A^{(N,N)} = \begin{pmatrix} -\frac{4}{h} & \frac{2}{h} \\ \frac{2}{h} & -\frac{4}{h} \end{pmatrix}, \quad \mathbf{b}^1 = \begin{pmatrix} \frac{4}{h} \\ -\frac{2}{h} \end{pmatrix}\beta, \quad \mathbf{b}^N = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\gamma.$$

Case 4: $s = 1$, the block tridiagonal matrices are reduced to three scalar numbers,

$$A^{(j,j)} = -\frac{2}{h}, \quad A^{(j,j+1)} = A^{(j,j-1)} = \frac{1}{h},$$

$$A^{(N,N)} = -\frac{1}{h}, \quad \mathbf{b}^1 = \beta, \quad \mathbf{b}^N = \gamma.$$

4. Fully discretized spectral-DG method for Schrödinger–Poisson equations

As Eqs. (2.8) and (2.9) are a set of 1-D differential equations in (z, t)-variables, the discretization of these equations is similar to that of the following two equations:

$$\mathrm{i}\frac{\partial}{\partial t}u(z,t) = -\frac{\partial^2}{\partial z^2}u(z,t) + v(z,t)u(z,t), \tag{4.1}$$

$$\frac{\partial^2}{\partial z^2}v(z,t) = -\bar{u}(z,t)u(z,t) \tag{4.2}$$

with appropriate boundary conditions (Dirichlet or Neumann). The discretization of (4.2) is the same as (3.1), we have the following linear system similar to (3.30):

$$D_{sN}\begin{pmatrix} \mathbf{v}^1 \\ \mathbf{v}^2 \\ \vdots \\ \mathbf{v}^N \end{pmatrix} + \overrightarrow{\mathbf{b}} = \begin{pmatrix} \mathbf{g}^1 \\ \mathbf{g}^2 \\ \vdots \\ \mathbf{g}^N \end{pmatrix}, \tag{4.3}$$

where D_{sN} is defined in (3.31) or (3.38), vector $\overrightarrow{\mathbf{b}} = (\mathbf{b}^1, \mathbf{b}^2, 0, \ldots, 0, \mathbf{b}^{N-1}, \mathbf{b}^N)^{\mathrm{T}}$ is the boundary terms corresponding to either Dirichlet or Neumann boundary conditions and $\mathbf{v}^j = (v_1^j, v_2^j, \ldots, v_s^j)^{\mathrm{T}}$ are the coefficients of the basis functions on the element I_j and $v(z,t) = \sum_{i=1}^{s} v_i^j \phi_i$ on I_j, and $\mathbf{g}^j = (g_1^j, g_2^j, \ldots, g_s^j)^{\mathrm{T}}$. On the element I_j, we can write out $g_k^j,\ k = 1, 2, \ldots, s$ as

$$g_k^j = (\overline{\mathbf{u}^j})^{\mathrm{T}} Q_k^j \mathbf{u}^j,$$

where $\mathbf{u}^j = (u_1^j, u_2^j, \ldots, u_s^j)^{\mathrm{T}},\ j = 1, 2, \ldots, N$ and $u(z,t) = \sum_{i=1}^{s} u_i^j \phi_i$ on element I_j and the matrices $Q_k^j,\ k = 1, 2, \ldots, s$ are given by

$$Q_k^j = \begin{pmatrix} \int_{I_j} \phi_1\phi_1\phi_k\,\mathrm{d}z & \int_{I_j} \phi_1\phi_2\phi_k\,\mathrm{d}z & \cdots & \int_{I_j} \phi_1\phi_s\phi_k\,\mathrm{d}z \\ \int_{I_j} \phi_2\phi_1\phi_k\,\mathrm{d}z & \int_{I_j} \phi_2\phi_2\phi_k\,\mathrm{d}z & \cdots & \int_{I_j} \phi_2\phi_s\phi_k\,\mathrm{d}z \\ \vdots & \vdots & \ddots & \vdots \\ \int_{I_j} \phi_s\phi_1\phi_k\,\mathrm{d}z & \int_{I_j} \phi_s\phi_2\phi_k\,\mathrm{d}z & \cdots & \int_{I_j} \phi_s\phi_s\phi_k\,\mathrm{d}z \end{pmatrix}. \tag{4.4}$$

By using the same discretization of the z-derivative, we can get a semi-discretization of time-dependent Schrödinger equation (4.1) as a system of ordinary differential equations

$$\mathrm{i}\begin{pmatrix} M^1 & 0 & \cdots & 0 \\ 0 & M^2 & \cdots & 0 \\ 0 & 0 & \ddots & \vdots \\ 0 & 0 & \cdots & M^N \end{pmatrix}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \mathbf{u}^1 \\ \mathbf{u}^2 \\ \vdots \\ \mathbf{u}^N \end{pmatrix} = -D_{sN}\begin{pmatrix} \mathbf{u}^1 \\ \mathbf{u}^2 \\ \vdots \\ \mathbf{u}^N \end{pmatrix} - \overrightarrow{\mathbf{b}} + \begin{pmatrix} \mathbf{f}^1 \\ \mathbf{f}^2 \\ \vdots \\ \mathbf{f}^N \end{pmatrix}, \tag{4.5}$$

where M^j, $j = 1, 2, \ldots, N$ is the element mass matrix over the element I_j

$$M^j = \begin{pmatrix} \int_{I_j} \phi_1\phi_1 \,\mathrm{d}z & \int_{I_j} \phi_1\phi_2 \,\mathrm{d}z & \cdots & \int_{I_j} \phi_1\phi_s \,\mathrm{d}z \\ \int_{I_j} \phi_2\phi_1 \,\mathrm{d}z & \int_{I_j} \phi_2\phi_2 \,\mathrm{d}z & \cdots & \int_{I_j} \phi_2\phi_s \,\mathrm{d}z \\ \vdots & \vdots & \ddots & \vdots \\ \int_{I_j} \phi_s\phi_1 \,\mathrm{d}z & \int_{I_j} \phi_s\phi_2 \,\mathrm{d}z & \cdots & \int_{I_j} \phi_s\phi_s \,\mathrm{d}z \end{pmatrix}.$$

And $\mathbf{u} = (\mathbf{u}^1, \mathbf{u}^2, \ldots, \mathbf{u}^N)^{\mathrm{T}}$ is the solution vector while $\mathbf{u}^j = (u_1^j, u_2^j, \ldots, u_s^j)^{\mathrm{T}}$ is the unknown on interval I_j and $u(z,t) = \sum_{i=1}^{s} u_i^j \phi_i$. And $\mathbf{f}^j = (f_1^j, f_2^j, \ldots, f_s^j)^{\mathrm{T}}$ on the element I_j where f_k^j, $k = 1, 2, \ldots, s$ is given by

$$f_k^j = (\mathbf{v}^j)^{\mathrm{T}} Q_k^j \mathbf{u}^j, \tag{4.6}$$

with $\mathbf{v}^j$ being the coefficients of $v(z,t)$, and Q_k^j defined in (4.4). We rewrite (4.5) as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = B\mathbf{u} + \mathbf{F}(\mathbf{u}), \tag{4.7}$$

where $B = \mathrm{i}M^{-1}D_{sN}$ and $\mathbf{F} = -\mathrm{i}M^{-1}[(\mathbf{f}^1, \mathbf{f}^1, \ldots, \mathbf{f}^N)^{\mathrm{T}} - \overrightarrow{\mathbf{b}}]$. This system of ordinary differential equations can be numerically solved by various time integration schemes such as a fourth-order Runge–Kutta method.

4.1. ETD method

Recently, ETD method [8] has been investigated to handle the linear term in ODE systems in (4.7) with high accuracy through an integrating factor e^{-Bt}, which is assumed to be calculated with enough accuracy. In [1], an improved approach is proposed for the computation of a matrix exponential that includes an automatic correction of rounding errors without much extra cost. The idea of ETD is described briefly as follows.

For the nonlinear system (4.7), after multiplying the integrating factor e^{-Bt} and integrating the equation over a time step from $t = t_n$ to $t = t_{n+1} = t_n + \Delta t$, we have

$$\mathbf{u}(t_{n+1}) = \mathrm{e}^{Bh}\mathbf{u}(t_n) + \mathrm{e}^{Bh} \int_{t_n}^{t_{n+1}} \mathrm{e}^{-B\tau}\mathbf{F}(\mathbf{u}(t+\tau), t+\tau)\,\mathrm{d}\tau.$$

Here $\mathbf{F}$ can be time dependent.

We can then use a Runge–Kutta method to approximate the integration part of the formula [8]. A third-order RK ETD (ETDRK3) method is given by

$$\begin{aligned} \mathbf{a}_n &= \mathbf{u}_n\mathrm{e}^{Bh/2} + (\mathrm{e}^{Bh/2} - I)\mathbf{F}(\mathbf{u}_n, t_n)/B, \\ \mathbf{b}_n &= \mathbf{u}_n\mathrm{e}^{Bh/2} + (\mathrm{e}^{Bh} - I)(2\mathbf{F}(\mathbf{a}_n, t_n + h/2) - F(\mathbf{u}_n, t_n))/B, \\ \mathbf{u}_{n+1} &= \mathbf{u}_n\mathrm{e}^{Bh} + \{\mathbf{F}(\mathbf{u}_n, t_n)[-4 - Bh + \mathrm{e}^{Bh}(4 - 3Bh + B^2h^2)] \\ &\quad + 4\mathbf{F}(\mathbf{a}_n, t_n + h/2)[2 + Bh + \mathrm{e}^{Bh}(-2 + Bh)] \\ &\quad + \mathbf{F}(\mathbf{b}_n, t_n + h)[-4 - 3Bh - B^2h^2 + \mathrm{e}^{Bh}(4 - Bh)]\}/B^3h^2, \end{aligned}$$

while a fourth-order RK ETD (ETDRK4) method is given by

$$\begin{aligned} \mathbf{a}_n &= \mathbf{u}_n\mathrm{e}^{Bh/2} + (\mathrm{e}^{Bh/2} - I)\mathbf{F}(\mathbf{u}_n, t_n)/B, \\ \mathbf{b}_n &= \mathbf{u}_n\mathrm{e}^{Bh/2} + (\mathrm{e}^{Bh/2} - I)\mathbf{F}(\mathbf{a}_n, t_n + h)/B, \\ \mathbf{c}_n &= \mathbf{a}_n\mathrm{e}^{Bh/2} + (\mathrm{e}^{Bh/2} - I)(2\mathbf{F}(\mathbf{b}_n, t_n + h/2) - F(\mathbf{u}_n, t_n))/B, \end{aligned}$$

$$\mathbf{u}_{n+1} = \mathbf{u}_n \mathrm{e}^{Bh} + \{\mathbf{F}(\mathbf{u}_n, t_n)[-4 - Bh + \mathrm{e}^{Bh}(4 - 3Bh + B^2h^2)] + 2(\mathbf{F}(\mathbf{a}_n, t_n + h/2) + \mathbf{F}(\mathbf{b}_n, t_n + h/2))[2 + Bh + \mathrm{e}^{Bh}(-2 + Bh)] + \mathbf{F}(\mathbf{c}_n, t_n + h)[-4 - 3Bh - B^2h^2 + \mathrm{e}^{Bh}(4 - Bh)]\}/B^3h^2,$$

where $\mathbf{u}_n \doteq u(n\Delta t)$.

5. Numerical results

5.1. Boundary conditions

In this subsection, we will address the issues of the boundary treatment for computing the coupled Schrödinger–Poisson equations (1.1) and (1.2) over unbounded domains. We will use the method of perfect matched layer (PML) developed for Maxwell equations [5] to truncate the computational domain to a finite size. For the coupled nonlinear system (1.1) and (1.2), we ignore the Poisson equation of self-consistency near the boundary, which is assumed far away enough from the quantum device where the self-consistent potential $V_{\mathrm{ch}}(x, y, z, t)$ from charges is important. So, in principle only the linear Schrödinger equation is to be used near the PML regions. Also, in order to use the PML formulation, a combination of total wave and scattering wave approaches will be used with the former for the internal computational domain and the latter for the PML regions.

5.1.1. PML for the Schrödinger equation

For non-dispersive waves, wave velocity is independent of the wave frequencies, so an one-way wave equation corresponding to that velocity can provide a good absorbing boundary condition. For a dispersive system such as the Schrödinger equation, we need to provide an absorbing boundary condition valid for all frequencies. Perfectly matched layer (PML) was proposed by Berenger for electromagnetic wave [5]. This method has many advantages over the transmitting boundary method (QTBM) [13] and the transparent boundary condition [24] and Schmidt's method [20]. The PMLs surrounding the computational domain allow wave to propagate outward with exponential attenuation and negligible reflections back into the computational domains. We introduce the PML in 1-D case by starting from the time-independent Schrödinger equation

$$\left[-\frac{1}{\varepsilon}\frac{\partial}{\partial z}\frac{1}{\varepsilon}\frac{1}{m}\frac{\partial}{\partial z} + V(z)\right]\Psi = E\Psi, \tag{5.1}$$

where m is the electron mass and ε is an artificial parameter. If $\varepsilon = 1$, the equation reduces to the original form in the physical medium. If $\varepsilon = (1 + \mathrm{i}\sigma)$ and σ is a suitable real number, the wave will decay exponentially when it propagates into the PML medium. This can be seen from the fact that the wave satisfying the above equation is of the form

$$\Psi = \exp(\mathrm{i}k\varepsilon z) = \exp(\mathrm{i}k(1 + \mathrm{i}\sigma)z) = \exp(\mathrm{i}kz)\exp(-k\sigma z), \tag{5.2}$$

where $k = \sqrt{m(E - V)}$.

As a result, for a wave incident from a region with m to a region with εm, there is no reflection if the two regions have the same potentials. Because the PML is valid for each frequency, it can be used for time domain simulations.

5.1.2. Total-scattering formula for the Schrödinger equation

As the PML is designed for outgoing scattering waves, a combination of total and scattering wave formulation will be used for our problem. We will compute the scattering wave in the PML regions and the total wave in the computational domain. When the flux on the interface of the PML and the computation domains is needed, the incident wave is subtracted or added in either domain to make the fluxes consistent between two domains [23].

As shown in Fig. 1, scattering wave Ψ^{scat} is computed in the PML domain, and Ψ^{tot} is computed in the computational domain. We denote the elements by $I_{-2}, I_{-1}, I_0, I_1, I_2$, respectively. The total wave is

$$\Psi^{\mathrm{tot}} = \Psi^{\mathrm{scat}} + \Psi^{\mathrm{inc}}, \tag{5.3}$$

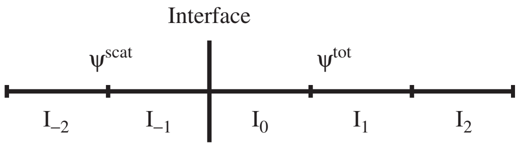

Fig. 1. The total-scattering formula for the Schrödinger equation.

Table 1
L^2 error for the solution of Eq. (5.5) with the central numerical flux (3.17) and (3.18)

	$s = 0$ (order)	$s = 1$ (order)	$s = 2$ (order)	$s = 3$ (order)	$s = 4$ (order)
$N = 10$	3.33E − 3 (–)	3.43E − 4 (–)	3.64E − 4 (–)	2.69E − 6 (–)	4.88E − 7 (–)
$N = 20$	7.53E − 4 (1.63)	1.55E − 4 (1.14)	2.47E − 6 (3.88)	2.26E − 7 (3.57)	3.27E − 8 (3.90)
$N = 40$	3.46E − 4 (1.12)	7.57E − 5 (1.04)	2.26E − 7 (3.45)	2.66E − 8 (3.09)	8.97E − 10 (5.19)

Table 2
L^2 error for the solution of Eq. (5.5) with the upwinding numerical flux (3.34) and (3.35)

	$s = 0$ (order)	$s = 1$ (order)	$s = 2$ (order)	$s = 3$ (order)	$s = 4$ (order)
$N = 10$	1.37E − 3 (–)	2.28E − 4 (–)	2.03E − 5 (–)	2.01E − 6 (–)	3.00E − 7 (–)
$N = 20$	6.78E − 4 (1.02)	5.74E − 5 (1.99)	2.61E − 6 (2.96)	1.45E − 7 (3.80)	1.40E − 8 (4.42)
$N = 40$	3.38E − 4 (1.00)	1.43E − 5 (2.00)	3.29E − 7 (2.99)	9.63E − 9 (3.91)	3.97E − 10 (5.14)

where we assume that the incident wave Ψ^{inc} is a known function. When we update Ψ^{tot} in element I_0, we need to use Ψ^{tot} in elements I_{-2} and I_{-1} according to the discretized formula equations (3.28a)–(3.28e). We compute Ψ^{inc} in elements I_{-2} and I_{-1}, then get Ψ^{tot} in these two elements by using Eq. (5.3). When we update Ψ^{scat} in element I_{-1}, we need to compute Ψ^{inc} in elements I_0 and I_1, then get Ψ^{scat} in these two elements by using

$$\Psi^{\text{scat}} = \Psi^{\text{tot}} - \Psi^{\text{inc}}. \tag{5.4}$$

5.2. Accuracy of derivative matrices D_{sN} for the Poisson equation

To test the accuracy of the derivative matrices, we compute the solution to

$$\begin{aligned} u''(z) &= \exp\left(\frac{1}{z(z-1)}\right)\frac{6z^4 - 12z^3 + 12z^2 - 6z + 1}{z^4(z-1)^4}, \quad z \in [0, 1], \\ u(0) &= u(1) = 0 \end{aligned} \tag{5.5}$$

with an exact solution representing two boundary layers at the $z = 0, 1$,

$$u(z) = \exp\left(\frac{1}{z(z-1)}\right). \tag{5.6}$$

The computational domain [0, 1] is equally divided into N elements. The order of the basis functions s is set to be 0, 1, 2, 3 or 4. The L^2 errors are given in Tables 1 and 2 for two different types of numerical flux, respectively. The errors are not scaled by the maximum of $u(z)$ which is approximately 0.018.

Next, we compute the problem

$$u''(z) = -4\pi^2 \cos(2\pi z), \quad z \in [0, 1] \tag{5.7}$$

with the exact solution

$$u(z) = \cos(2\pi z), \quad z \in [0, 1]. \tag{5.8}$$

Table 3
L^2 error for the solution of Eq. (5.7) with the central numerical flux (3.17) and (3.18)

	$s=0$ (order)	$s=1$ (order)	$s=2$ (order)	$s=3$ (order)	$s=4$ (order)
$N=10$	1.96E − 1 (–)	3.78E − 2 (–)	6.21E − 4 (–)	8.52E − 5 (–)	7.73E − 7 (–)
$N=20$	7.51E − 2 (1.38)	1.65E − 2 (1.19)	7.12E − 5 (3.13)	9.60E − 6 (3.15)	2.21E − 8 (5.12)
$N=40$	3.35E − 2 (1.16)	7.68E − 3 (1.11)	8.69E − 6 (3.03)	1.12E − 8 (3.09)	6.78E − 10 (5.03)

Table 4
L^2 error for the solution of Eq. (5.7) with the upwinding numerical flux (3.34) and (3.35)

	$s=0$ (order)	$s=1$ (order)	$s=2$ (order)	$s=3$ (order)	$s=4$ (order)
$N=10$	1.33E − 1 (–)	2.42E − 2 (–)	8.99E − 4 (–)	5.67E − 5 (–)	1.13E − 6 (–)
$N=20$	4.47E − 2 (1.04)	6.02E − 3 (2.01)	1.08E − 4 (3.05)	3.63E − 6 (3.97)	3.30E − 8 (5.10)
$N=40$	3.21E − 2 (1.01)	1.49E − 3 (2.01)	1.34E − 5 (3.01)	2.28E − 7 (3.99)	1.01E − 9 (5.03)

The boundary condition is provided by assuming that the solution outside the region [0, 1] is known. First we got the L^2 errors given in Table 3 by using the flux (3.17) and (3.18).

Then we use the flux (3.34) and (3.35) and get the errors in Table 4.

From the two examples, we can see that the numerical flux (3.34) and (3.35) are slightly better than (3.17) and (3.18), and, as the derivative matrix for the former numerical flux has a smaller bandwidth, we will use it for the rest of our numerical tests.

5.3. Time integrations for the Schrödinger equation

In this section, we will study various time integration schemes including Runge–Kutta, Crank–Nicholson, and ETD for the linear time-dependent Schrödinger equation. We consider an 1-D Schrödinger equation with a piecewise constant electron mass

$$\mathrm{i}\frac{\partial}{\partial t}\Psi(z,t) = -\frac{\partial}{\partial z}\frac{1}{m}\frac{\partial}{\partial z}\Psi(z,t), \tag{5.9}$$

where the effective mass is a piecewise constant function

$$m = \begin{cases} 1.5625 & \text{if } 0.3 < z < 0.7, \\ 1 & \text{otherwise.} \end{cases}$$

With interface boundary conditions $[\Psi]=0$ and $[(1/m)(\partial/\partial z)\Psi]=0$ at $z=0.3$ and 0.7, we can find a solution of Eq. (5.9) in the form $\Psi(z,t)=\psi(z)\mathrm{e}^{-\mathrm{i}\omega t}$ where $\omega=4\pi^2$

$$\Psi(z,t) = \begin{cases} (0.809017 - \mathrm{i}0.588785)\mathrm{e}^{\mathrm{i}(2\pi z - 4\pi^2 t)} & \text{if } z < 0.3, \\ (0.510739 - \mathrm{i}1.00238)\mathrm{e}^{\mathrm{i}(4\pi z - 4\pi^2 t)} + (0.111376 + \mathrm{i}0.0567488)\mathrm{e}^{\mathrm{i}(-4\pi z - 4\pi^2 t)} & \text{if } 0.3 < z < 0.7, \\ \mathrm{e}^{\mathrm{i}(2\pi z - 4\pi^2 t)} & \text{if } z > 0.7. \end{cases}$$

After the space discretization, we have an ordinary differential system

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = A\mathbf{u} + \mathbf{F}(t),$$

where the time-dependent term $\mathbf{F}(t)$ comes from the boundary condition.

The computational domain [0, 1] is divided into N elements equally, and a fourth order Runge–Kutta method is used up to a final time $T=0.0253$. The L^2 errors are listed in Table 5. The time steps are 64E − 6, 16E − 6, 4E − 6, respectively.

Though Crank–Nicholson method is easy to implement, it is only second-order accurate. So we can choose $\Delta t = c\Delta x^2$ with c constant to get a fourth-order accurate numerical discretization. The L^2 errors are listed in Table 5. The time steps are 2E − 5, 1E − 5, 4E − 6, respectively.

Table 5
L_2 error for the solution of RK4, Crank–Nicholson (CN) and exponential time difference (ETDRK4) with central flux defined in (3.34) and (3.35)

	RK4 (order)	CN (order)	ETR4 (order)
$M = 10$	1.01E − 4 (–)	1.04E − 4 (–)	1.23E − 4 (–)
$N = 20$	6.79E − 6 (3.90)	6.82E − 6 (3.94)	7.29E − 6 (4.08)
$N = 40$	3.90E − 7 (3.88)	3.94E − 7 (4.04)	4.35E − 7 (4.07)

The polynomial order is $s = 3$.

A larger time step can be used with the ETDRK4 method. The L^2 errors are listed in Table 5. The time steps are 1E − 3, 5E − 4, 2.5E − 4, respectively. Here we choose $\Delta t = c\Delta x$ with a constant c. But the exponential matrix and the coefficients used by the ETDRK4 are harder to calculate accurately for large non-diagonal matrices.

We obtained the numerical examples in Table 5 on a PC with a TM 2 Duo E6600 CPU. And the CPU time for the time integration part on the finest mesh for RK4, CN, and ETDRK4 is 0.77, 0.76, 0.11 s, respectively. For the example in Table 5, we calculated the exponential with the software, Mathematica. Based on numerical experiments, the size for non-diagonal matrices is 3200 × 3200 on a mesh of $N = 80$ points with third-order basis functions when the expected fourth-order accuracy of the ETDRK4 was not achieved. We also tried the algorithms of computing matrix exponentials given in [1] and observed degeneracy of accuracy when the size of matrix is bigger than 40 × 40. The L_2 errors are 1.10E − 4 and 1.60E − 5 for the meshes of points $N = 10$ and 20, respectively.

5.4. 3-D nonlinear time-dependent Schrödinger–Poisson equations

Finally, we apply the Fourier spectral-DG method for a 3-D time-dependent problem modelling electron wave function through quantum supperlattices. The self-consistent calculation of time-dependent Schrödinger–Poisson equations in 3-D is a challenging problem computationally. Here, we consider a 3-D problem

$$\begin{aligned} i\hbar\frac{\partial \Psi(\mathbf{x}\ ,t)}{\partial t} &= -\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial z^2}\right)\Psi(\mathbf{x},t) \\ &\quad + (V_{\text{in}}(\mathbf{x})+V_{\text{ch}}(\mathbf{x},t))\Psi(\mathbf{x},t), \quad \mathbf{x}=(x,y,z)\in[0,20\pi]^2\times R, \end{aligned} \tag{5.10}$$

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial z^2}\right)V_{\text{ch}}(\mathbf{x},t) = -|\psi(\mathbf{x},t)|^2, \quad \mathbf{x}\in[0,20\pi]^2\times[z_1,z_4], \tag{5.11}$$

$$V_{\text{in}}(\mathbf{x}) = \begin{cases} 10(\exp(0.9)-\exp(-\cos(x/10)/2-\cos(y/10)/2)) & \text{if } z\in[z_2,z_3], \\ 0 & \text{otherwise}, \end{cases} \tag{5.12}$$

where z_1, z_2, z_3, z_4 satisfy $z_1 < z_2 < z_3 < z_4$. The intrinsic potential $V_{\text{in}}(x, y, z, t)$ is discontinuous along the propagation z-direction and provides quantum confinement of electron waves along the (x, y) plane such as arrays of quantum dots [10].

Based on the accuracy study above of the three types of time integrations, the Crank Nicholson gives the best numerical results with the most efficiency and will be used for the 3-D problem here. With time discretization by the Crank Nicholson method and Fourier spectral method in (x, y) directions, (5.10) and (5.11) become

$$\begin{aligned} & i\frac{u_{m,n}(z,(n+1)\Delta t)-u_{m,n}(z,(n-1)\Delta t)}{2\Delta t} \\ &\quad = -\frac{1}{\varepsilon}\frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{u_{m,n}(z,(n-1)\Delta t)+u_{m,n}(z,(n+1)\Delta t)}{2}\right) \\ &\qquad + \frac{1}{100}(m^2+n^2)\frac{u_{m,n}(z,(n-1)\Delta t)+u_{m,n}(z,(n+1)\Delta t)}{2} \\ &\qquad + \sum_{m=-M}^{M}\sum_{n=-M}^{M} V_{\text{in}}(m,n,z)\frac{u_{m,n}(z,(n-1)\Delta t)+u_{m,n}(z,(n+1)\Delta t)}{2} \\ &\qquad + \sum_{m_1+m_2=m,n_1+n_2=n} v_{m_1,n_1}(z,n\Delta t)u_{m_2,n_2}(z,n\Delta t), \\ &\qquad m,n=-M,\ldots,M, \quad z\in[-0.25,4.25], \end{aligned} \tag{5.13}$$

$$\frac{\partial^2}{\partial z^2} v_{m,n}(z, n\Delta t) = -\sum_{n_2-n_1=n, m_2-m_1=m} \bar{u}_{m_1,n_1}(z, n\Delta t) u_{m_2,n_2}(z, n\Delta t) + \frac{1}{100}(m^2+n^2) v_{m,n}(z, n\Delta t), \quad m, n = -2M, \ldots, 2M, \quad z \in [z_1, z_4]. \tag{5.14}$$

• Incident wave: The linear Schrödinger equation when $z \notin [z_1, z_4]$ admits a solution of the following form, which will be used as the incident wave impinging from $z < z_1$ to the intrinsic potential barrier created by (5.12),

$$\Psi^{\text{inc}}(x, y, z, t) = \sum_{m,n} u_{m,n}(z, t) \exp(\mathrm{i}(mx + ny)), \tag{5.15}$$

where

$$u_{m,n}(z, t) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} f_{m,n}(\omega) \exp(\mathrm{i}(k_{m,n}(\omega) z - \omega t))\, \mathrm{d}\omega,$$

$$k_{m,n} = \sqrt{\omega - (m^2 + n^2)},$$

$$f_{m,n}(\omega) = c_{m,n} \frac{t_{\text{decay}}}{\sqrt{2}} \exp\left(-\frac{(\omega_c - \omega)^2 t_{\text{decay}}^2}{4}\right) \exp(\mathrm{i} t_0 \omega),$$

where $c_{m,n}$, t_{decay}, t_0 and ω_c are arbitrary constants. In our numerical example, we select

$$c_{m,n} = \begin{cases} 1 & \text{if } n = m = 0, \\ 0 & \text{otherwise} \end{cases}$$

and $\omega_c = 1$, and $t_{\text{decay}} = 10$, and $t_0 = 4t_{\text{decay}}$. The incident wave represents a Gaussian pulse along the propagation z-direction, as shown in Fig. 2, with a periodic profile over (x, y) plane. For the selected parameters, the incident wave takes constant value over the (x, y) plane.

The computational domain is set to be $[0, 4]$, and two PMLs with a thickness 0.625 are added to both ends of the computational domain, and $z_1 = 1$ and $z_2 = 2$ and $z_3 = 2.5$ and $z_4 = 3$. As (5.15) is a localized pulse, so we can also use $\Psi(x, y, z, t = 0)$ as the initial condition. We will use the numerical solution got by using the finest mesh and the maximum M_0 as a reference solution, then calculate the error between the numerical solution

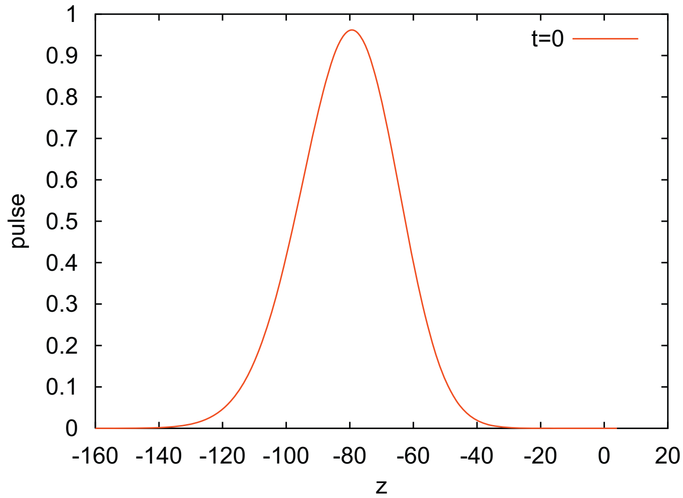

Fig. 2. The incident Gaussian pulse along the propagation direction (constant magnitude over (x, y) plane).

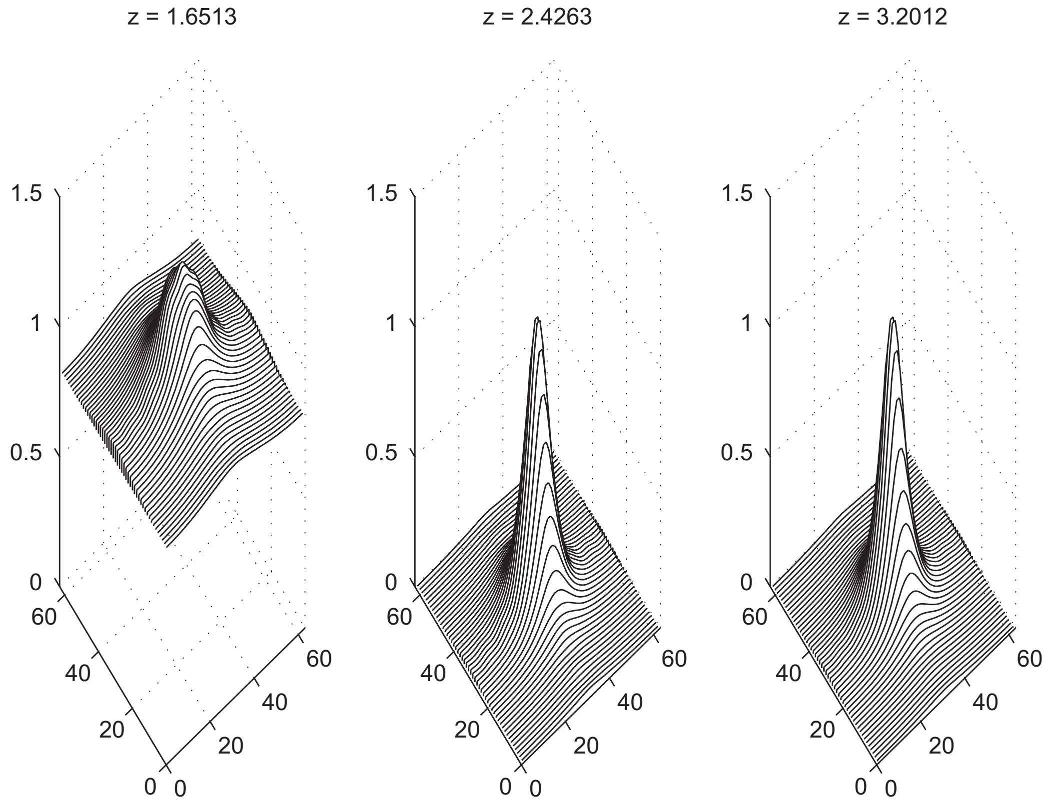

Fig. 3. The magnitude of the wave function at three planes along the z-direction. The wave is confined in the center of the region after it passes through a potential barrier.

$\Psi_1(x, y, z, t) = \sum_{m=-M}^{M}\sum_{n=-M}^{M} u_{m,n}(z, t)\exp(\mathrm{i}(mx+ny))$ and the reference solution $\Psi_2(x, y, z, t)=\sum_{m=-M_0}^{M_0}\sum_{n=-M_0}^{M_0} f_{m,n}(z, t)\exp(\mathrm{i}(mx+ny))$ using the following formula:

$$\mathrm{Error}^2 = \sum_{m=-M_0}^{M_0}\sum_{n=-M_0}^{M_0}\int_0^4 \mathrm{d}z|u_{m,n}(z, t) - f_{m,n}(z, t)|^2,$$

where we assume $M \geqslant N$ and $u_{m,n}(z, t) = 0$ if $|m| > M$ or $|n| > M$.

The computational domain [0, 4] is divided into 64 equally spaced meshes. We compute the self-consistent solution up to $T = 40$ with a time step $\Delta t = 0.00390625$, and $M = 0, 1, 2, 4$, and the degree of the basis function set to be 3. Due to the computational cost of 3-D problems, we limit the size of the mode number in (x, y) directions to $M_0 = 6$ as a reference solution. The relative L^2 errors for $M = 0, 1, 2, 3, 4, 5$ are 0.210744, 0.159648, 0.110236, 0.0740385, 0.0487261, 0.0255488, respectively. The magnitude of the wave function at various z-locations is plotted in Fig. 3, which shows the expected quantum confinement of the electron waves from the intrinsic potential $V_{\mathrm{in}}(x, y, z)$.

6. Conclusion

In this paper, we have proposed a Fourier spectral-discontinuous Galerkin method for coupled nonlinear time-dependent Schrödinger–Poisson equations and provided the explicit formulas for the derivative matrices for the wave function, which can be readily used for exponential time difference and other implicit time discretizations. Numerical results in 3-D problems show the potential of this method for problems where potentials are known to be discontinuous along material interfaces in heterojunction and quantum supperlattice structures. Future work will be carried out for cases when the potentials are also time dependent for transient excitations in laser physics.

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Appendix A.

In the following, double index k or m implies summation over $1 \leqslant k \leqslant s$, $1 \leqslant m \leqslant s$, respectively. No summation is assumed for the element j index.

When $3 \leqslant j \leqslant N-2$, $a_{n,k}^{j,l}$, $l = j-2, j-1, \ldots, j+2$ are given as

$$\begin{aligned} a_{n,k}^{j,j} = {} & \frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j}[2M_{mk}^{z,j} - \phi_m^j(z_{j+1/2})\phi_k^j(z_{j+1/2}) + \phi_m^j(z_{j-1/2})\phi_k^j(z_{j-1/2})] \\ & + \frac{1}{2}\phi_n^j(z_{j+1/2})\left[-\frac{\varepsilon_j}{c_{j,m}} M_{mk}^{z,j}\phi_m^j(z_{j+1/2}) + \frac{\varepsilon_j}{2c_{j,m}}\phi_k^j(z_{j+1/2})\phi_m^j(z_{j+1/2})\phi_m^j(z_{j+1/2})\right. \\ & \left. -\frac{\varepsilon_j}{2c_{j,m}}\phi_k^j(z_{j-1/2})\phi_m^j(z_{j-1/2})\phi_m^j(z_{j+1/2}) - \phi_k^j(z_{j+1/2})\phi_m^{j+1}(z_{j+1/2})\phi_m^{j+1}(z_{j+1/2})\frac{\varepsilon_{j+1}}{2c_{j+1,m}}\right] \\ & - \frac{1}{2}\phi_n^j(z_{j-1/2})\left[-\frac{\varepsilon_j}{c_{j,m}} M_{mk}^{z,j}\phi_m^j(z_{j-1/2}) + \frac{\varepsilon_{j-1}}{2c_{j-1,m}}\phi_k^j(z_{j-1/2})\phi_m^{j-1}(z_{j-1/2})\phi_m^{j-1}(z_{j-1/2})\right. \\ & \left. + \frac{\varepsilon_j}{2c_{j,m}}\phi_m^j(z_{j-1/2})(\phi_k^j(z_{j+1/2})\phi_m^j(z_{j+1/2}) - \phi_k^j(z_{j-1/2})\phi_m^j(z_{j-1/2}))\right], \end{aligned} \tag{A.1}$$

$$\begin{aligned} a_{n,k}^{j,j+1} = {} & -\frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j}\phi_m^j(z_{j+1/2})\phi_k^{j+1}(z_{j+1/2}) + \frac{1}{2}\phi_n^j(z_{j+1/2})\left[-\frac{\varepsilon_{j+1}}{c_{j+1,m}} M_{mk}^{z,j+1}\phi_m^{j+1}(z_{j+1/2})\right. \\ & + \frac{\varepsilon_j}{2c_{j,m}}\phi_m^j(z_{j+1/2})\phi_m^j(z_{j+1/2})\phi_k^{j+1}(z_{j+1/2}) + \frac{\varepsilon_{j+1}}{2c_{j+1,m}}\phi_m^{j+1}(z_{j+3/2})\phi_m^{j+1}(z_{j+1/2})\phi_k^{j+1}(z_{j+3/2}) \\ & \left. -\frac{\varepsilon_{j+1}}{2c_{j+1,m}}\phi_m^{j+1}(z_{j+1/2})\phi_m^{j+1}(z_{j+1/2})\phi_k^{j+1}(z_{j+1/2})\right] \\ & - \frac{1}{2}\phi_n^j(z_{j-1/2})\varepsilon_j\frac{1}{c_{j,m}}\left[\frac{1}{2}\phi_m^j(z_{j+1/2})\phi_m^j(z_{j-1/2})\phi_k^{j+1}(z_{j+1/2})\right], \end{aligned} \tag{A.2}$$

$$\begin{aligned} a_{n,k}^{j,j-1} = {} & \frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j}\phi_m^j(z_{j-1/2})\phi_k^{j-1}(z_{j-1/2}) - \frac{\varepsilon_j}{4c_{j,m}}\phi_n^j(z_{j+1/2})\phi_m^j(z_{j-1/2})\phi_m^j(z_{j+1/2})\phi_k^{j-1}(z_{j-1/2}) \\ & - \frac{1}{2}\phi_n^j(z_{j-1/2})\left[-\frac{\varepsilon_{j-1}}{c_{j-1,m}} M_{mk}^{z,j-1}\phi_m^{j-1}(z_{j-1/2}) + \frac{\varepsilon_{j-1}}{2c_{j-1,m}}\phi_m^{j-1}(z_{j-1/2})\phi_m^{j-1}(z_{j-1/2})\phi_k^{j-1}(z_{j-1/2})\right. \\ & - \frac{\varepsilon_{j-1}}{2_{j-1,m}}\phi_m^{j-1}(z_{j-3/2})\phi_m^{j-1}(z_{j-1/2})\phi_k^{j-1}(z_{j-3/2}) \\ & \left. -\frac{\varepsilon_j}{2c_{j,m}}\phi_m^j(z_{j-1/2})\phi_m^j(z_{j-1/2})\phi_k^{j-1}(z_{j-1/2})\right], \end{aligned} \tag{A.3}$$

$$a_{n,k}^{j,j+2} = \frac{1}{2}\phi_n^j(z_{j+1/2})\left[\frac{1}{2}\varepsilon_{j+1}\frac{1}{c_{j+1,m}}\phi_m^{j+1}(z_{j+3/2})\phi_m^{j+1}(z_{j+1/2})\phi_k^{j+2}(z_{j+3/2})\right], \tag{A.4}$$

$$a_{n,k}^{j,j-2} = \frac{1}{2}\phi_n^j(z_{j-1/2})\left[\frac{1}{2}\varepsilon_{j-1}\frac{1}{c_{j-1,m}}\phi_m^{j-1}(z_{j-3/2})\phi_m^{j-1}(z_{j-1/2})\phi_k^{j-2}(z_{j-3/2})\right]. \tag{A.5}$$

When $j = 1, 2, N-1, N$, $A^{(j,l)}$ will be modified due to the boundary condition. Using the flux Eq. (3.19) and $j = 1$, we have

$$\begin{aligned} a_{n,k}^{j,j} =& \varepsilon_j \frac{1}{c_{j,m}} M_{nm}^{z,j} M_{mk}^{z,j} - \frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j+1/2}) \phi_k^j(z_{j+1/2}) + \frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j-1/2}) \phi_k^j(z_{j-1/2}) \\ &+ \frac{1}{2} \phi_n^j(z_{j+1/2}) \left[-\frac{\varepsilon_j}{c_{j,m}} M_{mk}^{z,j} \phi_m^j(z_{j+1/2}) + \frac{\varepsilon_j}{2c_{j,m}} \phi_k^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \right. \\ &\left. - \frac{\varepsilon_j}{2c_{j,m}} \phi_k^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j+1/2}) - \frac{\varepsilon_{j+1}}{2c_{j+1,m}} \phi_k^j(z_{j+1/2}) \phi_m^{j+1}(z_{j+1/2}) \phi_m^{j+1}(z_{j+1/2}) \right] \\ &- \phi_n^j(z_{j-1/2}) \left[-\frac{\varepsilon_j}{c_{j,m}} M_{mk}^{z,j} \phi_m^j(z_{j-1/2}) + \frac{\varepsilon_j}{2c_{j,m}} \phi_k^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j-1/2}) \right. \\ &\left. - \frac{\varepsilon_j}{2c_{j,m}} \phi_k^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \right], \end{aligned} \tag{A.6}$$

$$\begin{aligned} a_{n,k}^{j,j+1} =& -\frac{1}{2} \varepsilon_j \frac{1}{c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j+1/2}) \phi_k^{j+1}(z_{j+1/2}) + \frac{1}{2} \phi_n^j(z_{j+1/2}) \\ &\times \left[-\varepsilon_{j+1} \frac{1}{c_{j+1,m}} M_{mk}^{z,j+1} \phi_m^{j+1}(z_{j+1/2}) + \frac{1}{2} \varepsilon_j \frac{1}{c_{j,m}} \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \phi_k^{j+1}(z_{j+1/2}) \right. \\ &\left. + \frac{\varepsilon_{j+1}}{2c_{j+1,m}} \phi_m^{j+1}(z_{j+1/2}) (\phi_m^{j+1}(z_{j+3/2}) \phi_k^{j+1}(z_{j+3/2}) - \phi_m^{j+1}(z_{j+1/2}) \phi_k^{j+1}(z_{j+1/2})) \right] \\ &- \phi_n^j(z_{j-1/2}) \frac{\varepsilon_j}{2c_{j,m}} \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j-1/2}) \phi_k^{j+1}(z_{j+1/2}), \end{aligned} \tag{A.7}$$

$$\begin{aligned} b_n^j =& \frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j-1/2}) \beta - \frac{1}{2} \phi_n^j(z_{j+1/2}) \frac{\varepsilon_j}{2c_{j,m}} \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j+1/2}) \beta + \phi_n^j(z_{j-1/2}) \\ &\times \frac{\varepsilon_j}{2c_{j,m}} \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \beta. \end{aligned} \tag{A.8}$$

The expression of $a_{n,k}^{j,j+2}$ is the same as that of (A.4). Using the flux Eq. (3.19) and $j = 2$, we have

$$b_n^j = \frac{1}{2} \phi_n^j(z_{j-1/2}) \left[\frac{1}{2} \varepsilon_{j-1} \frac{1}{c_{j-1,m}} \phi_m^{j-1}(z_{j-3/2}) \phi_m^{j-1}(z_{j-1/2}) \beta \right]. \tag{A.9}$$

The expressions of $a_{n,k}^{j,j}$, $a_{n,k}^{j,j+1}$, $a_{n,k}^{j,j-1}$ and $a_{n,k}^{j,j+2}$ are the same as that of (A.1), (A.2), (A.3) and (A.4), respectively. Using the flux Eq. (3.20) and $j = N$, we have

$$\begin{aligned} a_{n,k}^{j,j} =& \frac{\varepsilon_j}{c_{j,m}} M_{nm}^{z,j} M_{mk}^{z,j} - \frac{\varepsilon_j}{c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j+1/2}) \phi_k^j(z_{j+1/2}) + \frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j-1/2}) \\ &\times \phi_k^j(z_{j-1/2}) + \frac{1}{2} \phi_n^j(z_{j+1/2}) \left[-\varepsilon_j \frac{1}{c_{j,m}} M_{mk}^{z,j} \phi_m^j(z_{j+1/2}) + \varepsilon_j \frac{1}{c_{j,m}} \phi_k^j(z_{j+1/2}) \right. \\ &\left. \times \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) - \frac{\varepsilon_j}{2c_{j,m}} \phi_k^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j+1/2}) \right] - \frac{1}{2} \phi_n^j(z_{j-1/2}) \\ &\times \left[-\varepsilon_j \frac{1}{c_{j,m}} M_{mk}^{z,j} \phi_m^j(z_{j-1/2}) + \varepsilon_{j-1} \frac{1}{c_{j-1,m}} \frac{1}{2} \phi_k^j(z_{j-1/2}) \phi_m^{j-1}(z_{j-1/2}) \phi_m^{j-1}(z_{j-1/2}) \right. \\ &\left. + \frac{\varepsilon_j}{c_{j,m}} \phi_k^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j-1/2}) - \frac{\varepsilon_j}{2c_{j,m}} \phi_k^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \phi_m^j(z_{j-1/2}) \right], \end{aligned} \tag{A.10}$$

$$b_n^j = \tfrac{1}{2} \phi_n^j(z_{j+1/2}) \gamma. \tag{A.11}$$

The expressions of $a_{n,k}^{j,j-1}$ and $a_{n,k}^{j,j-2}$ are the same as that of (A.3) and (A.5), respectively. Using the flux Eq. (3.20) and $j = N - 1$, we have

$$\begin{aligned} a_{n,k}^{j,j+1} = & -\frac{\varepsilon_j}{2c_{j,m}} M_{nm}^{z,j} \phi_m^j(z_{j+1/2}) \phi_k^{j+1}(z_{j+1/2}) + \frac{1}{2}\phi_n^j(z_{j+1/2}) \\ & \times \left[-\frac{\varepsilon_{j+1}}{c_{j+1,m}} M_{mk}^{z,j+1} \phi_m^{j+1}(z_{j+1/2}) + \frac{\varepsilon_j}{2c_{j,m}} \phi_m^j(z_{j+1/2}) \phi_m^j(z_{j+1/2}) \phi_k^{j+1}(z_{j+1/2}) \right. \\ & \left. + \frac{\varepsilon_{j+1}}{2c_{j+1,m}} \phi_m^{j+1}(z_{j+1/2}) (2\phi_m^{j+1}(z_{j+3/2}) \phi_k^{j+1}(z_{j+3/2}) - 1\phi_m^{j+1}(z_{j+1/2}) \phi_k^{j+1}(z_{j+1/2})) \right] \qquad \text{(A.12)} \\ & - \frac{1}{2}\phi_n^j(z_{j-1/2}) \varepsilon_j \frac{1}{c_{j,m}} \left[\frac{1}{2}\phi_m^j(z_{j+1/2}) \phi_m^j(z_{j-1/2}) \phi_k^{j+1}(z_{j+1/2}) \right], \qquad \text{(A.13)} \end{aligned}$$

$$b_n^j = 0. \qquad \text{(A.14)}$$

The expressions of $a_{n,k}^{j,j}$, $a_{n,k}^{j,j-1}$and $a_{n,k}^{j,j-2}$ are the same as that of (A.1), (A.3) and (A.5), respectively.

References

[1] F. Aluffi-Pentini, V. De Fronzo, V. Parisi, A novel algorithm for the numerical integration of systems of ordinary differential equations arising in chemical problems, J. Math. Chem. 33 (1) (2003) 1–15.

[2] W. Bao, N.J. Mauser, H.P. Stimming, Effective one particle quantum dynamics of electrons: a numerical study of the Schrödinger–Poisson-X_α model, Comm. Math. Sci. 1 (4) (2003) 809–828.

[3] C. Bardos, L. Erdos, F. Golse, N. Mauser, H. Yau, Derivation of the Schrödinger–Poisson equation from the quantum N-body problem, C. R. Acad. Sci. t Sér. I Math. 334 (6) (2002) 515–520.

[4] N. Ben Abballah, P. Degond, P.A. Markowich, On a one-dimensional Schrödinger–Poisson scattering model, ZAMP 48 (1997) 35–55.

[5] J.P. Berenger, A perfectly matched layer for the absorption of electromagnetic waves, J. Comput. Phys. 114 (2) (1994) 185–200.

[6] M. Cahay, M. McLennan, S. Datta, M.S. Lundstrom, Importance of space-charge effects in resonant tunneling devices, Appl. Phys. Lett. 50 (1987) 612–614.

[7] C. Cheng, Q. Liu, J. Lee, H.Z. Massoud, Spectral element method for the Schrödinger–Poisson system, J. Comput. Electron. 3 (2004) 417–421.

[8] S.M. Cox, P.C. Matthews, Exponential time differencing for stiff systems, J. Comput. Phys. 176 (2002) 430–455.

[9] M. Ehrhardt, A. Zisowsky, Fast calculation of energy and mass preserving solutions of Schrödinger–Poisson systems on unbounded domains, J. Comput. Appl. Math. 187 (1) (2006) 1–28.

[10] D. Ferry, S. Marshall Goodnick, Transport in Nanostructures, Cambridge University Press, Cambridge, UK, New York, 1997.

[11] D. Gottlieb, S. Orszag, Numerical Analysis of Spectral Methods: Theory and Applications, SIAM, Philadelphia, PA, 1977.

[12] E.K.U. Gross, W. Kohn, Local density-functional theory of frequency-dependent linear response, Phys. Rev. Lett. 55 (1985) 2850–2852.

[13] G.R. Haldley, Transparent boundary condition for the beam propagation method, IEEE J. Quantum Electron. 28 (1992) 363–370.

[14] R. Harrison, I. Moroz, K.P. Tod, A numerical study of the Schrödinger–Newton equation 2: the time-dependent problem, math-ph/0208046, 2002.

[15] R. Harrison, I. Moroz, K.P. Tod, A numerical study of the Schrödinger–Newton equations, Nonlinearity 16 (2003) 101–122.

[16] T. Lu, W. Cai, P.W. Zhang, Conservative local discontinuous Galerkin methods for time dependent Schroedinger equation, Internat. J. Numer. Anal. Modeling 1 (2005) 45–65.

[17] J.H. Luscombe, A.M. Bouchard, M. Luban, Electron confinement in quantum nanostructures: self-consistent Poisson–Schrödinger theory, Phys. Rev. B 46 (1992) 10262–10268.

[18] P. Markowich, C. Ringhofer, C. Schmeiser, Semiconductor Equations, Springer, Berlin, 1990.

[19] H. Ohnishi, T. Inata, S. Muto, N. Yokoyama, A. Shibatomi, Self-consistent analysis of resonant tunneling current, Appl. Phys. Lett. 49 (1986) 1248–1250.

[20] F. Schmidt, D. Yevick, Discrete transparent boundary conditions for Schrödinger-type equations, J. Comput. Phys. 134 (1997) 96–107.

[21] F. Siddhartha Guzman, L. Arturo Urena-Lopez, Gravitational cooling of self-gravitating Bose-Condensates, astro-ph/0603613, 2006.

[22] F. Stern, Iteration methods for calculating self-consistent fields in semiconductor inversion layers, J. Comput. Phys. 6 (1) (1970) 56–67.

[23] A. Taflove, S.C. Hagness, Computational Electromagnetics: The Finite-Difference Time-Domain Method. second ed., Artech House, Boston, London, 2000.

[24] M. Talebian, W. Pötz, Open boundary conditions for a time-dependent analysis of the resonant tunneling structure, Appl. Phys. Lett. 69 (1996) 1148–1150.

[25] J. Werschnik, E.K.U. Gross, K. Burke, Time-dependent density functional theory: past, present, and future, cond-mat/0410362, 2004.

[26] Y. Xu, C.W. Snhu, Local discontinuous Galerkin methods for nonlinear Schrödinger equations, J. Comput. Phys. 205 (2005) 72–97.