Efficient Calculation of Quasi-bound States for the Simulation of Direct Tunneling

Markus Karner, A. Gehring, S. Holzer, and H. Kosina

Institute for Microelectronics, TU Vienna,
Gußhausstraße 27–29, A-1040 Wien, Austria
Karner@iue.tuwien.ac.at

Abstract. We study the calculation of quasi-bound states (QBS) in MOS inversion layers, which represent the major source of tunneling electrons. The calculation of QBS is performed by the perfectly matched layer (PML) method. Introducing a complex coordinate stretching enables us to apply artifical absorbing layers at the boundaries. This allows us to determine the QBS as the eigenvalues of a linear non-Hermitian Hamiltonian where the QBS lifetimes are directly related to the imaginary part of the eigenvalues. The PML formalism has been compared to other established methods and it has proven to be as an elegant, numerically stable, and efficient method to calculate QBS lifetimes.

1 Introduction

The continuous progress in the development of MOS field-effect transistors within the last years goes hand in hand with down-scaling the device feature size and therefore, they feature gate oxide thicknesses below two nanometers. Thus, quantum mechanical tunneling has significant effects on the characteristics of state-of-the-art electrical devices. The major source of tunneling electrons in the inversion layers of MOS-structures is due to quasi-bound states (QBS) [4, 1]. Since QBS in the potential well have a finite lifetime, they give rise to a quantum mechanical tunneling current out of the well into the oxide. The contribution of the QBS to the tunneling current is given by

$$J_{\mathrm{2D}} = \frac{\mathrm{k_B}T\mathrm{q}}{\pi\hbar^2} \sum_{i,\nu} \frac{g_\nu m_\parallel}{\tau_\nu(\mathcal{E}_{\nu,i}(m_\mathrm{q}))} \ln\left(1 + \exp\left(\frac{\mathcal{E}_\mathrm{F} - \mathcal{E}_{\nu,i}}{\mathrm{k_B}T}\right)\right) \tag{1}$$

where $\mathcal{E}_\mathrm{F}$ denotes the Fermi level, g_ν the valley degeneracy, $m_\parallel$ the parallel mass, m_q the quantization masses, and $\tau_\nu(\mathcal{E}_{\nu,i})$ the lifetime of the quasi-bound state $\mathcal{E}_{\nu,i}$. For the calculation of direct tunneling in silicon MOS structures, assuming [100] orientation, (1) have to be evaluated two times using $g_\nu = 2$, $m_\parallel = m_\mathrm{t}$, $m_\mathrm{q} = m_\mathrm{l}$, and $g_\nu = 4$, $m_\parallel = \sqrt{m_\mathrm{l} m_\mathrm{t}}$, $m_\mathrm{q} = m_\mathrm{t}$.

Hence, the calculation of direct tunneling currents is based on the accurate determination of the QBS. Several approaches have been established for the calculation of the lifetime broadening of QBS but there are still no generally accepted and efficient algorithms. Within this work, a semi-classical approximation as well as a method based on scanning the derivative of the reflection

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coefficient are compared with a new method based on the perfectly matched layer formalism.

2 Calculation of Quasi-bound States

The potential well used for the further considerations was acquired from a self-consistent quantum-mechanical Schrödinger-Poisson solver. The calculation has been performed for an n-MOS structure with a poly gate doping of N_{D}=1 × $10^{18}\mathrm{cm}^{-3}$ and a substrate doping of N_{A}=1 × $10^{17}\mathrm{cm}^{-3}$ at a gate bias of 1.5 V resulting in a potential well as displayed in Fig. 1.

The calculation of tunneling currents is based on the accurate determination of the QBS which are obtained from the time-independent effective mass Schrödinger equation:

$$-\frac{\hbar^2}{2}\nabla\cdot\left(\tilde{m}^{-1}\nabla\Psi(\mathbf{x})\right)+V(\mathbf{x})\Psi(\mathbf{x})=\mathcal{E}\Psi(\mathbf{x})\,. \tag{2}$$

Here, $V(x)$ denotes the potential energy, and $\tilde{m}^{-1}$ denotes the inverse effective mass tensor. For the simulation of silicon within the effective mass approximation, two different quantization masses occur, and therefore (2) has to be solved twice. Note that three different valley sorts occur, but for one-dimensional simulations two of them have the same quantization mass. Then, the QBS are determined as the eigenstates of the Hamiltonian. The QBS lifetimes are directly related to the imaginary parts of the eigenvalues: $\tau_i = \hbar/2\mathcal{E}_i$. Assuming closed boundaries, we obtain a linear Hermitian eigenvalue problem. Some of the eigenstates are displayed in Fig. 1. Since the wavefunction of a closed quantum system does not carry current, open boundary conditions have to be applied for an accurate description of tunneling electrons.

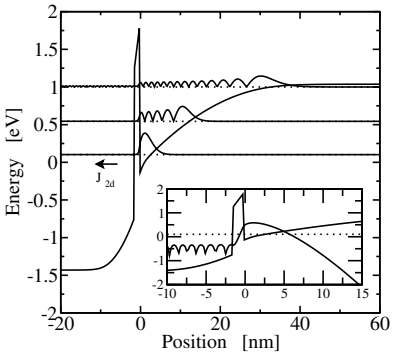

Fig. 1. The potential well that arises at an nMOS inversion layer and its eigenstates assuming closed boundary conditions. The inset displays the wavefunction of the first QBS at a logarithmic scale.

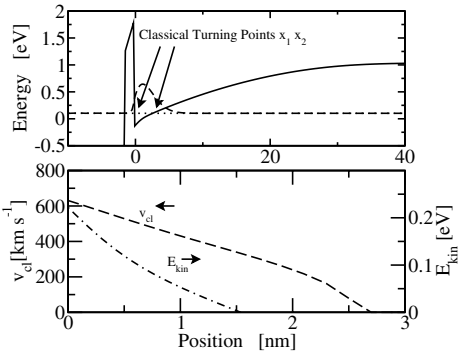

Fig. 2. The energy level and the classical turning points x_1, x_2 of the first eigenstate. In the lower figure, the kinetic energy and the velocity (assuming classical behavior of the particles) are displayed.

2.1 Semiclassical Approximation

However, it has been found that in practice the closed boundary eigenvalues are close to the eigenvalues of the open system [4]. This allows us to take the closed boundary eigenvalues, and determine a particle velocity [2] for each eigenstate under the assumption of classical behavior of the particle as displayed in Fig. 2. This implies that the electrons are bouncing between two classical turning points x_1 and x_2. At the oxide, the electrons are partially reflected according the transmission coefficient of the barrier. This gives rise to an exponential decay in time. For the i$^{\text{th}}$ QBS, the classical velocity $v_{\text{cl},i}$ and the QBS lifetimes τ_i follow

$$v_{\text{cl},i}(x) = \sqrt{\frac{\mathcal{E}_i - V(x)}{m(x)}} \qquad (3) \qquad \tau_i = \frac{1}{TC(\mathcal{E}_i)} \int_{x_1,i}^{x_2,i} \frac{\mathrm{d}x}{v_{\text{cl},i}(x)} \qquad (4)$$

where the transmission coefficient $TC(\mathcal{E}_i)$ can be determined using the quantum transmitting boundary method (QTBM) or a WKB approximation.

2.2 The QTB Method

A more rigorous way to determine the energetic position and the lifetime broadening of the QBS is the quantum-transmitting boundary method (QTBM) [3] where a scanning of the transmission coefficient yields the lifetimes. Since the transmission coefficient is zero for half open system, it has been shown [5], that the phase of the reflection coefficient $\phi(\mathcal{E})$, defined as $\mathrm{RC}(\mathcal{E}) = \exp(\imath\phi(\mathcal{E}))$, follows $\phi(\mathcal{E}) \approx c + 2\arctan(\Gamma/2(\mathcal{E} - \mathcal{E}_i))$ near to the resonances and therefore its derivative has Lorentzian form

$$\frac{\partial\phi}{\partial\mathcal{E}} = \frac{\Gamma}{(\mathcal{E} - \mathcal{E}_i)^2 + \Gamma^2/4} \quad . \qquad (5)$$

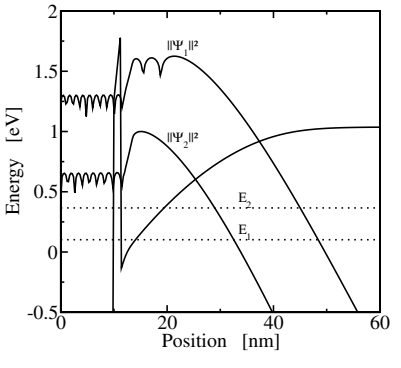

Fig. 3. The potential well and the energy levels of the first and third resonance which represent QBS, calculated with the QTB method. The wavefunctions at the resonances are displayed in a logarithmic scale.

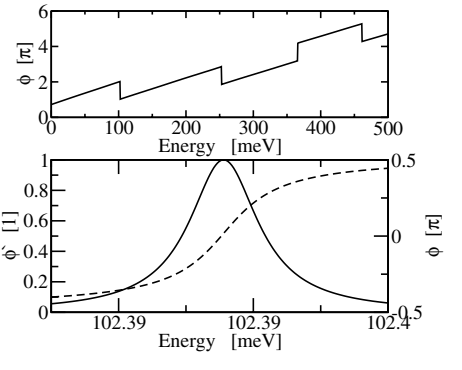

Fig. 4. The upper plot shows the phase of the reflection coefficient as a function of the electron energy. The second plot zooms in the first resonance peak and displays the phase and the derivative of the phase coefficient.

This is shown in Fig. 4. However, for the energy barriers of MOS capacitors, energy resolutions in the peV regime are necessary to accurately resolve the full-width half maximum (FWHM) value, which is required to calculate the QBS lifetime: $\tau_i = \hbar/\mathrm{FWHM}_i$.

2.3 The PML Method

Within this work, a novel method to determine QBS, proposed in [6] is applied, using the perfectly matched layers formalism which is often used in electromagnetic theory. The idea is to add non-physical absorbing layers at the boundary of the simulation region (physical region). This procedure prevents reflection at the boundary of the physical region.

The newly introduced artifical absorbing layers allow application of Dirichlet boundary conditions, and the QBS are determined by the eigenvalues of the non-Hermitian, but linear Hamiltonian of the system. Some of the resulting eigenenergies and the corresponding wavefunctions are displayed in Fig. 5. The absorbing property of the PML region is achieved by introducing stretched coordinates in (2). The evaluation of the ∇ in one dimension yields:

$$\tilde{x} = \int_0^x s_x(\tau)\,\mathrm{d}\tau \qquad (6) \qquad\qquad \frac{\partial}{\partial \tilde{x}} = \frac{1}{s_x(x)}\frac{\partial}{\partial x} \qquad (7)$$

Within the PML region, the stretching function $s_x(x)$ is given as $s_x(x) = 1+(\alpha+\imath\beta)x^n$, with $\alpha = 1$, $\beta = 1.4$, and $n = 2$, while it is unity in the physical region as displayed in Fig. 6. Assuming a constant potential $V(z)$ within the PML regions, the wavefunctions can be written as a plane wave $\Psi(x) = \Psi_0 \exp(\imath\tilde{k_x}x)$ with the wave vector $\tilde{k_x} = k_x/s_x$. Considering two points in the PML region x_1, $x_2 = x_1 + \mathrm{d}x$ the wave vector at the point x_2 can be approximated as

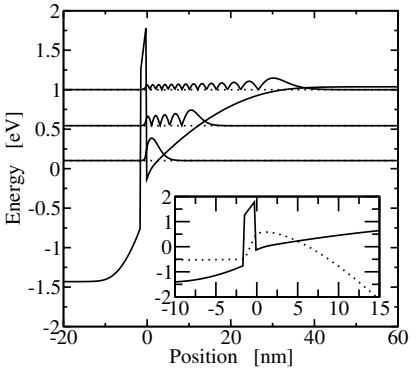

Fig. 5. The potential barrier and its eigenstates assuming open boundary conditions using the PML technique. The inset shows the wavefunction of the first QBS at logarithmic scale.

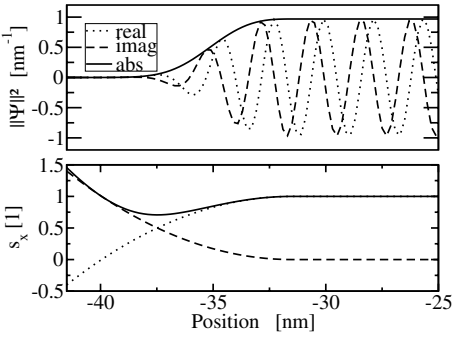

Fig. 6. The wavefunction of the first QBS and the complex stretching function are displayed in the perfectly matched layer region as well as its transition to the physical region

$$k_x(x_2) \approx \frac{s_x(x_2)}{s_x(x_1)} k_x(x_1) = (1 + (\alpha + \imath\beta)\,\mathrm{d}x) \quad . \tag{8}$$

The parameter α scales the phase velocity of the plane wave, while β acts as a damping parameter. Since this damping coefficient is greater than zero within the absorbing region the envelope of the wavefunctions is pinned to zero as shown in Fig. 6. These parameters, as well as the thickness of the absorbing layer can be varied over a wide range with virtual no influence on the results.

However, using QTBM or assuming closed boundary conditions yields a superposition of two moving plane waves in opposite directions. This can be seen as an envelope of the resulting wavefunctions displayed in the insets of Fig. 1 and Fig. 3. In contrast, using PML techniques yields no reflected wave into the well, and therefore the wavefunction is a plane traveling wave with constant envelope function as displayed in Fig. 5. The QBS, however, are reproduced correctly.

3 Results and Conclusions

Three methods for determining energetic positions and the lifetime broadening of QBS have been presented. The results are compared in Table 1. For the semiclassical method, it is still necessary to solve the closed system in order to get the eigenenergies of the well. Using closed eigenvalues together with the assumption of a classical velocity might result in inaccurate lifetimes. This is also true for the QTBM method since good initial values are needed in order to find the resonances. However, there is a perfect agreement with eigenvalues obtained from PML techniques. The PML formalism yields the desired eigenvalues in a natural way without any additional assumptions. Solving the eigenvalue problem directly yields the energetic positions and the lifetime of the QBS. Although the dimension of the system increases due to the additional points in the PML region, the computational effort of the PML has shown to be lower compared to QTBM as shown in Fig. 7. Thus, the PML formalism represents an efficient, and numerically stable method to determine QBS which is appropriate for integration in a device simulator for the investigation of direct tunneling phenomena.

Table 1. The resulting energy levels and lifetimes of the QBS for the semiclassical approximation, QTB method, and PML technique

Classical	E_{real} [meV]	τ_l [ns]
1	102.3	57.10
2	252.5	40.34
3	360.0	35.78

QTBM	E_{real} [meV]	FWHM [eV]	τ_l [ns]
1	102.3	1.245×10^{-6}	52.8
2	252.5	1.428×10^{-6}	46.0
3	365.9	1.735×10^{-6}	37.9

PML	E_{real} [meV]	E_{imag} [eV]	τ_l [ns]
1	102.3	-6.14×10^{-7}	53.5
2	252.5	-7.12×10^{-7}	46.2
3	365.9	-8.83×10^{-7}	37.2

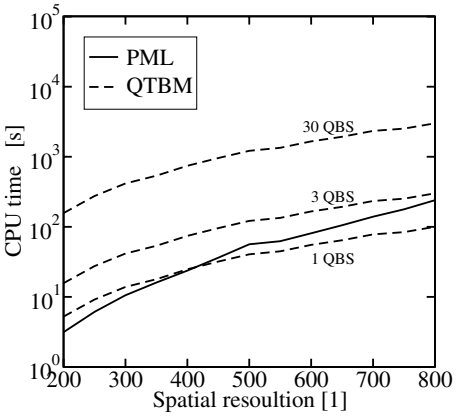

Fig. 7. Comparison of the CPU demand for the PML, and QTB methods with a given set of QBS

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