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An improved transient algorithm for resonant tunneling

N. Ben Abdallah*, A. Faraj†

Abstract

The simulation of the time dependent evolution of the resonant tunneling diode is done by a multiscale algorithm exploiting the existence of resonant states. After revisiting and improving the algorithm developed in [N. Ben Abdallah, O. Pinaud, J. Comp. Phys. 213 (2006) 288-310] for the stationary case, the time dependent problem is dealt with. The existence of two resonances corresponding to the initial potential and to the local time potential lead to the decomposition of the wave function into a non resonant part and two resonant ones. The resonant parts are dealt with by a projection method. The simulation times are shown to be reduced by a factor two.

Keywords: Schrödinger equation; numerical scheme; resonant tunneling diode; resonant states; time dependent.

Subject classifications: 35Q41, 35Q55, 65M99, 65P99, 65Z05, 81-08, 81V99

1 Introduction

We are interested in the simulation of open resonant systems, typically the resonant tunneling diode. Because of the small size of these devices, quantum effects are observed and the Schrödinger equation is required for the modeling. Classical observables like electronic and current densities are given by integrals on the energy involving generalized eigenfunctions. The resonant tunneling diode presents resonances and the variation of generalized eigenfunctions tends to be singular in the vicinity of resonant energies. Therefore, to compute correctly the densities, the integral on the energy variable needs a refined mesh next to these resonances and a big number of Schrödinger equations needs to be solved. Adaptive refinement was developed in [16] in the stationary regime for a resonant tunneling diode. The method does however not extend to the transient case since the resonant energies do move as time varies. Lately, inspired by an idea for the transient case from [17], an algorithm was proposed by [5] for the discretization of the stationary case. The method consists in decomposing the wave function in a part living in the well between the double barrier and a second part which is mostly localized outside this well. The latter is called the non resonant part and the former is the resonant one. The non resonant part is smooth with respect to the energy variable and only requires a coarse energy mesh. At variance, the resonant part has sharp peaks at resonant energies. It is computed by a projection method after a precomputation of resonant states. In the present work, we first present an improvement of [5], the resonance being computed more precisely by solving the non-linear eigenvalue problem verified by the resonance and written in [14]. Then we present a transient algorithm inspired by the idea of [17]. More precisely, the algorithm consists in the computation of the resonance at each time step, the resonant information is therefore captured and the frequency mesh can be chosen coarse enough thus reducing the simulation time. The resonant part of the wave function has two components, one which corresponds to the dissipation of the initial resonance and one which is proportional to the resonant mode. Let us mention that in [5], a new finite element method using the WKB approximation was developed to reduce the numerical cost (see also [3, 13]). Since we want to

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concentrate on the energy discretization we will use a standard finite difference method for the space discretization.

2 The model

The considered device is assumed to occupy the domain $[0, L]$, $L > 0$. The model consists in an infinite number of Schrödinger equations coupled to the Poisson equation. The Schrödinger equation involves the time dependent Hamiltonian

$$H(t) = -\frac{\hbar^2}{2m}\partial_x^2 + U(t) + V(t),$$

where \hbar is the reduced Planck constant, m is the effective mass of the electron and $x \in \mathbb{R}$ is the position variable.

The external potential $U(t) = V_0 + \mathcal{B}(t)$ is given as if a data of the problem where

$$V_0 = v_0 \mathbf{1}_{[a_2, b_2]} + W,$$

the well W is given by

$$W = -v_0 \mathbf{1}_{[a_3, b_3]},$$

and the applied bias by

$$\mathcal{B}(t) = -B(t) \left(\frac{x - a_1}{b_1 - a_1} \mathbf{1}_{[a_1, b_1[} + \mathbf{1}_{[b_1, +\infty[} \right),$$

with $v_0 \geq 0$ and $B(t) \geq 0$ scalars representing respectively the height of the barrier and the amplitude of the applied bias in eV , and we have:

$$0 < a_1 < a_2 < a_3 < b_3 < b_2 < b_1 < L.$$

The points a_1 and b_1 are the extremities of the diode.

Such a potential $U(t)$ is represented in Figure 1.

The nonlinear potential $V(t)$ is due to Coulomb interaction and satisfies the Poisson equation:

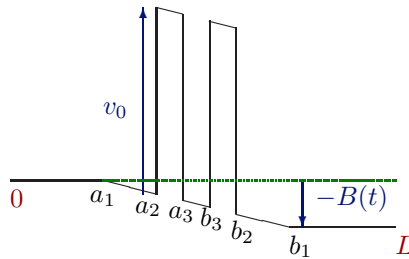


Figure 1: External potential $U(t)$.

$$\begin{cases} -\partial_x^2 V = \frac{q^2}{\varepsilon} (n[V] - n_D), & (0, L) \\ V(0) = V(L) = 0, \end{cases} \quad (2.1)$$

where q is the elementary charge of the electron, ε is the dielectric constant, n_D is the doping equal to

$$n_D = n_D^1 (\mathbf{1}_{[0, a_1[} + \mathbf{1}_{[b_1, L]}) + n_D^2 \mathbf{1}_{[a_1, b_1]},$$

with $n_D^1 > n_D^2 \geq 0$, and the electron density $n[V]$ is given by:

$$n[V](x) = \int_{\mathbb{R}} g(k) |\Phi_k(x)|^2 dk, \quad x \in [0, L], \quad (2.2)$$

in the stationary regime and

$$n[V](t, x) = \int_{\mathbb{R}} g(k) |\Psi_k(t, x)|^2 dk, \quad x \in [0, L], \quad (2.3)$$

in the time dependent regime. Here g is the injection profile and the Φ_k , resp. the $\Psi_k(t)$, are the wave functions corresponding to the Hamiltonian $H(0)$, resp. $H(t)$, for a wave vector $k \in \mathbb{R}$. We will choose the function g to be the one dimensional Fermi-Dirac integral :

$$g(k) = \frac{mk_B T}{2\pi^2 \hbar^2} \ln \left(1 + \exp \left(\frac{E_F - \frac{\hbar^2 k^2}{2m}}{k_B T} \right) \right),$$

where k_B is the Boltzmann constant, T is the temperature of the semiconductor and E_F is the Fermi level.

In the stationary case, for a given initial bias $B_I = B(0)$, we will note $U_I = U(0)$ the corresponding initial exterior potential and V_I a corresponding solution to (2.1)(2.2), then, the wave functions are the restriction to $[0, L]$ of the solutions to the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Phi_k + (U_I + V_I) \Phi_k = E_k \Phi_k, \quad x \in \mathbb{R}, \quad (2.4)$$

with scattering conditions

$$\begin{cases} \Phi_k(x) = e^{ikx} + r(k)e^{-ikx}, & x < 0 \\ \Phi_k(x) = t(k)e^{i\sqrt{k^2 + 2mB_I/\hbar^2}x}, & x > L, \end{cases} \quad \text{for } k \geq 0$$

and

$$\begin{cases} \Phi_k(x) = t(k)e^{-i\sqrt{k^2 - 2mB_I/\hbar^2}x}, & x < 0 \\ \Phi_k(x) = e^{ikx} + r(k)e^{-ikx}, & x > L, \end{cases} \quad \text{for } k < 0,$$

where

$$E_k = \begin{cases} \frac{\hbar^2 k^2}{2m}, & k \geq 0 \\ \frac{\hbar^2 k^2}{2m} - B_I, & k < 0. \end{cases} \quad (2.5)$$

In the transient case, the wave functions are the restriction to $[0, L]$ of the solutions to the time-dependent Schrödinger equation

$$\begin{cases} i\hbar \partial_t \Psi_k(t) = -\frac{\hbar^2}{2m} \partial_x^2 \Psi_k(t) + (U(t) + V(t)) \Psi_k(t), & x \in \mathbb{R} \\ \Psi_k(0) = \Phi_k, \end{cases} \quad (2.6)$$

where $V(0) = V_I$.

3 The stationary algorithm revisited

3.1 Recalling the standard algorithm

To solve the stationary non-linear Schrödinger-Poisson system (2.1)(2.2)(2.4), we will use the same algorithm as in [16]. It is based on a Gummel iteration, see [11], which consists in the computation of a sequence V_I^l , $l \geq 0$ where the potential V_I^{l+1} at step $l+1$ is deduced from the potential V_I^l at step l by solving the following non-linear equation:

$$\begin{cases} -\frac{d^2}{dx^2} V_I^{l+1} = \frac{q^2}{\epsilon} (n[V_I^l] \exp((V_I^l - V_I^{l+1})/V_{ref}) - n_D), & (0, L) \\ V_I^{l+1}(0) = V_I^{l+1}(L) = 0, \end{cases} \quad (3.1)$$

for a fixed reference potential V_{ref} .

The repartition function g being exponentially decreasing at infinity, the integral in (2.2) can be restricted, in computations, to a domain $[-k_M, k_M]$ where k_M is chosen to be big enough. We consider a uniform discretization $x_0 = 0, x_1, \dots, x_j, \dots, x_J = L$ of the interval $(0, L)$ with fixed mesh size Δx and a (non-necessarily uniform) discretization $k_0 = -k_M, k_1, \dots, k_p, \dots, k_P = k_M$ of the interval $[-k_M, k_M]$. Then, for a given initial potential V_I^0 , the algorithm writes:

Algorithm 3.1 (Gummel algorithm).

Fix $l = 0$.

Do While $\|V_I^{l+1} - V_I^l\|_2 \geq \varepsilon$:

Computation of the density

S1. For $p = 0, \dots, P$: computation of Φ_p^l wave function corresponding to the potential V_I^l and the frequency k_p .

S2. Numerical integration: for $j = 0, \dots, J$

$$n_j^l = \sum_{p=0}^{P-1} I_{p,j}^l, \quad \text{where} \quad I_{p,j}^l = \int_{k_p}^{k_{p+1}} g(k) \left| (\Phi_k^l)_j \right|^2 dk.$$

Coupling to the Poisson equation : Gummel iteration

Computation of the potential V_I^{l+1} from the potential V_I^l and the density n^l by solving equation (3.1).

Set $l = l + 1$.

End Do.

The equation (3.1) is nonlinear and it is solved using a Newton method where the Laplacian is discretized with finite differences.

Because of the peaked form of the transmission near resonances, the method used to compute the density $n[V_I^l]$ from the potential V_I^l (steps *S1* and *S2*) is of major importance, and the Gummel algorithm may fail to converge if a non accurate method is used.

In [16], the steps *S1* and *S2* are performed without particular treatment of resonances: the wave functions are computed on $[0, L]$ solving the Schrödinger equation with transparent boundary conditions and the integrals $I_{p,j}^l$ are computed with a trapezoidal rule. In that case, the convergence is provided by the choice of the frequency mesh $\{k_p, p = 0, \dots, P\}$: the mesh size $k_{p+1} - k_p$ is refined when a resonance peak is detected. As said in the introduction, this forces to solve a big number of Schrödinger equations and increases the numerical cost. However, this process, that we will call Direct Resolution, gives good results and will be used to evaluate the performance of the One Mode Approximation algorithm presented in what follows.

As proposed in [5], the One Mode Approximation consists in decomposing the wave function in a non-resonant part and a resonant part proportional to the first resonant mode. In [5], using a WKB interpolation to compute each part of the wave function, an adapted treatment of the step *S1* is realized and the convergence of the Gummel method is possible.

In the present work, we do not use the WKB interpolation, however the accuracy required at step *S1* is reached by an improvement of the computation of the first resonance. In particular, a precise computation of its imaginary part is essential. A simple reconstitution of the wave functions not allowing to modify the frequency mesh, we obtain convergence with a large frequency mesh by adapting the step *S2* such that all the resonant information is taken into account. It is done by an explicit integration of the coefficient of proportionality with the resonant mode instead of the trapezoidal rule.

3.2 Accurate computation of resonances

In the founder work [1], see also [12], resonances of a sel-adjoint operator are defined using analytic transformations, and it is a common fact that it correspond to an eigenvalue in a modified L^2 space [9]. Using the second approach, it is shown in [8] and [14] that the resonances of the Hamiltonian:

$$-\frac{\hbar^2}{2m}\partial_x^2 + Q,$$

where the potential Q verifies:

$$Q(x) = 0, x \leq 0, \quad \text{and} \quad Q(x) = Q_L, x \geq L,$$

are the complex values z such that $\exists u \in H^2(0, L)$ verifying $\|u\|_{L^2(0, L)} = 1$ and:

$$\begin{cases} [-\frac{\hbar^2}{2m}\partial_x^2 + Q]u = zu, & (0, L), \\ \frac{\hbar}{\sqrt{2m}}u'(0) + is(z)u(0) = 0, \\ \frac{\hbar}{\sqrt{2m}}u'(L) - is(z + Q_L)u(L) = 0. \end{cases} \quad (3.2)$$

Here $s(z)$ denotes the determination of the square root which is holomorphic on $\mathbb{C} \setminus i\mathbb{R}_-$ and defined as follows: for $z = \rho e^{i\theta}$, with $\rho > 0$ and $\theta \in (-\frac{\pi}{2}, \frac{3\pi}{2})$, $s(z) = \sqrt{\rho}e^{i\frac{\theta}{2}}$. This determination is different from the one used in [5] and leads to a convergent Newton algorithm as will be illustrated herebelow. In [5], the computation of the resonance is done by an iterative method which converges slowly. The homogeneous transparent boundary conditions in the problem above give a restriction of the eigenproblem for the resonant mode to the domain $(0, L)$ and allows to make numerical computations. In particular, we introduce a variational formulation for problem (3.2) including the boundary conditions such that the discretization leads to a non-linear eigenvalue problem solved with a Newton-like algorithm.

Multiplying the first equation in (3.2) by the conjugate of a function $v \in H^1(0, L)$ and integrating by part, we get the following equation on the resonant mode:

$$\begin{aligned} \frac{\hbar^2}{2m} \int_0^L u' \bar{v}' dx + \int_0^L Q u \bar{v} dx - i \frac{\hbar}{\sqrt{2m}} [s(z)(u\bar{v})(0) + s(z + Q_L)(u\bar{v})(L)] \\ - z \int_0^L u \bar{v} dx = 0, \end{aligned}$$

where the boundary conditions were considered. The discretization is performed using a finite element method with P^1 function basis: p_j , $j = 0, \dots, J$ defined by $p_j(x_{j'}) = \delta_{jj'}$. This leads to the following problem: find $(\mathbf{u}, \mathbf{z}) \in \mathbb{C}^{J+1} \times \mathbb{C}$ such that:

$$\begin{cases} M(\mathbf{z})\mathbf{u} = 0 \\ \mathbf{u}^H \mathbf{u} = 1, \end{cases} \quad (3.3)$$

where $M(z)$ is a non-linear matrix valued function of z defined by:

$$M(z) = M_1 + s(z)M_2 + s(z + Q_L)M_3 - zM_4,$$

and the matrices $M_1, \dots, M_4 \in \mathcal{M}_{J+1}(\mathbb{C})$ are given in Appendix A. This kind of problem was studied in [15] and [10]. The term $\mathbf{u}^H \mathbf{u}$ appearing in problem (3.3) is not differentiable with respect to \mathbf{u} , therefore a Newton method must be modified to be used here. Following [15], for a given iterate $(\mathbf{u}^n, \mathbf{z}^n)$ verifying $(\mathbf{u}^n)^H \mathbf{u}^n = 1$, we are looking for a direction $(\delta \mathbf{u}^n, \delta \mathbf{z}^n)$ such that $(\mathbf{u}^n + \delta \mathbf{u}^n, \mathbf{z}^n + \delta \mathbf{z}^n)$ is solution to problem (3.3). Using $(\mathbf{u}^n)^H \mathbf{u}^n = 1$ the system:

$$\begin{cases} M(\mathbf{z}^n + \delta \mathbf{z}^n)(\mathbf{u}^n + \delta \mathbf{u}^n) = 0 \\ (\mathbf{u}^n + \delta \mathbf{u}^n)^H (\mathbf{u}^n + \delta \mathbf{u}^n) = 1 \end{cases}$$

gives at order 2:

$$\begin{aligned} M(\mathbf{z}^n)\delta\mathbf{u}^n + \delta\mathbf{z}^n M'(\mathbf{z}^n)\mathbf{u}^n &= -M(\mathbf{z}^n)\mathbf{u}^n, \\ (\mathbf{u}^n)^H \delta\mathbf{u}^n + (\delta\mathbf{u}^n)^H \mathbf{u}^n &= 0. \end{aligned} \quad (3.4)$$

As remarked earlier, there is a problem with the second equation, however, it is enough to impose $(\mathbf{u}^n)^H \delta\mathbf{u}^n = 0$ in order to verify (3.4). Therefore, we obtain the following linear system:

$$\begin{bmatrix} M(\mathbf{z}^n) & M'(\mathbf{z}^n)\mathbf{u}^n \\ (\mathbf{u}^n)^H & 0 \end{bmatrix} \begin{bmatrix} \delta\mathbf{u}^n \\ \delta\mathbf{z}^n \end{bmatrix} = \begin{bmatrix} -r^n \\ 0 \end{bmatrix}, \quad \text{where } r^n = M(\mathbf{z}^n)\mathbf{u}^n. \quad (3.5)$$

Its resolution corresponds to an iteration of our Newton-like method to compute the resonant mode. The assumption $(\mathbf{u}^n)^H \mathbf{u}^n = 1$ that we made to obtain this system is verified at order 2 as long as $(\mathbf{u}^0)^H \mathbf{u}^0 = 1$.

3.3 The One Mode Approximation

We start with the description of the step *S1*, in the One Mode Approximation, of the computation of a wave function Φ_k solution to the stationary Schrödinger equation (2.4) for a given frequency k . Following the works [5] and [17], the One Mode Approximation consists in the decomposition:

$$\Phi_k = \Phi_k^{nr} + \Phi_k^r,$$

where the non-resonant part Φ_k^{nr} solves the stationary Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_{I,fill} + V_I\right] \Phi_k^{nr} = E_k \Phi_k^{nr}, \quad x \in \mathbb{R}, \quad (3.6)$$

with filled potential $U_{I,fill} = U_I + v_0 \mathbf{1}_{[a_3, b_3]}$, and where we omit the indice l appearing in Algorithm 3.1 to simplify notations. The function Φ_k^{nr} is computed on $[0, L]$ by the resolution of (3.6) with the exact transparent boundary conditions:

$$\begin{cases} (\Phi_k^{nr})'(0) + ik\Phi_k^{nr}(0) = 2ik, \\ (\Phi_k^{nr})'(L) - i\sqrt{k^2 + 2mB_I/\hbar^2}\Phi_k^{nr}(L) = 0, \end{cases}$$

for $k \geq 0$, and:

$$\begin{cases} (\Phi_k^{nr})'(0) + i\sqrt{k^2 - 2mB_I/\hbar^2}\Phi_k^{nr}(0) = 0, \\ (\Phi_k^{nr})'(L) + ik\Phi_k^{nr}(L) = 2ike^{ikL}, \end{cases}$$

for $k < 0$. This resolution is performed with a RK4 method as it is done to compute Φ_k in the Direct Resolution, see [16]. The statistic g being fastly decreasing at infinity, the resonant part Φ_k^r is searched, on $(0, L)$, proportional to the resonant mode u_I of minimal resonant energy $\text{Re}(z_I)$ where $[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_I + V_I]u_I = z_I u_I$ and $\int_0^L |u_I(x)|^2 dx = 1$. In other words, we look for Φ_k^r of the form:

$$\Phi_k^r(x) = \theta_k u_I(x), \quad x \in (0, L).$$

Like in [5], the condition that Φ_k verifies the stationary Schrödinger equation (2.4) gives the following explicit value of the proportionality coefficient:

$$\theta_k = \frac{1}{z_I - E_k} v_0 \int_{a_3}^{b_3} \Phi_k^{nr} \overline{u_I} dx. \quad (3.7)$$

The resonance and the resonant mode are computed using the method presented in section 3.2 with the potential $Q = U_I + V_I$. The method is initialized at the fundamental energy and fundamental mode of the Hamiltonian

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_I + V_I\right] \quad (3.8)$$

equipped with homogeneous Dirichlet boundary conditions at a_2 and b_2 . It's shown in [6][7] that the real part of resonances are well approached by the eigenvalues of the Dirichlet Hamiltonian (3.8). The imaginary part of resonances being small, such an initialization guaranties that the algorithm converges to the resonance with smaller energy. This achieves the step $S1$. For the step $S2$, the peaked form (3.7) of the coefficient of proportionality with the resonant mode is used in the computation of the intregal:

$$I_{p,j} = \int_{k_p}^{k_{p+1}} g(k) \left| (\Phi_k)_j \right|^2 dk.$$

Using an argument of localisation of support, see [17], the cross term in the development of $\left| (\Phi_k^{nr} + \theta_k u_I)_j \right|^2$ can be neglected, which gives the approximation:

$$I_{p,j} = \int_{k_p}^{k_{p+1}} g(k) \left| (\Phi_k^{nr})_j \right|^2 dk + \int_{k_p}^{k_{p+1}} g(k) |\theta_k|^2 dk |(u_I)_j|^2.$$

The non resonant part being regular with respect to k , the first integral can be computed with a simple trapezoidal rule. The keypoint is then the approximation of $J_p := \int_{k_p}^{k_{p+1}} g(k) |\theta_k|^2 dk$. Using (3.7), we have:

$$J_p = \int_{k_p}^{k_{p+1}} R_k \frac{1}{|E_k - z_I|^2} dk,$$

where

$$R_k = g(k) v_0^2 \left| \int_{a_3}^{b_3} \Phi_k^{nr} \overline{u_I} dx \right|^2.$$

The wave function Φ_k^{nr} has no resonance peak and therefore, R_k is regular with respect to k . Then, we can make the linear interpolation on $[k_p, k_{p+1}]$:

$$R_k = \alpha_p k + \beta_p,$$

where

$$\alpha_p = \frac{R_{p+1} - R_p}{\Delta k} \quad \text{and} \quad \beta_p = \frac{R_p k_{p+1} - R_{p+1} k_p}{\Delta k}. \quad (3.9)$$

This gives

$$J_p = \alpha_p \int_{k_p}^{k_{p+1}} \frac{k}{|E_k - z_I|^2} dk + \beta_p \int_{k_p}^{k_{p+1}} \frac{1}{|E_k - z_I|^2} dk. \quad (3.10)$$

Using (2.5) and writing $z_I = E_I - i\frac{\Gamma_I}{2}$ with $E_I, \Gamma_I > 0$, a direct computation gives:

$$\int_{k_p}^{k_{p+1}} \frac{k}{|E_k - z_I|^2} dk = \gamma^2 \chi^1(k_p, k_{p+1}, c_I, d_I), \quad \text{and} \quad \int_{k_p}^{k_{p+1}} \frac{1}{|E_k - z_I|^2} dk = \gamma^2 \chi^0(k_p, k_{p+1}, c_I, d_I) \quad (3.11)$$

where the function χ^n is given in Appendix C and

$$\gamma = \frac{2m}{\hbar^2}, \quad c_I = \gamma(E_I + B_I \mathbf{1}_{\{k_p \leq 0\}}), \quad d_I = \gamma \frac{\Gamma_I}{2}.$$

This approximation has the advantage to be peaked around the resonance.

Remark 3.2. In numerical applications, the computation of the resonance is done only one time at each step of the integer l , the resonance is the same for all integer p . We note also that the integral J_p can be computed only one time at each step of the integer p , it is the same for all integer j .

4 The time-dependent algorithm

4.1 The algorithm

As in the stationary regime, we first present the algorithm proposed in [16] to solve the time-dependent non-linear Schrödinger-Poisson system (2.1)(2.3)(2.6). Then, we give the details of a time-dependent one-mode approximation algorithm.

The space and frequency meshes are defined as in section 3.1. For a given exterior potential $U(t)$ and time step Δt , the algorithm corresponds to the computation of the sequence V^l of approximations of the self-consistent potential at time $t_l = l\Delta t$. The initial potential V^0 and wave functions Ψ_p^0 are given by V_I , and respectively Φ_p , discret solution to the stationary non-linear Schrödinger-Poisson system (2.1)(2.2)(2.4) with exterior potential equal to U_I . The resolution of the Schrödinger equation (2.6) involves a Crank-Nicolson scheme which is semi-implicit and insures stability. Therefore, the value of the intermediary potential $V^{l+\frac{1}{2}}$ must be computed to perform the algorithm. It is done by an extrapolation using the Gummel iteration (3.1). Then, the algorithm writes:

Algorithm 4.1 (Transient algorithm).

Do For $l \geq 0$:

Computation of the intermediary potential

Computation of the potential $V^{l+\frac{1}{2}}$ from the potential V^l and the density n^l by the resolution of the non-linear equation:

$$\begin{cases} -\frac{d^2}{dx^2}V^{l+\frac{1}{2}} = \frac{q^2}{\epsilon}(n[V^l] \exp((V^l - V^{l+\frac{1}{2}})/V_{ref}) - n_D), & (0, L) \\ V^{l+\frac{1}{2}}(0) = V^{l+\frac{1}{2}}(L) = 0, \end{cases} \quad (4.1)$$

for a fixed reference potential V_{ref} .

Computation of the density

S1. For $p = 0, \dots, P$: computation of Ψ_p^{l+1} wave function at time t^{l+1} and frequency k_p using the potential $V^{l+\frac{1}{2}}$ and the wave function Ψ_p^l .

S2. Numerical integration: for $j = 0, \dots, J$

$$n_j^{l+1} = \sum_{p=0}^{P-1} I_{p,j}^{l+1}, \quad \text{where} \quad I_{p,j}^{l+1} = \int_{k_p}^{k_{p+1}} g(k) \left| (\Psi_k^{l+1})_j \right|^2 dk.$$

Coupling, Poisson equation

Computation of the potential V^{l+1} from the density n^{l+1} by solving the Poisson equation (2.1):

$$\begin{cases} -\frac{d^2}{dx^2}V^{l+1} = \frac{q^2}{\epsilon}(n^{l+1} - n_D), & (0, L) \\ V^{l+1}(0) = V^{l+1}(L) = 0. \end{cases} \quad (4.2)$$

End Do.

As in the stationary case, the equation (4.1) is solved using a Newton method. The linear equation (4.2) is discretized with finite differences and solved by a simple matrix inversion. Due to the presence of resonances, the steps *S1* and *S2* to compute density will be crucial here also.

In the algorithm proposed in [16], which we will call equally Direct Resolution, the steps *S1* and *S2* are performed without particular treatment of resonances: the wave functions are computed on $[0, L]$ solving the Schrödinger equation using a Crank-Nicolson Scheme with discrete transparent

boundary conditions and the integrals $I_{p,j}^l$ are computed with a trapezoidal rule. In that case, the accuracy of the method is provided by the imposition of a uniform frequency mesh with a small mesh size everywhere (an other strategy would be to choose a small frequency mesh size only in the region where will live the resonant energy). Indeed, if the mesh size is small only near the initial resonant energy then, because of the time evolution of the resonance, the refined mesh will loose its relevance. Therefore, for the Direct Resolution, the number of Schrödinger equations to solve in the time dependent regime is more important than in the stationary regime. Moreover, the Crank-Nicolson method to solve one Schrödinger equation requires a matrix inversion of big size (equal to $J + 1$) and is numerically much more expensive than the RK4 stationary method. In this context, it is important to look for an adapted treatment of the resonance peaks to reduce the number of frequency points.

In the following section, we propose a one-mode approximation method which extends the method proposed in section 3.3 to the time-dependent case.

4.2 The time dependent One Mode Approximation

Recall first that in the initial work [17], the One Mode Approximation was presented in the time dependent case with a simplified model. Then, let us start with the description, in the One Mode Approximation, of the decomposition of a wave function $\Psi_k(t)$ solution to the transient Schrödinger equation (2.6) for a given frequency k . The One Mode Approximation consists in the decomposition:

$$\Psi_k(t) = \Psi_k^{nr}(t) + \Psi_k^r(t), \quad (4.3)$$

where the non-resonant part $\Psi_k^{nr}(t)$ solves the transient Schrödinger equation:

$$\begin{cases} i\hbar\partial_t\Psi_k^{nr}(t) = [-\frac{\hbar^2}{2m}\partial_x^2 + U_{fill}(t) + V(t)]\Psi_k^{nr}(t), & x \in \mathbb{R} \\ \Psi_k^{nr}(0) = \Phi_k^{nr}, \end{cases} \quad (4.4)$$

with filled potential $U_{fill}(t) = U(t) + v_0\mathbf{1}_{[a_3,b_3]}$, where Φ_k^{nr} is solution to (3.6) with the initial potential $U_{I,fill} + V_I$. In comparison with the stationary algorithm, it seems natural to look for $\Psi_k^r(t)$ proportional to the resonant mode $u(t)$ corresponding to the first resonance $z(t)$ of the Hamiltonian $H(t)$ at time t which verifies

$$[-\frac{\hbar^2}{2m}\partial_x^2 + U(t) + V(t)]u(t) = z(t)u(t) \quad (4.5)$$

and $\int_0^L |u(t,x)|^2 dx = 1$. However, since the change of potential at time $t = 0$ is abrupt, the adiabaticity hypothesis of [17] is not satisfied and one expects two peaks at both the energy of the resonant mode at time $t = 0^-$ and the resonant energy at time t . This is what happens numerically. Indeed, if denoting $z(t) = E(t) - i\frac{\Gamma(t)}{2}$, where $E(t)$, $\Gamma(t) > 0$, in Figure 2 are plotted the logarithm $C(t, k)$ of the charge in the well for one wave function with respect to the frequency k :

$$C(t, k) = \log \left(\int_{a_2}^{b_2} |\Psi_k(t, x)|^2 dx \right) \quad (4.6)$$

and the frequencies corresponding to the resonant energy

$$k_R^-(t) = -\sqrt{\frac{2m}{\hbar^2}(E(t) + B(t))}, \quad k_R^+(t) = \sqrt{\frac{2m}{\hbar^2}E(t)}, \quad (4.7)$$

at different time t . The resolution is performed with the external potential $U(t)$ corresponding to the bias $B(t)$ defined as follows: for the biases $B_I = 0 eV$ and $B_\infty = 0.1 eV$, and for the time $t_0 = 10^{-12} s$, we have $B(t) = B_I$ for $t \leq 0$, $B(t) = B_\infty$ for $t \geq t_0$ and on $(0, t_0)$, $B(t)$ is the polynomial of degree 3 such that $B(t)$ is a C^1 function on \mathbb{R} . The method used is the Direct Resolution with the numerical parameters $J = 300$, $P = 1500$, $\Delta t = 10^{-15} s$ and the physical

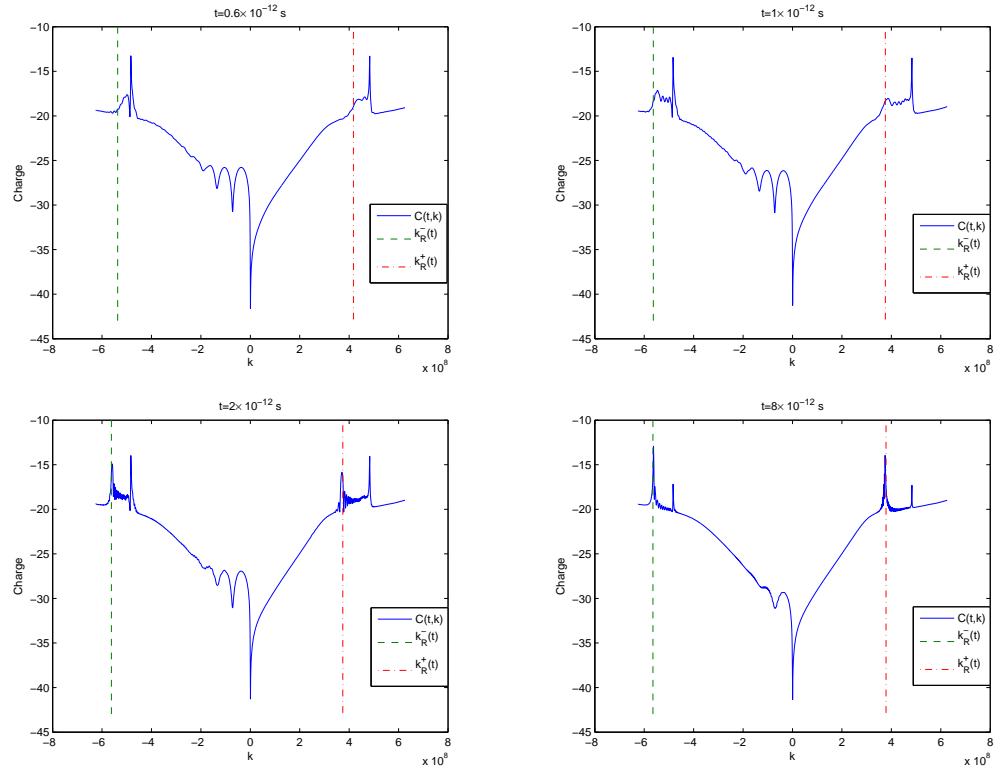


Figure 2: Logarithm $C(t, k)$ of the charge in the well for one wave function with respect to the frequency k and frequencies, $k_R^-(t)$ and $k_R^+(t)$, corresponding to the resonant energy, at different time t , for a time dependent bias.

parameters given in section 5.

We see that for small time the resonance peak is not localised at the resonant energy $E(t)$ at time t but it's localised at the initial resonant energy E_I . Then, the initial peak vanishes while a peak grows at $E(t)$. Therefore, we look for Ψ_k^r of the form:

$$\Psi_k^r(t, x) = \theta_k v(t, x) + \lambda_k(t) u(t, x), \quad x \in (0, L), \quad (4.8)$$

where $v(t)$ is the propagation of the initial resonant mode by the Schrödinger equation:

$$\begin{cases} i\hbar \partial_t v(t) = [-\frac{\hbar^2}{2m} \partial_x^2 + U(t) + V(t)] v(t), & x \in \mathbb{R}, \\ v(0) = u_I \end{cases} \quad (4.9)$$

and θ_k is the proportionality coefficient in the stationary regime corresponding the initial data such that:

$$\Phi_k(x) = \Phi_k^{nr}(x) + \theta_k u_I(x), \quad x \in (0, L). \quad (4.10)$$

Comparing (4.3)(4.8) and (4.10), the initial condition in (2.6) implies $\lambda_k(0) = 0$. Moreover, injecting (4.3)(4.8) in the transient Schrödinger equation (2.6) and using equations (4.4),(4.5) and (4.9) we get the following equation on $\lambda_k(t)$:

$$[i\hbar \lambda_k'(t) - z(t) \lambda_k(t)] u(t, x) + i\hbar \lambda_k(t) \partial_t u(t, x) = -v_0 \mathbf{1}_{[a_3, b_3]}(x) \Psi_k^{nr}(t, x).$$

Multiplying the previous equation by $\bar{u}(t, x)$ and integrating on $(0, L)$, it follows:

$$\begin{cases} \lambda_k'(t) + [\frac{i}{\hbar} z(t) + \int_0^L \partial_t u(t, x) \bar{u}(t, x) dx] \lambda_k(t) = S_k(t) \\ \lambda_k(0) = 0, \end{cases} \quad (4.11)$$

where $S_k(t) = \frac{i}{\hbar} v_0 \int_{a_3}^{b_3} \Psi_k^{nr}(t, x) \bar{u}(t, x) dx$.

Remark 4.2. Equation (4.11) is an ODE which homogeneous solution oscillates at the energy $E(t)$ and which source term oscillates at the energy $\varepsilon_k(t)$ defined by:

$$\varepsilon_k(t) = \begin{cases} \frac{\hbar^2 k^2}{2m}, & k \geq 0 \\ \frac{\hbar^2 k^2}{2m} - B(t), & k < 0 \end{cases} \quad (4.12)$$

Therefore $\lambda_k(t)$ has a peak at the frequencies k such that $\varepsilon_k(t) = E(t)$.

4.2.1 Step S1

The aim here is to compute the wave function at step $l + 1$ making the decomposition:

$$\Psi_k^{l+1} = (\Psi_k^{nr})^{l+1} + \theta_k v^{l+1} + \lambda_k^{l+1} u^{l+1}.$$

However, at this point of the algorithm, we do not have the value of the potential V^{l+1} and the resonant mode u^{l+1} can not be computed. Therefore, we will make the following approximation:

$$\Psi_k^{l+1} = (\Psi_k^{nr})^{l+1} + \theta_k v^{l+1} + \lambda_k^{l+1} u^{l+\frac{1}{2}}. \quad (4.13)$$

Then the step S1 writes as follows.

Suppose that the quantities $(\Psi_k^{nr})^l$, v^l and λ_k^l are known (at $l = 0$, it is given by the initial decomposition (4.10)).

As it is done in the Direct Resolution for Ψ_k^{l+1} , see [16], the function $(\Psi_k^{nr})^{l+1}$ is computed on $[0, L]$ using $(\Psi_k^{nr})^l$ and $V^{l+\frac{1}{2}}$ by the resolution of (4.4) with the Crank-Nicolson scheme (B.2), where the potential Q is equal to $U_{fill} + V$. Since the initial data Φ_k^{nr} is not supported in $(0, L)$, the

suitable boundary conditions are the non-homogeneous discrete transparent boundary conditions presented in Appendix B. More precisely, if the bias is equal to

$$B(t) = \begin{cases} B_I, & t = 0 \\ B_\infty, & t > 0 \end{cases} \quad (4.14)$$

then we will use the boundary conditions (B.8)(B.7) and for general biases $B(t)$ we will use the boundary conditions (B.8)(B.9).

The function v^{l+1} is computed by the Crank Nicolson scheme (B.2) on $[0, L]$ starting from v^l and using for $V^{l+\frac{1}{2}}$ the solution to (4.1). The initial data u_I is almost equal to 0 at $x = 0$ and $x = L$ and the homogeneous boundary conditions (B.3)(B.4) can be applied directly.

The resonance $z^{l+\frac{1}{2}}$ and resonant mode $u^{l+\frac{1}{2}}$ are computed using the method presented in section 3.2 where the potential Q is equal to $U^{l+\frac{1}{2}} + V^{l+\frac{1}{2}}$. The initial guess for $(u^{l+\frac{1}{2}}, z^{l+\frac{1}{2}})$ are the first eigenfunction and eigenenergy of the Hamiltonian

$$\left[-\frac{\hbar^2}{2m}\partial_x^2 + U^{l+\frac{1}{2}} + V^{l+\frac{1}{2}}\right]$$

with homogeneous Dirichlet boundary conditions at a_2 and b_2 .

To achieve the step $S1$, we have to compute the coefficient λ_k^{l+1} . It is obtained from λ_k^l , $(\Psi_k^{nr})^l$, $(\Psi_k^{nr})^{l+1}$, $z^{l+\frac{1}{2}}$ and $u^{l+\frac{1}{2}}$ by the resolution of equation (4.11). The resolution is performed with a Crank-Nicolson scheme, which leads to the following iteration:

$$\begin{aligned} (\lambda_k^{l+1} - \lambda_k^l)/\Delta t + \left[\frac{i}{\hbar}z^{l+\frac{1}{2}} + \int_0^L \partial_t u^{l+\frac{1}{2}} \overline{u^{l+\frac{1}{2}}} dx\right](\lambda_k^l + \lambda_k^{l+1})/2 \\ = (S_k^{l+\frac{1}{2},l} + S_k^{l+\frac{1}{2},l+1})/2, \end{aligned} \quad (4.15)$$

where $S_k^{l,m} = \frac{i}{\hbar}v_0 \int_{a_3}^{b_3} (\Psi_k^{nr})^m \overline{u^l} dx$.

By adequately fixing the resonant mode phase, the quantity

$$\mu^{l+1/2} := \int_0^L \partial_t u^{l+1/2} \overline{u^{l+1/2}} dx$$

appearing in (4.15) is fitted to zero. Indeed, we consider $\tilde{u}(t)$ solution to (4.5) such that $\|\tilde{u}(t)\|_{L^2(0,L)} = 1$ and we look for $u(t)$ of the form $u(t) = \tilde{u}(t)e^{i\varphi(t)}$ where $\varphi(t) \in \mathbb{R}$. We note first that we have the approximation

$$\mu^{l+1/2} = \frac{1}{2\Delta t} \int_0^L (u^{l+1/2} - u^{l-1/2}) \overline{(u^{l+1/2} + u^{l-1/2})} dx,$$

which becomes

$$\mu^{l+1/2} = \frac{i}{\Delta t} \text{Im} \left[\int_0^L u^{l+1/2} \overline{u^{l-1/2}} dx \right] \quad (4.16)$$

under the condition $\|u^{l-1/2}\|_{L^2(0,L)} = \|u^{l+1/2}\|_{L^2(0,L)} = 1$. Then, defining

$$\omega^{l+1/2} = \int_0^L \tilde{u}^{l+1/2} \overline{u^{l-1/2}} dx,$$

we choose

$$e^{i\varphi^{l+1/2}} = \frac{\overline{\omega^{l+1/2}}}{|\omega^{l+1/2}|}$$

and it follows:

$$\int_0^L u^{l+1/2} \overline{u^{l-1/2}} dx = e^{i\varphi^{l+1/2}} \int_0^L \tilde{u}^{l+1/2} \overline{u^{l-1/2}} dx = \omega^{l+1/2} e^{i\varphi^{l+1/2}} = |\omega^{l+1/2}| \in \mathbb{R}.$$

As a consequence, $\text{Im}[\int_0^L u^{l+1/2} \overline{u^{l-1/2}} dx] = 0$ and equation (4.16) shows that $u^{l+1/2}$ is such that $\mu^{l+1/2}$ is almost equal to 0.

4.2.2 Step S2

In this section, we use the decomposition (4.13) to find an approximation of

$$n_j^{l+1} = \int_{-k_M}^{k_M} g(k) \left| (\Psi_k)_j^{l+1} \right|^2 dk$$

which is adapted to the resonant peaks. Like in section 3.3, we make the approximation:

$$\left| \Psi_k^{l+1} \right|^2 = \left| (\Psi_k^{nr})^{l+1} \right|^2 + \left| \theta_k v^{l+1} \right|^2 + \left| \lambda_k^{l+1} u^{l+\frac{1}{2}} \right|^2 + 2\text{Re} \left(\theta_k v^{l+1} \overline{\lambda_k^{l+1} u^{l+\frac{1}{2}}} \right). \quad (4.17)$$

The coefficient θ_k has a peak at E_I given by formula (3.7) and as noted in Remark 4.2 the coefficient $\lambda_k(t)$ has a peak at $E(t)$. It follows that the cross term in the previous equation can be neglected for biases of the form (4.14) with $B_I \neq B_\infty$ since the initial resonance and the resonance at time t are not in the same domain of frequency. We write here the step S2 in the corresponding framework (the method for general biases follows the same line). Therefore, equation (4.17) writes

$$\left| \Psi_k^{l+1} \right|^2 = \left| (\Psi_k^{nr})^{l+1} \right|^2 + \left| \theta_k v^{l+1} \right|^2 + \left| \lambda_k^{l+1} u^{l+\frac{1}{2}} \right|^2.$$

The wave function $\Psi_k^{nr}(t)$ being regular with respect to the frequency k , the non resonant part of the density can be computed with a large frequency mesh size, as it is done in the stationary regime in [5]. Suppose that the discretisation $k_0 = -k_M, k_1, \dots, k_p, \dots, k_P = k_M$ of the interval $[-k_M, k_M]$ is uniform with mesh size Δk and suppose that there exists two integers P' and ν such that $\frac{P}{P'} = \nu$. Then, the approximation for the density is

$$\begin{aligned} n_j^{l+1} &= \sum_{p'=0}^{P'-1} \left(g(k_{\nu p'}) \left| (\Psi_{\nu p'}^{nr})_j^{l+1} \right|^2 + g(k_{\nu(p'+1)}) \left| (\Psi_{\nu(p'+1)}^{nr})_j^{l+1} \right|^2 \right) \frac{\nu \Delta k}{2} \\ &+ \sum_{p=0}^{P-1} \left(g(k_p) |\theta_p|^2 + g(k_{p+1}) |\theta_{p+1}|^2 \right) \frac{\Delta k}{2} |v_j^{l+1}|^2 \\ &+ \sum_{p=0}^{P-1} \left(g(k_p) |\lambda_p^{l+1}|^2 + g(k_{p+1}) |\lambda_{p+1}^{l+1}|^2 \right) \frac{\Delta k}{2} |u_j^{l+\frac{1}{2}}|^2. \end{aligned}$$

The number of Schrödinger equations to solve is reduced: P' equations instead of P equations for the Direct Resolution, which induces a reduction of the numerical cost. However, this reduction implies that we have only access to the functions $(\Psi_{\nu p'}^{nr})^{l+1}$ for $p' = 0, \dots, P'$ and the computation of the coefficient λ_p^{l+1} , for $p = 0, \dots, P$, requires an interpolation of the non resonant wave function to evaluate the source term in (4.15). Following Remark 4.2, the picked form of the coefficient λ_p^{l+1} is obtained numerically only if the approximation of the source term at the frequency k oscillates in time at the energy $\varepsilon_k(t)$. This implies that a polynomial interpolation is not adapted. Therefore, we propose the suitable algorithm below: from the scheme (4.15), we have for $p = 1, \dots, P$

$$\lambda_p^{l+1} = \frac{1}{1 + i \frac{\Delta t z^{l+\frac{1}{2}}}{2\hbar}} \left[\left(1 - i \frac{\Delta t z^{l+\frac{1}{2}}}{2\hbar} \right) \lambda_p^l + \frac{\Delta t}{2} (S_p^{l+\frac{1}{2}, l} + S_p^{l+\frac{1}{2}, l+1}) \right],$$

where the source term is given by the interpolation:

$$\text{for } 0 \leq p' \leq P' - 1 \text{ and } 1 \leq j \leq \nu - 1, \quad S_{\nu p'+j}^{l,m} = \frac{i}{\hbar} v_0 \int_{a_3}^{b_3} (\tilde{\Psi}_{\nu p'}^{nr})^m e^{-\frac{i}{\hbar} \varepsilon_{\nu p'+j}^\infty t^m} \overline{u^l} dx,$$

with

$$(\tilde{\Psi}_p^{nr})^m = (\Psi_p^{nr})^m e^{\frac{i}{\hbar} \varepsilon_p^\infty t^m}$$

and

$$\varepsilon_p^\infty = \begin{cases} \frac{\hbar^2 k_p^2}{2m}, & k_p \geq 0 \\ \frac{\hbar^2 k_p^2}{2m} - B_\infty, & k_p < 0. \end{cases}$$

Remark 4.3. It is numerically verified that the method presented in this section is stable in time and allows long time simulations, see section 5.4. It is not the case of the time dependent version of the method presented in 3.3 which corresponds to the explicitely computation of the integral $\int_{k_p}^{k_p+1} g(k)|\lambda_k(t)|^2 dk$ with the Briet-Wigner formula for $\lambda_k(t)$ of the form (3.7).

5 Results

The physical parameters used for the numerical computations are gathered in the following array:

Rel. el. mass	0.067	Rel. permittivity	11.44
Temperature	300 K	Fermi level E_F	$6,7097 \times 10^{-21}$ J
Donor density n_D^1	$10^{24} m^{-3}$		
Donor density n_D^2	$5 \times 10^{21} m^{-3}$		

For all the tests, the two barriers has the same size which is equal to the size of the well. The data concerning the external potential are gathered in the following array:

L (nm)	a_1 (nm)	a_2 (nm)	a_3 (nm)	b_3 (nm)	b_2 (nm)	b_1 (nm)	v_0 (eV)
135	50	60	65	70	75	85	0.3

In all the simulations, we took the number of space points to be $J = 300$ which is such that the stability condition $\frac{\hbar^2}{2m\Delta x^2} > 1$ is verified. And we fixed $k_M = \sqrt{\frac{2m}{\hbar^2}(E_F + 7k_B T)}$.

5.1 Computation of resonances

In this section we give the numerical values of the resonance of lower energy obtained using the algorithm presented in section 3.2 for different biases B_I . The potential Q is equal to $U_I + V_I$ where U_I is the external potential and V_I the solution to the Schrödinger-Poisson system (2.1)(2.2)(2.4) corresponding to B_I . The number of iterations before convergence N_{cv} denotes the iteration n such that $\|M(\mathbf{z}^n)\mathbf{u}^n\|_2 < 10^{-15}$. We obtain the following results:

B_I (eV)	N_{cv}	E_0 (meV)	E_I (meV)	Γ_I/E_I
0	3	126.83	127.55	2.58×10^{-3}
0.1	3	80.29	81.00	4.40×10^{-3}

where the resonance is equal to $z_I = E_I - i\frac{\Gamma_I}{2}$ and E_0 denotes the fundamental energy of the Dirichlet Hamiltonian (3.8). The modulus of the normalized resonant mode $\frac{|u_I(x)|}{\|u_I\|_2}$ for $B_I = 0.1$ eV is represented in Figure 3.

5.2 The stationary regime

We show here a comparison of the Direct Resolution and of our One Mode Approximation algorithm presented in section 3 with respect to a Reference Resolution. The latest corresponds to the Direct Resolution with a uniformly refined frequency mesh where $P = 4000$.

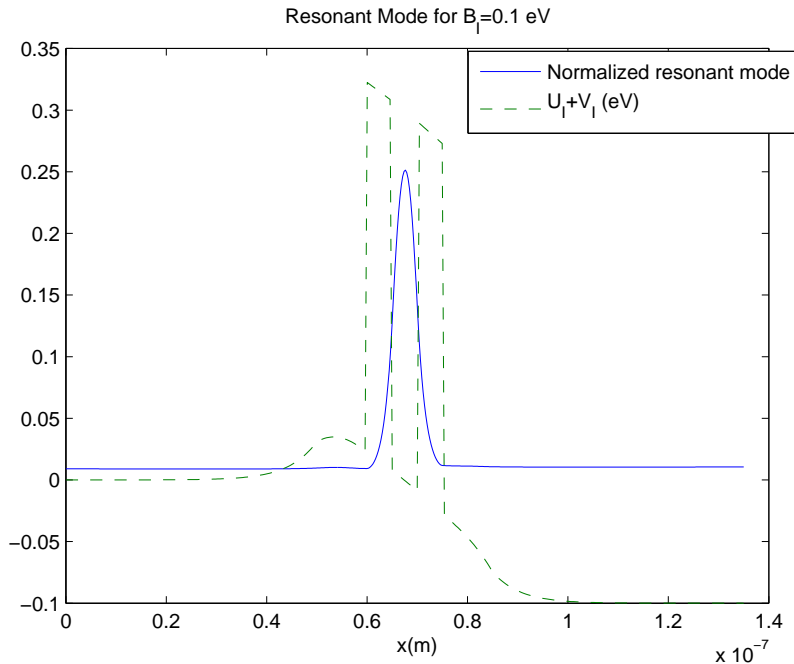


Figure 3: Representation of the potential $U_I + V_I$ (dashed line) and the corresponding normalized resonant mode (full line) for $B_I = 0.1 \text{ eV}$ and $J = 300$.

Remark 5.1. For the bias $B_I = 0$ the Gummel method can be initialized at the potential $V_I^0 = 0$. Such an initialization does not converge for $B_I > 0$, we have convergence when initializing at the solution given by the method when $B_I = 0$.

For the One Mode Approximation, the method to compute the resonance at the first iteration of the Gummel algorithm is initialized at the fundamental energy and fundamental mode of the Dirichlet Hamiltonian (3.8). For the following iteration, it can be initialized at the resonance and resonant mode of the previous iteration to decrease the numerical cost.

The results we obtained for two different values of the bias B_I are given in the array of Figure 4. The number of iterations before convergence N_{cv} denotes the iteration l such that

$$e^l := \frac{\|V^l - V^{l-1}\|_2}{\|V^l\|_2} < 10^{-15}. \quad (5.1)$$

The integer P is the number of frequency points, CPU is the time spent by the processor to realize the computation. The column L_2 error denotes the relative error for the potential in L^2 norm given by:

$$100 \frac{\|V^{N_{cv}} - V_{ref}\|_2}{\|V_{ref}\|_2},$$

where V_{ref} is the potential of the Reference Resolution. In the Direct Resolution, the number of frequency points changes from an iteration to the other, however it stays around a fixed number which we wrote with the symbol \approx . The One Mode Approximation algorithm converges and needs less frequency points than the Direct Resolution. Nevertheless, the first algorithm doesn't cost much less than the second because the computation cost of one resonance is much bigger than the resolution of one Schrödinger equation. In the time-dependent case, it is not possible to use an adaptative frequency mesh and the numerical cost for the computation of one resonance is comparable to the resolution of one Schrödinger equation, therefore the One Mode Approximation will be much more interesting.

		N_{cv}	P	CPU(s)	L_2 error(%)
$B_I = 0$ eV	Reference	36	4000	69.47	/
	Direct	37	≈ 916	16.47	4.59×10^{-3}
	One Mode	37	50	5.53	1.26
$B_I = 0.1$ eV	Reference	34	4000	65.10	/
	Direct	34	≈ 896	14.80	3.03×10^{-3}
	One Mode	34	50	4.34	2.04

Figure 4: Comparison of the Direct Resolution and One Mode Approximation algorithms for the resolution of the stationary Schrödinger-Poisson system.

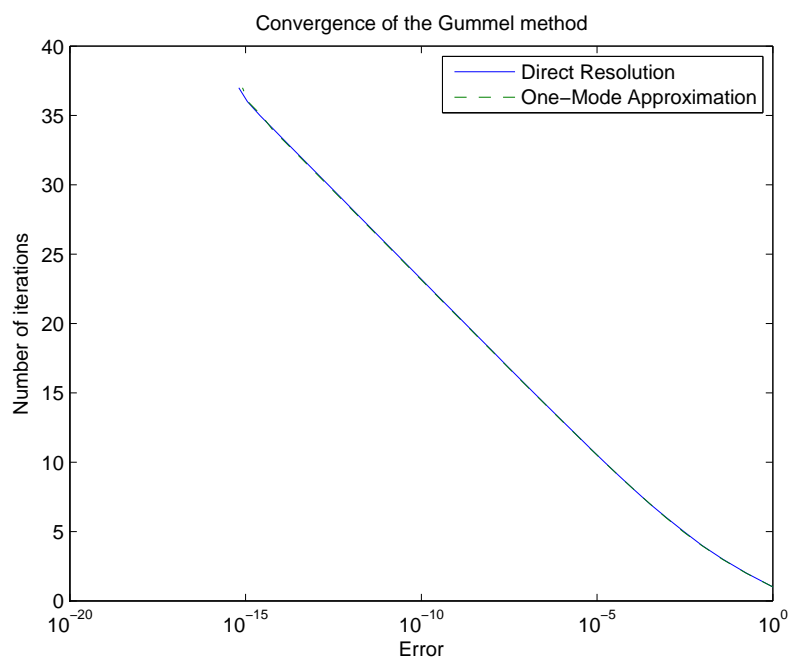


Figure 5: Relative error with respect to the number of iterations for $B_I = 0$ eV.

In Figure 5 is represented the error e^l defined by (5.1) with respect to the number of iterations l for the Direct Resolution and the One Mode Approximation. The bias is equal to $B_I = 0$ eV which corresponds to the upper part of the array of Figure 4. We see that the One Mode Approximation algorithm reaches the accuracy 10^{-15} in 37 iterations and converges as fast as the Direct Resolution.

In Figure 6, are represented the self-consistent potential and the density after convergence for the part $B_I = 0$ eV of the array of Figure 4 and for the three methods. We see that the three methods give very similar results.

5.3 The transient regime: step S1

We present here a validation of the step S1 described in section 4.2. It is realized using a comparison of the One Mode Approximation algorithm described in this section, where only the step S1 is performed, with the Direct Resolution. For this One Mode Approximation algorithm, the integrals $I_{p,j}^l$ are computed with a trapezoidal rule instead of using the step S2 and the number of frequency points has to be the same than for the Direct Resolution.

The external potential $U(t)$ is the time dependent external potential corresponding to the bias

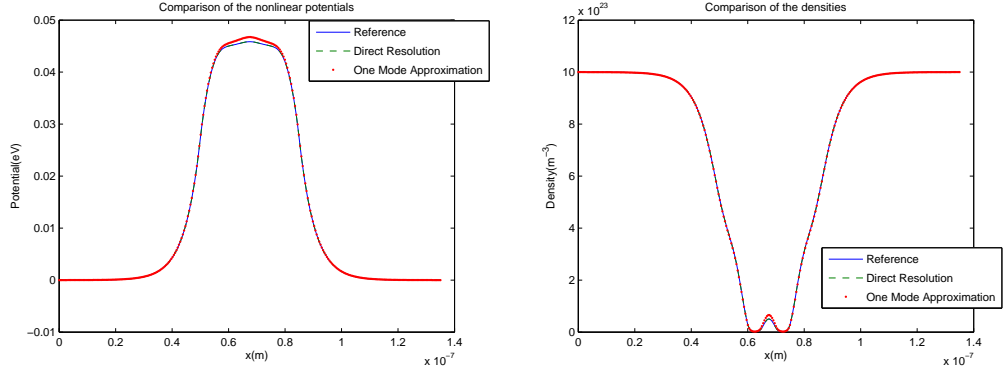


Figure 6: Nonlinear potential and density for $B_I = 0 eV$.

$B(t)$ defined in (4.14) where $B_I = 0 eV$ and $B_\infty = 0.1 eV$.

For the two methods, the number of frequency points is equal to $P = 1500$. In order to have stability, we took a time step $\Delta t = 10^{-15} s$ and the final time of the simulation is $t = 8 \times 10^{-12} s$. The time spent by the processor to complete the simulation is 66853.45 s for the Direct Resolution and 97329.36 s for the One Mode Approximation. The decomposition of the wave function at each frequency and time step makes the computational time more important for the One Mode Approximation, therefore, this method is not interesting without a reduction of the number P . The left plot of Figure 7 is the representation, for the two methods, of the evolution of the charge in the well:

$$\int_{a_2}^{b_2} n(t, x) dx \quad (5.2)$$

with respect to time t . We see that for the One Mode Approximation and for the Direct Resolution the charge in the well increases from the charge corresponding to B_I to the one corresponding to B_∞ .

On the right plot of Figure 7, is represented the relative distance in L2 norm d^l between the density n^l and the density n_∞ corresponding to the stationary solution with the bias B_∞ :

$$d^l = 100 \frac{\|n^l - n_\infty\|_{L^2(a_2, b_2)}}{\|n_\infty\|_{L^2(a_2, b_2)}} \quad (5.3)$$

with respect to time t^l . The relevant variation of the density being in the well, the norm is considered only on the interval (a_2, b_2) . We remark that for both methods, the density converges to a density close to the stationary density corresponding to B_∞ . The difference between the asymptotic density and the stationary density corresponding to B_∞ is due to the fact that the methods used to perform the integration in k for the time dependent and for the stationary algorithms are different.

In the left plot of Figure 8, are represented, at time $t = 3 \times 10^{-12} s$, the functions

$$C_\theta(t, k) = \log \left(\int_{a_2}^{b_2} |\theta_k v(t, x)|^2 dx \right), \quad C_\lambda(t, k) = \log \left(\int_{a_2}^{b_2} |\lambda_k(t) u(t, x)|^2 dx \right), \quad (5.4)$$

the function $C(t, k)$ defined by (4.6) and the frequencies $k_R^-(t)$, $k_R^+(t)$ defined by (4.7) with respect to the frequency k . This picture confirms that the step $S1$ corresponds to a decomposition of the wave function Ψ_k in a function $\theta_k v$ peaked at the frequency related to the initial resonant energy E_I and a function $\lambda_k u$ peaked at the frequency related to the resonant energy $E(t)$.

In the right plot of Figure 8, is represented the square of the L2 norm of $v(t)$ in the well, defined by:

$$N(t) = \int_{a_2}^{b_2} |v(t, x)|^2 dx,$$

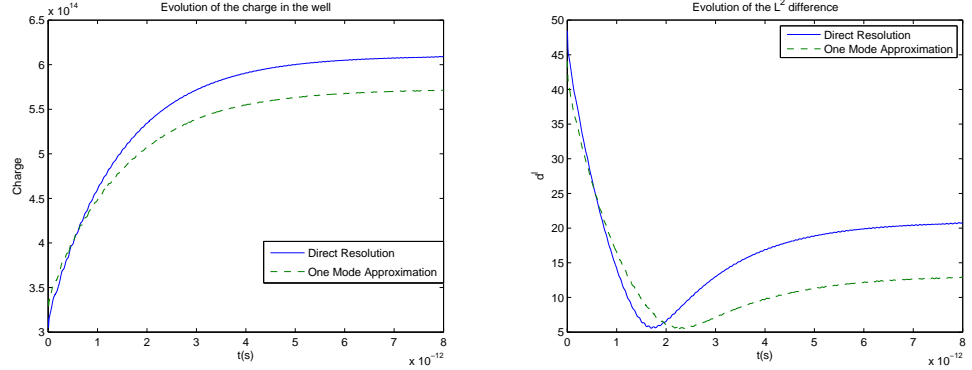


Figure 7: Evolution of the charge in the well (left) and of the L^2 difference d^l (right) for the Direct Resolution and One Mode Approximation algorithms.

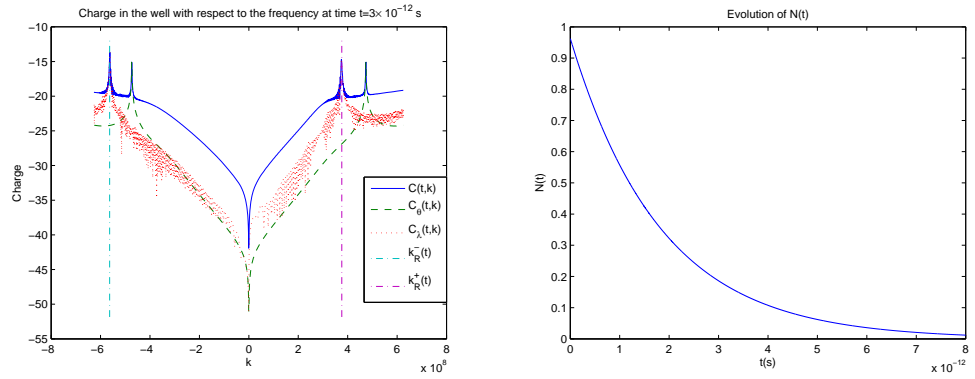


Figure 8: Functions $C(t, k)$, $C_\theta(t, k)$, $C_\lambda(t, k)$ and resonant frequencies $k_R^-(t)$, $k_R^+(t)$ at time $t = 3 \times 10^{-12} s$ (left) and time evolution of $N(t)$ (right).

as a function of the time t . We observe that $v(t)$ vanishes in the well for times larger than $5 \times 10^{-12} s$. This corresponds to the extinction of the resonant peak at energy E_I observed in Figure 2. Moreover, the decay of $N(t)$ is theoretically given by the imaginary part of the resonance following the approximation:

$$\frac{N(t_0 + T)}{N(t_0)} \approx e^{-\frac{1}{\hbar} \int_{t_0}^{t_0+T} \Gamma(s) ds}.$$

This is verified numerically since we have for $t_0 = 10^{-12} s$ and $T = 10^{-12} s$:

$$\frac{N(t_0 + T)}{N(t_0)} = 0.578$$

and

$$e^{-\frac{1}{\hbar} \int_{t_0}^{t_0+T} \Gamma(s) ds} = 0.582.$$

5.4 The transient regime: reduction of the number of frequency points

We present here a comparison of the One Mode Approximation algorithm described in section 4.2, where the steps $S1$ and $S2$ are performed, with the Direct Resolution.

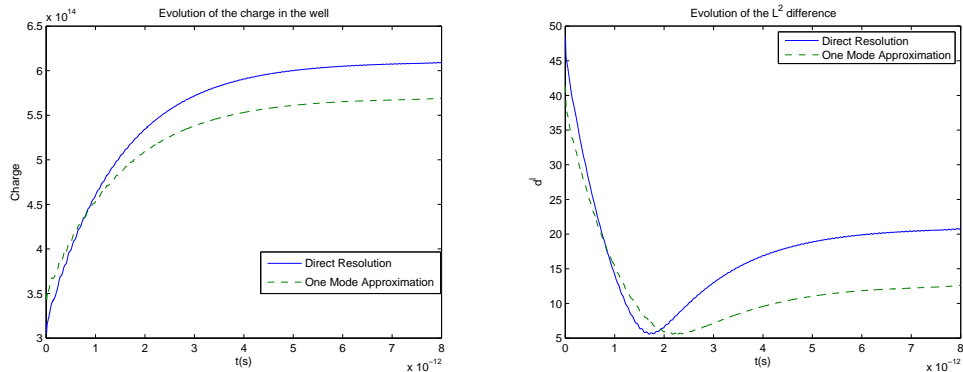


Figure 9: Evolution of the charge in the well (left) and of the L^2 difference d^l (right) for the Direct Resolution and One Mode Approximation algorithms.

The external potential $U(t)$ is the time dependent external potential corresponding to the bias $B(t)$ defined in (4.14) where $B_I = 0 \text{ eV}$, $B_\infty = 0.1 \text{ eV}$. The number of frequency points is $P = 1500$ for the Direct Resolution. For the One Mode Approximation, the number of frequency points for the non resonant part is $P' = 750$ and $P = 1500$ for the resonant part. As in the previous section, we took a time step $\Delta t = 10^{-15} \text{ s}$ to have stability. The final time of the simulation is $t = 8 \times 10^{-12} \text{ s}$. The left plot of Figure 9, is the representation, for both methods, of the charge evolution in the well defined by (5.2). We see that for the One Mode Approximation and for the Direct Resolution the charge in the well increases from the charge corresponding to B_I to this corresponding to B_∞ . On the right plot of Figure 9, is represented the L^2 difference d^l , defined by (5.3), as a function of time t^l . We remark that for both methods, the density converges to the stationary density corresponding to B_∞ .

For the One Mode Approximation the simulation is possible with a half less Schrödinger equations at each time step and the computational time is divided by two. The method we propose for the step $S2$ presents the two following properties: first, the resolution is stable and allows long time simulations, second, the picked form of the coefficient is reconstructed and allows at time increase of the charge in the well. These two properties, that we set as a validity criterion for the One Mode Approximation algorithm, are still verified after a reduction of the frequency points similar to the stationary algorithm by taking $P' = 50$ and $P = 1500$. However, for such a simulation, the initial value of the density and the long time value of the density are poorly evaluated. Nevertheless, this lack of precision can be probably overcome by improving the interpolation of the exterior wave functions and replacing the trapezoidal rule to compute the initial resonant pic $\int_{k_p}^{k_{p+1}} g(k) |\theta_k|^2 dk$ by its explicit value given in section 3.3.

We represented in Figure 10 the logarithm $C(t, k)$ of the charge at frequency k , the frequencies $k_R^-(t)$ and $k_R^+(t)$ defined by (4.6) and (4.7) computed with the Direct Resolution and at different values of the time t . As noted for Figure 2, for small times the peak is localized at the initial resonant energy E_I . Then, the initial resonance peak vanishes while a resonance peak grows around $E(t)$. However, the two cases are different: in Figure 2 the resonant energy $E(t)$ moves with the bias $B(t)$ for $t \in (0, t_0)$. In that case, the resonance peak corresponding to $E(t)$ appears at the same frequency as the initial one and the two peaks split. In the present case, the peak, when it appears, is already far from the initial one.

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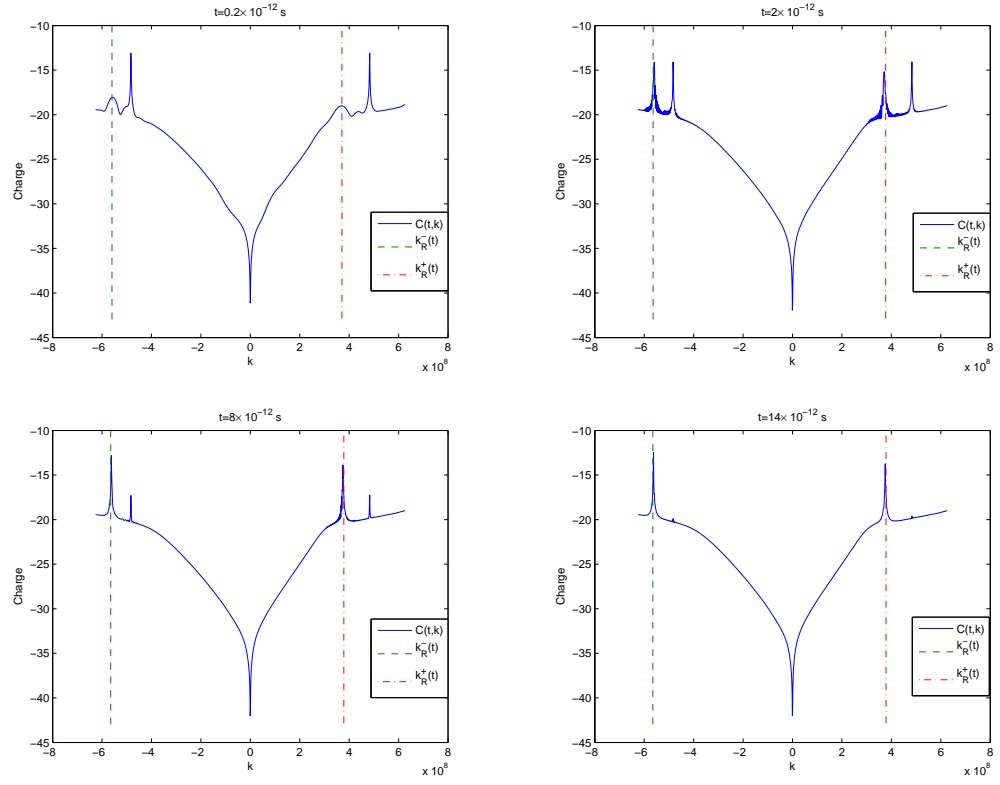


Figure 10: Logarithm $C(t, k)$ of the charge in the well for one wave function with respect to the frequency k and frequencies, $k_R^-(t)$ and $k_R^+(t)$, corresponding to the resonant energy at different time t .

A Computation of resonances: FEM matrices

The matrices appearing in section 3.2 are given as follows:

$$M_2 = \begin{pmatrix} -i\frac{\hbar}{\sqrt{2m}} & 0 & \dots & 0 \\ 0 & & & \\ \vdots & & 0 & \\ 0 & & & \end{pmatrix}, \quad M_3 = \begin{pmatrix} & & & 0 \\ & & & \vdots \\ & 0 & & 0 \\ 0 & \dots & 0 & -i\frac{\hbar}{\sqrt{2m}} \end{pmatrix}, \quad M_4 = \Delta x \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & & & \\ \frac{1}{6} & \frac{2}{3} & & & \\ & \ddots & \frac{1}{6} & & \\ 0 & & \ddots & \frac{1}{6} & \\ & & & \frac{2}{3} & \frac{1}{3} \\ & & & \frac{1}{6} & \frac{1}{3} \end{pmatrix}$$

$$M_1 = \frac{\hbar^2}{2m\Delta x} \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix} + \Delta x \begin{pmatrix} \xi_0 & \zeta_0 & & & \\ \zeta_0 & \xi_1 & \zeta_1 & & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & & \zeta_{J-2} & \xi_{J-1} & \zeta_{J-1} \\ & & & \zeta_{J-1} & \xi_J \end{pmatrix},$$

where

$$\zeta_j = \frac{Q_j + Q_{j+1}}{12}, \quad j = 0, \dots, J-1,$$

$$\xi_0 = \frac{Q_0}{4} + \frac{Q_1}{12}, \quad \xi_j = \frac{Q_{j-1} + Q_{j+1}}{12} + \frac{Q_j}{2}, \quad j = 1, \dots, J-1, \quad \xi_J = \frac{Q_J}{4} + \frac{Q_{J-1}}{12}$$

and Q_j are the approximations of the nodal values of the potential: $Q(x_j)$.

B Resolution of the time dependent Schrödinger equation

B.1 The homogeneous case

In this section, we recall the scheme proposed in [2] to solve on the bounded domain $[0, L]$ a time dependent Schrödinger equation

$$\begin{cases} i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\partial_x^2\Psi + Q\Psi, & t > 0, x \in \mathbb{R} \\ \Psi(0, x) = \Phi(x), & x \in \mathbb{R}, \end{cases} \quad (\text{B.1})$$

with the following hypothesis:

H1. The initial condition Φ is supported in $0 < x < L$.

H2. The potential Q verifies: for $t > 0$

$$Q(t, x) = 0, \quad x \leq 0, \quad \text{and} \quad Q(t, x) = Q_L, \quad x \geq L.$$

Considering the time and space discretization defined in section 4.1, we note Ψ_j^l the approximation of the solution $\Psi(t^l, x_j)$. Then, equation (B.1), is solved with the Crank-Nicolson method:

$$-iR(\Psi_j^{l+1} - \Psi_j^l) = \Delta_{xx}\Psi_j^{l+1} + \Delta_{xx}\Psi_j^l + wQ_j^{l+1/2}(\Psi_j^{l+1} + \Psi_j^l), \quad j = 1, \dots, J-1, \quad l \geq 0, \quad (\text{B.2})$$

where $\Delta_{xx}\Psi_j = \Psi_{j+1} - 2\Psi_j + \Psi_{j-1}$, $R = \frac{4m\Delta x^2}{\hbar\Delta t}$ and $w = -\frac{2m\Delta x^2}{\hbar^2}$.

The equation (B.2) comes with the discrete transparent boundary conditions:

$$\Psi_1^l - s_0^0\Psi_0^l = \sum_{k=1}^{l-1} s_0^{l-k}\Psi_0^k - \Psi_1^{l-1}, \quad l \geq 1, \quad (\text{B.3})$$

$$\Psi_{J-1}^l - s_J^0 \Psi_J^l = \sum_{k=1}^{l-1} s_J^{l-k} \Psi_J^k - \Psi_{J-1}^{l-1}, \quad l \geq 1, \quad (\text{B.4})$$

where, we have for $j = 0$ and $j = L$:

$$s_j^l = \left[1 - i \frac{R}{2} + \frac{\sigma_j}{2} \right] \delta_l^0 + \left[1 + i \frac{R}{2} + \frac{\sigma_j}{2} \right] \delta_l^1 + \alpha_j \exp \left(-il \varphi_j \frac{P_l(\mu_j) - P_{l-2}(\mu_j)}{2l-1} \right), \quad (\text{B.5})$$

and

$$\varphi_j = \arctan \frac{2R(\sigma_j + 2)}{R^2 - 4\sigma_j - \sigma_j^2}, \quad \mu_j = \frac{R^2 + 4\sigma_j + \sigma_j^2}{\sqrt{(R^2 + \sigma_j^2)[R^2 + (\sigma_j + 4)^2]}}$$

$$\sigma_j = \frac{2\Delta x^2}{\hbar^2} Q_j, \quad \alpha_j = \frac{i}{2} ((R^2 + \sigma_j^2)[R^2 + (\sigma_j + 4)^2])^{1/4} \exp \left(i \frac{\varphi_j}{2} \right).$$

Here P_l denotes the Legendre polynomials, with the convention $P_{-1} = P_{-2} = 0$, and δ_l^j the Kronecker symbol related to the integers j and l .

The boundary conditions above are available only for initial data supported in $(0, L)$ and therefore it is called homogeneous discrete transparent boundary conditions.

B.2 The non homogeneous case

For the initial potential Q_I such that $Q(0, x) = Q_I(x)$ and

$$Q_I(x) = 0, \quad x \leq 0, \quad \text{and} \quad Q_I(x) = Q_{I,L}, \quad x \geq L,$$

we consider the problem (B.1) where the initial condition Φ is solution to

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Phi + Q_I \Phi = E_I \Phi, \quad x \in \mathbb{R}, \quad (\text{B.6})$$

for a given energy E_I . Like in section B.1, we will use the Crank-Nicolson scheme (B.2), however, the hypothesis $H1$ is not verified and we can not apply (B.3)(B.4).

Nevertheless, using equations (B.1) and (B.6), the function

$$\varphi = \Psi - \Phi e^{-i \frac{E_I}{\hbar} t} \quad \text{where} \quad E_L = E_I + (Q_L - Q_{I,L})$$

is solution to:

$$i \hbar \partial_t \varphi = \left[-\frac{\hbar^2}{2m} \partial_x^2 + Q \right] \varphi, \quad x \geq L$$

and verifies $\varphi(0, x) = 0$. Thus, we can write the homogeneous boundary condition (B.4) for φ which gives the following boundary condition at $x = L$ for Ψ :

$$\Psi_{J-1}^l - s_J^0 \Psi_J^l = \sum_{k=1}^{l-1} s_J^{l-k} \Psi_J^k - \Psi_{J-1}^{l-1} - \Phi_J \sum_{k=1}^l s_J^{l-k} e^{-i \frac{E_I}{\hbar} k \Delta t} + \Phi_{J-1} e^{-i \frac{E_I}{\hbar} (l-1) \Delta t} (1 + e^{-i \frac{E_I}{\hbar} \Delta t}), \quad l \geq 1, \quad (\text{B.7})$$

where the coefficients s_j^l are given by (B.5). We proceed similarly at $x = 0$ by setting

$$\varphi = \Psi - \Phi e^{-i \frac{E_0}{\hbar} t} \quad \text{where} \quad E_0 = E_I.$$

We obtain the following boundary condition at $x = 0$:

$$\Psi_1^l - s_0^0 \Psi_0^l = \sum_{k=1}^{l-1} s_0^{l-k} \Psi_0^k - \Psi_1^{l-1} - \Phi_0 \sum_{k=1}^l s_0^{l-k} e^{-i \frac{E_0}{\hbar} k \Delta t} + \Phi_1 e^{-i \frac{E_0}{\hbar} (l-1) \Delta t} (1 + e^{-i \frac{E_0}{\hbar} \Delta t}), \quad l \geq 1. \quad (\text{B.8})$$

B.3 Time dependent potential

In this section, we consider the same problem than in section B.2 and in addition, we suppose that the potential verifies: for $t \geq 0$

$$Q(t, x) = 0, \quad x \leq 0, \quad \text{and} \quad Q(t, x) = Q_L(t), \quad x \geq L,$$

instead of the hypothesis *H2*. As we did in section B.2, we will use the Crank-Nicolson scheme (B.2). The boundary condition (B.8) at $x = 0$ obtained there can also be applied in our case. At $x = L$, the time dependance of the potential must be considered. To this aim, we introduce the function:

$$\varphi = \Psi e^{\frac{i}{\hbar} \int_0^t Q_L(s) ds} - \Phi e^{-i \frac{E_L}{\hbar} t} \quad \text{where} \quad E_L = E_I - Q_{I,L}.$$

Using equations (B.1) and (B.6), it is verified that $\varphi(0) = 0$ and

$$i\hbar \partial_t \varphi = -\frac{\hbar^2}{2m} \partial_x^2 \varphi, \quad x \geq L,$$

where we got rid of the time dependent potential. Therefore, φ verifies at $x = L$ the boundary condition (B.4) with potential equal to 0. This gives the following boundary condition for Ψ : $\forall l \geq 1$

$$\begin{aligned} \varepsilon^l \Psi_{J-1}^l - \tilde{s}_J^0 \varepsilon^l \Psi_J^l = & \sum_{k=1}^{l-1} \tilde{s}_J^{l-k} \varepsilon^k \Psi_J^k - \varepsilon^{l-1} \Psi_{J-1}^{l-1} - \Phi_J \sum_{k=1}^l \tilde{s}_J^{l-k} e^{-i \frac{E_L}{\hbar} k \Delta t} \\ & + \Phi_{J-1} e^{-i \frac{E_L}{\hbar} (l-1) \Delta t} (1 + e^{-i \frac{E_L}{\hbar} \Delta t}), \end{aligned} \quad (\text{B.9})$$

where

$$\varepsilon^l = e^{\frac{i}{\hbar} \sum_{k=0}^{l-1} (Q_L^k + Q_L^{k+1}) \Delta t / 2}$$

and \tilde{s}_J^l is given by (B.5) when replacing σ_J by 0.

C Explicit value of some useful integrals

The aim of this section is to give, for $n = 0, 1$, the explicit value of the integral

$$\chi^n(a, b, c, d) = \int_a^b \frac{x^n}{(x^2 - c)^2 + d^2} dx,$$

where $a < b$, $c > 0$ and $d > 0$.

- Case $n=0$:

We have the decomposition

$$\begin{aligned} \frac{1}{(x^2 - c)^2 + d^2} &= \frac{-1}{2id} \left(\frac{1}{x^2 - c + id} - \frac{1}{x^2 - c - id} \right) \\ &= \frac{-1}{d} \text{Im} \left(\frac{1}{x^2 - c + id} \right) \end{aligned}$$

and

$$\frac{1}{x^2 - c + id} = \frac{-1}{2z_0} \left(\frac{1}{x + z_0} - \frac{1}{x - z_0} \right), \quad (\text{C.1})$$

where $z_0 = \sqrt{c - id}$ and \sqrt{z} denotes the square root holomorphic on $\mathbb{C} \setminus \mathbb{R}_-$. It is defined by $z = \rho e^{i\theta}$ and $\sqrt{z} = \sqrt{\rho} e^{i\frac{\theta}{2}}$ where $\rho \geq 0$, $\theta \in (-\pi, \pi]$.

This leads to:

$$\begin{aligned} \chi^0(a, b, c, d) &= \frac{1}{2d} \operatorname{Im} \left[\frac{1}{z_0} \left(\int_a^b \frac{1}{x + z_0} dx - \int_a^b \frac{1}{x - z_0} dx \right) \right] \\ &= \frac{1}{2d} \operatorname{Im} \left[\frac{1}{z_0} (\ln(b + z_0) - \ln(a + z_0) - \ln(b - z_0) + \ln(a - z_0)) \right], \end{aligned}$$

where the logarithm is defined by $z = \rho e^{i\theta}$ and $\ln z = \ln \rho + i\theta$ where $\rho > 0$, $\theta \in (-\pi, \pi]$.

- Case n=1:
We have

$$\begin{aligned} \chi^1(a, b, c, d) &= \frac{1}{2} \int_{a^2-c}^{b^2-c} \frac{1}{x^2 + d^2} dx \\ &= \frac{1}{2d} \left(\arctan \left(\frac{b^2 - c}{d} \right) - \arctan \left(\frac{a^2 - c}{d} \right) \right). \end{aligned}$$

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