On the Efficient Calculation of Quasi-Bound States for the Simulation of Direct Tunneling

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Quantum mechanical tunneling has significant affects on the characteristics of state of the art electrical devices. The major source of tunneling electrons in resonant-tunneling diodes (RTDs) and in the inversion layers of MOS-structures represent quasi-bounds states (QBS). The contribution of each QBS to the tunneling current follows

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

where g_ν denotes the valley degeneracy, $m_\parallel$ the parallel mass, and m_q the quantization masses, and $\tau_\nu(\mathcal{E}_{\nu,i})$ is the lifetime of the quasi-bound state $\mathcal{E}_{\nu,i}$. Thus, the calculation of tunneling currents is based on the accurate determination of the QBS which follows from the SCHRÖDINGER equation:

$$-\frac{\hbar^2}{2} \nabla \cdot (\tilde{m}^* \nabla \Psi(\mathbf{x})) + V(\mathbf{x}) \Psi(\mathbf{x}) = E \Psi(\mathbf{x}) \; . \tag{2}$$

Since the wavefunction of a closed quantum system cannot carry any current open boundary conditions have to be applied for an accurate description of tunneling electrons. Then, the QBS are determined by the eigenstates of the Hamiltonian. The QBS lifetimes are related to the imaginary parts of the eigenvalues: $\tau_i = \hbar/2\mathcal{E}_i$.

A widely used method to introduce open boundaries for (2) is the quantum-transmitting boundary method (QTBM) where the Hamiltonian becomes non-Hermitian and non-linear. The energetic position and the lifetime broadening of the QBS follows from an scanning of the derivative of the phase of the reflection coefficient or the reflection coefficient itself. However, these method's are hardly applicable to the energy barriers of MOS capacitors because energy resolutions in the peV regime would be necessary to accurately resolve the full-width half maximum (FWHM) value, which is necessary to calculate the QBS lifetime: $\tau_i = \hbar/\mathrm{FWHM}_i$.

Within this work, the determination of QBS is performed by 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 in order to avoid the influence to the wavefunction in the physical region. This is achieved by introducing the stretched coordinate $\tilde{x} = \int_0^x s_x(\tau)\,\mathrm{d}\tau$ which leads to $\partial/\partial\tilde{x} = 1/s_x(x)\partial/\partial x$. 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. These artifical absorbing layers enable us to apply Dirichlet boundary conditions and the QBS are determined by the eigenvalues of the non-Hermitian, but still linear Hamiltonian of the system. 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. The PML formalism has been proven as an elegant, efficient, and numerical stable method to determine QBS.