THz displacement current in tunneling devices with coherent electron-photon interaction

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Abstract

For frequencies comparable to the inverse of the electron transit time, the measured total current in electron devices needs to include not only the particle but also the displacement current. Typically, in most quantum transport simulators, the displacement current is ignored, or simply computed from Gauss’ law involving only the longitudinal (zero rotational) electric field. In this work, the role of the transverse (zero divergence) electromagnetic field in the evaluation of the displacement current in resonant tunneling diodes is analyzed within either classical or quantum models of such fields. In the quantum case, the peaks of the original transmission coefficient, without interaction with photons, split into two new peaks due to the resonant electron-photon interaction leading to Rabi oscillations. Such phenomenon, that mimics known effects predicted by a Jaynes-Cummings model in closed systems, exemplifies how a full quantum treatment of electrons and electromagnetic fields opens unexplored paths for engineering new THz electron devices. The computational burden involved in the multi-time measurements of THz currents is minimized by invoking a Bohmian description of the light-matter interaction. As an additional result, we show that the traditional transmission coefficient used to characterize DC quantum electron devices has to be substituted by a new displacement current coefficient in high frequency AC scenarios.

keywords: Matter-light interaction; Resonant Tunnelling Diode; Bohmian conditional wavefunction; Rabi Oscillation; Jaynes-Cummings model.

1 Introduction

In the transition from microelectronics to nanoelectronics, thirty years ago, a revolution appeared in the way electron devices were modeled. The classical treatment of electrons had to be definitively abandoned and substituted by a quantum view to account for new phenomena like electron tunneling and energy quantization. Such a transition was envisioned by Landauer as early as 1957 [1]. Nowadays, as electron devices reach low nanometer scales, most typical electron device models have adopted a quantum treatment of electrons [2–10]. Most of our understanding of the interaction of matter with electromagnetic fields is accounted for by solving Gauss’ law coupled to an electron transport equation under an electrostatic approximation. However, this electrostatic assumption fails for nanoelectronic devices operating at frequencies of hundreds of GHz or even few THz [5–7,17,18] and novel modeling approaches are required. The development of quantum transport models for electron nanodevices at such frequencies is important, for example, in the so called THz gap, around the frequency range 0.1-30 THz. Such a gap is now being explored by a growing number of technologies, from frequency down-conversion of photon sources [19] as in [20–25] to frequency up-conversion of electron sources [26] as in [27–30]. The closure of this gap, with electron devices working at room temperature, would enable a large body of applications with significant societal impacts [37], such as non-ionizing imaging of human tissues [38,39] including cancer screening [40,41], security imaging [37], and higher data rates associated to the use of higher carrier frequencies for wireless information transmission [17,22,23,25,42].

Therefore, a proper quantum modeling of electron transport is required beyond the electrostatic approximation, as for example, for dealing with collective oscillations of electrons (plasmons) [43–46]. In addition, the effect of external magnetic fields on the dynamics of electron devices is something well studied in the literature [47–49]. In fact, at GHz or THz frequencies, not only the particle current, but also the displacement current [50–52] needs to be properly taken into account, which is not an easy task. The simplest solution is mixing an electrostatic quantum treatment for the electron transport with a compact model that includes not only resistors, but also capacitors and/or inductors to account, among others, for the displacement current component [53–55]. Such procedure enormously simplifies the computational burden of modeling high-frequency effects. Meanwhile, it has also been demonstrated experimentally that displacement currents play a dominant role in Resonant Tunneling Diodes (RTDs) [56] and in RTD oscillators [57,58], when they are operated in a high-frequency regime. In addition, at frequencies of tens of THz, the photon energies start to be comparable to the energy of the electrons even at room temperature, and the fact that the energy of the electromagnetic field is quantized can no longer be avoided. Typically, the treatment of quantized
electromagnetic fields is done by including collisions into the equation of transport of the electrons. In each collision it is assumed that the electron absorbs or emits the energy of a photon according to the Fermi Golden Rule. This perturbative technique has been successfully included in many quantum simulators [8–16], but it neglects the possible coherent behaviour of the interaction among electron and electromagnetic field.

In this paper we will explore if, as already done for electrons thirty years ago, one needs a full quantum treatment of the electromagnetic fields too to develop the next generation of THz electron devices. We notice that the quantum treatment of the electromagnetic field interacting with matter is a topic as old as the quantum theory of the electron itself. In 1927, Dirac already described the quantization of the electromagnetic field as an ensemble of harmonic oscillators [60]. Later, Tomonaga, Schwinger and Feynman developed the so-called quantum electrodynamics theory [57–59]. Nowadays, due to recent experimental advances, there is a renewed interest on the light-matter coupling in nanoscale systems with few or many particles, opening a path to new research topics like polaritonic chemical reactions [60–61] or light-induced states of matter [62–65]. The many-body systems are studied, for example, through extensions of the density-functional theory within the quantum electrodynamic framework [60] reaching DC dynamics through the linear Kubo approximation [67]. In order to reach non-linear predictions of the (out-of-equilibrium) electron device performance at THz frequencies, our computational approach will be much simpler: an electron in the conduction band in the effective mass approximation interacting with one mode of the electromagnetic field. We will show that a fully coherent quantum treatment of such electron interacting with electromagnetic fields in a RTD can lead to phenomena well-known in quantum optics [65–70], but mostly ignored by the electronics community. One of the novelties of the present work is that we see the electron-photon coupling signatures in the measured displacement current, which is the typical output parameter in the electronic device community, rather than in other output parameters common in the quantum optics community.

The structure of the paper is the following. Section 2 discusses Maxwell’s equations in terms of longitudinal and transverse fields; only the transverse fields, which are usually ignored in electron device modeling, require new degrees of freedom apart from the electronic ones. Section 3 shows the Hamiltonian of an electron interacting with a single mode of the electromagnetic field written in terms of canonical variables, which allows us to develop semiclassical, orthodox quantum and Bohmian quantum viewpoints [71] for the electron-photon interaction. In Section 4 the Bohmian framework allows us to describe the displacement current for a large number of electrons in the active region of a RTD, minimizing the computational complications of the orthodox measurement; we then present the displacement current coefficient, which is the analogous to the transmission coefficient, in scenarios where the displacement current becomes relevant. In Section 5 we present some results for both transmission and displacement current coefficients for both semiclassical and quantum modelings of a RTD. We then conclude in Section 6 and some Appendices explain, for quantum optics (closed systems), phenomena that are analogous to the ones described in the main text for electronic devices (open systems).

2 Maxwell equations in terms of transverse and longitudinal electromagnetic fields

In this section we review Maxwell’s equations by distinguishing longitudinal and transverse components of the electromagnetic field. We explain the so-called Darwin approximation which will be later used in the computation of the displacement current, allowing a tradeoff between increasing predictive power and controllable computational burden. Despite being interested in electromagnetic fields inside semiconductors, to simplify our discussion following the typical nomenclature used in quantum optics literature [68–70], we will present our developments in terms of the electric \( E(r, t) \) and magnetic fields \( B(r, t) \) in vacuum. The generalization of our results in terms of the electric displacement field \( D(r, t) \) and \( H(r, t) \) is straightforward under the assumption that the latter are just proportional to the former.

The Helmholtz decomposition of vector fields into solenoidal and irrotational components allows one to write the total electric field \( E(r, t) \) in terms of transverse \( E_{\perp}(r, t) \) (zero divergence) and longitudinal \( E_{\parallel}(r, t) \) (zero rotational) components as \( E(r, t) = E_{\perp}(r, t) + E_{\parallel}(r, t) \). The transverse field satisfies

\[
\nabla \cdot E_{\perp}(r, t) = 0, \\
\n\nabla \times E_{\perp}(r, t) = -\frac{∂B(r, t)}{∂t},
\]

where the last equation couples it to the magnetic field \( B(r, t) \).

The longitudinal field satisfies

\[
\nabla \times E_{\parallel}(r, t) = 0, \\
\n\nabla \cdot E_{\parallel}(r, t) = \frac{ρ(r, t)}{ε_0},
\]

in which the last equation couples it to the charge density \( ρ(r, t) \), defined by

\[
ρ(r, t) = \sum_{j=1}^{N} ϵ_δ(r - r_j[t])
\]

for a closed system with \( N \) particles, each one with (unsigned) charge \( e \) located at \( r_j[t] \), with \( ε_0 \) the vacuum permeability. The magnetic field, on the other hand, has only a transverse component, that is, \( B_{\perp}(r, t) \equiv B(r, t), B_{\parallel}(r, t) = 0 \), and it satisfies

\[
\nabla \cdot B(r, t) = 0, \\
\n\nabla \times B(r, t) = μ_0 ε_0 \frac{∂E(r, t)}{∂t} + μ_0 J_{\perp}(r, t),
\]

with \( μ_0 \) the vacuum magnetic permeability and \( c = \frac{1}{√μ_0 4πε_0} \) the speed of light, and where the particle current density is defined by

\[
J_{\perp}(r, t) = \sum_{j=1}^{N} εv_j(t)δ(r - r_j[t]),
\]
with \( \mathbf{v}_j(t) \) the velocity of particle \( j \). Notice that (9) and (10) are valid definitions of charge and current densities not only when classical mechanics is used, but also when Bohmian quantum mechanics [71,73] is invoked as done in Section 3.4, where each particle has well-defined position \( \mathbf{r}_j(t) \) and velocity \( \mathbf{v}_j(t) \).

Maxwell equations imply the existence of vector \( \mathbf{A}(\mathbf{r}, t) \) and scalar \( U(\mathbf{r}, t) \) potentials, which characterize completely the fields through

\[
\mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{A}(\mathbf{r}, t)}{\partial t} - \nabla U(\mathbf{r}, t), \quad (9)
\]

\[
\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t). \quad (10)
\]

However, since distinct potential pairs \([\mathbf{A}(\mathbf{r}, t), U(\mathbf{r}, t)]\) may yield the same field pairs \([\mathbf{E}(\mathbf{r}, t), \mathbf{B}(\mathbf{r}, t)]\) one needs to impose a gauge to uniquely define the electromagnetic field. Hereafter we employ the Coulomb gauge (which is the typical gauge used in electronics [74]), where \( \mathbf{A}(\mathbf{r}, t) \) is also a transverse vector satisfying \( \nabla \cdot \mathbf{A}(\mathbf{r}, t) = 0 \), and which allows one to write (10) as

\[
\begin{align*}
\mathbf{E}_\perp(\mathbf{r}, t) &= -\frac{\partial \mathbf{A}(\mathbf{r}, t)}{\partial t}, \\
\mathbf{E}_\parallel(\mathbf{r}, t) &= -\nabla U(\mathbf{r}, t),
\end{align*} \quad (11, 12)
\]

so that Gauss’ law [4] can be rewritten in terms of \( U(\mathbf{r}, t) \) as the well-known and common in electronics Poisson equation,

\[
\nabla^2 U(\mathbf{r}, t) = -\frac{\rho(\mathbf{r}, t)}{\epsilon_0}. \quad (13)
\]

The continuity equation, valid for any choice of the gauge, in the case of the Coulomb gauge can be obtained from the Ampere law [11] as

\[
0 = \frac{\partial \rho(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{J}_c(\mathbf{r}, t), \quad (14)
\]

which leads to the definition of the total current \( \mathbf{J}(\mathbf{r}, t) \) as the sum of three contributions,

\[
\mathbf{J}(\mathbf{r}, t) = \mathbf{J}_c(\mathbf{r}, t) + \epsilon_0 \frac{\partial \mathbf{E}_\parallel(\mathbf{r}, t)}{\partial t} + \epsilon_0 \frac{\partial \mathbf{E}_\perp(\mathbf{r}, t)}{\partial t}, \quad (15)
\]

in which the last two terms yield the displacement current density. By construction, the total current satisfies the relevant property

\[
\nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0, \quad (16)
\]

which ensures that the total current predicted on a surface of the active region of an electron device (see \( I(t) \) in Fig. 1) is equal to that measured on a surface of the ammeter (see \( I'(t) \) in Fig. 1) when radiation outside the cable connecting it is assumed negligible.

In other words, at high frequency, the particle current \( \mathbf{J}_c(\mathbf{r}, t) \) on the surface of the active region is not equal to the particle current \( \mathbf{J}_c(\mathbf{r}_M, t) \) on a surface of the ammeter at the position \( \mathbf{r}_M \). Thus, in high frequency electronics, what has to be predicted is the total current in the active region, \( \mathbf{J}(\mathbf{r}, t) \), and not only the particle current \( \mathbf{J}_c(\mathbf{r}, t) \).

### 2.1 Darwin approximation

An equation of motion for the particles needs to be specified to determine \( \rho(\mathbf{r}, t) \) and \( \mathbf{J}_c(\mathbf{r}, t) \) in the previous section, which will depend, in turn, on electric- and magnetic-field solutions of Maxwell’s equations, making a quite complicated self-consistent loop. Thus, reasonable approximations are mandatory to be able to provide practical predictions. The simplest one is the static approximation, which assumes that all time derivatives in Maxwell’s equations are zero. Then, the equations involving electric and magnetic fields are decoupled, and electrostatics/magnetostatics is reached. The
electric field can be computed from Gauss’ law \([11]\), together with an equation of motion for particles to find \(\rho(r, t)\).

A less crude option is to employ one of the quasi-static approximations, which assumes that only some of the time-derivatives in Maxwell’s equations are zero. If one neglects only the time-derivative of the electric field \(\frac{\partial E(r, t)}{\partial t} \approx 0\) in Ampère’s law \([12]\), one arrives at quasi-magnetostatics, but this is not an appropriate approximation for high-frequency electronics in semiconductor devices because it directly ensures a macroscopic steady-state current, \(\nabla \cdot J(r, t) = 0\), which neglects both the displacement current and a possible time dependence in the continuity equation \([13]\). If instead one neglects only the time derivative of the magnetic field \(\frac{\partial B(r, t)}{\partial t} \approx 0\) in Faraday’s law \([2]\), one reaches quasi-electrostatics, which does provide displacement current and it also satisfies the continuity equation \([14]\), being a reasonable approximation for semiconductors.

But there is yet another approximation even less invasive, and it is the one we consider in our discussion. The so-called Darwin approximation \([16]\) fits better with our attempt to keep the displacement current and the vector potential \(A(r, t)\) into consideration at a small computational cost. It does not neglect the magnetic field but instead it assumes that the time derivative of only the transverse electric field, \(\frac{\partial E_{\perp}(r, t)}{\partial t}\), is negligible in comparison with the other terms of the total current \([15]\), which then in Darwin approximation becomes

\[
J(r, t) \approx J_{e}(r, t) + e_{0} \frac{\partial E_{\parallel}(r, t)}{\partial t}. \tag{17}
\]

Notice that such approximation satisfies conservation of current in \([12]\) because Gauss’ law \([2\text{I}]\) depends only on the longitudinal electric field \(E_{\parallel}(r, t)\).

By using the magnetic field \([16]\) together with the transverse \([11\text{I}]\) and longitudinal \([12\text{I}]\) components of the electric field into Ampère’s law \([7\text{I}]\), and by employing the identity \(\nabla \times \nabla \times A(r, t) = \nabla (\nabla \cdot A(r, t)) - \nabla^{2} A(r, t)\) in the Coulomb gauge, one arrives at

\[
\nabla^{2} A(r, t) - \frac{\partial^{2} A(r, t)}{c^{2} \partial t^{2}} = \nabla \frac{\partial U(r, t)}{\partial t} - \mu_{0} J_{e}(r, t). \tag{18}
\]

The Darwin approximation also implies that the second time derivative of the vector potential, \(\frac{\partial^{2} A(r, t)}{\partial t^{2}}\), is negligible in comparison with the other terms in \([18\text{I}]\). This implies eliminating retardation effects in the definition of electromagnetic fields. Thus the Darwin approximation assumes that \(t - |r - r'|/c \approx t\), with \(r'\) the source location and \(r\) the point where the fields are evaluated. Neglecting the time step \(\Delta t = |r - r'|/c\) is acceptable if we are interested in the dynamics involving angular frequencies \(\omega\) much slower than the maximum angular frequency \(\omega_{\text{max}} = 2\pi/\Delta t, \omega \ll \omega_{\text{max}}\). We also need to define the active region of length \(L\), as seen in Fig. \(\text{I}\) where we want to provide accurate predictions. As a result, the necessary condition for the Darwin approximation to be valid in the active region is

\[
\omega \ll \frac{2\pi c}{L} \quad \text{or} \quad L \ll \lambda, \tag{19}
\]

where \(\lambda = 2\pi c/\omega\) is the wavelength linked to \(\omega\). If a nanoelectronic scenario is considered, with maximum device length \(L = 50 \text{ nm}\), one realizes that the maximum frequencies where the Darwin approximation for the transverse fields is acceptable are as high as several tens of THz.

### 3 Hamiltonian for an electron interacting with a single mode of the electromagnetic field

Since we want to deal with light-matter interaction, when looking for some Hamiltonian to move particles, we will have to include the energies of both particles and electromagnetic field, plus the interaction among them. Such global Hamiltonian will provide an equation of motion not only for the particles but also for the electromagnetic field (i.e. Maxwell’s equations from the previous section), in either classical or quantum scenarios. After developing such global Hamiltonian, at the end of this section we compare the four possible approaches for the light-matter coupling: classical, semiclassical, orthodox quantum, and Bohmian quantum equations of motion.

Hereafter, since we deal with electronic devices, the only particles that we explicitly consider are electrons. The first approximation in our attempt to develop a general Hamiltonian that describes the dynamics of electrons and electromagnetic fields in a manageable way is to assume that the many-body Hamiltonian of all \(N\) electrons interacting with the electromagnetic field can be studied as a sum over \(N\) simpler Hamiltonian of an individual electron interacting with the electromagnetic field only. In the context of electronic devices this is typically invoked as an assumption of ballistic transport. Notice that such type of simplification (a \(N\)-body problem studied as a sum of \(N\) single-particle problems) is conceptually exact in terms of the Bohmian conditional wave functions \([70]\) as far as some complicated terms, analogous to the exchange-correlation potential in the Kohn-Sham equations, are included as mentioned in Appendix \(\text{E}\).

The Hamiltonian for a single-electron in the conduction band (in the effective mass approximation for a semiconductor with parabolic energy-wave vector dispersion) interacting with the electromagnetic field is described by,

\[
H = \frac{[p - eA(r, t)]^{2}}{2m^{*}} + eU(r, t) + V_{r}(r, t) + H_{\omega}, \tag{20}
\]

with \(m^{*}\) the effective mass of the electron, \(e\) its charge, and \(H_{\omega}\) the energy of the electromagnetic field,

\[
H_{\omega} = \frac{\epsilon_{0}}{2} \int d^{3}r |E_{\perp}(r, t) + c^{2}B^{2}(r, t)|. \tag{21}
\]

The term \(V_{r}(r, t)\) accounts for the band structure seen by the electron, which results from the interaction of the simulated electron with the other non-simulated degrees of freedom (the atoms of the device within the Born-Oppenheimer approximation and all the other electrons). In principle, other ‘external’ potentials are needed to take into account the many-body correlations among simulated and non-simulated electrons which, for simplicity, are not considered here. See Appendix \(\text{E}\) or \([70]\) for an enlarged explanation on this description of the simulated degrees of freedom, and the treatment of the many-body
problem within the Bohmian conditional wave function. Notice that $p$ and $r$ in (20) are to be considered as degrees of freedom, needed to specify the state of the electron.

In the Coulomb gauge considered here, the scalar potential $U(r, t)$ is just the Coulomb potential among electrons. Thus, in our single-electron system, we get $U(r, t) = 0$ because we discard the electron interacting with itself [77]. Then, from [9], [11], and [12], $E_\| (r, t) = 0$ and $E(r, t) = E_{\perp} (r, t) = -\frac{\partial A_\perp (r, t)}{\partial t}$. We see in (21) that only $E_{\perp} (r, t)$ and $B(r, t)$ play a role in the discussion of a quantized electromagnetic field [74].

We now notice that the approximation [19] implies that $A(r, t) \approx A(r_0, t)$, i.e., the so-called dipole approximation. Altogether, by using the gauge transformation $A' = A + \nabla \chi$ and $U' = U + \frac{\partial \chi}{\partial t}$, with $\chi(r, t) = -eA(r_0, t) \cdot r/h$, one can rewrite (20) as

$$H = \frac{p^2}{2m^*} + V_e(r, t) - e r \cdot E_{\perp} (r_0, t) + H_\omega,$$

where $H_e = p^2/(2m^*) + V_e(r, t)$ is the electron Hamiltonian and $H_\omega = -e r \cdot E_{\perp} (r_0, t)$ the light-matter coupling Hamiltonian. Thus, the equation of motion for electrons required to compute the displacement current also requires the knowledge of the transverse electric field $E_{\perp} (r_0, t)$, as well as of the magnetic field $B(r_0, t)$ present in $H_\omega$. As a result, $E_{\perp} (r_0, t)$ and $B(r_0, t)$ are the genuine degrees of freedom needed to specify the state of the electromagnetic field [78]. Although $r$ and $p$ are conjugate degrees of freedom for matter, in the sense that they satisfy Hamilton equation, the same is not true for $E_{\perp} (r_0, t)$ and $B(r_0, t)$ in (21) for the electromagnetic field. To look for canonical degrees of freedom of the electromagnetic fields too it is convenient to work in the reciprocal space, where Maxwell’s equations are local, and define

$$\tilde{E}_{\perp} (k, t) = \int d^3 r \frac{1}{(2\pi)^3/2} E_{\perp} (r, t) e^{-i k r} = \frac{i}{c} N(k) \left[g(k, t) - g^* (-k, t)\right],$$

and

$$\tilde{B}(k, t) = \int d^3 r \frac{1}{(2\pi)^3/2} B(r, t) e^{-i k r} = \frac{i}{c} N(k) \left[\frac{k}{|k|} \times g(k, t) + \frac{k}{|k|} \times g^* (-k, t)\right],$$

where $N(k)$ is a constant specifying the strength of the field (the units of the product $N(k) g(k, t)$ are energy divided by charge multiplied by length squared). Such definitions satisfy Maxwell’s equations in the reciprocal space (see [79]) when the so-called normal variable $g(k, t)$ satisfies

$$\frac{\partial g(k, t)}{\partial t} + i \omega g(k, t) = \frac{\frac{\hbar}{2}\pi N(k)}{e_0},$$

with $\omega = c k$. Notice that $g(k, t)$ is truly an independent variable coupling electric and magnetic fields. Without electrons (i.e., $\tilde{J}_{\perp}(k, t) = 0$), the trivial solution is $g(k, t) = \frac{g(0)}{e^{i \omega t}}$, and $\tilde{J}_{\perp}(k, t)$ would then resemble a simple harmonic oscillator motion, with solutions describing fully decoupled normal vibrational modes of the free field. With such definitions (21) becomes

$$H_\omega = e_0 \int d^3 k N(k) \left[|g(k, t)|^2 + |g^*(k, t)|^2\right].$$

In principle, the number of normal modes is infinite. Hereafter, for simplicity, we consider that light-matter interaction happens around one frequency $\omega$ with an uncertainty $\Delta \omega$ so that only one mode is relevant, with a wave vector $k$ and an uncertainty $\Delta k = \Delta \omega / e$ in each direction. To simplify the final equation, we consider that the transverse electric field has a linear polarization in $x$-direction so that $g(k, t) \approx g(k, t) \hat{x}$. As seen in Fig. (1a), we have defined $\hat{x}$, $\hat{y}$ and $\hat{z}$ as three orthonormal vectors in our real space. Then, (20) can be simplified as

$$H_\omega \approx e_0 \Delta k^3 N(k) [g(k, t) g^*(k, t) + g^*(k, t) g(k, t)],$$

where we keep the order in the two products involving the degrees of freedom $g(k, t)$ and $g^*(k, t)$ anticipating the fact that they will not commute in the quantum case. Identically, the transverse electric field from (23) reads

$$E_{\perp} (r, t) = \int d^3 k \frac{1}{(2\pi)^3/2} \tilde{E}_{\perp} (k, t) e^{i k r} \approx \frac{\Delta k^3}{(2\pi)^3/2} \tilde{E}_{\perp} (k, t) \hat{x},$$

where the dipolar approximation in (19) is employed as $e^{i k r} \approx 1$. One can now define $g(k, t)$, $g^*(k, t)$ in terms of new canonical degrees of freedom $q_g$ and $s_g$ as

$$g(k, t) = \frac{1}{2N(k)} \sqrt{\frac{\omega}{e_0 \Delta k^3}} (s_g - i q_g),$$

$$g^*(k, t) = \frac{1}{2N(k)} \sqrt{\frac{\omega}{e_0 \Delta k^3}} (s_g + i q_g).$$

With them, (28) gives $E_{\perp} (r, t) = q_g \sqrt{\frac{\omega}{e_0 \Delta k^3}} \hat{x}$ and (27) yields $H_\omega = \omega (q_g^2 + s_g^2)/2$. We use the subindex $g$ in $q_g$ and $s_g$ to indicate that they are ‘general’ degrees of freedom valid for classical or quantum scenarios. Altogether, with $r = x \hat{x} + y \hat{y} + z \hat{z}$, (22) reads

$$H = \frac{p^2}{2m^*} + V_e(x, t) - \frac{\alpha}{\sqrt{\omega}} x q_g + \frac{\alpha}{\sqrt{\omega}} \frac{\omega}{2} (q_g^2 + s_g^2),$$

where the value of the coupling constant in $H_1$ is $\alpha = \omega \sqrt{\frac{\Delta k^3}{(2\pi)^3/2}}$, being the responsible for the interaction of both transverse fields with the electron [80]. In (30) we have also considered the typical situation in RTDs (a lateral dimension of the active region much larger than $L^2$) so that the $y$, $z$ degrees of freedom of the electron are decoupled from the $x$ degree, and as such we have assumed $r \equiv x$ and $p \equiv p_x$ in (22). The canonical electron degrees of freedom $x$ and $p_x$ are relevant in $H_e$, while the new canonical variables $q_g$ and $s_g$ take care of the electromagnetic field in $H_\omega$. Despite being a standard procedure in quantum optics, since it is unusual for the electronics community, we have written here explicitly the steps from [79] until [80]. In such development, we have followed mainly Refs. [81][82].

It is important to remind that (30) describes just one electron interacting with the transverse electromagnetic field. However, in a typical RTD, there is a huge number of electrons
traversing the device simultaneously. We have eliminated the interaction among electrons through the typical mean field approximation. But, certainly, we will take them into account in Section 4 when computing the electric current measured by an ammeter. One should remember that, at any frequency, the electrons are affected by the longitudinal part of the electric field through Gauss’ equation [1], which here is included in the external potential $V_e(x, t)$. Notice that the longitudinal electric field is fully determined once we know the positions of all electrons, and does not require any additional degrees of freedom.

Up to here the discussion of the full Hamiltonian (30) in terms of the degrees of freedom $x, p_x, q_g, s_g$ is valid for either classical or quantum scenarios. In what follows we distinguish four different scenarios.

### 3.1 Classical solution

In a classical scenario, the degrees of freedom $x$ and $p_x$ (for position and momentum of the electron) and $q_g$ and $s_g$ (for the amplitude and phase of the transverse electric and magnetic fields) lead to algebraic Hamilton equations. The practical solution of a classical light-matter interaction problem just requires solving such Hamilton equations, fixing the initial conditions for all the variables $x(0), p_x(0), q_g(0), s_g(0)$, to get the trajectories $x(t), p_x(t), q_g(t), s_g(t)$ specifying the evolution of the system.

### 3.2 Semiclassical solution

The previous classical solution misses a very important ingredient for devices at the nanoscale: the quantum coherence or non-local quantum wholeness of the electron [81]. It is well known that any solution of (30) will include the quantum wholeness if the degrees of freedom are considered as non-commuting operators. The standard approach for the electron is defining non-commuting operators in the position representation,

$$ x \rightarrow x, \quad p_x \rightarrow -i\hbar \frac{\partial}{\partial x}. $$

(31)

The semiclassical treatment of light-matter interaction consists in using the previous quantum operators for the electrons while keeping the other degrees of freedom as well-defined variables for the classical electromagnetic fields. As such the Hamiltonian (30) becomes

$$ H_S = \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V_e(x, t) - \frac{\alpha}{\sqrt{\omega}} q_g(t) x, $$

(32)

where the electromagnetic energy $\omega(q_g^2(t) + s_g^2(t))/2$ is not included since it is a pure time-dependent potential with no spatial dependence, having no practical effect on the electron dynamics. The state of the system is given by a wave function $\Psi(x, t)$ which depends parametrically on $q(t)$, which can be understood as the amplitude of the transverse electromagnetic field. Thus, the transverse electric field affects the electron, but the opposite is not taken into account in such semiclassical approximation.

A typical discussion of the semiclassical light-matter interaction is done in Appendix A using, not a position representation as in (32), but an energy representation for a closed system with only two energy eigenstates relevant for the electron.

### 3.3 Orthodox quantum solution

In the orthodox coherent quantum scenario both electromagnetic field and electron are quantum elements, that is, besides the non-commuting operators in (31) for the electron, one also has to consider similar terms for the transverse fields,

$$ q_g \rightarrow \sqrt{\omega} q, \quad s_g \rightarrow -i \frac{\hbar}{\sqrt{\omega}} \frac{\partial}{\partial q}, $$

(33)

so that the new Hamiltonian from (30) becomes

$$ H_Q = \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V_e(x, t) - \alpha x q - \frac{\hbar^2}{2} \frac{\partial^2}{\partial q^2} + \frac{\omega^2}{2} q^2. $$

(34)

The state of the system is now described by a wave function with degrees of freedom for both electron and transverse fields as $\Psi(x, q, t)$, whose evolution follows from the Schrödinger equation

$$ i\hbar \frac{\partial \Psi(x, q, t)}{\partial t} = \left( -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V_e(x, t) \right) \Psi(x, q, t) $$

$$ + \left( -\frac{\hbar^2}{2} \frac{\partial^2}{\partial q^2} + \frac{\omega^2}{2} q^2 \right) \Psi(x, q, t) $$

$$ - \alpha x q \Psi(x, q, t). $$

(35)

From a mathematical point of view, (35) is just a 2D Schrödinger equation whose numerical solution will be carried out in this work. Instead of (33), the standard way of dealing with light-matter interaction is through annihilation $\hat{a}$ and creation $\hat{a}^\dagger$ operators, which is approached in Appendix B there we also describe the Jaynes-Cummings model, common in quantum optics [65] [70] and that builds on a closed two-level model, in energy representation, for the coupled electron-photon problem as shown in Appendix C and which will be useful to interpret the numerical results of the RTD in Section 6. The reason why we prefer the $xq$-representation in (35) will become evident in the next section, where the Bohmian viewpoint is presented.

Let us now discuss what type of solutions can be expected from (35). One can define the single-electron eigenstates $\phi_n^{(e)}(x)$, $n = 1...N_e$, as solution of the Hamiltonian

$$ H_e = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V_e(x, t). $$

(36)

In our electron device scenario, understood as an open system, the Landauer scattering states are such eigenstates. In a closed system as we discuss in Appendices B and C one could consider that only the $n = 0$ and $n = 1$ states, for the ground and excited state respectively, are relevant. In the RTD considered here, as an open system, the number of electron eigenstates is, in principle, infinite. On the other hand, the field Hamiltonian,

$$ H_\omega = -\frac{\hbar^2}{2} \frac{\partial^2}{\partial q^2} + \frac{\omega^2}{2} q^2, $$

(37)

is that of an harmonic oscillator, whose eigenstates $\phi_m^{(\omega)}(q)$, $m = 1...N_\omega$, are well-known (e.g. the Fock number basis),
with energies $\hbar \omega (m + 1/2)$. In fact, for each given harmonic mode (here we focus on a single mode cavity), each discrete excitation is a photon of the quantum field. As such, a general solution of (35) can be written as

$$\Psi(x, q, t) = \sum_{n} \sum_{m} c_{n,m}(t) \phi_{n}^{(x)}(x) \phi_{m}^{(q)}(q), \quad \text{(38)}$$

which can be recast into

$$\Psi(x, q, t) = \sum_{m} \Phi_{m}(x, t) \phi_{m}^{(q)}(q), \quad \text{(39)}$$
$$\Phi_{m}(x, t) = \sum_{n} c_{n,m}(t) \phi_{n}^{(x)}(x). \quad \text{(40)}$$

Using (39) in (35) and integrating out the photon degree of freedom (by multiplying by $\phi^{(q)}_{n}(q)$ and using the orthogonality of the harmonic eigenstates), one obtains

$$i \hbar \frac{\partial}{\partial t} \Phi_{n}(x, t) = [H_{c} + \hbar \omega (n + 1/2)] \Phi_{n}(x, t) + \alpha x \sqrt{n+1} \Phi_{n+1}(x, t) + \sqrt{n} \Phi_{n-1}(x, t), \quad \text{(41)}$$

with $\alpha = \alpha \sqrt{\hbar / (2m)}$ (the units of $\alpha$ are energy divided by length). Equation (41) explicates how the interaction term,

$$H_{I} = \alpha x q, \quad \text{(42)}$$

introduces a set of coupled equations for the electron dynamics, each one referring to a specific photon number and connected to two neighboring states. So, if one assumes that, in our single mode model, only two consecutive photon states are relevant, say, $l$ and $l+1$ for any $l$, (39) reads

$$\Psi(x, q, t) = \Phi_{l}(x, t) \phi_{l}^{(q)}(q) + \Phi_{l+1}(x, t) \phi_{l+1}^{(q)}(q), \quad \text{(43)}$$

while (41) yields

$$i \hbar \frac{\partial}{\partial t} \Phi_{l}(x, t) = \left[ H_{c} + \hbar \omega (l + 1/2) \right] \Phi_{l}(x, t) + \sqrt{l+1} \alpha x \Phi_{l+1}(x, t), \quad \text{(44a)}$$
$$i \hbar \frac{\partial}{\partial t} \Phi_{l+1}(x, t) = \left[ H_{c} + \hbar \omega (l + 3/2) \right] \Phi_{l+1}(x, t) + \sqrt{l} \alpha x \Phi_{l}(x, t). \quad \text{(44b)}$$

As such, (44a) and (44b) describe processes involving emission ($l \rightarrow l+1$) and absorption ($l+1 \rightarrow l$) of a photon. Results for the particular case, $l = 0$, are shown in Section 3 (and in Appendix D for a closed system).

### 3.4 Bohmian quantum solution

According to the orthodox theory, the wave function $\Psi(x, q, t)$ solution of (35) provides the evolution of the system while it is not being measured. The measurement requires the introduction of collapse as an additional element of state evolution (22). There are, however, other formulations of quantum phenomena where the measurements do not need to be introduced in an ad-hoc manner and the evolution of both electrons and electromagnetic fields are always given by (35).

One of such formulations is the Bohmian theory [71, 73, 83], where the position of the electron and the amplitude of the electromagnetic field are taken as well-defined at all times (with or without measurements), and given by $x(t)$ and $q(t)$ respectively. Then, from a computational point of view, the evaluation of the displacement current at THz frequencies can be done in a natural way without invoking the collapse, as it will be shown in Section 4.

The unitary evolution of $\Psi(x, q, t)$ in (35) ensures that there is a global conservation of probability [71]. In fact, a straightforward manipulation of (35) shows that the probability locally conserved through the continuity equation,

$$0 = \frac{\partial |\Psi|^{2}}{\partial t} + \frac{\partial J_{c}}{\partial x} + \frac{\partial J_{q}}{\partial q}, \quad \text{(45)}$$

where $J_{c} = J_{c}(x, q, t)$ is the particle current linked to the electron velocity

$$v_{x} \equiv \frac{v_{x}(x, q, t)}{|\Psi(x, q, t)|^{2}} = \frac{J_{c}(x, q, t)}{|\Psi(x, q, t)|^{2}} = \frac{1}{m^{*}} \frac{\partial S(x, q, t)}{\partial x}, \quad \text{(46)}$$

while $J_{q} = J_{q}(x, q, t)$ is the single-mode current in the $q$-space of the electromagnetic field, whose velocity is

$$v_{q} \equiv v_{q}(x, q, t) = \frac{J_{q}(x, q, t)}{|\Psi(x, q, t)|^{2}} = \frac{\partial S(x, q, t)}{\partial q}. \quad \text{(47)}$$

In these expressions we have rewritten the complex wave function in polar form, $\Psi(x, q, t) = R(x, q, t) e^{i S(x, q, t)/\hbar}$, with $R$ and $S$ real functions. From such velocities it is straightforward to redefine the coupled trajectories

$$x^{j}(t) = x^{j}(0) + \int_{0}^{t} v_{x}(x^{j}(t'), q^{j}(t'), t') dt', \quad \text{(48a)}$$
$$q^{j}(t) = q^{j}(0) + \int_{0}^{t} v_{q}(x^{j}(t'), q^{j}(t'), t') dt'. \quad \text{(48b)}$$

The superindex $j$ specifies the initial variables $x^{j}(0)$ and $q^{j}(0)$, that are different in each experiment. Since all experiments are considered to be described by the same identically prepared wave function $\Psi(x, q, 0)$, the distribution of the different values $x^{j}(0)$ and $q^{j}(0)$ has to be consistent with $|\Psi(x, q, 0)|^{2}$. In fact, it can be demonstrated that for a large number $M \rightarrow \infty$, of experiments, at any time $t$ the identity [72]

$$|\Psi(x, q, t)|^{2} = \lim_{M \rightarrow \infty} \sum_{j=1}^{M} \delta(x - x^{j}(t)) \delta(q - q^{j}(t)) \quad \text{(49)}$$

is satisfied. Similarly, the particle current density in (45) can be written as

$$J_{c}(x, q, t) = \lim_{M \rightarrow \infty} \sum_{j=1}^{M} v_{x}(x^{j}(t)) \delta(q - q^{j}(t)). \quad \text{(50)}$$

An identical expression holds for $J_{q}(x, q, t)$ in terms of $v_{q}$. Notice that $x^{j}(t)$ is really a trajectory in the physical space, while $q^{j}(t)$ is just a trajectory in the (abstract) space of the
amplitude of the electromagnetic field. Since we are describing here a system with one electron and one electromagnetic mode, the sum over $M$ in (19) and (50) is different from the sum over $N$ in (5) and (8). The former (superindex $j$) is a sum over $M$ experiments in a system with only two degrees of freedom $x$ and $q$, while the latter (subindex $j$) is a sum over a system with $N$ degrees of freedom in a single experiment. This discussion will be important in next section when we compute the displacement current in a RTD with $N$ electrons simultaneously in each experiment.

4 Displacement current in nanodevices

After discussing the equation of motion for an electron and a single mode electromagnetic field in a quantum scenario, we can compute the total current in (17) under the Darwin approximation when $N$ particles are involved. In particular, we will show that the Ramo-Shockley-Pellegrini theorem [84] [86] allows the computation of the total current in a quite simple manner.

4.1 The Ramo-Shockley-Pellegrini theorem

We consider an arbitrary volume $\Omega$ with length $L_\Omega$, height $H_\Omega$, and width $W_\Omega$ as depicted in Fig. 1(a), limited by a closed surface $\mathcal{S}$ which, in turn, is composed of six rectangular surfaces $\mathcal{S} = \{S_1, ..., S_N\}$. Notice that $\Omega$ is not a physical volume, but just an arbitrary mathematical volume used in the computation of the displacement current (black dashed lines in Fig 1(a)). The total current $I_\Omega(t) = \int_{\mathcal{S}} J(x, t) \cdot ds$ is computed on one of the surfaces $\mathcal{S}_\eta$. We define a set of functions (one for each particular surface $\mathcal{S}_\eta$) as scalar functions $G_\eta(r)$ and vector functions $F_\eta(r)$ through

$$F_\eta(r) = -\nabla G_\eta(r),$$

and fulfilling

$$\nabla \cdot [\epsilon_0 F_\eta(r)] = -\nabla \cdot [\epsilon_0 \nabla G_\eta(r)] = 0.$$  

For reasons that will be later clear, the following particular Dirichlet boundary conditions on the definition of $G_\eta(r)$,

$$G_\eta(r) = 1 \ \forall r \in \mathcal{S}_\eta \ \text{and} \ G_\eta(r) = 0 \ \forall r \in \mathcal{S}\eta' \neq \eta,$$

are considered, meaning that $G_\eta(r) = 1$ on the surface $\mathcal{S}_\eta$ and zero on the other surfaces. With (52) and (53), the total current $I_\eta(t)$ on $\mathcal{S}_\eta$ can be written as

$$I_\eta(t) = \int_{\mathcal{S}} G_\eta(r) J(r, t) \cdot ds = -\int_{\Omega} F_\eta(r) \cdot J(r, t) dv.$$  

Then, from the total current density in (17) under the Darwin approximation we get

$$I_\eta(t) = -\int_{\Omega} F_\eta(r) \cdot J_x(r, t) dv + \epsilon_0 \int_{\Omega} F_\eta(r) \cdot \frac{\partial U(r, t)}{\partial t} dv.$$  

Notice that the the first term cannot be identified with the particle current only, because it includes the displacement current too. From [8] plugged into the first term of right hand side of (54), we see that an electron far from the surface $\mathcal{S}_\eta$ has a contribution to the total current given by $e v(t_j(t), t) \cdot F_\eta(r_j(t))$. Such contribution cannot be the particle current because the electron is not crossing the surface $\mathcal{S}_\eta$, so that it is displacement current. The last term can be rewritten as

$$\int_{\Omega} F_\eta(r) \cdot \frac{\partial U(r, t)}{\partial t} dv = \int_{\mathcal{S}} \frac{dU(r, t)}{dt} F_\eta(r) \cdot ds \approx 0,$$

which we consider negligible by assuming that the volume $\Omega$ is large enough so that the surfaces $\mathcal{S} = \{S_1, ..., S_N\}$ are either touching the metallic reservoirs that connect the active region or are located very far from the active region or contacts, as depicted in the volume $\Omega$ in Fig 1(a). Thus, finally, we get that the total current in the surface $\mathcal{S}_\eta$ can be computed as

$$I_\eta(t) = -\int_{\Omega} F_\eta(r) \cdot J_x(r, t) dv,$$

which depends on the particle current density $J_x(r, t)$ in (8). This expression is a well-known expression found by Ramo [83], Shockley [85], and later by Pellegrini [86]. We consider now the current described from (8) to obtain

$$I_\eta(t) = -e \sum_{j=1}^{N} F_\eta(r_j(t)) \cdot \nu_j(t),$$

where $\nu_j(t)$ is the Bohmian velocity of the $j$ particle in our $N$ particle system. Notice that, because of the spatial integral in (55) over the volume $\Omega$, the symbol $N$ does only take into account the electrons inside the volume $\Omega$ at time $t$. Now we consider, as seen in Fig. 1(a), that the lateral dimensions of $\Omega$ are much larger than the transport direction, $L_\Omega \ll H_\Omega, W_\Omega$. As such, from (52), it can be shown that $F_\eta(r) = -\frac{1}{\epsilon} \hat{x}$ and then (55) becomes

$$I_\eta(t) = e \sum_{j=1}^{N} \nu_j(t) \cdot \hat{x}. $$

when $\eta$ is considered as the surface, of the volume $\Omega$, which is perpendicular to the transport direction $\hat{x}$ and closer to the ammeter. If $\eta$ was the other perpendicular surface, for symmetry, we will get just $F_\eta(r) = \frac{1}{\epsilon} \hat{x}$ meaning that the total current entering for one perpendicular surface is the same as the total current leaving the other perpendicular surface. This is the typical scenario for a two-contact device considered here. Hereafter, we will eliminate the subindex $\eta$ from the current by understanding that we refer to the current in any of the two perpendicular surfaces.

4.2 Displacement current coefficient

The transmission coefficient $T$ is the typical link between the macroscopic current in the device and the microscopic dynamics of the electrons. However, it assumes that the potential profile is constant during all the time $\tau$ that the electron takes to traverse the active region (typically a tunneling region). Such approximation is valid as far as the external frequencies $f$ involved in the performance of the device are much smaller than $1/\tau$. At THz frequencies we can no longer assume that $f \ll 1/\tau$ and the link of the current with the transmission coefficient can be misleading. Another way of understanding
Thus, inside the active region. The integral on a fixed central position is not present at time \( t \)= 0 will see different time evolutions of \( \Psi(x,q,t;\tau_i,E) \), so that the wave packet injected at \( E \) or at \( E \) \( t \) or at \( E \) \( t \) or at \( E \) \( t \) evolves [87–91]. We consider the double barrier static potential \( V(x,t) \) and \( V(x,t) \) or AC \( \omega \) frequency \( \Omega \). The underlines that superindex \( f \) is the external frequency of the potential, which affects \( \psi(x,q,t;\tau_i,E) \) and derived Hamiltonians, as we will see in the numerical results. We define the displacement current coefficient \( D \) as the quotient between the current \( I^{(f)}(t) \) in [59] and the current injected from the contact \( e\Omega(E) \), that is

\[
D^{(f)}(E,t) = \frac{I^{(f)}(t,E)}{e\Omega(E)} \tag{60}
\]

which takes the role of the transmission coefficient \( T \) for scenarios where \( V_e(x,t) \) varies in time intervals comparable to the electron transit time, i.e., when \( \Psi(x,q,t;\tau_i,E) \neq \Psi(x,q,0;\tau_i,E) \).

For time-independent scenarios where \( V_e(x,t) \approx V_e(x) \) we can assume \( \Psi(x,q,t;\tau_i,E) = \Psi(x,q,t;\tau_i,E) \), and then \( J_e(x,q,t;\tau_i,E) = J_e(x,q,t;\tau_i,E) \), so that \( 60 \) can be rewritten with a change of variables \( t' = t - t \) as

\[
D^{(f)}(E,t) = \frac{1}{L} \int_{-L/2}^{L/2} dx \int_{-\infty}^{\infty} dq \int_{0}^{\infty} dt' J_e(x,q,t';0,E) \tag{61}
\]

which provides a time-independent displacement current coefficient. The transmission coefficient \( T(E) \) is defined, independently of \( D^{(f)}(E,t) \), as

\[
T(E) = \int_{-\infty}^{\infty} dq \int_{0}^{\infty} dt J_e(x,q,t;0,E) \tag{62}
\]

which is independent on any \( x \) in the active region because, at \( t = 0 \), the wave packet was located far from such region and, at \( t \to \infty \), it has been either fully transmitted or reflected, with zero probability in the active region. Notice that \( T(E) \) does not depend on time, while in general \( D^{(f)}(E,t) \) does.

To reach the final result one has to consider all types of wave packets involved in the transport, e.g., one has to include all relevant central energies. From [60] the total current in [59], when taking into account all relevant energies, can be written in a Landauer-like shape as

\[
I^{(f)}(t) = \int_{-\infty}^{\infty} dE T(E) \cdot f_{EF}(E) \cdot D^{(f)}(E,t) \tag{63}
\]

where \( f_{EF}(E) \) is the Fermi distribution function and \( T(E) \) is the density of states. We consider positive energy for electrons injected from the left, and negative from the right. The superindex \( f \) is the external frequency of the potential, which underlines that \( D^{(f)}(E,t) \) can be computed in DC \( (f \ll 1/\tau) \) or AC \( (f \geq 1/\tau) \) conditions.

5 Results

Since its invention, due to its relatively easy fabrication, the RTD has been the prototypical tunneling device where new physical phenomena are predicted and experimentally explored [57,91]. We consider the double barrier static potential \( V_e(x) = V_e(x,t) \) of Fig. 2(a) as a sketch of our RTD.
Later on, in Section 5.3, we will include a time-dependent external signal to the potential profile of this structure. The barrier width is 2 nm, the symmetric well length is \( L_W = 16 \) nm and the barrier height is 500 meV. These parameters and potential profile are typical of a RTD built with InGaAs for the well and AlAs for the barriers. For simplicity we consider only one effective mass \( m^* = 0.041 m_0 \), where \( m_0 \) is the mass of the electron in free space. The transmission coefficient \( T(E) \) in Fig. 2(b) shows two resonant energies, \( E_0 = \hbar \omega_0 = 28 \) meV and \( E_1 = \hbar \omega_1 = 106 \) meV, whose separation \( \hbar \omega_c = E_1 - E_0 = 78 \) meV is linked to a resonant oscillation frequency \( \nu = \omega_c/(2\pi) \approx 18.8 \) THz. As mentioned in our introduction, the effect of the electromagnetic field on the electric current in such devices has been studied through simple collision/scattering models that account for spontaneous emission and absorption processes, neglecting the coherence of electron and electromagnetic fields. In this work, on the contrary, we want to explore the effect of the electromagnetic field on the total current by taking into account a full quantum treatment with back action.

The transverse fields we consider are defined by ground (zero photon) \( \phi_0^{(0)}(q) \) and first excited (one photon) \( \phi_1^{(1)}(q) \) states, meaning that we take \( l = 0 \) in \( 43 \), and the electron-photon state can be written as

\[
\Psi(x, q, t) = \Phi_0(x, t)\phi_0^{(1)}(q) + \Phi_1(x, t)\phi_1^{(1)}(q),
\]

where \( \Phi_0(x, 0) \) and \( \Phi_1(x, 0) \) are initial Gaussian electron wave packets deep inside the reservoirs (with no probability presence in the active region) with spatial dispersion \( \sigma_x = 150 \) nm and initial central position \( x_{left} = 3.5 \sigma_x \) from the active region, as shown schematically in Fig. 1(b). The spatial uncertainty corresponds to standard deviation of the energy distribution (in the initial flat potential) of around 5 meV, such that each initial electron wave packet has a well-defined \( E \). The evolution of \( 64 \) implies the solution of the two coupled Schrödinger-like equations from \( 44 \) with \( l = 0 \),

\[
\begin{align*}
    i\hbar \frac{\partial}{\partial t} \Phi_0(x, t) &= \left[ H_e + \frac{\hbar \omega}{2} \right] \Phi_0(x, t) + \bar{\alpha} x \Phi_1(x, t), \\
    i\hbar \frac{\partial}{\partial t} \Phi_1(x, t) &= \left[ H_e + \frac{3\hbar \omega}{2} \right] \Phi_1(x, t) + \bar{\alpha} x \Phi_0(x, t),
\end{align*}
\]

since for \( l = 0 \) one can write \( \bar{\alpha} = \frac{l+1}{\sqrt{l+1}} \). As seen in Fig. 1(b), the simulation box for both wave packets is 2 \( \mu \)m, much larger than the active region. We emphasize that the numerical simulation has physical meaning only inside the active region. The time-evolution done inside the simulation box, but outside the active region, has to be understood as a mathematical technique to get correct boundary conditions at the borders of the active region (avoiding spurious reflections when electrons leave it and providing a reasonable description on what type of wave function enters it). Thus, only inside the active region we include light-matter interaction through \( H_Q \) in \( 34 \), while outside electrons just evolve following \( H_e \) in \( 36 \), decoupled from the electromagnetic fields which follow \( H_\omega \) in \( 37 \).

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**Figure 2:** (a) Potential profile of the simulated RTD device as function of position \( x \). (b) Transmission probability \( T(E) \) as defined in \( 42 \). Only ground and first excited electron states are shown at energies \( E_0 = 28 \) meV and \( E_1 = 106 \) meV.

### 5.1 Wave packet evolution for a static potential profile

From the quantum model in \( 64 \)-\( 65 \), where we take \( \bar{\alpha} = 1.33 \) meV/nm, we evolve \( \Psi(x, q, t) \) and compute the electron prob-
ability $P_Q(x,t)$ as function of time and position by integrating the degree of freedom $q$.

$$P_Q(x,t) = \int dq |\Psi(x,q,t)|^2 = |\Phi_0(x,t)|^2 + |\Phi_1(x,t)|^2.$$  (66)

We also evolve a single electron wave packet $\Psi(x,t)$ with the semiclassical model $H_S$ in \ref{eq:32}. By taking $(\alpha/\sqrt{\hbar})q_0(t) = \hat{\alpha}(\sqrt{2/\hbar})q_0(t) = 1.33\sin(\omega t)\text{meV/nm}$, we compute the probability $P_S(x,t) = |\Psi(x,t)|^2$. We underline that the oscillation of $(\alpha/\sqrt{\hbar})q_0(t)$ is related to an internal electromagnetic field that is different from the external signal that will be applied to the potential profile $V_e(x,t)$ later in Section \ref{sec:5.3}. Both models, semiclassical and quantum, are computed in a resonant case where $\omega = \omega_e$, and are compared with the no light-matter interaction probability $P_0(x,t) = |\Psi(x,t)|^2$, this last one obtained by evolving $\Psi(x,t)$ with only $H_e$ in \ref{eq:36}. In all cases, the initial energy of the electron wave packet equals the resonant electron energy $E = E_1 = 106\text{ meV}$. In the quantum case, we assume that initially only $\Phi_0(x,0)$, linked to zero photon, is present; $\Phi_1(x,t)$ will be activated through the term $\hat{\alpha}x\Phi_0(x,t)$ in \ref{eq:36}.

In Fig. \ref{fig:3}a), the no light-matter interaction probability $P_0(x,t)$, shows that inside the quantum well only the first excited state remains occupied, and the wavefunction gets mostly transmitted. Figure \ref{fig:3}b), for $P_S(x,t)$, shows two different frequencies: first, there is a fast oscillation of the charge at roughly 18.8 THz due to the resonant term $q_0(t) \approx \sin(\omega_e t)$ in $H_S$ in \ref{eq:32}, which is adiabatically activated when the wave packet enters the well; second, there is a slower natural oscillation, the so-called Rabi oscillation.

By comparing the closed system in \ref{eq:74} with \ref{eq:32}, we can identify $\hbar\gamma_S \sin(\omega t) \approx 1.33 \sin(\omega t) |d_x|$, with the dipole $|d_x| \approx 2.9\text{ nm}$ estimated in Appendix \ref{app:D} for a symmetric infinite well with same $L_W$. With such values, the theoretical Rabi frequency predicted in Appendix \ref{app:A} is $\gamma_S \approx 5.8\text{ THz}$, which approaches the numerical one seen in Fig. \ref{fig:3}b).

On the other hand, for the quantum case $P_Q(x,t)$ in Fig. \ref{fig:3}c), only the Rabi oscillation seems to play a role by periodically transitioning between the two RTD states with a frequency that is the double of the semiclassical one. Notice that, by comparing the closed system in \ref{eq:34} with \ref{eq:36}, we have $\hbar\gamma \approx 1.33|d_x|$, yielding $\gamma \approx 5.8\text{ THz}$ from the same previous value of $|d_x|$. However, the Rabi oscillation in the quantum case (see Appendix \ref{app:B}) is $\gamma_{m=0} = 2\sqrt{m+1}\gamma \approx 11.6\text{ THz}$, which is confirmed by the fact that such natural oscillation in the quantum model in Fig. \ref{fig:3}c) is twice the oscillation of the semiclassical model in Fig. \ref{fig:3}b). On the other hand, we notice the absence of the fast resonant $\omega = \omega_e$ oscillations. Electrons do not evolve as a superposition of such eigenstates $E_{n,0,1}$ of $H_e$ but instead of the eigenstates $E_{\pm}$ of $H_Q$, the so-called light-dressed states of matter, as explained in Appendix \ref{app:C}. The behavior of Figs. \ref{fig:3}b) and \ref{fig:3}c) can be explained with the (closed system) models described respectively in Appendices \ref{app:A} and \ref{app:B} (with the results plotted in Appendix \ref{app:D}).

Figure 3: (a) Evolution of $P_0(x,t)$ from no light-matter interaction Hamiltonian $H_e$ in \ref{eq:34}. (b) Evolution of $P_S(x,t)$ from the semiclassical equation of motion $H_S$ in \ref{eq:32}. (c) Evolution of $P_Q(x,t)$ from the quantum equation of motion $H_Q$ in \ref{eq:34}, or to be more precise the simplified version of $H_Q$ \ref{eq:34}. Each one interacting with the double barrier structure shown in Fig. \ref{fig:2}a).
5.2 Transmission coefficient for a static potential profile

We now address the transmission coefficient $T(E)$ from for the same profile $V_e(x)$ in Fig. 2(a), with same parameters of Fig. 3 and once more with $\Phi_0(x,0)$ as the initial wave packet in the quantum scenario. Following the same situations as described by $P_{0,S,Q}(x,t)$ in the previous section, we compare the three scenarios for $T(E)$, that is, $T_0(E)$, $T_S(E)$, and $T_Q(E)$, which refer respectively to no light-matter, semiclassical, and quantum interaction scenarios.

In Fig. 4(a) we compare $T_0(E)$ (black) with $T_S(E)$ (red, resonant $\omega = \omega_e$). No important differences are observed, apart from a higher transmission coefficient for $T_S(E)$. This small difference can be explained knowing that in this semiclassical picture the bottom of the well is oscillating, at $\nu \approx 18.8$ THz, so that electrons with an initial low energy $E$ are, at some times, aligned with the resonant energies of the well, and this provides more transmission than with a $\nu = 0$ potential.

In Fig. 4(b) we compare $T_Q(E)$ (black) with $T_Q(E)$ (in red for the resonant $\omega = \omega_e$ and in blue for the nonresonant $\omega = 0.01 \omega_e$). The striking new feature is the appearance, for the resonant photon case (red), of two peaks around the second resonant RTD energy of the no light-matter interaction case; the reason can qualitatively be understood from the arguments mentioned in Appendix C. The light-dressed eigenstates $E_{\pm}$ of $H_Q$ are not the same as $E_{0,1}$ of $H_e$, and have, at resonance, an avoided crossing $E_+ - E_- \approx 2\hbar \gamma_{m=0}$; since $\gamma_{m=0} \approx 11.6$ THz in our system, such energy spacing is roughly 15 meV. The energy difference of that double peak in Fig. 4(b) is a bit larger due to the role of the finite height barriers and the following broadening of the states.

This double-peak feature does not occur for the nonresonant photon (blue) in Fig. 4(b) because of lack of conservation of energy, since the initial $E_1 + h\omega/2$ and final $E_0 + 3h\omega/2$ energy states are near-degenerate only if $\omega \approx \omega_e$. As discussed in Appendix C away from resonance the coupling term, whose strength is given by $\alpha$, is not able to correlate such doublet states, and the avoided crossing is not observed.

Notice that no such double-peak splitting appears in the first resonant RTD level (for both red and blue lines), since the initial energy related to $\Phi_0(x,0)$ is so low that it cannot activate $\Phi_1(x,0)$, which requires an increment of $h\omega_e = 78$ meV; in other words, $\Phi_0(x,0)$ evolves as if $H_Q \approx H_e$ since $\Phi_1(x,0) \approx 0$. Such energy conservation restriction applies only to the case when $l = 0$ photons are involved at the beginning of the simulation; for $l \neq 0$ the electromagnetic field has enough energy to allow $\Phi_l(x,0)$ to create $\Phi_{l+1}(x,0)$. So, in general, such level splitting feature will occur for any resonant RTD state in the well.

In Fig. 4(c) we show the same study as in Fig. 4(b) for photons with different frequencies. In general, by looking at the eigenenergies of the simulation box for $H_e$ (quantum...
As such, the conduction band ing an additional oscillating external potential seen at 145 meV. In other words, the eigenstates of this system. Another additional peak related to the resonant energies above the window plotted in Fig. 4(c), so that we only see the photon eigenstate with an initial electron energy given by \( E_{\omega} \). This means that the new energy eigenvalues of the whole electron and electromagnetic system, when the double-peak splitting seen in Fig. 4(b) is not relevant, that is, away from resonance, are roughly given by \( E_0 + \hbar \omega/2, E_1 + \hbar \omega/2 \) and \( E_1 + 3\hbar \omega/2 \). Notice also that the injection energy in the horizontal axis of Fig. 3 is not the total energy, but only the initial electron energy \( E \). Since the initial global wave function \( \Psi(x,q,0) = \Phi_0(x,t)\phi_0^{(e)}(q) \) has zero photons \( \phi_0^{(e)}(q) \), the initial electromagnetic energy is \( \hbar \omega/2 \), so that the total initial energy is just \( E + \hbar \omega/2 \), and if we want to represent Fig. 4 as function of the total energy we could simply add \( \hbar \omega/2 \) to the horizontal axis. The green line in Fig. 4(c) shows the result when the photon frequency is \( \omega = 2 \omega_c \). This means that \( E_0 + 3\hbar \omega/2 \) and \( E_1 + 3\hbar \omega/2 \) energies are above the window plotted in Fig. 4(c), so that we only see the resonant energies \( E_0 + \hbar \omega/2 \) and \( E_1 + \hbar \omega/2 \). The blue line in Fig. 4(c) shows the case \( \omega = \omega_c/2 \). Now, we see a new peak at \( \approx 67 \text{meV} \), which corresponds to the electron-photons eigenstate with an initial electron energy given by \( E_0 + \hbar \omega = 28 \text{meV} + \hbar \omega = 67 \text{meV} \). We have subtracted the energy of the vacuum state of the electromagnetic field). Another additional peak related to \( E_1 + 3\hbar \omega/2 \) is also seen at 145 meV. In other words, the eigenstates of this system, as mentioned in [25], are not the electron energy eigenstates of the quantum well, but are the electron-photons eigenstates coming from both the quantum well and the harmonic oscillator.

### 5.3 Displacement current coefficient \( D^{(f)}(E,t) \) in oscillating potential profiles

We now include in our model an external battery providing an additional oscillating external potential \( V_{\text{ext}}(t) = V_A \cos(2\pi f t + \Theta_i) \) at the drain side of the active region. As such the conduction band \( V_c(x,t) \) of the RTD device becomes time-dependent,

\[
V_c(x,t) = V_c(x) + V_A \cos(2\pi f t + \Theta_i) \frac{x + L/2}{L},
\]

where we have defined \( V_c(x) \) as the static potential profile seen in Fig. 4(a), and we will consider values of \( f \) ranging from 0.2 THz to 2 THz; the role of the phase \( \Theta_i \) will be explained later. Notice that \( V_{\text{in}}(t) \) has no relation at all with the semiclassical oscillation \( q_{\text{osc}}(t) \) present in \( H_S \). The former is an external signal applied to the device while the latter provides the light-matter interaction. The term \( \frac{x + L/2}{L} \) in [67] is an ad-hoc interpolation of what would be the potential profile solution of Gauss’ equation in [11] if all the electron charges in [15] were considered. This self-consistent procedure between the charge and the scalar potential is avoided here because it would not provide any conceptually different conclusion. Gauss’ law deals only with the longitudinal electric field, while in this paper we are interested in the effects of the transverse electromagnetic fields on the displacement current. As noticed previously, in the Coulomb gauge, the scalar potential \( V_c(x,t) \) is linked to the longitudinal electrical field that does not need any quantization procedure, as opposed to the transverse field [74, 77]. In all the following cases, we consider the electron injection energy as \( E = 106 \text{meV} \), which corresponds to the maximum transmission of the second resonant energy for \( T_0(E) \) and \( T_0(E) \) in Fig. 4(a), and to the minimum of transmission in the quantum case in resonance for \( T_0(E) \). This also means that the initial state will be \( \Psi(x,q,0) = \Phi_0(x,t)\phi_0^{(e)}(q) \).

To understand how we will represent \( D^{(f)}(E,t) \), we briefly introduce the concept of complex small-signal conductance \( Y_{11}(f) \). This is typical in the study of high-frequency electron devices, and it is defined by

\[
(I_R^{(f)}(t) - I_{DC}) + i(I_I^{(f)}(t) - I_{DC}) = Y_{11}(f)V_A e^{i2\pi ft},
\]

where \( I_R(t) \) and \( I_I(t) \) are respectively the device current when the external voltage is \( V_A \cos(2\pi f t) \) and \( V_A \cos(2\pi f t + \pi/2) \). The two external signals can be represented by a unique \( V_A \cos(2\pi f t + \Theta_i) \) with \( \Theta_i = 0 \) for \( I_R(t) \) and \( \Theta_i = -\pi/2 \) for \( I_I(t) \). In both cases we subtract \( I_{DC} \) to deal with a small signal analysis. We define the real and imaginary parts of the conductance \( Y_{11}(f) = Re(Y_{11}(f)) + i Im(Y_{11}(f)) \), as

\[
Y_{11}(f) = \left( \frac{I_R^{(f)}(0) - I_{DC}}{V_A} \right) + i \left( \frac{I_I^{(f)}(0) - I_{DC}}{V_A} \right) = \left( \frac{I_R^{(f)}(0) - I_{DC}}{V_A} \right) + i \left( \frac{I_I^{(f)}(0) - I_{DC}}{V_A} \right).
\]

In principle, the computation of \( I^{(f)}(t) \) in [25] requires an energy integral of \( D^{(f)}(E,t) \). However, for simplicity, we have considered here that the current is due to just a flux of electrons, with different initial times, injected from the left all at the same energy \( E \). Thus, the energy integral is ignored and only the integrals on \( x, q \) and \( t_i \) are explicitly computed to evaluate \( D^{(f)}(E,t) \). As such we identify \( I^{(f)}(t) \rightarrow D^{(f)}(E,t) \) and \( I_{DC} = T(E) \), so that

\[
Re(Y_{11}(f)) = \left( \frac{D_0^{(f)}(E,0) - T(E)}{V_A} \right),
\]

\[
Im(Y_{11}(f)) = \left( \frac{D^{(f)}(-\pi/2,0) - T(E)}{V_A} \right).
\]

As we will see in the results below, when the small-signal implies a finite small value of \( V_A \) (but not infinitesimally small), the electron device is not linear at very high frequencies [30]. In a linear system, one can anticipate the output values \( D^{(f)}(E,0) = -D^{(f)}(E,0) \) for \( \Theta_i = 0 \) and \( \Theta_i = -\pi \), because the input values satisfy \( \cos(2\pi f t - \pi) = -\cos(2\pi f t) \). However, we will see that the condition \( D^{(f)}(E,0) = -D^{(f)}(E,0) \) is not valid for all frequencies in our RTD, because this device is not linear at THz frequencies. For more details about the possibilities opened by the use of non-linearity in high frequency nanodevices, see Ref. [50].

Since we are only interested in \( t = 0 \) and only one \( E \) is involved, hereafter we will not write explicitly their dependence (unless needed). We analyze below the dependence of \( D^{(f)} \) on \( f \) for the three scenarios discussed so far, that is, no light-matter, semiclassical, and quantum interactions,
which we will refer to as $D_{0,\epsilon_1}^{(j)}$, $D_{S,\epsilon_1}^{(j)}$, and $D_{Q,\epsilon_1}^{(j)}$, respectively. For each scenario, we consider three different phases $\Theta_i = 0, -\pi/2, -\pi$.

The key point to understand the following results is, as discussed in Section 4, that the current measured at time $t = 0$ is due to a flux of electrons that have entered in the active region in the time interval $[0 - \tau, 0]$, being $\tau$ the (average) electron transit time. Thus, the last electron entering the active region at time $t$ has seen only the external potential $V_{e}(x, 0)$, while the first electron entering it at time $0 - \tau$ has seen the time evolution of the potential profile from $V_{e}(x, 0 - \tau)$ until $V_{e}(x, 0)$. If the external frequency $f$ is smaller than the inverse of the electron transit time, then there is no big difference between $V_{e}(x, t)$ and $V_{e}(x, t - \tau)$. Thus, all electrons see the same potential profile while traversing the active region because they evolve much faster than the rate of change of the external signal. This in electronic devices is the typical scenario where $D^{(j)}(E, t) \rightarrow T(E)$, as mentioned in [61].

Then, the displacement current discussed in this paper has no big role in such a regime.

On the contrary, for $\tau \approx 1/f$, the evolution of $V_{e}(x, t)$ in the time interval $[0 - \tau, 0]$ is relevant for the value of the current measured at time $t = 0$. One can say that the electrons entering at time $0 - \tau$ have a memory about the evolution of the potential profile before $t = 0$. The electric current at $t = 0$ does not only depend on the voltage at time $t = 0$, but also on the voltages at previous times. So, in this scenario, it is mainly the displacement current of electrons that controls the measured electric current, and one gets novel results, since $D^{(j)} \neq T$.

Figure 4 shows $D^{(j)}$ for three phases with an external frequency $f$ running from 0.2 THz to 2 THz. Similar to what happens with $T(E)$ in Fig. 4 the semiclassical and no-light-matter interaction results have similar tendencies, while the behavior of the quantum case is quite different. For $\Theta_i = -\pi/2$, we get $D^{(j)}_{-\pi/2} \approx 0$ at low frequencies in the three scenarios, since the potential profile in (67) becomes $V_{e}(x, 0) = V_{e}(x)$ because $V_{A} \cos(-\pi/2) = 0$. So, as indicated in (61), we get $D^{(j)}_{-\pi/2} \approx T(E)$ at low frequencies. When $f \approx 1/\tau$, the coefficients $D^{(j)}_{0, -\pi/2}$ and $D^{(j)}_{S, -\pi/2}$ tend to decrease as the frequency increases. The reason is that the applied signal respects the relationship $V_{A} \cos(2\pi f (0 - \tau - \pi/2) < V_{A} \cos(0 - \pi/2) = 0$, so that the electrons entering at time $0 - \tau$ have a tendency to provide lower current (even at $t = 0$) because they have seen a negative voltage increment at the drain (positive conduction band increment in the drain). Another way of understanding this increment of the current for electrons injected at $0 - \tau$ is that a higher conduction band in the drain corresponds to looking for the transmission coefficient in energies lower than 106 meV in Fig. 4 which implies lower current (transmission). On the contrary $D^{(j)}_{-\pi/2}$ increases because here, any negative applied voltage in the drain (increment of the conduction band in the drain) corresponds to looking for transmission at energies lower than 106 meV which implies, now, higher current (transmission) because $E = 106$ meV is the energy for the minimum of $T(E)$ for the red curve in Fig. 4. Then, applying a negative small voltage in the potential profile implies that now $E = 106$ meV is no longer the energy corresponding to the minimum of transmission, so that $D^{(j)}_{Q, -\pi/2} > T(E)$ in (69).

For $\Theta_i = 0$, at low frequency, we get $D^{(j)}_{0}$ negative for the non-interacting $D^{(j)}_{0,0}$ and semiclassical $D^{(j)}_{S,0}$ cases. Now, at low frequency, we have $V_{A} \cos(0) = V_{A} > 0$ so that the electrons at energy $E = 106$ meV see a positive applied voltage (negative conduction band increment in the drain) that corresponds to looking for a transmission coefficient at higher energies in Fig. 4. Thus, we get less transmission because now $E = 106$ meV is no longer the resonant energy (maximum transmission). For the quantum case $D^{(j)}_{Q,0}$ the situation is just the contrary than for $D^{(j)}_{0,0}$ and $D^{(j)}_{S,0}$ because the applied bias implies that $E = 106$ meV is no longer a minimum of transmission so that $D^{(j)}_{Q,0} > T(E)$ in (69). The tendency of $D^{(j)}_{0}$ when the frequency $f$ is increased is just the contrary to what was explained for $D^{(j)}_{-\pi/2}$. Now, $V_{A} \cos(2\pi f (0 - \tau))$ has a positive voltage, but smaller than $V_{A} \cos(0) = V_{A}$ so less current is expected from electrons injected at $0 - \tau$ than from the ones injected at $t = 0$ for $D^{(j)}_{0, -\pi/2}$ and $D^{(j)}_{S, -\pi/2}$. As before $D^{(j)}_{Q, -\pi/2}$ has an opposite tendency.

For $\Theta_i = -\pi$, the results are quite similar to the ones for $\Theta_i = 0$. The differences can be understood by noticing that $V_{A} \cos(-\pi) = -V_{A} < 0$ so that we have now a small negative applied voltage (rather than positive). Thus, we have to look for a transmission of electrons corresponding to energies lower than $E = 106$ meV in Fig. 4. So that, we can expect less transmission than when the value of the input signal was positive.
We finally notice that the qualitative arguments provided above just confirm the physical soundness of the results in Fig. 5 for low and intermediate frequencies. For much higher frequencies, the computational scenarios are quite complex (strictly speaking there are no resonant energies in a double barrier with time-dependent potential profiles), so that simple and intuitive explanations of the results are not evident. In any case, our results show that there is plenty of room for engineering new THz applications in electron devices when displacement current with coherent electron-photon interactions is taken into account.

6 Conclusions

The physical simulation of the performance of an electron device, understood as a many-body open system far from thermodynamic equilibrium, is one of the most difficult computational tasks. Thus, important simplifications are present in the history of computational electronics. A first revolution in the modeling of devices appeared thirty years ago when the classical view of electrons was substituted by a quantum perspective. In this paper, we have explored whether a second revolution is needed to change the typical classical view of electromagnetic fields by a quantum approach. Typically, for DC predictions, an electrostatic approximation is used in the modeling of electron devices, where only Gauss’ law is invoked to link the charge distribution to the longitudinal electric field. However, when we are interested in getting information on the dynamic behavior of the electron device at frequencies comparable or greater than the inverse of the electron transit time in the active region, the electrostatic approximation is no longer valid. At such frequencies, what is measured is the total current, defined as the sum of the particle plus displacement components, and not only the particle current. One solution to go beyond the electrostatic approximation is considering a time-dependent scenario, where the time-dependent charge generating time-dependent longitudinal electric fields are taken into account, to include the displacement current, but still neglecting the role of the transverse electromagnetic field.

In the Coulomb gauge, the longitudinal electric field is just a function of the electron degrees of freedom, so it does not require new degrees of freedom (neither new quantization) for its proper modeling. On the contrary, the transverse electric field and the magnetic field require their own degrees of freedom. Notice that we are not only discussing external electromagnetic fields, but also the internal ones present in the active region because electrons and electromagnetic fields share the same quantum wave function $\Psi(x,q,t)$. The spontaneous emission of light from electrons is a clear evidence of such deep connection between electrons and electromagnetic fields even when no external electromagnetic fields are applied to the RTD. In particular, in this paper we have checked if such new degrees of freedom of the electromagnetic field require classical or quantum treatment. The results on the electron transmission coefficient in a double barrier structure in Fig. 4 provide two clear answers. First, in resonance, when there is no detuning between the frequencies of the electromagnetic field and the energy separation of the involved electronic levels, a quantum treatment of the electron-photon coupling is...
required. The eigenenergies of the electron-photon system are not just the sum of the uncoupled eigenenergies of the electron system (alone) plus the photon system (alone), giving rise to (Rabi) oscillations of the charge inside the quantum well of a RTD. At such resonant frequencies, ignoring the transverse electromagnetic fields or treating them in a semiclassical way seems not accurate. On the other hand, when the detuning is nonzero and one is then in a out-of-resonance situation, the deep connection between electrons and photons is no longer relevant and simplified treatments of electrons and photons, which consider them without interaction, seems accurate enough. We have also shown that the treatment of the interaction of electrons and photons from a collision model, where electrons just gain or lose the energy of the photon according to some scattering rates, misses important phenomena present in Fig. 4 like the avoided energy crossing.

The language (and some of the modeling) used in this work for the quantum case assumes that electrons have well-defined positions in the active region, and also that the amplitude of the electromagnetic field inside the active region is well-defined. Such assumptions are not rigorous within the orthodox quantum theory because such knowledge is only real, strictly speaking, when a measuring apparatus of the amplitude of the electromagnetic field or the position of electrons in the active region is explicitly considered (the so-called eigenstate-eigenvalue-link). On the contrary, a Bohmian interpretation of such quantum phenomena [71, 73, 75] allows a rigorous justification of the language used in this paper. Identically, our use of a pure wave function do not have to be understood as a naive way of studying an open quantum system (which requires the use of the reduced density matrix in the orthodox language), because the concept of Bohmian conditional wave function shows [76] that such pure states are a perfectly valid conceptual tool to understand an open quantum system, as mentioned in Appendix E. In addition, the computational burden involved in the multi-time measurements of THz currents is minimized by invoking a Bohmian description of the light-matter interaction. We have shown that the typical transmission coefficient used to characterize DC quantum electron devices has to be substituted by a new displacement current coefficient in AC scenarios.

The main approximation done in the present paper is that the treatment of the interaction between electrons and light inside the RTD was developed for a single mode of the electromagnetic field interacting with a single electron in the conduction band (in the effective mass approximation for a semiconductor with parabolic energy-wave vector dispersion). In principle, a quantitative understanding of the phenomena described here requires a many-body generalization, with several modes and many electrons, which is far from the scope of this work and of our computing capabilities. We have pointed that the main physical phenomena explained in our work for the interaction of photons and electrons in RTDs mimic well-known results predicted by a Jaynes-Cummings model for closed light-matter systems, which are summarized in the Appendices. Thus, the present qualitative results are not surprising for the quantum optics community [89, 92], but we do believe they open an unexplored path for engineering new electron devices and new applications in the THz gap.

A Analytical solution for the semiclassical scenario in a two-level closed system

The simplest analytical model for the semiclassical Hamiltonian in (62) is obtained when the wave function \( \Psi(x,t) \) is described by a closed two-level system, with electron eigenstates \( \phi_0(x) \) (ground) and \( \phi_1(x) \) (excited) of \( H_e \). That is, by neglecting the photon degree of freedom in (65), \( \Psi(x,t) = c_0(t)\phi_0(x) + c_1(t)\phi_1(x) \). The electromagnetic field, in a single-mode approximation with frequency \( \omega \), is given by (25) when \( \mathbf{J}(k,t) = 0 \) because the semiclassical approximation assumes that matter has no backaction towards the electromagnetic field. Then its trivial solution is \( g(k,t) = |g(k,0)|e^{i\theta e^{-i\omega t}} \), so that the transverse electric field in (25) is, in dipole approximation, \( E_x(r,t) = 2N(k)\Delta k^3 |g(k,0)|/(2\pi)^{3/2}\sin(\omega t - \theta) \mathbf{x} \). The matrix representation of (62), in the energy basis of \( H_e \), with \( \phi_0(x) = \langle x|0 \rangle \) and \( \phi_1(x) = \langle x|1 \rangle \) and with energies \( \hbar\omega_0 \) and \( \hbar\omega_1 \), renders obviously \( H_e \) as the diagonal part,

\[
H_e = \hbar\omega_0|0\rangle\langle 0| + \hbar\omega_1|1\rangle\langle 1|,
\]

while the interaction Hamiltonian, as derived from \( H_I = -\varepsilon x E_x(x_0,t) \) and since \( \langle 0|x_0|0 \rangle = \langle 1|x_0|1 \rangle = 0 \), yields the off-diagonal part

\[
H_I(t) = -\hbar\gamma_S\sin(\omega t) \left| 0 \right\rangle \left\langle 1 \right| + \left| 1 \right\rangle \left\langle 0 \right|,
\]

where the so-called semi-classical Rabi frequency is \( \gamma_S = -e\varepsilon d_2N(k)\Delta k^3 |g(k,0)|/(2\pi)^{3/2} \hbar \), and we have supposed a real dipole matrix element \( d_2 = \langle 0|x_0|1 \rangle \) and \( \theta = 0 \). As such, by writing the full Hamiltonian \( H = H_e + H_I(t) \) in the \( H_e \) basis, one sees that \( H_I(t) \) may induce transitions - the Rabi oscillations - within the two-level subspace, where the full wavefunction can be written, by factoring out the energy terms, as

\[
|\Psi(t)\rangle = c_0(t)e^{-i\omega_0 t}|0\rangle + c_1(t)e^{-i\omega_1 t}|1\rangle.
\]

By using (70), (71), and (72) in the Schrödinger equation \( i\hbar d|\Psi(t)\rangle/dt = H(t)|\Psi(t)\rangle \), the coefficients evolution has analytical solutions [69, 71] given by

\[
c_0(t) = \left\{ c_0(0) \left[ \cos \left( \frac{\Omega_s t}{2} \right) + i \frac{\Delta}{\Omega_s} \sin \left( \frac{\Omega_s t}{2} \right) \right] + c_1(0) \frac{\gamma_s}{\Omega_s} \sin \left( \frac{\Omega_s t}{2} \right) \right\} e^{-i\Delta t/2},
\]

\[
c_1(t) = \left\{ c_1(0) \left[ \cos \left( \frac{\Omega_s t}{2} \right) - i \frac{\Delta}{\Omega_s} \sin \left( \frac{\Omega_s t}{2} \right) \right] + c_0(0) \frac{\gamma_s}{\Omega_s} \sin \left( \frac{\Omega_s t}{2} \right) \right\} e^{i\Delta t/2},
\]

where the new frequencies are the detuning \( \Delta = \omega_e - \omega \), with the electronic level spacing \( \omega_e = \omega_1 - \omega_0 \), and the generalized classical Rabi frequency \( \Omega_s = \sqrt{\gamma_s^2 + \Delta^2} \). The normalization of \( |\Psi(t)\rangle \) implies \( |c_0(t)|^2 + |c_1(t)|^2 = 1 \), and imposes a condition on the initial values of the coefficients. So if one starts the dynamics in the excited state, \( (c_0(0), c_1(0)) = (0, 1) \),
simplifies to
\begin{align*}
  c_0(t) &= i\gamma_S \sin\left(\frac{\Omega_S t}{2}\right) e^{-i\Delta t/2}, \\
  c_1(t) &= \left[\cos\left(\frac{\Omega_S t}{2}\right) - i\Delta \Omega_S \sin\left(\frac{\Omega S t}{2}\right)\right] e^{i\Delta t/2},
\end{align*}
\tag{74}
so that the probability of inverting the system to the ground state is 
\( P_I(t) = |c_1(t)|^2 - |c_0(t)|^2 = (\Delta^2 + \gamma_S^2 \cos(\Omega_S t))/\Omega_S^2 \); at resonance \((\Delta = 0)\) one simply has \(c_0(t) = \sin(\gamma_S t/2)\) and \(c_1(t) = \cos(\gamma_S t/2)\), such that \(P_I(t) = \cos(\gamma_S t)\) and the system gets fully inverted within oscillations as given by the Rabi frequency \(\gamma_S\). Notice the crossed terms when calculating expectation values from \(\langle \Psi(t)|H_e + H_I(t)\rangle\Psi(t)\rangle\) for each \(j\) and \(|0\rangle\langle 1|\hat{a}_j\rangle\langle 1|\hat{a}_j^\dagger\rangle\) has a similar form to \(\gamma_S\) in \(\langle \Psi(t)\rangle\), they have different origins. Out of the four terms in \(H_I\) for each \(j\), \(|0\rangle\langle 1|\hat{a}_j^\dagger\rangle\langle 1|\hat{a}_j\rangle\) stands for a transition from excited to ground electron state via emission of a photon in mode \(j\), while \(|1\rangle\langle 0|\hat{a}_j\rangle\langle 0|\hat{a}_j^\dagger\rangle\) stands for the opposite process, both conserving the total electron-photon energy. On the other hand, the terms \(|0\rangle\langle 1|\hat{a}_j\rangle\langle 1|\hat{a}_j\rangle\) (net loss) and \(|1\rangle\langle 0|\hat{a}_j^\dagger\rangle\langle 0|\hat{a}_j\rangle\) (net gain) do not conserve total energy (higher order processes): if one is not far from resonance, in the RWA spirit, they can be neglected.

Assuming a single-mode field in \(\langle \Psi(t)\rangle\) and in \(\langle \Psi(t)|\rangle\) under RWA, together with \(\langle \hat{N}|\rangle\) for the electron, the diagonal part of the full Hamiltonian \(H\) is given by the sum of the uncoupled electron and photon energies, \(H_{e\omega} = H_e + H_\omega\), that is,
\begin{align*}
  H_{e\omega} &= \hbar \omega_0 |0\rangle\langle 0| + \hbar \omega_1 |1\rangle\langle 1| + \hbar \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right),
\end{align*}
\tag{79}
while its now time-independent off-diagonal is
\begin{align*}
  H_I &= -\hbar \gamma |\langle 0|\hat{a}_j + |1\rangle\rangle\langle 1|\hat{a}_j\rangle\rangle, \tag{80}
\end{align*}
with \(\gamma \equiv \gamma_1\). The state vector \(\langle \Psi(t)\rangle\) of the full \(H = H_{e\omega} + H_I\) is a linear combination of the possible products of electron-photon states of \(H_{e\omega}\). That is, from \(\langle \Psi(t)\rangle\) in energy representation with \(\phi_{\alpha\beta}(q) = \langle q|m\rangle\) and \(n = 0, 1\), by factoring out the energy terms,
\begin{align*}
  |\Psi(t)\rangle &= \sum_m N_m \left\{ e^{-i(m+\frac{1}{2})\omega t} e^{-i\omega_0 t} c_{0,m=1}(t) |0, m+1\rangle \\
  &\quad + e^{-i(m+\frac{1}{2})\omega t} e^{-i\omega_1 t} c_{1,m}(t) |1, m\rangle \right\},
\end{align*}
\tag{81}
In writing \(\langle \Psi(t)|\rangle\) we have anticipated the fact that \(H_I\) can only induce transitions between states \(|1, m\rangle\) and \(|0, m+1\rangle\), since \(\hat{a}\) and \(\hat{a}^\dagger\) have no units. Then, the electromagnetic field Hamiltonian from \(\langle \Psi(t)|\rangle\), generalized to many modes \(j\), can be written as
\begin{align*}
  H_\omega &= \sum_j \hbar \omega_j \left(\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2}\right) = \sum_j \hbar \omega_j \left(\hat{m}_j + \frac{1}{2}\right), \tag{77}
\end{align*}
where we have used the commutation relation \(\hat{a}_j, \hat{a}_j^\dagger = \delta_{j,j'}\), and defined \(\hat{m}_j = \hat{a}_j^\dagger \hat{a}_j\) as the number of photons in mode \(j\), which also labels the eigenstates \(\{|m_j\}\) of \(H_\omega\) with eigenenergies \(\hbar \omega_j (m_j + 1/2)\). On the other hand, in the interaction term \(H_I = -e\mathbf{E}_\perp (\mathbf{r}_0, t)\), the now time-independent electric field \(\mathbf{E}_\perp (\mathbf{r}_0)\) from the dipole approximation in \(\langle \Psi(t)|\rangle\) reads \(\mathbf{E}_\perp (\mathbf{r}_0) = -\sum_j (\hat{a}_j + \hat{a}_j^\dagger) \sqrt{\frac{\hbar \omega_j \Delta k^j}{2\hbar c \epsilon_0 (2\pi)^3}} \hat{r}_j\). So, by considering the same two-level basis of \(H_e\) for the electrons as done in Appendix A in the \(|0\rangle, |1\rangle\) energy representation, \(H_I\) reads
\begin{align*}
  H_I &= -\hbar \sum_j \gamma_j |\langle 0|\hat{a}_j + |1\rangle\rangle\langle 1|\hat{a}_j\rangle\rangle.
\end{align*}
\tag{78}

B Analytical solution for the orthodox quantum scenario in a two-level closed system

In the manuscript we have employed the operators \(\sqrt{\omega}q\) and \(-i\sqrt{\omega}q\) in \(\langle \Psi(t)\rangle\) and reached a simple 2D Hamiltonian in \(\langle \Psi(t)|\rangle\). In the literature, however, the typical operators used for quantizing the electromagnetic field are the annihilation \(\hat{a}_j\) and creation \(\hat{a}_j^\dagger\) operators, defined as
\begin{align*}
  \hat{a}_j &= \frac{1}{\sqrt{2\hbar}} (q_{g,j} + i s_{g,j}), \\
  \hat{a}_j^\dagger &= \frac{1}{\sqrt{2\hbar}} (q_{g,j} - i s_{g,j}),
\end{align*}
\tag{76}
with \(q_{g,j}, s_{g,j}\) in terms of \(g(k,t)\) and \(g^*(k,t)\) for each \(j\) mode as in \(\langle \Psi(t)|\rangle\). Notice that \(\hat{a}_j\) and \(\hat{a}_j^\dagger\) have no units. Then, the electromagnetic field Hamiltonian from \(\langle \Psi(t)|\rangle\), generalized to many modes \(j\), can be written as
\begin{align*}
  H_\omega &= \sum_j \hbar \omega_j \left(\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2}\right) = \sum_j \hbar \omega_j \left(\hat{m}_j + \frac{1}{2}\right),
\end{align*}
\tag{77}
analytical solutions [69,70] given by
\[
c_{0,m+1}(t) = \left\{ c_{0,m+1}(0) \left[ \cos \left( \frac{\Omega m t}{2} \right) + i \frac{\Delta}{\Omega m} \sin \left( \frac{\Omega m t}{2} \right) \right] - c_{1,m}(0) \frac{\gamma_m}{\Omega m} \sin \left( \frac{\Omega m t}{2} \right) \right\} e^{-i \Delta t/2},
\]
\[
c_{1,m}(t) = \left\{ c_{1,m}(0) \left[ \cos \left( \frac{\Omega m t}{2} \right) - i \frac{\Delta}{\Omega m} \sin \left( \frac{\Omega m t}{2} \right) \right] - c_{0,m+1}(0) \frac{\gamma_m}{\Omega m} \sin \left( \frac{\Omega m t}{2} \right) \right\} e^{i \Delta t/2},
\]
with the quantized Rabi frequency \( \gamma_m = 2\sqrt{m + 1} \gamma \) yielding the generalized quantized Rabi frequency \( \Omega_m = \sqrt{\gamma_m^2 + \Delta^2} \). The normalization of \( \Psi(t) \) now implies \( \Sigma_m p(m) = 1 \), with \( p(m) = |c_{0,m}(t)|^2 + |c_{1,m}(t)|^2 \) the probability of \( m \) photons in the field, while the inversion probability now becomes
\[
P_I(t) = \Sigma_m |c_{1,m}(t)|^2 - |c_{0,m}(t)|^2.
\]

Although expressions [82] and [83] look similar, let us point out two main novelties present in this so-called Jaynes-Cummings model. If one starts the dynamics in the electronic excited state, \( (c_{0,m}(0),c_{1,m}(0)) = (0,c_m(0)) \) with \( c_m(0) \) the probability amplitude of the field alone, [82] simplifies to
\[
c_{0,m+1}(t) = -c_m(0) i \frac{\gamma_m}{\Omega_m} \sin \left( \frac{\Omega m t}{2} \right) e^{-i \Delta t/2},
\]
\[
c_{1,m}(t) = c_m(0) \left[ \cos \left( \frac{\Omega m t}{2} \right) - i \frac{\Delta}{\Omega m} \sin \left( \frac{\Omega m t}{2} \right) \right] e^{i \Delta t/2},
\]
so that \( P_I(t) = \Sigma_m |c_m(0)|^2 [\Delta^2 + \gamma_m^2 \cos(\Omega_m t)/\Omega_m^2] \). One can envision two cases: i) for an initial vacuum field, that is, \( |c_m(0)|^2 = \delta_{m,0} \), and under resonance (\( \Delta = 0 \)), one simply has the coefficients \( c_{0,1}(t) = -i \sin(\gamma_1 t/2) \) and \( c_{1,0}(t) = \cos(\gamma_0 t/2) \), so that \( P_I(t) = \cos(\gamma t) \) and the system can be fully inverted, even without an external field, due to spontaneous photon emission; ii) by using a typical coherent initial Poisson distribution around the average photon number \( \langle m \rangle \), that is, \( |c_m(0)|^2 = \langle m \rangle^m e^{-\langle m \rangle} / m! \), as \( \langle m \rangle \) increases, one obtains collapses and revivals of \( P_I(t) \) as caused by interferences among the different terms in the sum over \( m \), which oscillate at their own distinct frequencies. Notice that, although a continuous photon distribution or even a classical random field could also induce a collapse in \( P_I(t) \), the revivals are a pure quantum feature. We focus here only on case i).

As it will become clear in Appendix E the light-matter coupling creates a doublet structure in the spectrum of the full Hamiltonian; if one only has photon states \( m = 0,1 \), since \( |0,0 \rangle \) is unaffected while \( |1,0 \rangle \) only couples to a higher doublet, the lowest doublet has from [81] the full wavefunction
\[
|\Psi(t)\rangle = e^{-i \frac{\Delta}{\Omega} t} e^{-i \omega_0 t} c_{0,1}(t)|0,1\rangle + e^{-i \frac{\Delta}{\Omega} t} e^{-i \omega_0 t} c_{1,0}(t)|1,0\rangle,
\]
which couples the excited electron state with no photon to the ground electron state with a single photon. For the case where the system is initiated in the excited state without photons one simply has
\[
c_{0,1}(t) = i \frac{\gamma_0}{\Omega_0} \sin \left( \frac{\Omega_0 t}{2} \right) e^{-i \Delta t/2},
\]
\[
c_{1,0}(t) = \left[ \cos \left( \frac{\Omega_0 t}{2} \right) - i \frac{\Delta}{\Omega_0} \sin \left( \frac{\Omega_0 t}{2} \right) \right] e^{i \Delta t/2}.
\]

Notice that [84] and [85] resemble [72] and [74].

Expectation values however have distinct features with regard to the semiclassical case. The energy becomes
\[
\langle \Psi(t)| H_{ew} + H_I |\Psi(t)\rangle = (\hbar \omega_0 + 3\hbar \omega/2)|c_{0,1}(t)|^2
\]
\[
+ (\hbar \omega_1 + \hbar \omega/2)|c_{1,0}(t)|^2 - 2\hbar \gamma \Re \left[ c_{0,1}(t) c_{1,0}(t) e^{-i \Delta t} \right],
\]
which, at resonance, is conserved as expected since the crossed term vanishes; at \( \Delta > 0 \) tough the same may not be true. Both position and momentum vanish, \( \langle \Psi(t)|x|\Psi(t)\rangle = \langle \Psi(t)|x|\Psi(t)\rangle - i \hbar d/dx \langle \Psi(t) \rangle = 0 \), due to the orthogonality of the photon states. And the same happens for their counterparts, \( \langle \Psi(t)|q|\Psi(t)\rangle = \langle \Psi(t)|q|\Psi(t)\rangle - i \hbar dq/dq \langle \Psi(t) \rangle = 0 \), due to the orthogonality of the electron states. Only bilinear terms involving \( xq \) (or \( d/dx \ d/dq \)), at \( \Delta > 0 \), may be non-zero, as \( \langle \Psi(t)|xq|\Psi(t)\rangle = 2d_x dq \Re \left[ c_{0,1}(t)c_{1,0}(t) e^{-i \Delta t} \right] \), with \( d_x \) a similar definition to \( dx \) but for the photons, \( d_q = (0|q|0) - (1|q|1) = 0 \). As such, expected terms in the Real part above are the same ones found in [85], since the Hamiltonian [80] is derived from such a bilinear term.

C Light-dressed states of the matter

Having in mind that in the Jaynes-Cummings model of Appendix E the full Hamiltonian \( H \) is time independent, and that \( H_I \) can only induce \( |0,m + 1\rangle \leftrightarrow |1,m\rangle \) transitions in \( H_{ew} \) (such that state \( |0,0\rangle \) is unaffected), one realizes that the spectrum of \( H \) is given by a set of energy doublets \( D_m \) if one is not far from resonance; that is, \( D_1 \) contains states \( |0,1\rangle - |1,0\rangle \), \( D_2 \) builds on \( |0,2\rangle - |1,1\rangle \), and so on. As such, the Hamiltonian of each doublet subspace
\[
H_{D_m} = h \left[ \omega_0 + (m + 3/2) \omega - \frac{\gamma_m}{\omega_1 + (m + 1/2) \omega} \right],
\]
can easily be diagonalized, yielding the eigenvalues \( E_{\pm,m} \),
\[
E_{\pm,m} = h(\omega_0 + \omega_1/2 + (m + 1) \omega) \pm \sqrt{(\Delta/2)^2 + \gamma_m^2},
\]
and the eigenvectors \( |\psi_{\pm,m}\rangle \),
\[
|\psi_{-m}\rangle = -\sin(\theta_m/2)|0,m + 1\rangle + \cos(\theta_m/2)|1,m\rangle,
\]
\[
|\psi_{+m}\rangle = \cos(\theta_m/2)|0,m + 1\rangle + \sin(\theta_m/2)|1,m\rangle,
\]
with \( \tan(\theta_m) = 2\gamma_m/\Delta \), \( \theta_m < \pi \). Notice that \( E_{+m} - E_{-m} = 2h \sqrt{(\Delta/2)^2 + \gamma_m^2} \), so that even at resonance (\( \Delta = 0 \), \( \theta_m = \pi/2 \)), where the bare levels of \( H_{ew} \) are degenerated, the coupling term \( \gamma_m \) induces an avoided crossing in its own doublet, and creates fully entangled matter-radiation states \( |\psi_{\pm,m}\rangle = 1/\sqrt{2}|\pm[0,m+1] + |1,m\rangle \), the so-called light-dressed states of the matter. As \( \Delta \) increases so that
\( \theta_m \) approaches 0 or \( \pi \), \( |\psi_{\pm,m}\rangle \) tends to the uncorrelated bare states \( |0, m + 1\rangle \) or \( |1, m\rangle \). So the Rabi oscillations can be understood from the dressed state picture: one inverts \( |\phi_n^{(c)}(x)\rangle \) in (88)-(90), one can project (111) in \( \psi_{j,k}(x) \) as to also integrate out the electron degree of freedom, resulting

\[
H = \sum_n \left[ \sqrt{k} \alpha c_n \right] \langle j | x | n \rangle.
\]

(90)

Usual confining potentials will have symmetries like parity dictating selection rules for real dipole matrix elements, so

\[
\begin{align*}
\langle j | x | n \rangle & = \langle |0, n+1\rangle + \langle |1, n-1\rangle, \\
\langle j | x | n \rangle & = \langle \delta_j, n+1 + \delta_{j-1, n-1} \rangle, \\
\end{align*}
\]

that is, only two neighboring electronic states are connected, and as such \( |\phi_0^{(c)}(x)\rangle \) becomes

\[
\begin{align*}
H & = [E_j + \hbar \omega (k + 1/2)] c_{j,k}(t) \\
& + \alpha \sum_n \left[ \sqrt{k} + 1 \right] [d_{j,j-1} c_{j-1,k} + d_{j,j+1} c_{j+1,k}] \\
& + \alpha \hbar k [d_{j,j-1} c_{j-1,k} + d_{j,j+1} c_{j+1,k}] \\
& = [E_j + \hbar \omega (k + 1/2)] c_{j,k}(t) \\
& + \alpha \sqrt{k} [d_{j,j-1} c_{j-1,k} + d_{j,j+1} c_{j+1,k}].
\end{align*}
\]

(91)

By employing the RWA and so neglecting the terms \( c_{j-1,k-1} \) and \( c_{j+1,k+1} \) that do not conserve the number of electron-photon excitations, (91) becomes

\[
\begin{align*}
H & = [E_j + \hbar \omega (k + 1/2)] c_{j,k}(t) \\
& + \alpha \sqrt{k} [d_{j,j-1} c_{j-1,k-1} + d_{j,j+1} c_{j+1,k-1}].
\end{align*}
\]

(92)

As an example, in the case of a two-level system for the electrons as considered in our work \( j = 0, 1 \), for the two lowest photon states \( k = 0, 1 \), (92) yields

\[
\begin{align*}
\frac{d}{dt} c_{0,0}(t) & = [E_0 + \hbar \omega / 2] c_{0,0}(t), \\
\frac{d}{dt} c_{1,0}(t) & = [E_1 + \hbar \omega / 2] c_{1,0}(t) + \alpha d_x c_{0,1}, \\
\frac{d}{dt} c_{0,1}(t) & = [E_0 + 3\hbar \omega / 2] c_{0,1}(t) + \alpha d_x c_{1,0}, \\
\frac{d}{dt} c_{1,1}(t) & = [E_1 + 3\hbar \omega / 2] c_{1,1}(t) + \alpha \sqrt{2} d_x c_{0,2},
\end{align*}
\]

(93)

with \( d_x \) as defined before, and in the last equation the term \( \alpha d_x c_{2,0} \) is neglected as it refers to the electron state \( j = 2 \).

So, as expected in an isolated system, we recover the results from the Jaynes-Cummings model since the equations for \( c_{1,0}(t) \) and \( c_{0,1}(t) \) are the same obtained in the development of (82) (having those same solutions). They constitute the doublet \( D_1 \), and as we have just seen \( c_{0,0}(t) \) is decoupled, while \( c_{1,1}(t) \), by coupling with \( c_{0,2}(t) \), would build the next doublet \( D_2 \). We emphasize, however, that (111) is more general for dealing with open transport scenarios, since it does not dwell on the specific information of an isolated system basis.

### D Results for Semiclassical, Orthodoxy and Bohmian isolated two-level scenarios

We show some illustrative results of the analytical models developed so far, by considering a simple isolated electronic system defined by an 1D infinite symmetric quantum well, with \( m^* = 0.041 m_0 \), \( L_W = 16 \) nm, basis functions \( \phi_0^{(c)}(x) = \sqrt{2/L_W \cos(\pi x / L_W)} \) and \( \phi_1^{(c)}(x) = -\sqrt{2/L_W \sin(2\pi x / L_W)} \), dipole \( d_x \approx -2.9 \) nm, dipole \( d_p \approx -0.11 \) nm\(^{-1}\), energies \( \hbar \omega_0 \approx 35 \) meV and \( \hbar \omega_1 \approx 140 \) meV, so that \( \omega_x \approx 160 \) THz. In the quantum case we also consider a two-level scheme for the photon with \( m = 0 \) and resonant energy \( \hbar \omega / 2 \approx 52 \) meV, where the simple harmonic basis functions are \( \phi_0^{(w)}(q) = (1/(\pi l_0^2))^{1/4} e^{-q^2/(2l_0^2)} \) and \( \phi_1^{(w)}(q) = (1/(\pi l_0^2))^{1/4} e^{-q^2/(2l_0^2)} \sqrt{2} q / l_0 \), with \( l_0 = \sqrt{\hbar / \omega} \). A single-mode resonant field \( \omega = \omega_x \), then as frequency \( \nu = \omega / (2\pi) \approx 25 \) THz, implying \( \Delta = 0 \) and \( \Omega_S = \gamma_S (\Omega_0 = \gamma_0) \) for the semiclassical (quantum) scenario in equations (92), (93), (94), (95); the dynamics starts from the excited electron state, without photon. In practical terms, the Rabi inversion frequency can be taken as a parameter - smaller than \( \omega_x \), dictating the intensity of coupling \( \gamma_S (\gamma) \) between electron and electromagnetic fields (photons) in the semiclassical (quantum) picture in equation (111). Since \( \gamma_0 = 2\sqrt{0 + \gamma_0 \gamma} \), for a meaningful comparison, we define a common numerical Rabi frequency

\[
\gamma_R \equiv \gamma_S (\gamma_0 = 2\gamma), \text{ and take } \gamma_R / \omega_x \approx 32 \text{ THz.}
\]

Figures 6 and 7 each with five panels, deal respectively with the semiclassical Rabi model and with the quantum Jaynes-Cummings model. Results in general show what one expects from the discussion in the previous Appendices, with Rabi oscillations with period \( 2\pi / \gamma_R \approx 0.2 \) ps.

Since we are considering only a resonant \( \Delta = 0 \) case, panel (a) in both figures presents a periodic full inversion of the system, from the respective excited to ground states. In panel (b), the distinct look of \( |\Psi(x,t)\rangle^2 \) from the semiclassical to the quantum scenarios has a clear origin: the phases \( e^{i\omega_0 t} \) in (72) create the ‘noisy’ semiclassical pattern due to the crossed terms; on the other hand, \( |\Psi(x,t)\rangle^2 \) in the quantum case has the photon degree integrated so that its orthogonality eliminates the crossing terms in (84). Notice tough that, had we considered the semiclassical case without those phases its evolution would look exactly the same as the quantum case, alternating between double (excited state) to single (ground state) peaks. In panel (c), for the semiclassical model, the expectation value for the position \( \langle \Psi(t) | x | \Psi(t) \rangle \) oscillates in between \( \pm d_x \), while for the momentum \( \langle \Psi(t) | -i\hbar d_x / dt | \Psi(t) \rangle \) oscillates in between \( \pm \hbar d_p \) (scaled by 20 in the figure); one sees that frequencies other than the Rabi one are playing a role in the dynamics. On the other hand, in panel (c) for the quantum model, due to the orthogonality of the photon degree, both expectations are zero; similarly, had we plot-
\[ \langle \Psi(t) | q | \Psi(t) \rangle \] and \[ \langle \Psi(t) | -i \hbar d/dq | \Psi(t) \rangle \] the same would happen due to the orthogonality of the electron degree.

Figure 6: Time-evolution of the semiclassical Rabi model. (a) ground and excited state probabilities; (b) wavefunction distribution \( |\Psi(x, t)|^2 \); (c) expectation values of position \( \langle \Psi(t) | x | \Psi(t) \rangle \) and momentum (multiplied by 20) \( \langle \Psi(t) | p | \Psi(t) \rangle \); (d) “energy” \( E = \langle \Psi(t) | H_e + H_I(t) | \Psi(t) \rangle \); (e) spectral density of the electron energy \( E \) of the wavefunction in (b).

The energy expectation in panel (d) for the quantum picture, \( E = \langle \Psi(t) | H_e + H_I(t) | \Psi(t) \rangle \), which comes from a time-independent Hamiltonian, remains conserved at the initial excited electron plus zero photon energy of \( \approx 140 + 52 = 192 \) meV. On the other hand, the “energy” for the semiclassical picture, \( E = \langle \Psi(t) | H_e + H_I(t) | \Psi(t) \rangle \), follows the expected trend with the Rabi oscillations, remaining in between excited \( \approx 140 \) meV and ground \( \approx 35 \) meV state energies, with also a clear signature of extra frequencies.

From a Fourier Transform of \( E \), as seen in panel (e), the quantum case obviously has no peaks, while in the semiclassical case one clearly identifies the first peak at the Rabi frequency \( \gamma_R \approx 32 \) THz, while the other two peaks are located at \( 2 \omega - \gamma_R \approx 288 \) THz and \( 2 \omega + \gamma_R \approx 352 \) THz, being separated by \( 2 \gamma_R \) as explained in Appendix C. Curiously, for a slightly nonresonant case (say \( \omega = 0.9 \omega_e \), such that the analytical models are still valid and one is still in the avoided crossing region), the middle peak among these latter two peaks is also seen at \( 2 \omega = 320 \) THz but, of course, the Rabi oscillations are no longer able to fully invert the system.

In order to exemplify the use of the Bohmian trajectories as discussed in (48) of Section 3.4, we show in Fig. an example of two of such trajectories in the 2D \( xq \) space for the quantum picture; trajectories in the 1D \( x \) space for the classical

Figure 7: Time-evolution of the quantum Jaynes-Cummings model. (a) ground and excited state probabilities; (b) wavefunction distribution \( |\Psi(x, t)|^2 \); (c) expectation values of position \( \langle \Psi(t) | x | \Psi(t) \rangle \) and momentum (multiplied by 20) \( \langle \Psi(t) | p | \Psi(t) \rangle \); (d) energy \( E = \langle \Psi(t) | H_e + H_I(t) | \Psi(t) \rangle \); (e) spectral density of the electron energy \( E \) of the wavefunction in (b).
E Bohmian approach to open systems

In principle, following the development done in this work, the wave function describing an electron device including $N$ electrons (each one with the three spatial components $r_j = \{x_j, y_j, z_j\}$) interacting with an electromagnetic field composed by $N_A$ modes (each $j$-th electron with one degree of freedom $q$ linked to one frequency $\omega$) will need to be written as

$$\Psi(r_1, ..., r_N, q_1, ..., q_{N_A}, \beta_1, ..., \beta_{N_A}, t).$$

Notice that, in (94), we have also included $N_\beta$ extra degrees of freedom belonging to the atoms that build such electron device and to any other degrees of freedom that can be relevant for the description of the device. As such, since we have included all relevant degrees of freedom, we are dealing with a closed system and its description in terms of the wave function (94) is conceptually unproblematic. However, from a computational point of view, manipulating the wave function (94) defined in the huge configuration space of $N \times N_A \times N_\beta$ dimensions is totally inaccessible. Thus, it becomes mandatory to eliminate most of the degrees of freedom, to reach a practical discussion of a many-body problem.

The orthodox way of eliminating degrees of freedom is by dealing with the reduced density matrix [92,93]. Strictly speaking, a description of an open system with pure states as we have done in our paper is not possible within the orthodox theory. In this sense, the reader can assume that our description in the paper in terms of pure states is not adequate. This is true in the orthodox formulation of an open system, but false in its Bohmian formulation [71–73,83], as used in this work, where the concept of conditional wave function is the key element to describe open systems. In this Appendix, we explain the Bohmian conditional wave function linked to the system described by (94).

In a Bohmian description of a closed quantum system we require not only its wave function but also a well-defined position for each electron at any time $t$,

$$r_j(t) = r_j(0) + \int_0^t dt' v_{r_j},$$

and a well-defined amplitude for the different modes of the electromagnetic field at all times,

$$q_j(t) = q_j(0) + \int_0^t dt' v_{q_j},$$

plus, for any other extra degrees of freedom,

$$\beta_j(t) = \beta_j(0) + \int_0^t dt' v_{\beta_j},$$

where $v_{r_j}$ is the electron velocity in real space computed from $\Psi$ in (94), while $v_{q_j}$ and $v_{\beta_j}$ play similar roles, despite the fact that $q_j(t)$ and $\beta_j(t)$ do not need to be positions in real space.

With all such information on the closed quantum system, one can construct the wave function of the degrees of freedom $r_1$ and $q_1$ conditioned to some particular well-defined values on the other degrees of freedom, giving

$$\Psi(r_1, q_1, t) = \Psi(r_1, q_1, t) r_2(t), q_2(t), \beta_2(t), ..., r_{N_A}(t), q_{N_A}(t), \beta_{N_A}(t), t) \equiv \Psi(r_1, q_1, t), r_2(t), q_2(t), \beta_2(t), ..., r_{N_A}(t), q_{N_A}(t), \beta_{N_A}(t), t).$$
The conditional wave function $\Psi(r_1, q_1, t)$, without writing explicitly the elements $r_2(t), q_2(t), \beta_1(t), \ldots, r_N(t), q_N(t), \beta_N(t)$, is what we have used all along this paper. Certainly, a big avenue of research, far from the scope of the present paper, is what is the exact equation of motion for the conditional wave function $\Psi(r_1, q_1, t)$. See Refs. [76, 94] for additional details.

In this work, for simplicity, we have assumed that the equations of motion for $\Psi(r_1, q_1, t)$ are just the ones linked to the Hamiltonians as they are used in the paper. The only external potential due to the non-simulated degrees of freedom is $V_e(r, t)$ as mentioned in (20).

The short discussion in this Appendix is only conceptual, without any numerical or practical contribution. Its only role is to clarify that the treatment of light-matter interaction in terms of wave functions, within the framework of the Bohmian quantum mechanics, is a valid tool to describe the open quantum systems studied in this paper, and not only closed systems. In particular when said wave functions assume a conditional value.

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[78] The fact that $E_\perp(r,t)$ and $B(r,t)$ are the genuine degrees of freedom is not a consequence of our single-electron assumption. From Maxwell’s equations and the Coulomb gauge, we know that $E_\parallel(r,t)$ depends only on the positions of the electrons. Thus $E_\parallel(r,t)$ is not a genuine degree of freedom [68].
[79] The pertinent Maxwell’s equations in the reciprocal space are $\frac{\partial\mathbf{B}(k,t)}{\partial t} = -i\mathbf{k} \times \mathbf{E}_\perp(k,t)$, and $\frac{\partial\mathbf{E}_\perp(k,t)}{\partial t} = i\epsilon_0 \mathbf{k} \times \mathbf{B}(k,t) - \frac{1}{\epsilon_0} \mathbf{j}_\perp(k,t)$. 

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Here, $\alpha$ depends on the type of electromagnetic field considered through $\Delta k$ while, in the literature, such dependence is typically not present and it is substituted by an arbitrary dependence on the size of a mathematical cavity that contains the electromagnetic field inside. Our paper uses Fourier integrals, while the use of a mathematical cavity implies Fourier series. Such different approaches do not have any implications in the results of this paper.

An intuitive explanation of the non-local character of quantum phenomena in the Bohmian language is that an electron corresponding to some $a$-experiment guided by a Hamiltonian is affected by what happens to another electron in a different $b$-experiment also governed by the same Hamiltonian. In other words, the trajectory $x_a(t)$ is affected by the trajectory $x_b(t)$, even if they are different experiments and have (non-local) spatial separation. The appropriate element that can capture such non-classical (non-local) behavior is a wave function whose extension (coherence length) includes $x_a(t)$ and $x_b(t)$ in the relevant times.

According to the orthodox theory, the properties of the studied system such as the position of the electron or the amplitude of the electromagnetic field have no well-defined values while the system follows the unitary evolution. Such properties are only well-defined when a (strong) measurement is done and the system collapse into a state with well-defined properties. The orthodox theory states that the measurement process is not governed by the unitary evolution, but by a new law named wave function collapse (or state reduction), that provides a definite value of the position of the electron, if measured, or of the amplitude of the electromagnetic field, if measured. This relation between the measurement and the reality of the properties of the quantum system is known as the eigenstate-eigenvalue-link. When one gets information of a quantum system at THz frequencies, the system is measured at time steps lower than 1 ps. Within the orthodox theory, such multi-time measurement brings computational difficulties when changing from unitary to non-unitary evolutions of a quantum state that can be greatly simplified when using a Bohmian explanation of such measurement.

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