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Accurate mesh truncation for Schrödinger equations by a perfectly matched layer absorber: Application to the calculation of optical spectra

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Quasibound and continuum states are of particular importance for the numerical investigation of coherence properties and are sensitive with respect to the boundary condition chosen at the edge of the computational window. An open boundary condition will be derived which is particularly suitable for dynamical problems described by Schrödinger-type equations. With this approach, bound states as well as unbound states can be described adequately. The boundary condition is derived from a perfectly matched layer (PML) formalism commonly used in the field of electrodynamics. Consequently, the calculation domain is reduced leading to a calculation time reduction by orders of magnitude. From the physical point of view this formulation allows an adequate analysis of transport phenomena or absorption spectra, e.g., the results obtained by the PML formalism are compared with accurate numerical results calculated using a large mesh and show an excellent performance. For example, the Coulomb enhanced Franz-Keldysh effect is investigated, which cannot be analyzed adequately without using proper open boundary conditions. [S0163-1829(99)51332-5]

Numerical calculations are important for the design of semiconductor devices as well as in the investigation of novel effects like coherence properties. If one is not interested in bound states only, care must be taken at the boundary of the calculation window. If the boundary conditions are not appropriate, strong reflections occur, which can significantly affect the results. The usual solution is to choose a large calculation domain. Then, intrinsic losses lead to a vanishing wave amplitude at the mesh boundaries. However, this results in very long computation times, and, especially for multidimensional problems, the needed computer resources are not acceptable. Usually, all interactions take place within a limited area. Thus, computational efficiency can be enhanced by using open boundary conditions and more complex problems can be investigated.

In this paper we apply the perfectly matched layer (PML) technique to the calculation of optical spectra of semiconductor heterostructures. Generally, the semiconductor Bloch equation is formulated in a six-dimensional hyperspace. Assuming rotational symmetry, quantum wells and superlattices can be calculated within a three-dimensional computation domain. If one is interested in bound-state absorption only, an expansion into a few single particle wave functions is a fast computational approach.[1] Using the full three-dimensional semiconductor Bloch equation results in a wide range of possible applications,[2] but is numerically expensive without appropriate boundary conditions. For example, a mesh of up to 1 million discretization points has been used with about 10 points in the quantum well direction only.[2] This discretization is appropriate for demonstrating basic properties but is much too coarse for practical investigation purposes. We will show that using the PML boundary condition enhances the numerical efficiency, thus the range of applications will be enhanced. This is demonstrated by calculating the Franz-Keldysh absorption from the three-dimensional semiconductor Bloch equation.

It is quite complicated to develop open boundary conditions for the Schrödinger equation because it is of first order in time and of second order in space, compared to electrodynamic calculations using Maxwell's equations or the electromagnetic wave equation, which are both second order in space and time. In electromagnetic theory there is a long tradition of developing open or analytically absorbing boundary conditions (ABC) back to 1977.[3,4] They are based on an analytical one-dimensional estimation of the exterior points resulting from a factorization of the one-dimensional wave equation. Thus, for multidimensional problems, effective constants, depending on the incidence angle and material properties, must be estimated. Another approach is to model a physical absorber which attenuates the outgoing waves.[5] A drawback is that this kind of absorber is not reflection-free at the interface between the absorber and the calculation domain. Berenger[6] proposed the introduction of a nonphysical absorber which is matched to the calculation domain for all angles of incidence, called perfectly matched layer. It improved the accuracy of the boundary conditions by orders of magnitude introducing additional anisotropic losses, which is equivalent to a complex coordinate stretching.

For the Schrödinger equation, the most natural way to formulate open boundary conditions is to match the calculation space to an analytic solution of the exterior region. This approach has been called the quantum transmitting boundary method (QTBM),[7] and works quite accurately for simple structures and for stationary problems. It is related closely to Hadleys transparent boundary condition (TBC).[8] For dynamical problems, this method has been applied also,[9] but then the parameters have to be estimated from time derivatives. A more elegant method has been proposed by Schmidt[10] which results in a boundary condition similar to the ABC for electromagnetic problems. As the Schrödinger equation is of first order in time it results in a formulation which is nonlocal in time. Again, this estimation has been done for one dimension only, thus again effective constants must be estimated. In contrast, absorbers do not require a parameter estimation and are easy to implement. Physical absorbers have already been used for beam propagation

methods,[5,11] but had to be carefully adjusted to prevent reflections, as these absorbers were not matched.

In this paper we will derive a PML formalism for Schrödinger-type equations. This results in a boundary condition which is local in time and space. Additionally, even for multi-dimensional calculations, the formalism can be implemented easily, providing a very high accuracy. There are some differences compared to the formulation used for electromagnetic calculation because the wave functions obey different boundary conditions than those used in electromagnetic computations. Without loss of generality, we will present the development of the PML for the three-dimensional exciton equation which describes the optical absorption in quantum well structures. It can be extended to more dimensions or other Schrödinger-type equations.

In this section we will show that it is possible to develop an absorber which is ideally nonreflecting, independent of the angle of incidence. We start with the linear density matrix equation for excitons[2,12]

$$\left(\frac{\partial}{\partial t}+\mathrm{j}V_{eh}+\Gamma\right)\psi-\frac{\mathrm{j}\hbar}{2}\nabla\cdot\underbrace{\begin{pmatrix} m_e^{-1} & 0 & 0\\ 0 & m_h^{-1} & 0\\ 0 & 0 & m_r^{-1}\end{pmatrix}}_{\mathbf{m}^{-1}}\nabla\psi = \frac{\mathrm{j}M_0}{\hbar}\frac{\delta(z_e-z_h)\delta(r)}{2\pi r}E. \tag{1}$$

M_0 is the optical dipole matrix element, E is the electric field, and Γ is a dephasing rate due to scattering. The reduced electron-hole mass is $m_r=(1/m_e+1/m_h)^{-1}$, the electron-hole potential V_{eh} includes the dielectrically screened Coulomb potential

$$V_{eh}=e_0(V_e(z_e)-V_h(z_h))-\frac{e_0^2}{4\pi\epsilon_0\epsilon_r\sqrt{(z_e-z_h)^2+r^2}}. \tag{2}$$

Equation (1) is valid for parabolic bands and for the Nabla operator ∇ in cylindrical coordinates. At an arbitrarily located interface between two materials 1 and 2, the boundary conditions

$$\psi_1=\psi_2, \quad \mathbf{m}_1^{-1}\nabla\psi_1=\mathbf{m}_2^{-1}\nabla\psi_2, \tag{3}$$

hold.[13] This form conserves hermiticity of the Hamiltonian even in a discretized form.

To develop the PML-absorber, complex stretched coordinates are defined by stretching factors s_x with x standing for the coordinates z_e, z_h, or r:

$$\tilde{x}=\int_0^x s_x(x')dx', \tag{4}$$

resulting in

$$\frac{\partial}{\partial\tilde{x}}=\frac{1}{s_x}\frac{\partial}{\partial x}. \tag{5}$$

This results in a change of the Nabla operator. Clearly, for $s_x=1$, the original equations result and because of the integral form [Eq. 4] the coordinates transform gradually.

To show that these transformations lead to additional damping, we will calculate the dispersion relation. In a second step it is shown that modifying the stretching factors will not result in reflections. We will consider the case $r\gg 0$ due to simplicity. In this case the general solution can be written as a local superposition of plane waves with wave vectors $\vec{k}=(k_{z_e}k_{z_h}k_r)^T$:

$$\psi_1=a_i\mathrm{e}^{-\vec{k}_1\vec{r}-\mathrm{j}\,\omega t}+a_r\mathrm{e}^{\vec{k}_1\vec{r}-\mathrm{j}\,\omega t}, \quad \psi_2=a_t\mathrm{e}^{-\vec{k}_2\vec{r}-\mathrm{j}\omega t}, \tag{6}$$

with amplitudes a_i, a_r, and a_t of the incident, reflected, and transmitted wave, respectively. The two regions at the interface are labeled 1 and 2. The dispersion relation calculated from Eq. (1) results in

$$\frac{k_{z_e}^2}{s_{z_e}^2 m_e}+\frac{k_{z_h}^2}{s_{z_h}^2 m_h}+\frac{k_r^2}{s_r^2 m_r}=\frac{2}{\hbar}(-\omega+V_{eh}-\mathrm{j}\,\Gamma):=E_0. \tag{7}$$

This is the equation of an ellipsoid and solutions are of the form

$$k_{z_e}=s_{z_e}\sqrt{m_eE_0}\sin\theta\cos\phi,$$

$$k_{z_r}=s_{z_h}\sqrt{m_hE_0}\sin\theta\sin\phi,$$

$$k_r=s_r\sqrt{m_rE_0}\cos\theta. \tag{8}$$

Inserting the plane wave solution into Eq. (3), the condition for a vanishing reflected wave for identical materials and arbitrary stretching factors is

$$\frac{k_{x,1}}{s_{x,1}}=\frac{k_{x,2}}{s_{x,2}}. \tag{9}$$

For physical absorbers the stretching factors in Eq. (9) are equal to 1. Thus every change in the wave numbers (8) will lead to reflections. They can be minimized by the shape of the absorber.[5] With stretched coordinates, Eq. (9) is always valid for arbitrary angles and arbitrary stretching factors s_x.

While the absorber constructed above is theoretically reflection-free, numerical errors result from strong variations of the scaling parameters. A good choice would be a polynomial space dependence according to

$$s_x=\alpha+\mathrm{j}\,\beta=(\alpha_m+\mathrm{j}\,\beta_m)x^n, \tag{10}$$

with α_m and β_m as maximum values for the real and imaginary stretching, x is the normalized absorber length with $|x|\leqslant 1$. n is the shape parameter, values between 1 and 4 are reasonable. Figure 1 visualizes the introduction of complex stretching factors.

The most interesting interface is between the physical calculation domain and the absorber. We will show with very simple approximations how the propagation properties change across this interface. The vectorial properties are dropped for simplicity. Within the calculation domain, labeled with the index 1 in all subsequent equations, all stretching factors are 1. The absorber region is labeled with

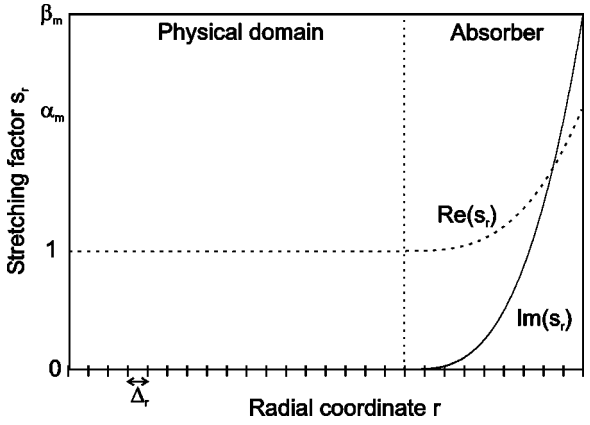

FIG. 1. Principal coordinate stretching.

the index 2. For a purely propagating wave with a dominant imaginary propagation constant $k_1 \approx -\mathrm{j}\, k_0''$, the propagation constant then is

$$k_2 \approx \beta k_0'' - \mathrm{j}\, \alpha k_0''. \tag{11}$$

This shows that the propagation speed is scaled by α and the wave is damped by β. If on the other hand the wave is of an evanescent type with a dominant real propagation constant $k_1 \approx k_0'$, the natural damping is enhanced by the scaling parameter α whereas β does not contribute to damping:

$$k_2 \approx \alpha k_0' + \mathrm{j}\, \beta k_0'. \tag{12}$$

The case $\alpha = 1$ yields the original PML formulation due to Berenger.[6] The PML absorber can be implemented using the finite difference (FD) or the finite element (FE) method. It is applicable to stationary boundary-value problems and eigenvalue problems as well as to time-dependent problems with the same amount of programming and calculation effort. This results from the fact that the Schrödinger equation is of first order in time. Because electromagnetic computations are second order in time, the coordinate stretching must be formulated energy dependent. This results in an increase of computational effort for time-dependent problems by a factor of 2.

All numerical examples are calculated using a finite element (FE) method with linear or trilinear base functions. Heavy hole–electron transitions are considered in our calculations, only. We will present some examples which demonstrate the effectiveness of the PML.

Ideal two-dimensional excitons. The first example is intended to show the influence of the proposed boundary condition in comparison to exact calculations. The absorption of an ideal quantum well consisting of $Ga_{0.4}In_{0.6}As_{0.9}P_{0.1}$ is calculated using a mesh size of 60 points with a constant mesh size of 1 nm. The resulting equation is obtained from Eq. (1) by letting $z_e = z_h = 0$ and neglecting derivatives in the z direction. To distinguish between discretization errors and errors due to mesh truncation the results are compared with a numerically exact calculation using a very large mesh of 1500 points.[2] In Fig. 2 the absorption spectrum of an ideal two-dimensional quantum well is shown for a damping rate $\hbar\Gamma = 2$ meV. The reduced mass is $m_r = 0.04$ and the dielectric constant is $\epsilon_r = 14$. This results in an exciton Bohr radius of $a_b = 14$ nm and an exciton Rydberg energy of $R = 2.8$ meV. Assuming a Dirichlet boundary condition[2] implies vanishing wave functions at the boundaries, which results in strong reflections due to the additional quantization. The results of an 18-point PML absorber with $\beta_m = 3$ and $n = 3$ cannot be distinguished from the exact numerical solution in the scale of Fig. 2, as the relative error of the calculation using the PML shown in Fig. 3 is less than 3%, which is appropriate for most applications. Additionally, the use of the analytic ABC (Ref. 10) is shown in Fig. 3. Independent of the boundary condition the bound excitons are properly modeled. The ABC has an overall error which is about twice that of the PML. Additionally, the error is independent of energy. The PML error decreases for higher energies. This is due to the simplification $r \gg 0$. For higher energies the wavelength reduces and the approximation improves. Thus a further improvement would be the extension of the PML formalism to true radial coordinates. For electromagnetic calculations this has already been done,[14] but for the Schrödinger equation this may result in additional terms.

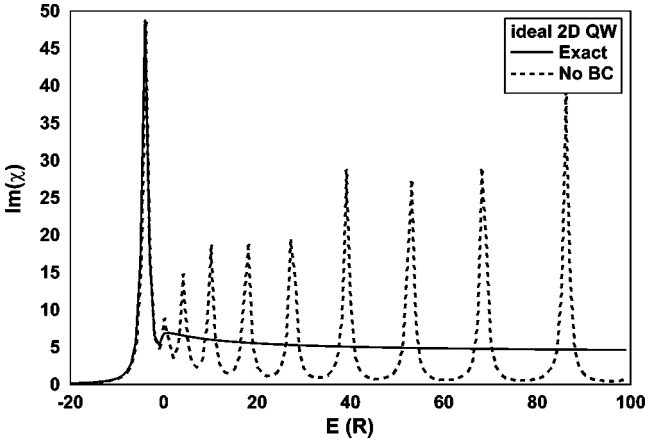

FIG. 2. Absorption of an ideal quantum well, exact and with vanishing wave functions (no boundary condition).

The use of the PML boundary condition results in reduced computation time by two orders of magnitude compared to a numerically exact solution. It is even more efficient for low damping rates since the computational domain must be enlarged to compensate for the small damping in this case. This will be especially interesting for modeling low-temperature experiments.

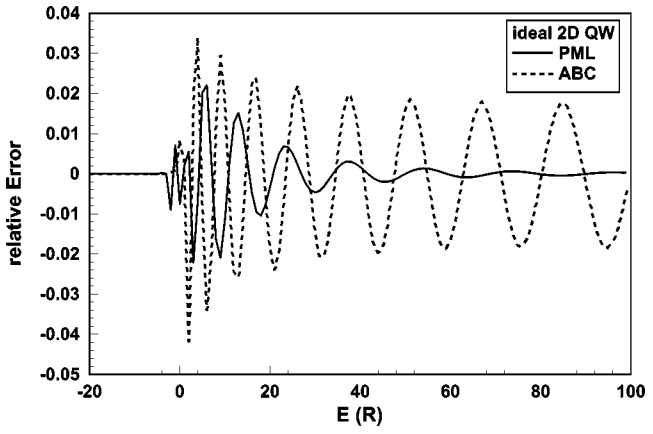

FIG. 3. Relative error of the solution including PML or ABC to exact solution.

Franz-Keldysh absorption. Using the PML, the optical absorption α of an arbitrary semiconductor structure can be calculated. It has been shown[2] that Eq. (1) can be used to calculate the optical properties of coupled quantum wells and superlattices. It is possible to calculate both type I and type II structures. Due to a great reduction in computation time using the PML boundary condition it is even possible to calculate the continuum absorption and to describe the absorption of very flat quantum wells whose absorption is close to a continuum. For example, the free particle absorption of $Ga_{0.202}In_{0.798}As_{0.446}P_{0.554}$ is calculated for room temperature which is modeled by a dephasing rate of $\hbar\Gamma = 10$ meV. In Fig. 4 the Coulomb enhanced Franz-Keldysh absorption is shown for different applied voltages. The Coulomb effect results in an enhanced absorption and a red shift. Due to the lack of a field dependent shift, all graphs pass through a single point. This typical feature of the Franz-Keldysh effect can be seen from measurements of practical devices used in optical communication systems. Because this model describes both the quantum confined stark effect (QCSE) and the Franz-Keldysh absorption, it will be of great practical interest, especially for the calculation of the modulator chirp which depends on transitions above the band gap.

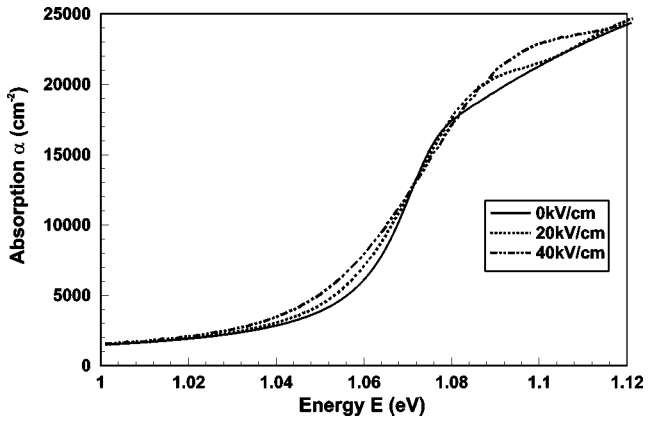

FIG. 4. Franz-Keldysh absorption.

We have presented an absorbing boundary condition for the Schrödinger equation which shows a very good performance and is local both in time and space. It can easily be implemented within FE and FD methods. Due to the substantial saving of computer resources, the direct calculation of the optical absorption is now possible for realistic structures and effects like the Coulomb enhanced Franz-Keldysh effect can be investigated for semiconductor heterostructures. The PML concept should also result in substantial computational savings for nonlinear problems.[15]

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