Quantum and Classical Simulation of Light and Matter: QC_slim guide for students and educators

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A software for simulating light-matter interacting systems in the classical and quantum regimes offering didactic explanations of different phenomena and a smooth transition between classcial and quantum explanations, through visual animations. The latest version of this document is available at the website of QC slim manual

Contents

1 Motivation:

Many textbooks explain quantum phenomena by emphasizing their differences from classical ones. However, in reality, quantum and classical mechanics are not so different. Indeed, it is not necessary to abandon all classical knowledge to properly understand quantum concepts; rather, one can make a smooth transition between the two.

1.1 Classical and quantum mechanics predictions are different, but they do not need to use different languages

Landau and Lifshitz in the introduction of their famous book on quantum mechanics wrote

> *Thus quantum mechanics occupies a very unusual place among physical theories: it contains classical mechanics as a limiting case, yet at the same time it requires this limiting case for its own formulation.* [1]

It seems evident that a more fundamental physical theory, such as quantum mechanics, includes a less fundamental one, like classical mechanics, as a particular case. In this sense, classical mechanics can be derived from the principles of quantum mechanics in specific scenarios, particularly those involving phenomena related to decoherence.

What is less common, however, is that a more fundamental theory is constructed using the concepts and elements of the less fundamental one as its foundational building blocks. For example, to predict the behavior of an electron inside a hydrogen atom, quantum mechanics employs the classical expression for kinetic energy (momentum squared divided by twice the mass) and the classical expression for potential energy (given by the Coulomb interaction between the electron and the proton). The quantum Hamiltonian, which is the fundamental element for predicting the dynamics of quantum systems, is essentially derived from these familiar classical concepts. The classical Hamiltonian becomes a quantum one when it undergoes a modification known as **canonical quantization**, where the variables of the classical Hamiltonian are transformed into operators [1–4].

The similarities between classical and quantum systems are not only found in the Hamiltonians involved but also in the elements used to describe these systems. Typically, trajectories are used to describe classical systems, while wave functions are used for quantum systems. However, the classical Hamilton-Jacobi theory demonstrates that it is possible to describe an ensemble of classical systems using a classical wave function [5]. Similarly, de Broglie and Bohm showed that it is possible to describe a single quantum system using a quantum trajectory [5–7].

The **main motivation** of this project is to emphasize the similarities between classical and quantum systems (rather than their differences) as a way to facilitate learning in the phenomena occurring when light interacts with matter. This idea of showing a smooth transition between classical and quantum concepts is particularly well-suited for studying the interaction between light and matter, not only because the quantum and classical Hamiltonian are the same, but also because, in many cases, only one part of the system —either the matter or the light— is treated quantum mechanically, while the other is approached classically. The phenomena that arise from the interaction of light and matter in classical, semiclassical, and fully quantum systems are distinct, yet they share many underlying similarities. By recognizing these similarities (borrowing concepts from one formalisms to the other), the understanding of the fundamental concepts and phenomena occurring when light interacts with matter can be significantly enhanced.

1.2 Different learning goals, theory sections and simulated experiments

After discussing the main motivation for this project, we provide an overview of what the sections are about and the learning goals. Apart from this section devoted to the motivation of this project, this document is divided into 4 additional section:

- The section Theoretical background in 2 develops the Hamiltonian dealing with light and matter that will be used in all classical and quantum examples. In particular, we consider a non-relativistic electron, whose kinetic energy is given by the momentum squared divided by twice the mass. The electromagnetic field is regarded as a single-mode monochromatic polarized light.

- The section Types of theories/models in 3 develops the classical and quantum equations of motion derived from this Hamiltonian. Particular attention is devoted to explaining the perturbative approximation, the absorption and stimulated emission processes, and the Rabi oscillations in the semiclassical formalism. Such concepts are later revisited in the full quantum formalism of ligth and matter.

- The section Simulated experiments in 4 provides a list of representative examples where the student can visualize through animations the theoretical concepts mentioned in the previous section. To run the examples, the student needs to install the software QCslim.exe.

In addition, at the end of the document, there is a list of solutions to several proposed exercises that detail some theorethical developments needed in the manuscript. The bibliography with referecne to books and articles is presented at the end of the document. In the table below, a list of the specific items discussed in this document and the link to the theorethical discussion and simulated experiments is presented.

Num	**Learning goal**	**Section**	**Simulated experiment**	Class. Matter	Class. Light	Quan. Matter	Quan. Light
1	A simple light-matter Hamiltonian	Sec. 2		✓	✓	✓	✓
	Energy of light in terms of canonical variables	Sec. 2.2		✓	✓	✓	✓
	The long wave-length approximation	Sec. 2.3		✓	✓	✓	✓
2	Classical regime: Hamilton equations	Sec. 3.1	simulation 4.1.1	✓	✓	✗	✗
	Classical light-matter interaction	Sec. 3.1	simulation 4.1.2	✓	✓	✗	✗
	Classical statistical description	Sec. 3.1	simulation 4.2.1	✓	✓	✗	✗
3	Semiclassical regime: electrons in an infinite well	Sec. 3.2	simulation 4.3.1	✗	✓	✓	✗
	Absorption and stimulated emission: exact, perturbative and rotating wave approximation	Sec. 3.2.2	simulation 4.4.1	✗	✓	✓	✗
	Semiclassical Rabi oscillations	Sec. 3.2.2	simulation 4.5.1	✗	✓	✓	✗
	Semiclassical statistical description	Sec. 3.3	simulation 4.6.1	✗	✓	✓	✗
4	Photon: a quantum of energy	Sec. 3.4	simulation 4.7.1	✓	✗	✗	✓
	Probability distribution of electromagnetic fields	Sec. 3.5	simulation 4.7.2	✓	✗	✗	✓
5	Quantum regime: strong light-matter interaction	Sec. 3.6	simulation 4.8.1	✗	✗	✓	✓
	Quantum Rabi oscillations	Sec. 3.6.1	simulation 4.8.1	✗	✗	✓	✓
	Spontaneous emission	Sec. 3.6	simulation 4.9.1	✗	✗	✓	✓
	Quantum statistical description and weak values	Sec. 3.6	simulation 4.10.1	✗	✗	✓	✓

Table 1: List of main learning goals and subgoals in the present documents. The involved theory section, simulated experiment and the quantum or classcial fromalism for light and matter are indicated.

2 Theoretical background

In this section, we develop the final Hamiltonian that defines the physical system consisting of an electron interacting with an electromagnetic field. In particular, we consider a non-relativistic electron, whose kinetic energy is given by the momentum squared divided by twice the mass, and an electromagnetic field described by a single-mode monochromatic polarized light. The final Hamiltonian will be the same for a classical or quantum phenomena discussed in this document.

2.1 General Hamiltonian

The electron has a mass m and charge $-e$. Its position is defined by $\mathbf{r}$ and its momentum by $\mathbf{p}$. Along this document, vectors are defined by **bold** letters. The electromagnetic field is define by the electric field:

$$\mathbf{E} = -\nabla A_0 - \frac{\partial \mathbf{A}}{\partial t} \tag{1}$$

and the magnetic field:

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{2}$$

where $\mathbf{A}$ and A_0 are the vector and scalar electromagnetic potentials, respectively. These electromagnetic potentials are gauge-dependent in the sense that any set of potentials (indicated by the superscript g) given by

$$\mathbf{A}^g = \mathbf{A} + \nabla g(\mathbf{r}, t) \quad \text{and} \quad A_0^g = A_0 - \frac{\partial g(\mathbf{r}, t)}{\partial t}, \tag{3}$$

keeps the overall observable properties identical in any gauge [2, 3]. Here, $g(\mathbf{r}, t)$ is any regular enough real function.

Exercise 2.1.1 — Guage invariance of the electromagnetic fields

Show that the electric and magnetic fields in Eq. (1) and Eq. (2) are not dependent on the selected gauge function $g(\mathbf{r}, t)$ in Eq. (3)
See the detailed solution of this exercise in 5.1 at page 45

The general classical or quantum Hamiltonian that describes the interaction of an electron (or another particle) of mass m_e with an electromagnetic field, in the so-called minimal coupling [2–4], is given by:

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m_e} + eA_0 + V(\mathbf{r}) + H_R, \tag{4}$$

where H_R is the energy of the electromagnetic field. The term $V(\mathbf{r})$ corresponds to an additional external potential energy seen by the electron. [1]

2.2 The energy of the electromagnetic field

The term H_R in Eq. (4) is the energy of the electromagnetic field [3] defined as:

$$H_R = \frac{\epsilon_0}{2} \int d^3r \left(\mathbf{E}_T^2 + c^2 \mathbf{B}^2 \right), \tag{5}$$

where ϵ_0 is the dielectric constant (permittivity) and μ_0 the permeability of free space, givin $c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}$ the speed of light. In writing Eq. (5), the electromagnetic field in Eq. (1) is defined as the sum of a transversal (zero divergence) component $\mathbf{E}_T$ plus a longitudinal (zero rotational) field $\mathbf{E}_L$, i.e., $\mathbf{E} = \mathbf{E}_L + \mathbf{E}_T$. The magnetic field, by construction, has only a transversal component. [2]

[1] For example, $V(\mathbf{r})$ can be the barriers of an infinite well. Strictly speaking, such barriers reflect some type of interaction of the electron with other particles, but we want to neglect such other particles to reduce the computational burden. Thus, the barriers are an external potential in the sense that the electron $\mathbf{r}$ is affected by the barrier, but the barrier is not affected by the electron.

[2] The energy in Eq. (5) only depends on the transversal component of the electric field because the energy linked to the longitudinal component is given (in the Coulomb gauge defined as the $g(\mathbf{r}, t)$ function that ensures $\nabla \cdot \mathbf{A} = 0$) by the scalar potential, A_0. We will see that for a single electron $A_0 = 0$ because one electron has no Coulomb interaction with itself.

Exercise 2.2.1 — Longitudinal and transversal electromagnetic fields

Show that the electric field in Eq. (1) defined as $\mathbf{E} = \mathbf{E}_L + \mathbf{E}_T = -\nabla A_0 - \frac{\partial \mathbf{A}}{\partial t}$ can be written as $\mathbf{E}_L = -\nabla A_0$ and $\mathbf{E}_T = -\frac{\partial \mathbf{A}}{\partial t}$ when the Coulomb gauge (defined as $\nabla \cdot \mathbf{A} = 0$) is used.
See the detailed solution of this exercise in 5.2 at page 45

To further develop Eq. (5) is useful to decompose the electric and magnetic fields into their Fourier components. In general, the transversal electric field can be written as a superposition of the spatial Fourier components as:

$$\mathbf{E}_T(\mathbf{r},t) = \sum_\gamma \mathbf{e}_\gamma \tilde{E}_\gamma(t) e^{i\mathbf{k}_\gamma \mathbf{r}} \quad \text{and} \quad \tilde{E}_\gamma(t) = \frac{1}{V}\int d^3r\, \mathbf{e}_\gamma \mathbf{E}_T(\mathbf{r},t) e^{-i\mathbf{k}_\gamma \mathbf{r}} \tag{6}$$

where γ labels the different components. The polarization vector $\mathbf{e}_\gamma$ is perpendicular to the direction of vector $\mathbf{k}_{gamma}$. Identically,

$$\mathbf{B}(\mathbf{r},t) = \sum_\gamma \mathbf{e'}_\gamma \tilde{B}_\gamma(t) e^{i\mathbf{k}_\gamma \mathbf{r}} \quad \text{and} \quad \tilde{B}_\gamma(t) = \frac{1}{V}\int d^3r\, \mathbf{e'}_\gamma \mathbf{B}(\mathbf{r},t) e^{-i\mathbf{k}_\gamma \mathbf{r}} \tag{7}$$

with $\mathbf{e'}_\gamma = \frac{\mathbf{k}_\gamma}{|\mathbf{k}_\gamma|} \times \mathbf{e}_\gamma$. By construction, each Fourier component has a well defined wave vector $\mathbf{k}_\gamma$ that implies a well-defined angular frequency ω_γ with $c = \omega_\gamma / |\mathbf{k}_\gamma|$.

Exercise 2.2.2 — Maxwell equation in the Fourier space

Using Eq. (6) and Eq. (7), show that the following Maxwell equation (for the transversal fields) can be written as:

$$\nabla \times \mathbf{E}_T(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t} \quad \text{and} \quad \frac{\partial \tilde{B}_\gamma(t)}{\partial t} = -i|\mathbf{k}_\gamma| \tilde{E}_\gamma(t) \tag{8}$$

and the following Maxwell equation (for the transversal fields) can be written as:

$$\nabla \times \mathbf{B}(\mathbf{r},t) = \mu_0 \left(\mathbf{J}(\mathbf{r},t) + \epsilon \frac{\partial \mathbf{E}_T(\mathbf{r},t)}{\partial t} \right) \quad \text{and} \quad \frac{\partial \tilde{E}_\gamma(t)}{\partial t} = -ic\omega_\gamma \tilde{B}_\gamma(t) - \frac{1}{\epsilon_0}\tilde{J}_\gamma(t) \tag{9}$$

where the (transversal) component of the current density $\mathbf{J}_T(\mathbf{r},t)$ is decomposed into:

$$\mathbf{J}_T(\mathbf{r},t) = \sum_\gamma \mathbf{e}_\gamma \tilde{J}_\gamma(t) e^{i\mathbf{k}_\gamma \mathbf{r}} \tag{10}$$

See the detailed solution of this exercise in 5.3 at page 45

The right hand of Eq. (8) and Eq. (9) is a coupled system of equations of motion. It is convenient to decouple the above two equations to describe the energy of the electromagnetic field in terms of canonical variables [2–4]. For that reason, we define:

$$\alpha_\gamma(t) = \frac{1}{2Z_\gamma}\left[-ic\tilde{B}_\gamma + i\tilde{E}_\gamma\right] \quad \text{and} \quad \beta_\gamma(t) = \frac{1}{2Z_\gamma}\left[-ic\tilde{B}_\gamma - i\tilde{E}_\gamma\right] \tag{11}$$

where Z_γ is an arbitrary function. Notice that we can use arbitrary units for $\alpha_\gamma(t)$ as far as the units of $\alpha_\gamma(t)2Z_\gamma$ are the units of electric field.

Exercise 2.2.3 — Maxwell equation in terms of $\alpha_\gamma(t)$ and $\beta_\gamma(t)$

Show that the equation of motion for $\alpha_\gamma(t)$ and $\beta_\gamma(t)$ in Eq. (11) are given by:

$$\frac{\partial \alpha_\gamma(t)}{\partial t} = i\omega_\gamma \alpha_\gamma(t) - i\frac{1}{2Z_\gamma \epsilon_0}\tilde{J}_\gamma \quad \text{and} \quad \frac{\partial \beta_\gamma(t)}{\partial t} = -i\omega_\gamma \beta_\gamma(t) + i\frac{1}{2Z_\gamma \epsilon_0}\tilde{J}_\gamma \tag{12}$$

See the detailed solution of this exercise in 5.4 at page 45

Exercise 2.2.4 — Electric and magnetic field in terms of $\alpha_\gamma(t)$

Show that the electric and magnetic fields can be written as:

$$\mathbf{E}_T(\mathbf{r},t) = i\sum_\gamma \mathbf{e}_\gamma Z_\gamma[\alpha_\gamma(t)e^{i\mathbf{k}_\gamma\mathbf{r}} - \alpha_\gamma^*(t)e^{-i\mathbf{k}_\gamma\mathbf{r}}] \tag{13}$$

and,

$$\mathbf{B}(\mathbf{r},t) = i\sum_\gamma \mathbf{e'}_\gamma \frac{Z_\gamma}{c}[\alpha_\gamma(t)e^{i\mathbf{k}_\gamma\mathbf{r}} - \alpha_\gamma^*(t)e^{-i\mathbf{k}_\gamma\mathbf{r}}] \tag{14}$$

See the detailed solution of this exercise in 5.5 at page 46

It can be straightforward demonstrated, using the orthogonality of the different $\mathbf{e}_\gamma$ involved, that expression Eq. (5) can be written as:

$$H_R = \frac{\epsilon_0}{2}\int d^3r\left(\mathbf{E}_T^2 + c^2\mathbf{B}^2\right) = 2\epsilon_0 V\sum_\gamma Z_\gamma^2|\alpha_\gamma(t)|^2 \tag{15}$$

Finally, by defining:

$$\tilde{q}_\gamma(t) = 2Z_\gamma\sqrt{\frac{\epsilon_0 V}{\omega_\gamma}}Im(\alpha_\gamma(t)) \tag{16}$$

$$\tilde{s}_\gamma(t) = 2Z_\gamma\sqrt{\frac{\epsilon_0 V}{\omega_\gamma}}Re(\alpha_\gamma(t)) \tag{17}$$

The radiation energy can be written as:

$$H_R = \frac{\epsilon_0}{2}\int d^3r\left(\mathbf{E}_T^2 + c^2\mathbf{B}^2\right) = \sum_\gamma \frac{\omega_\gamma}{2}(\tilde{q}_\gamma(t)^2 + \tilde{s}_\gamma(t)^2) \tag{18}$$

2.3 The long wave-length approximation

In usual experimental setups, the relevant wavelength of the external field λ is much larger than the spatial extent of the region where the electron can move. We may therefore expand the spatial dependence of the vector potential $\mathbf{A}(\mathbf{r},t)$ in powers of $\mathbf{r}$, which yields a series of multipole moments of increasing order, and in good approximation keep only the lowest-order term $\mathbf{A}(0,t)$. In this scenario, we can look for the following gauge transformation [2–4]

$$g(\mathbf{r},t) = -\mathbf{A}(0,t)\mathbf{r} \tag{19}$$

Then, the electromagnetic potentials from Eq. (3) can be written as

$$\mathbf{A}^g = \mathbf{A}(0,t) + \nabla g(\mathbf{r},t) = \cancel{\mathbf{A}(0,t)} - \cancel{\mathbf{A}(0,t)} = 0 \tag{20}$$

and using Eq. (1)

$$A_0^g = A_0 - \frac{\partial g(\mathbf{r},t)}{\partial t} = A_0 + \mathbf{r}\frac{\partial \mathbf{A}(0,t)}{\partial t}, \tag{21}$$

Finally, using Eq. (1) in the new gauge, we get:

$$\mathbf{E}^g = -\nabla A_0^g - \partial\mathbf{A}^g\partial t = -\frac{\partial \mathbf{A}(0,t)}{\partial t}. \tag{22}$$

Then, Eq. (4) can be written in the new gauge as:

$$H = \frac{\mathbf{p}^2}{2m_e} - e\mathbf{r}\mathbf{E}^g + V(\mathbf{r}) + H_R, \tag{23}$$

Thus the interaction between the light and the matter (the fact that they do not evolve independently) is due to the term $-e\mathbf{r}\mathbf{E}^g$ involving degrees of freedom of the matter and light. In our case with a single electron simulated explicitly, we notice that the term A_0 in Eq. (4) corresponds to the Coulomb interaction between electrons, which can be set to zero since there is no interaction of an electron with itself, and it is not included in Eq. (23).[3]

2.4 Single mode monochromatic polarized light

To further simplify the discussion we can assume that the electromagnetic field $\mathbf{E}_T(0,t) = \{-E, 0, 0\}$ has only dependence on the x direction. Then, if we are interested in the interaction of light and matter, we only need to deal with the 1D equation:

$$H = \frac{p^2}{2m_e} + V(x) + H_R + xE, \tag{24}$$

where we define $H_M = \frac{p^2}{2m_e}$ and $H_I = xE$. If we consider that we are just considering a monochromatic polarized traveling wave, then the energy of the electromagnetic field in Eq. (18) can be defined as

$$H_R = \sum_\gamma \frac{\omega_\gamma}{2}(\tilde{q}_\gamma(t)^2 + \tilde{s}_\gamma(t)^2) = \frac{\omega}{2}(\tilde{q}(t)^2 + \tilde{s}(t)^2) \tag{25}$$

We avoid the subscript γ because is now irrelevant and we use a tilde to emphasize that we are dealing with canonical variables of the electromagnetic field. The light is considered to be confined in an optical cavity of length L_c so that the optical frequency can be defined as:

$$\omega = \frac{c\pi}{L_c} \tag{26}$$

where we have assumed that $L_c = \lambda/2$ and the dielectric constant equal to the value in the vacuum in all the cavity.

Exercise 2.4.1 — Electric field in terms of the canonical variables $\tilde{q}(t)$

Show that the electric field in a Eq. (13) for a single mode under the long-wavelength approximation can be written as:

$$\mathbf{E}_T(\mathbf{r},t) = \mathbf{e}\sqrt{\frac{\omega}{\epsilon_0 V}}\tilde{q}(t) \tag{27}$$

with $\mathbf{e}$ the linear polarization vector.

See the detailed solution of this exercise in 5.6 at page 46

By using Eq. (27), we get the final Hamiltonian:

$$H = (H_M + H_R + H_I) = \frac{p^2}{2m_e} + V(x) + \frac{\omega}{2}(\tilde{s}^2 + \tilde{q}^2) + \frac{\alpha}{\sqrt{\hbar}}x\tilde{q}, \tag{28}$$

We see that the term $\frac{\omega}{2}(\tilde{s}^2 + \tilde{q}^2)$ has units of energy so that $\tilde{q}$ and $\tilde{s}$ have units of $\sqrt{\hbar}$ because $\hbar\omega$ already has units of energy. The following change of variables:

$$\tilde{s} \to s\sqrt{\hbar} \qquad \text{and} \qquad \tilde{q} \to q\sqrt{\hbar} \tag{29}$$

is considered. Then, the Hamiltonian with the new variables will lead to

$$H = (H_M + H_R + H_I) = \frac{p^2}{2m_e} + V(x) + \frac{\hbar\omega}{2}(s^2 + q^2) + \alpha x q, \tag{30}$$

where α is a parameter that controls the light-matter interaction and it is proportional to $\sqrt{\frac{\omega}{\epsilon_0 V}}$.[4]

[3] Strictly speaking, the origin of the electromagnetic field in Eq. (4) can also be attributed to other electrons interacting with the electron that we are explicitly simulating. However, including the other electrons in Eq. (4) would increase the computational burden enormously. To keep the computational burden under control and not to obscure the didactic explanation we avoid the simulation of other particles and keep the electromagnetic field without further discussing its physical origin.

[4] Notice that now, q and s do not have units in Eq. (30) because $\hbar\omega$ already gives units of energy. Unless indicated, we will use the Hamiltonian Eq. (30) so that the degrees of the electromagnetic field q and s will have no units. Of course, the units of the electric field in Eq. (27) is given by Volt/meter $\mathbf{E}_T(\mathbf{r},t) = -\mathbf{e}\sqrt{\frac{\omega}{\epsilon_0 V}}\tilde{q}(t) = -\mathbf{e}\sqrt{\frac{\omega}{\epsilon_0 V}}\sqrt{\hbar}\, q(t)$.

3 Types of theories/models

The final Hamiltonian in Eq. (30) is valid for either classical or quantum systems. In this section, we will evaluate the classical and quantum equations of motion derived from this Hamiltonian.

3.1 Matter as classical trajectory and light as classical trajectory

The dynamics of the degrees of freedom of light and matter in a classical scenario can be just computed from Hamilton's equations for the Hamiltonian in Eq. (28) in canonical variables x_{cl}, p_{cl}, $\tilde{q}_{cl}$ and $\tilde{s}_{cl}$ and we get:

$$\frac{dx_{cl}}{dt} = \frac{\partial H}{\partial p_{cl}} = \frac{p_{cl}}{m_e} \qquad \text{and} \qquad \frac{dp_{cl}}{dt} = -\frac{\partial H}{\partial x_{cl}} = -\frac{\partial V(x_{cl})}{\partial x_{cl}} - \frac{\alpha}{\sqrt{\hbar}}\tilde{q}_{cl}$$

where the subscript cl indicates that we are dealing with a classical variable. Identically, Hamilton's equations for the variables $\tilde{q}_{cl}$ and $\tilde{s}_{cl}$ are:

$$\frac{d\tilde{q}_{cl}}{dt} = \frac{\partial H}{\partial \tilde{s}_{cl}} = \omega \tilde{s}_{cl} \qquad \text{and} \qquad \frac{d\tilde{s}_{cl}}{dt} = -\frac{\partial H}{\partial \tilde{q}_{cl}} = -\omega\tilde{q}_{cl} - \frac{\alpha}{\sqrt{\hbar}}x_{cl} \tag{31}$$

We can recover the original variables, in Eq. (30) using Eq. (29), getting:

$$\frac{dx_{cl}}{dt} = \frac{p_{cl}}{m_e} \qquad \text{and} \qquad \frac{dp_{cl}}{dt} = -\frac{\partial V(x_{cl})}{\partial x_{cl}} - \alpha q_{cl} \tag{32}$$

Identically,

$$\frac{dq_{cl}}{dt} = \omega s_{cl} \qquad \text{and} \qquad \frac{ds_{cl}}{dt} = -\omega q_{cl} - \frac{\alpha}{\hbar}x_{cl} \tag{33}$$

The trajectories of the light $q_{cl}(t)$ or $\tilde{q}_{cl}(t)$ have to be understood as the time-dependent parameter that determines the amplitude of the electric field as described Eq. (27). The word "trajectory" for the light does not mean different locations in the physical space, but only how is the evolution of the variable q in different times in the $q-t$ space [3].

Exercise 3.1.1 — Electron and light in the case of no-interaction, i.e., $\alpha = 0$

In the case of $\alpha = 0$, show that the electron follows a Newton equation:

$$m_e \frac{d^2 x_{cl}}{dt^2} = -\frac{\partial V(x_{cl})}{\partial x_{cl}} \tag{34}$$

and the electromagnetic field is just a sinusoidal signal.

$$q_{cl}(t) = A_q \sin\left(\omega t + \theta_q\right) \tag{35}$$

See the detailed solution of this exercise in 5.7 at page 46

Exercise 3.1.2 — Conservation of the total energy

Show that the system's total energy is conserved,

$$\frac{dH}{dt} = \frac{p_{cl}}{m_e}\frac{dp_{cl}}{dt} + \frac{\partial V(x_{cl})}{\partial x_{cl}}\frac{dx_{cl}}{dt} + \hbar\omega s_{cl}\frac{ds_{cl}}{dt} + \hbar\omega q_{cl}\frac{dq_{cl}}{dt} + \alpha\frac{dx_{cl}}{dt}q_{cl} + \alpha x_{cl}\frac{dq_{cl}}{dt} = 0, \tag{36}$$

See the detailed solution of this exercise in 5.22 at page 55

3.2 Matter as quantum wave and light as classical trajectory

If we want to consider the quantum nature of the electrons, the so-called canonical quantization is the typical procedure to convert a classical Hamiltonian into a quantum one [1–4]. It involves promoting classical variables to quantum operators and

imposing commutation relations among these operators that reflect the underlying classical Poisson brackets. In our case, the variables x and p in the Hamiltonian Eq. (30) are already canonical variables. The following operators:

$$\hat{x} \to x \qquad \text{and} \qquad \hat{p} \to -i\hbar\frac{\partial}{\partial x} \tag{37}$$

satisfy the expected commutator $[\hat{x}, \hat{p}] = i\hbar\mathbb{1}$.

Finally, from Eq. (30), using a classical description of the light with $q_{cl}(t)$ and $s_{cl}(t)$, we get the following Hamiltonian:

$$H = (H_M + H_I) = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} + V(x) + \alpha x q_{cl}(t), \tag{38}$$

The simplest way to understand Eq. (38) is treating the light as an "external" element that can affect the quantum electron, but the electron does not affect the light. Then the term $\frac{\hbar\omega}{2}(s_{cl}(t)^2 + q_{cl}(t)^2)$ in Eq. (30) is just a pure time-dependent term, which creates an offset of energy that can be neglected [3, 4, 8]. Such "external" elements (for example an "external" laser acting on an atom) do not necessarily implies not imply a nonrecognition that the "external" element is a classic one, but only that it is affected by the system dynamics.

A global description of the quantum system is given by wave function $\Psi(x,t)$ solution of the following Schrödinger equation:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_e}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) + \alpha x q_{cl}(t)\Psi(x,t), \tag{39}$$

We emphasize that $\Psi(x,t)$ is not a description of a single experiment, but a description of the ensemble of all (identical) experiments. The differences between an ensemble of experiments and a single experiment will be emphasized in several numerical examples (see, for example, simulation 4.6.1 at page 32).

In our case, $V(x)$ is a well with infinite barriers and length L_x. A proper base for describing the system's dynamics can be obtained from a Hamiltonian without interaction with the light.

Exercise 3.2.1 — Quantum states in an infinite square well

Compute the energy eigenstates $\phi_n(x)$ of the electron in an infinite well with borders at $x = \pm\frac{L_x}{2}$ and show that their eigenenergies are given by:

$$E_n = \frac{\hbar^2\pi^2(n+1)^2}{2\ m\ L_x^2} \tag{40}$$

with $n = 0, 1, 2, 3, ..$ the index of the (normalized) eigenstate:

$$\begin{aligned}\phi_n(x) = \langle x|\phi_n\rangle &= \sqrt{\frac{2}{L_x}}\cos\left(\frac{(n+1)\pi x}{L_x}\right) \quad \text{n=0,2,3,4,...}\\ \phi_n(x) = \langle x|\phi_n\rangle &= \sqrt{\frac{2}{L_x}}\sin\left(\frac{(n+1)\pi x}{L_x}\right) \quad \text{n=1,3,5,7,...}\end{aligned} \tag{41}$$

See the detailed solution of this exercise in 5.9 at page 47

Then, we can rewrite the wave function $\Psi(x,t)$ solution of Eq. (39) as

$$\Psi(x,t) = \sum_{n=0}^{N} c_n(t)\phi_n(x), \tag{42}$$

with

$$c_n(t) = \int dx\ \phi_n^*(x)\Psi(x,t) \tag{43}$$

where $\phi_n(x)$ are the states of an infinite quantum well. The evolution of the weave function can be anticipated from the evolution of $c_n(t)$. The equation of motion of the coefficient $c_n(t)$ is:

$$i\hbar\sum_{n=0}^{N}\frac{dc_n(t)}{dt}\phi_n(x) = (H_M + H_I)\sum_{n=0}^{N}c_n(t)\phi_n(x) = \sum_{n=0}^{N}E_{n,e}c_n(t)\phi_n(x) + \alpha x q_{cl}(t)\sum_{n=0}^{N}c_n(t)\phi_n(x) \tag{44}$$

Finally, using the orthonormality of $\phi_n(x)$ we get:

$$i\hbar\frac{dc_n(t)}{dt} = E_{n,e}c_n(t) + \alpha\, q_{cl}(t)\sum_{n'=0}^{N} c_{n'}(t)\int dx\, \phi_n^*(x)\, x\, \phi_{n'}(x) \tag{45}$$

Exercise 3.2.2 — No conservation of the energy of the electron

Show that the energy of the electron is not conserved, i.e.,

$$\frac{d\langle H(t)\rangle}{dt} = \omega\alpha\langle x(t)\rangle s(t). \tag{46}$$

See the detailed solution of this exercise in 5.10 at page 48

3.2.1 Semi-classical Rabi Oscillations with a time-independent interaction

Let's consider the Eq. (45) up to $N = 1$, (i.e., $n = 0$ and $n = 1$) which means we only take into account the ground and the first excited state of the electron. In this manner, we can consider our problem as a two-level system with states $|0\rangle = |\phi_0(x)\rangle$ and $|1\rangle = |\phi_1(x)\rangle$, described as eigenstates of the Hamiltonian H_M in Eq. (38) with electron eigenvalues E_0 and E_1. Then, a general state can be written as:

$$|\Psi(t)\rangle = c_0(t)\,|0\rangle + c_1(t)\,|1\rangle\,, \tag{47}$$

The interacting field H_I is represented by an interacting matrix $\omega_{ab} = \begin{pmatrix}\omega_{00} & \omega_{10}\\ \omega_{01} & \omega_{11}\end{pmatrix}$ in Eq. (45), whose components can be computed by the frequencies:

$$\omega_{ab} = \langle a|\,\hat{H}_I\,|b\rangle = \frac{\alpha q_{cl}(t)\left\langle\phi_a^*\right|x\left|\phi_b\right\rangle}{\hbar}, \quad a, b = 0, 1 \tag{48}$$

We use the fact that $\langle 1|\,\hat{x}\,|1\rangle = \int dx\phi_1^*(x)x\phi_1(x) = \int dx\phi_0^*(x)x\phi_0(x) = \langle 0|\,\hat{x}\,|0\rangle = 0$ in Eq. (48), so that $\omega_{00} = \omega_{11} = 0$, letting only the off-diagonal components of w_{ab} be different from 0. In addition, $\langle 1|\,\hat{x}\,|0\rangle = \langle 0|\,\hat{x}\,|1\rangle = \int dx\ \phi_0^*(x)\ x\ \phi_1(x)$ because we use the real eigenstates in Eq. (41).Thus, we can define the **semiclassical interacting frequency** $\omega_I = \omega_{01} = \omega_{10}$ as:

$$\omega_I \equiv \frac{\alpha A_{cl}\left\langle\phi_1^*\right|x\left|\phi_0\right\rangle}{\hbar}. \tag{49}$$

To simplify the discussion, in this subsection, we also assume that $q_{cl}(t) = A_{cl}$ so that the interacting term is time-independent. Later, we will consider time-dependent (sinusoidal) interaction. With these approximations, the coupled system of equations in Eq. (45) can be rewritten:

$$\begin{cases} i\hbar\dfrac{dc_0(t)}{dt} = c_0(t)E_0 + c_1(t)\hbar\omega_I \\ i\hbar\dfrac{dc_1(t)}{dt} = c_1(t)E_1 + c_0(t)\hbar\omega_I \end{cases} \implies i\hbar\frac{d}{dt}\begin{pmatrix}c_0(t)\\ c_1(t)\end{pmatrix} = \begin{pmatrix}E_0 & \hbar\omega_I\\ \hbar\omega_I & E_1\end{pmatrix}\begin{pmatrix}c_0(t)\\ c_1(t)\end{pmatrix} \tag{50}$$

In this scenario, the Hamiltonian in Eq. (50) defined as $\hat{H} = \hat{H}_M + \hat{H}_I$ can be written in the bra-ket notation as:

$$\begin{aligned}\hat{H}_M &= E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|\\ \hat{H}_I &= \hbar\omega_I|0\rangle\langle 1| + \hbar\omega_I|1\rangle\langle 0|,\end{aligned} \tag{51}$$

Exercise 3.2.3 — Rabi oscillations for a degenerate system

Show that a solution of the system of equations in Eq. (50) can be obtained in the degenerate case, when $E_0 = E_1$, assuming the initial conditions $c_0(0) = 1, c_1(0) = 0$, as:

$$|\psi(t)\rangle = e^{-i\frac{E_0}{\hbar}t}\cos\left(\omega_I t\right)|0\rangle + e^{-i\frac{E_1}{\hbar}t}\sin\left(\omega_I t\right)|1\rangle \tag{52}$$

giving the result:

$$|\langle 1|\psi(t)\rangle|^2 = |c_1(t)|^2 = \sin^2(\omega_I t) \tag{53}$$

See the detailed solution of this exercise in 5.11 at page 48

Next, we follow a general strategy to find the evolution of the system in Eq. (50). This general strategy requires computing the eigenstates of the interacting Hamiltonian in Eq. (50). In next, exercise we diagonalize a general two-states matrix.

Exercise 3.2.4 — Eigenstates of a two-states interacting quantum system

Let us consider a general matrix $\hat{H}$ defined as

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \tag{54}$$

where H_{11} and H_{22} as real elements and H_{12} and H_{21} as complex elements satisfying $H_{12} = H_{21}^*$ so that the matrix is Hermitian. Show that the eigenvalues of such matrix are:

$$E_\pm = \frac{H_{11} + H_{22}}{2} \pm \frac{1}{2}\sqrt{4|H_{21}|^2 + (H_{22} - H_{11})^2} \tag{55}$$

and the eigenstates:

$$\begin{cases} |\phi_+\rangle = \cos(\theta)e^{-i\gamma/2}|0\rangle + \sin(\theta)e^{i\gamma/2}|1\rangle \\ |\phi_-\rangle = -\sin(\theta)e^{-i\gamma/2}|0\rangle + \cos(\theta)e^{i\gamma/2}|1\rangle \end{cases} \tag{56}$$

with

$$\tan(2\theta) = \frac{2|H_{21}|}{H_{22} - H_{11}} \tag{57}$$

See the detailed solution of this exercise in 5.12 at page 49

We have defined two additional frequencies. The **sum frequency** ω_s as:

$$\omega_s \equiv \frac{\omega_1 + \omega_0}{2} \tag{58}$$

with $E_1 = \hbar\omega_1$ and $E_0 = \hbar\omega_0$. The **rest frequency** ω_r is defined as:

$$\omega_r \equiv \frac{\omega_1 - \omega_0}{2} \tag{59}$$

with such definitions, comparing Eq. (54) and the matrix in Eq. (50), we get $\hbar\omega_s = \frac{H_{11}+H_{22}}{2} = \frac{E_0+E_1}{2}$, $\hbar\omega_r = \frac{H_{22}-H_{11}}{2} = \frac{E_1-E_0}{2}$, $\gamma = 0$ and $H_{12} = H_{21} = \hbar\omega_I$. Then, the mixing angle θ in Eq. (57) being:

$$\tan 2\theta = \frac{2\hbar\omega_I}{E_0 - E_1} = \frac{\omega_I}{\omega_r} \tag{60}$$

and their corresponding eigen-energies in Eq. (55) are:

$$E_\pm = \frac{1}{2}(E_0 + E_1) \pm \frac{1}{2}\sqrt{(E_0 - E_1)^2 + 4(\hbar\omega_I)^2} = \hbar\left(\omega_s \pm \sqrt{\omega_r + \omega_I}\right) \tag{61}$$

Now, using Eq. (56) the general state describing the system in Eq. (47) can also be rewritten as:

$$|\Psi(t)\rangle = c_+(t)\cdot e^{-iE_+/\hbar t}|\phi_+\rangle + c_-(t)\cdot e^{-iE_-/\hbar t}|\phi_-\rangle \tag{62}$$

where $c_+(t)$ and $c_-(t)$ are determined by the initial conditions of the problem. For arbitrary electron energies, E_1 and E_0, the *Rabi* formula defining the probability probability $|\langle 1|\psi(t)\rangle|^2$ can be computed as indicated in the exercise below.

Exercise 3.2.5 — Rabi formula for time independent interaction

For the initial conditions, $|\Psi(t=0)\rangle = |0\rangle$, show that probability $|\langle 1|\psi(t)\rangle|^2$ is given by:

$$\begin{aligned} |\langle 1|\psi(t)\rangle|^2 = |c_1(t)|^2 &= \frac{4(\hbar\omega_I)^2}{(E_0-E_1)^2+4(\hbar\omega_I)^2}\sin^2\left(\frac{1}{2\hbar}\sqrt{(E_0-E_1)^2+4(\hbar\omega_I)^2}t\right) \\ &= \frac{\omega_I^2}{\omega_r^2+\omega_I^2}\sin^2\left(\sqrt{\omega_r^2+\omega_I^2}t\right) \end{aligned} \tag{63}$$

See the detailed solution of this exercise in 5.13 at page 50

The final result Eq. (63) can also be found in Ref. [3]. The figure 1 shows the results from Eq. (63) for different values of $\Delta E = 2\hbar\omega_r$. Notice that Eq. (53) can be obtained from Eq. (63) by just demanding degenerate states (i.e. $E_0 = E_1$ giving $\omega_r = 0$).

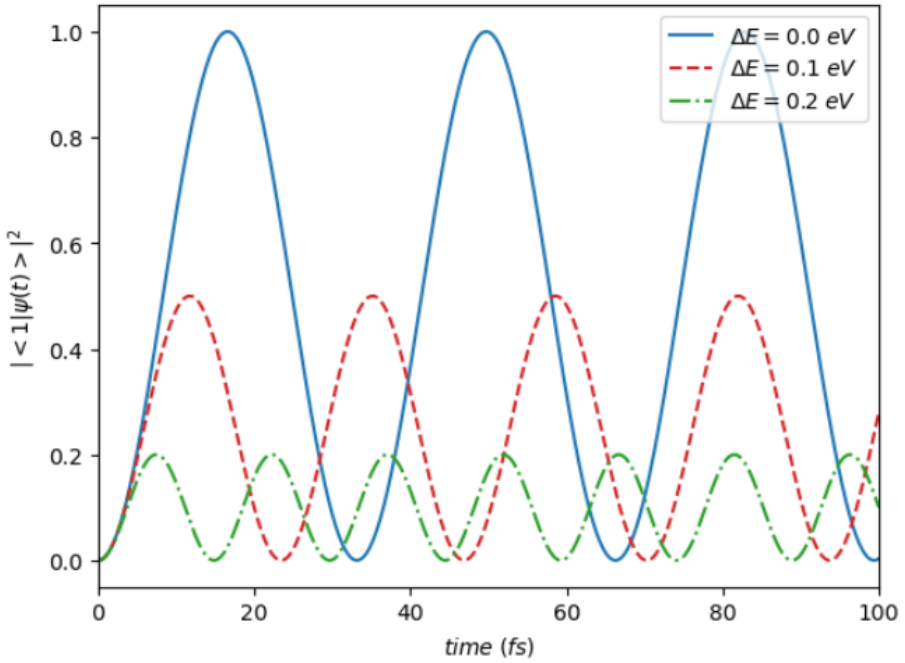

Figure 1: Rabi oscillations in the resonant case (blue line) and in off-resonant cases (red and green) for a system with $\omega_I = 98$ rad/ps (notice that $sin^2(x)$ oscillates at double the frequency of $sin(x)$). As the system moves further from resonance, the oscillation amplitude decreases while the oscillation frequency increases. Notice that $\Delta E = 0.1eV$ corresponds to $\omega_r = 75$ rad/ps and $\Delta E = 0.2eV$ corresponds to $\omega_r = 150$ rad/ps.

3.2.2 Semi-classical Rabi Oscillations with a time-dependent (sinusoidal) interaction

In the previous section, to simplify the mathematical developments, we assumed that the interaction W did not depend on time. However, we have seen in Exercise 3.1.1 that a typical description of a classical electromagnetic field is $q_{cl}(t) = A_{cl}\sin(\omega t)$ where we have defined the frequency of the oscillating electromagnetic field as ω (without subscripts). The value of ω is fixed by the optical cavity length as seen in Eq. (26)

Our Hamiltonian in Eq. (45) can be written as:

$$\begin{cases} i\hbar\dfrac{dc_0(t)}{dt} = c_0(t)\hbar w_0 + c_1(t)\hbar\omega_I\sin(\omega t) \\ i\hbar\dfrac{dc_1(t)}{dt} = c_1(t)\hbar w_1 + c_0(t)\hbar\omega_I\sin(\omega t) \end{cases} \implies i\hbar\frac{d}{dt}\begin{pmatrix} c_0(t) \\ c_1(t)\end{pmatrix} = \begin{pmatrix} \hbar\omega_0 & \hbar\omega_I\sin(\omega t) \\ \hbar\omega_I\sin(\omega t) & \hbar\omega_1\end{pmatrix}\begin{pmatrix} c_0(t) \\ c_1(t)\end{pmatrix} \tag{64}$$

with ω_I defined in Eq. (49). The whole Hamiltonian in Eq. (38), in the bra-ket notation, can be written now as $\hat{H} = \hat{H}_M + \hat{H}_I$

with:

$$\begin{aligned} \hat{H}_M &= \hbar\omega_0|0\rangle\langle 0| + \hbar\omega_1|1\rangle\langle 1|, \\ \hat{H}_I &= \hbar\omega_I \sin(\omega t)|0\rangle\langle 1| + \hbar\omega_I \sin(\omega t)|1\rangle\langle 0|), \end{aligned} \tag{65}$$

where $E_0 = \hbar\omega_0$ and $E_1 = \hbar\omega_1$. Compare the above time-dependent Hamiltonian in Eq. (65) with the time-independent one in Eq. (51). The general solution to this equation is:

$$|\Psi(t)\rangle = c_0(t)e^{-i\omega_0 t}|0\rangle + c_1(t)e^{-i\omega_1 t}|1\rangle. \tag{66}$$

Rewriting Eq. (64) by using the change $c_n(t) = \tilde{c}_n(t)e^{-w_n t}$, we end up with the following system:

$$\begin{cases} i\dfrac{d\tilde{c}_0(t)}{dt} = \dfrac{\tilde{c}_1(t)}{2i}\omega_I\left(e^{i(\omega-2\omega_r)t} - e^{-i(\omega+2\omega_r)t}\right) \\ i\dfrac{d\tilde{c}_1(t)}{dt} = -\dfrac{\tilde{c}_0(t)}{2i}\omega_I\left(e^{-i(\omega-2\omega_r)t} - e^{i(\omega+2\omega_r)t}\right) \end{cases} \tag{67}$$

where ω_r and ω_I defined in Eq. (59) and Eq. (49), and $\sin(\omega t) = \frac{e^{i\omega t} - e^{-i\omega t}}{2i}$. Here it is natural to define the **detuning parameter** Δ as:

$$\Delta \equiv 2\omega_r - \omega \tag{68}$$

and the **anti-detuning parameter** δ as:

$$\delta \equiv 2\omega_r + \omega \tag{69}$$

Note then that four terms in Eq. (67) behave like $e^{\pm i\Delta t}$ and $e^{\pm i\delta t}$. Since the latter oscillate much faster than the former, on average they yield a negligible contribution *if* one is not far from resonance. Neglecting the term $e^{\pm i\delta t}$ is the so called **rotating wave approximation** (RWA). Under this simplification, we end up with the following system:

$$\begin{cases} i\dfrac{d\tilde{c}_0(t)}{dt} = \dfrac{1}{2i}\tilde{c}_1(t)\omega_I e^{-i\Delta t} = \dfrac{1}{2}\tilde{c}_1(t)e^{i3\pi/2}\omega_I e^{-i\Delta t} \\ i\dfrac{d\tilde{c}_1(t)}{dt} = -\dfrac{1}{2i}\tilde{c}_0(t)\omega_I e^{i\Delta t} = \dfrac{1}{2}\tilde{c}_0(t)e^{-i3\pi/2}\omega_I e^{i\Delta t} \end{cases} \tag{70}$$

At this point, the excercise below shows the final Rabi oscillations for a time dependent (sinusoidal) signal.

Exercise 3.2.6 — Rabi formula with time-dependent interaction

Show that, starting from the excited state $|1\rangle$, we can evalute the transition probability to the state $|0\rangle$ at time t from Eq. (70) as:

$$|\langle 0|\Psi(t)\rangle|^2 = |c_0(t)|^2 = \frac{\omega_I^2}{\Delta^2 + \omega_I^2}\sin^2\left(\frac{\Omega}{2}t\right) \tag{71}$$

where Ω defined in Eq. (72).

See the detailed solution of this exercise in 5.14 at page 50

The Ω is defined as the **semiclassical Rabi angular frequency**:

$$\Omega = \sqrt{\Delta^2 + \omega_I^2} \tag{72}$$

The result in Eq. (71) has the same form as Eq. (63). Recovering the detuning parameter definition $\Delta = 2\omega_r - \omega = \omega_1 - \omega_0 - \omega$, we can see that even when the states are not degenerated ($\omega_1 \neq \omega_0$), we can still obtain a full oscillation among both states by tuning correctly the electromagnetic field frequency $\omega = \omega_1 - \omega_0$ giving $\Delta = 0$ and $\frac{\omega_I^2}{\Delta^2+\omega_I^2} = 1$ (See Fig. 2). Moreover, we see that the full width at half maximum is $2\omega_I$. Notice that Eq. (71) can also be found in Ref. [8]

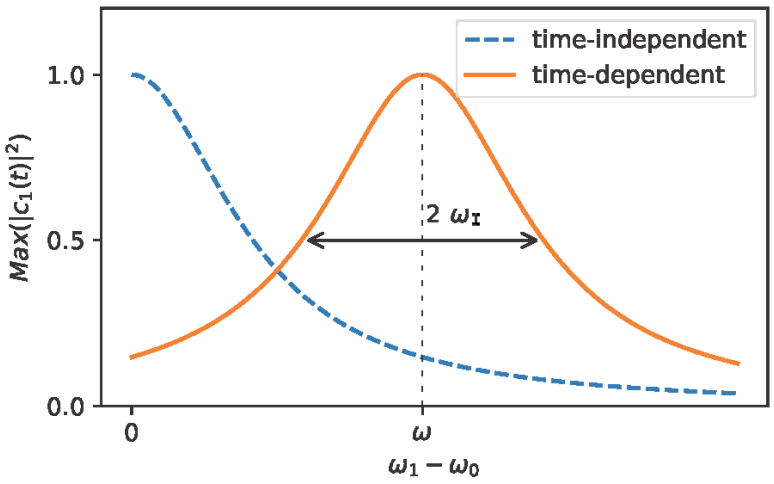

Figure 2: Comparison between the maximum transition probability from state $|0\rangle$ to state $|1\rangle$ for a time-independent (dotted blue) interaction and a time-dependent interaction (solid orange). We can see that the electromagnetic frequency ω can be used to tune the resonance, shifting the curve and centring it around ω.

Exercise 3.2.7 — Computation of the Rabi angular frequency ω_I

For a system with one electron with an effective 0.042 times the free electron mass and oscillating between the ground and excited state of a quantum well with a length $L_x = 16$ nm, and light described by a sinusoidal signal with an amplitude $A_{cl} = 1$ inside ann optical cavity with length $L_c = 5930$ nm , and with an interacting parameter between light and matter given by $\alpha = 0.01$ eV/nm, show that the **semiclassical Rabi angular frequency** in Eq. (72) gives the following value:

$$\Omega = \sqrt{\Delta^2 + \omega_I^2} = \omega_I \equiv \frac{\alpha A_{cl} \langle 0| \hat{x} |1\rangle}{\hbar} = 43 \text{ rad/ps}. \tag{73}$$

The angular frequency can be translated into a linear frequency, giving ≈ 7 THz. This computation of this frequency is used in simulation 4.5.1 at page 31.

See the detailed solution of this exercise in 5.15 at page 51

3.2.3 Perturbative Theory

In the previous section, we obtained the transition probability for going from state $|0\rangle$ to state $|1\rangle$ for a time-dependent (sinusoidal) interaction using the Rotating Wave Approximation. This approximation is valid when the system is not far from resonance and captures correctly the overall behaviour of the system. However, since it is neglecting the fast oscillating terms, it cannot be an exact solution. In this section, we will compute the transition probability using a perturbative approximation. We will arrive at a much more precise expression, but at the cost that it will be valid only for early times.

The perturbative approximation requires parametrizing the strength of the interaction in terms of the parameter β so that Eq. (45) now, becomes:

$$\begin{cases} i\hbar \dfrac{dc_0(t)}{dt} = c_0(t)\hbar w_0 + \beta c_1(t)\hbar\omega_I \sin(\omega t) \\ i\hbar \dfrac{dc_1(t)}{dt} = c_1(t)\hbar w_1 + \beta c_0(t)\hbar\omega_I \sin(\omega t) \end{cases} \tag{74}$$

We use now the change of variabes $\tilde{c}_n(t) = c_n(t)e^{-i\omega_n t}$ so that Eq. (74) can be rewritten as:

$$\begin{cases} i\hbar \dfrac{d\tilde{c}_0(t)}{dt} = \beta \tilde{c}_1(t)\hbar\omega_I \sin(\omega t)e^{-i2\omega_r t} \\ i\hbar \dfrac{d\tilde{c}_1(t)}{dt} = \beta \tilde{c}_0(t)\hbar\omega_I \sin(\omega t)e^{i2\omega_r t} \end{cases} \tag{75}$$

with ω_r is defined in Eq. (59). Then, Eq. (75) is a linear system of coupled equations. At this point, we expand the coefficients $\tilde{c}_n(t)$ in a power expansion of β:

$$\tilde{c}_n(t) = \beta^0 \tilde{c}_n^0 + \beta^1 \tilde{c}_n^1(t) + \beta^2 \tilde{c}_n^2(t) + \ldots \tag{76}$$

Then, putting Eq. (76) into Eq. (75), and setting equal order on β in both sides of the equation, we end up with several equations for different orders. For the zero order we have:

$$\beta^0 i\hbar \frac{d\tilde{c}_0^0(t)}{dt} = 0 \qquad \beta^0 i\hbar \frac{d\tilde{c}_1^0(t)}{dt} = 0 \tag{77}$$

and for the first order:

$$\beta i\hbar \frac{d\tilde{c}_0^1(t)}{dt} = \beta \tilde{c}_1^0(t)\hbar\omega_I \sin(\omega t) e^{-i2\omega_r t} \qquad \beta i\hbar \frac{d\tilde{c}_1^1(t)}{dt} = \beta \tilde{c}_0^0(t)\hbar\omega_I \sin(\omega t) e^{i2\omega_r t} \tag{78}$$

So we can see that by determining the zeroth order coefficient in the first place, higher order coefficients can be computed with the recurrent relation.

Exercise 3.2.8 — Perturbative evaluation of $c_0(t)$ and $c_1(t)$

If we set the initial conditions to be $c_0 = 1, c_1 = 0$, we get:

$$|\langle 1|\psi(t)\rangle|^2 = |c_1(t)|^2 = \frac{\omega_I^2}{4}\left|\frac{1-e^{i(\omega+2\omega_r)t}}{\omega+2\omega_r} - \frac{1-e^{-i(\omega-2\omega_r)t}}{2\omega_r-\omega}\right|^2 \tag{79}$$

On the other hand, starting from the excited state $c_0 = 0, c_1 = 1$, the transition probability to the ground state is:

$$|\langle 0|\psi(t)\rangle|^2 = |c_0(t)|^2 = \frac{\omega_I^2}{4}\left|\frac{1-e^{i(\omega+2\omega_r)t}}{\omega+2\omega_r} + \frac{1-e^{-i(\omega-2\omega_r)t}}{2\omega_r-\omega}\right|^2 \tag{80}$$

See the detailed solution of this exercise in 5.16 at page 52

The final result Eq. (79) includes both the rapid and the slow oscillating terms, without the rotating wave approximation, thus being much more precise than Eq. (71), but only as long the initial non-zero state $c_n(t)$ remains similar to $c_n(0) = 1$. This means that $t << \hbar/E_0$ for $c_0(t) \to c_1(t)$ and $t << \hbar/E_1$ for $c_1(t) \to c_0(t)$. To extend the solution to larger times, higher-order solutions should be computed. The final result Eq. (79) and Eq. (80) can also be found in [9]. This perturbative approximation are discussed in simulation 4.4.1 at page 30.

3.3 Matter as quantum trajectory and light as classical trajectory

In classical mechanics, typically, the electron is represented by a trajectory $x(t)$ as seen in Section 3.1. An ensemble of $j = 1, 2, ..., N$ (identical) experiments, each one described by its trajectory $x_j(t)$, can be used to define a classical probability density $\rho_{cl}(x,t)$ as:

$$\rho_{cl}(x,t) = \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta(x - x_j(t)) \tag{81}$$

If required, a similar distribution can be defined for a classical current probability distribution:

$$J_{x,cl}(x,t) = \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta(x - x_j(t))\frac{dx_j(t)}{dt}. \tag{82}$$

According to the Hamilton-Jacobi theorem, such probability densities can be translated into a classical wave function solution of a classical wave equation [5]. Thus, the concept of wave function is also applicable to classical systems. See the simulation 4.1.2 at page 24.

In quantum mechanics typically, the electron is represented by a wave function $\Psi(x,t)$ as seen in Section 3.2, whose density probability $|\Psi(x,t)|^2$ can be understood as the probability distribution when many (identical) experiments are considered. According to Hydrodynamic (or Bohmian) formulation of quantum mechanics, a description of quantum phenomena in terms of quantum trajectories is also possible [5–7]. In particular, the time-evolution of $\rho(x,t) = |\Psi(x,t)|^2$ can be defined from a set of quantum trajectories, $\{x_j(t)\}$, satisfying at all times:

$$\rho(x,t) = |\Psi(x,t)|^2 = \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta(x - x_j(t)) \tag{83}$$

Next, we show how to define such set of trajectories that satisfy Eq. (83).

Exercise 3.3.1 — Continuity equation in quantum mechanics

Show that there is a *local* continuity equation associated with the Hamiltonian in Eq. (38) given by:

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x} J_x(x,t) = 0 \tag{84}$$

with

$$J_x(x,t) = i\frac{\hbar}{2m_e}\left(\psi(x,t)\frac{\partial \psi^*(x,t)}{\partial x} - \psi^*(x,t)\frac{\partial \psi(x,t)}{\partial x}\right) = \frac{\hbar}{m_e} Im\left(\frac{\Psi(x,t)}{dx}\Psi^*(x,t)\right) \tag{85}$$

See the detailed solution of this exercise in 5.17 at page 52

If we define the velocity of such trajectories from Eq. (85) as:

$$v(x,t) = \frac{J_x(x,t)}{|\psi(x,t)|^2} = \frac{\hbar}{m_e} Im\left(\frac{\frac{\Psi(x,t)}{dx}}{\Psi(x,t)}\right) \tag{86}$$

them the trajectory can be defined as:

$$x_j(t) = x_j(t_0) + \int_{t_0}^{t} v(x_j(t'),t')dt' \tag{87}$$

where $x_j(t_0)$ is the initial position. Two trajectories representing the same experiment ("guided" by the same wave function) are different if they have different initial conditions, and they are labeled by a different subscript j. Then, the continuity equation in Eq. (84) can be rewritten as:

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x}(\rho(x,t)v(x,t)) = 0 \tag{88}$$

Finally, we realize that if a set of (infinite) Bohmian trajectories $\{x_j(t_0)\}$ satisfies the distribution $|\psi(x,t_0)|^2$ at the initial time t_0, then, these trajectories exactly reproduce the quantum probability at any time as described by Eq. (83) because of the continuity equation in Eq. (88). See Ref. [5–7]. Notice that Eq. (86) can be written also as $J_x(x,t) = |\psi(x,t)|^2 v(x,t)$, then, using Eq. (83) we get:

$$J_x(x,t) = |\psi(x,t)|^2 v(x,t) = \lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}\delta(x - x_j(t))v(x_j(t),t). \tag{89}$$

which has the same structure as Eq. (82), but the classical and quantum velocities (and so the trajectories) are different giving different classical and quantum distributions. [5]

3.4 Matter as classical trajectory and light as quantum wave

Similarly to what we have done in Section 3.2 for a quantum electron interacting with a classical light, we consider here a classical electron interacting with a classical light. We use again the canonical quantization. We promote the classical variables q and s used to describe the light in Eq. (30) to quantum operators and impose commutation relations among them:

$$\hat{q} \to q \qquad \text{and} \qquad \hat{s} \to -i\frac{\partial}{\partial q} \tag{90}$$

that satisfy the commutation relations $[\hat{s},\hat{q}] = i\mathbb{1}$. From Eq. (30), we get $p = p(t)$ and $x = x(t)$ so that:

$$H = (H_R + H_I) = \frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial q^2} + q^2\right) + \alpha x(t) q \tag{91}$$

[5] The quantum uncertainty is satisfied by these trajectories because of Eq. (83). Despite each experiment is described by a trajectory, we cannot know which trajectory is associated to each experiment because there are many possible initial positions $x_j(t_0)$ associated with the same wave function probability $|\psi(x,t_0)|^2$. The only experiment were it would be possible to anticipate the initial position with certainty is an experiment where the initial wave function probability is described by $|\psi(x,t_0)|^2 = \delta(x - x_0)$. Then, all initial positions in all experiments will be $x_j(t_0) = x_0$, but this is not a typical initial conditions in quantum experiments, and the delta function $\delta(x - x_0)$ is just a mathematical limit that cannot be achieved in the laboratory.

where $\frac{p(t)^2}{2m} + V(x(t))$ is just a pure time-dependent term related with an offset of energy. The Hamiltonian Eq. (91) contains the energy of the radiation, plus a time dependent interaction Hamiltonian reflecting that the effect of the matter on the light is treated as an external potential. The matter affects the light, but the light does not affect the matter.

Exercise 3.4.1 — Radiation energy in terms of creation and annihilation operators

Show that the part of the Hamiltonian in Eq. (91) related to the electromagnetic energy can be written as:

$$\frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial q^2} + q^2\right) \qquad \rightarrow \qquad \hat{H}_R = \hbar\omega\left(\frac{1}{2} + \hat{a}^\dagger\hat{a}\right) \tag{92}$$

in terms of the so-called creation $\hat{a}^\dagger$ and the annihilation operators $\hat{a}$.
See the detailed solution of this exercise in 5.18 at page 53

A description of an ensemble of experiments is encapsulated from the wave function , which is a solution of the following Schrodinger equation:

$$i\hbar\frac{\partial\Psi(q,t)}{\partial t} = -\frac{\hbar\omega}{2}\frac{\partial^2\Psi(q,t)}{\partial q^2} + \frac{\hbar\omega}{2}q^2\Psi(q,t) + \alpha x(t) q\Psi(q,t), \tag{93}$$

The term $|\Psi(q,t)|^2$ is a probability distribution of q (proportional to the amplitude of the electric field). It will be very enlightening to discuss $\Psi(q,t)$ when we neglect the interaction with the matter. Then, we deal with a the well-known quantum harmonic oscillator.

Exercise 3.4.2 — Quantum states in a parabolic well

Compute the energy eigenstates $\psi_m(q)$ of the light in a parabolic well and show that their eigenenergies are given by:

$$E_m = \hbar\omega\left(m + \frac{1}{2}\right) \tag{94}$$

with $m = 0, 1, 2, 3, ..$ the index of the (normalized) eigenstate:

$$\psi_m(q) = \left(\frac{1}{\pi}\right)^{1/4}\frac{H_m(q)}{\sqrt{2^m m!}}e^{-q^2/2} \tag{95}$$

See the detailed solution of this exercise in 5.19 at page 53

Then, we can rewrite the wave function $\Psi(q,t)$ solution of Eq. (39) as

$$\Psi(q,t) = \sum_{m=0}^{M} c_m(t)\psi_m(q), \tag{96}$$

with

$$c_m(t) = \int dx\ \psi_m^*(q)\Psi(q,t) \tag{97}$$

where $\phi_m(q)$ are the states of an infinite quantum well studied before. The equation of motion of the coefficient $c_m(t)$ is:

$$i\hbar\sum_{m=0}^{M}\frac{dc_m(t)}{dt}\psi_m(q) = (H_R + H_I)\sum_{m=0}^{M}c_m(t)\psi_m(q) = \sum_{m=0}^{M}E_{m,p}c_m(t)\psi_m(q) + \alpha x(t) q\sum_{m=0}^{M}c_m(t)\psi_m(q) \tag{98}$$

Finally, we get:

$$i\hbar\frac{dc_m(t)}{dt} = E_{m,p}c_m(t) + \alpha x(t)\sum_{m'=0}^{M}c_{m'}(t)\int dq\psi_m^*(q)q\psi_{m'}(q) \tag{99}$$

Exercise 3.4.3 — No conservation of the energy of the electron

Show that the energy of the light interacting is not conserved, i.e., $\frac{d\langle H(t)\rangle}{dt} = \frac{\alpha}{m_e}\langle q(t)\rangle p(t)$.

See the detailed solution of this exercise in 5.20 at page 54

3.5 Matter as classical trajectory and light as quantum trajectory

Identically to what we have done in section 3.3, for the classical light, an ensemble of (identical) experiments, each one described by the same optical cavity but different initial conditions for $q_{cl}(t)$, can be used to define a classical probability density $\rho_{cl}(q_{cl}, t)$ as:

$$\rho_{cl}(q,t) = \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta(q - q_{j,cl}(t)) \tag{100}$$

If required, a similar distribution can be defined for a classical current probability distribution related to $q(t)$ as:

$$J_{q,cl}(q,t) = \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta(q - q_{j,cl}(t))\frac{dq_{j,cl}(t)}{dt}. \tag{101}$$

According to the Hamilton-Jacobi theorem, such probability densities can be translated into a classical wave function solution of a classical wave equation. Thus, the concept of wave function is also applicable to classical systems. See the simulation 4.1.2 at page 24.

Identically to what we have done in section 3.3, according to the hydrodynamic (or Bohmian) formulation of quantum mechanics, the time evolution of $|\Psi(q,t)|^2$ mentioned in section 3.4 can be described in terms of quantum trajectories [8]. The description of the time-evolution of $\rho(q,t) = |\Psi(q,t)|^2$ is given as a sum of quantum trajectories by:

$$\rho(q,t) = |\Psi(q,t)|^2 = \lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} \delta(q - q_j(t)) \tag{102}$$

Next, we show how to define such set of trajectories that satisfy Eq. (102).

Exercise 3.5.1 — Continuity equation in quantum mechanics

Show that there is a *local* continuity equation associated with Eq. (93) given by:

$$\frac{\partial\rho(q,t)}{\partial t} + \frac{\partial}{\partial q}J_q(q,t) = 0 \tag{103}$$

with

$$J_q(q,t) = i\frac{\omega}{2}\left(\psi(q,t)\frac{\partial\psi^*(q,t)}{\partial q} - \psi^*(q,t)\frac{\partial\psi(q,t)}{\partial q}\right) = \omega Im\left(\frac{\Psi(q,t)}{dq}\Psi^*(q,t)\right) \tag{104}$$

See the detailed solution of this exercise in 5.21 at page 55

If we define the velocity of such trajectories from Eq. (104) as:

$$v_q(q,t) = \frac{J_q(q,t)}{|\psi(q,t)|^2} = \omega Im\left(\frac{\frac{\Psi(q,t)}{dq}}{\Psi(q,t)}\right) \tag{105}$$

them the trajectory can be defined as:

$$q_j(t) = q_j(t_0) + \int_{t_0}^{t} v_q(q_j(t'),t')dt' \tag{106}$$

where $q_j(t_0)$ is the initial position. Two trajectories representing the same experiment ("guided" by the same wave function) are different if they have different initial conditions, and they are labeled by a different subscript j. Then, the continuity equation in Eq. (103) can be rewritten as:

$$\frac{\partial\rho(q,t)}{\partial t} + \frac{\partial}{\partial q}(\rho(q,t)v_q(q,t)) = 0 \tag{107}$$

Finally, we realize that if a set of (infinite) Bohmian trajectories $\{q_j(t_0)\}$ satisfies the distribution $|\psi(q,t_0)|^2$ at the initial time t_0, then, these trajectories exactly reproduce the quantum probability at any time as described by Eq. (103) because of the continuity equation in Eq. (107). Notice that the current density can be written from Eq. (105) cas $J_q(x,t) = |\psi(q,t)|^2 v_q(q,t)$, then, using Eq. (102) we get:

$$J_q(q,t) = |\psi(q,t)|^2 v_q(q,t) = \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} \delta(q - q_j(t)) v_q(q_j(t),t). \tag{108}$$

which has the same structure as Eq. (101), but the classical and quantum velocities (and so the trajectories) are different giving different classical and quantum distributions.[6]

3.6 Matter as quantum wave and light as quantum wave

Finally, by using the canonical quantization in Eq. (37) and Eq. (90) to describe the quantum nature of electrons and electromagnetic field simultaneously, the following Hamiltonian is found:

$$H = (H_M + H_R + H_I) = -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} + V(x) + \frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial q^2} + q^2\right) + \alpha x q \tag{109}$$

which involves the two-dimensional Schrödinger equation,

$$i\hbar\frac{\partial\Psi(x,q,t)}{\partial t} = -\frac{\hbar^2}{2m_e}\frac{\partial^2\Psi(x,q,t)}{\partial x^2} + V(x)\Psi(x,q,t) - \frac{\hbar\omega}{2}\frac{\partial^2\Psi(x,q,t)}{\partial q^2} + \frac{\hbar\omega}{2}q^2\Psi(x,q,t) + \alpha x q\Psi(x,q,t), \tag{110}$$

The wave function $\Psi(x,q,t)$ is defined in the x-q configuration space. Then, by using the eigenenergies Eq. (40) and eigenstates Eq. (41) as a base of the the degree of freedom of the electron, and the eigenenergies Eq. (94) and eigenstates Eq. (95) as a base of the degree of freedom of the light, we can rewrite the wave function $\Psi(x,q,t)$ solution of Eq. (110) as

$$\Psi(x,q,t) = \sum_{n=0}^{N}\sum_{m=0}^{M} c_{n,m}(t)\phi_n(x)\psi_m(q), \tag{111}$$

with

$$c_{n,m}(t) = \int dq \int dx\ \phi_n^*(x)\psi_m^*(q)\Psi(x,q,t) \tag{112}$$

The equation of motion of the coefficient $c_{n,m}(t)$ is:

$$\begin{aligned} i\ \ \hbar\sum_{n=0}^{N}\sum_{m=0}^{M}\frac{dc_{n,m}(t)}{dt}\phi_n(x)\psi_m(q) &= (H_M + H_R + H_I)\sum_{n=0}^{N}\sum_{m=0}^{M} c_{n,m}(t)\phi_n(x)\psi_m(q) \\ = \sum_{n=0}^{N}\sum_{m=0}^{M} E_{n,e}c_{n,m}(t)\phi_n(x)\psi_m(q) &+ \sum_{n=0}^{N}\sum_{m=0}^{M} E_{m,p}c_{n,m}(t)\phi_n(x)\psi_m(q) + \alpha x q\sum_{n=0}^{N}\sum_{m=0}^{M} c_{n,m}(t)\phi_n(x)\psi_m(q) \end{aligned} \tag{113}$$

Finally, we get:

$$i\hbar\frac{dc_{n,m}(t)}{dt} = (E_{n,e} + E_{m,p})c_{n,m}(t) + \alpha\sum_{n'=0}^{N}\sum_{m'=0}^{M} c_{n',m'}(t)\int dx\phi_n^*(x)x\phi_{n'}(x)\int dq\psi_m^*(q)q\psi_{m'}(q) \tag{114}$$

Exercise 3.6.1 — Conservation of the energy of the electron and photon

Show that the energy of the electron plus light is conserved,

$$\frac{d\langle H(t)\rangle}{dt} = 0. \tag{115}$$

[6] The quantum trajectory $q_j(t)$ is not a trajectory in physical space, but just a description of the evolution of the parameter q, related to the amplitude of the electromagnetic field, as a function of time in the q space.

See the detailed solution of this exercise in 5.22 at page 55

3.6.1 Quantum Rabi Oscillations

In Sec. 3.2 we have already studied the Rabi oscillations from a semi-classical viewpoint. The same phenomena of the Rabi oscillations are revisited with a full quantum treatment. For example, if we consider Eq. (114) up to $N = 1$ and $M = 1$, which means we only take into account the ground and the first excited state of the electron and the light. We can describe this problem with the following four eigenstates of the Hamiltonian $H_M + H_R$ of Eq. (109):

$$\begin{aligned} \langle x, q|0,0\rangle &= \phi_0^*(x)\psi_0^*(q), \\ \langle x, q|0,1\rangle &= \phi_0^*(x)\psi_1^*(q), \\ \langle x, q|1,0\rangle &= \phi_1^*(x)\psi_0^*(q), \\ \langle x, q|1,1\rangle &= \phi_1^*(x)\psi_1^*(q) \end{aligned} \tag{116}$$

with energy eigenvalues:

$$\hat{H}_M + \hat{H}_R \,|n,m\rangle = (E_{n,e} + E_{m,p})\,|n,m\rangle \tag{117}$$

where $E_{n,e}$ is the eigenenergy of the electron and $E_{m,p}$ of the light. Now we introduce the interaction term H_I between the electron and the photon as an additional term to the full Hamiltonian $H = H_M + H_R + H_I$ of Eq. (109) so that we define the matrix component components $H_{i,n,m}$ can be computed by:

$$H_{i,n,m} = \alpha \sum_{n'=0}^{1} \sum_{m'=0}^{1} \int dx \phi_n^*(x) x \phi_{n'}(x) \int dq \psi_m^*(q) q \psi_{m'}(q) \tag{118}$$

This problem, with no approximations, is solved numerically in the simulation 4.8.1 at page 37. Under some approximation, an analytical model for the Rabi oscillations can be found through the so-called *Jaynes-Cummings* model as discussed in next section.

3.6.2 Jaynes-Cummings model

The so-called Jaynes-Cummings model describes a two-level atom with a ground state $|0\rangle$ and an excited state $|1\rangle$, interacting with an electromagnetic field inside an optical cavity. In this simplified case, we consider the complete system using the four possible states $|0,m\rangle, |0,m+1\rangle, |1,m\rangle, |1,m+1\rangle$ as an orthonormal basis of our Hilbert space, where m represents the number of photons in the system. For convenience, we can rewrite the the full Hamiltonian $H = H_M + H_R + H_I$ of Eq. (109) in terms of the photon creation, $\hat{a}^\dagger$ and annihilation, $\hat{a}$, operators:

$$\begin{aligned} \hat{H}_M &= \hbar\omega_0 |0\rangle\langle 0| + \hbar\omega_1 |1\rangle\langle 1|, \\ H_R &= \hbar\omega (a^\dagger a + \frac{1}{2}), \\ H_I &= \hbar\omega_{I,m} (|0\rangle\langle 1| + |1\rangle\langle 0|)(a + a^\dagger). \end{aligned} \tag{119}$$

where $E_{0,e} = \hbar\omega_0$ and $E_{1,e} = \hbar\omega_1$ of Eq. (119) are the electron energy of the ground and excited states, respectively. Looking at Eq. (118), we defined now a new interacting frequency for the quantum case defined as **quantum interacting frequency** $\omega_{I,m}$ as

$$\omega_{I,m} \equiv \frac{\alpha \left\langle \phi_1^* \right| x \left| \phi_0 \right\rangle \left\langle \psi_m^* \right| q \left| \psi_{m+1} \right\rangle}{\hbar}. \tag{120}$$

In the definition of $\omega_{I,m}$ we have assume that the electron can have states $|0\rangle$ and $|1\rangle$, while the light can be described by $|m\rangle$ and $|m+1\rangle$. The operator $\hat{a}^\dagger \hat{a}\,|m\rangle = m\,|m\rangle$ gives the number of photons as discussed in Exercise 3.4.1 at page 18. The H_I term is able to induce transitions among the electron+photon states Out of its four terms, $|0\rangle\langle 1|\hat{a}^\dagger$ stands for a transition from $|1,m\rangle$ to $|0,m+1\rangle$ through the absorption of a photon, while $|1\rangle\langle 0|\hat{a}$ stands for the opposite process, both conserving the total electron-photon energy:

$$\begin{aligned} |0\rangle\langle 1|\hat{a}^\dagger\,|1,m\rangle &= \sqrt{m+1}\,|0,m+1\rangle \\ |1\rangle\langle 0|\hat{a}\,|0,m+1\rangle &= \sqrt{m+1}\,|1,m\rangle \end{aligned} \tag{121}$$

If one is not far from resonance, in the rotating wave approximation spirit, the the terms $|0\rangle\langle 1|\hat{a}$ and $|1\rangle\langle 0|\hat{a}^\dagger$ can be neglected, so that Eq. (119) becomes:

$$H_I = \hbar\omega_{I,m}(|0\rangle\langle 1|a^\dagger + |1\rangle\langle 0|a). \tag{122}$$

with ω_I defined in Eq. (49) (using $A_{cl} = 1$). Then, the general solution becomes (again) a two-level system:

$$|\Psi(t)\rangle = c_{0,m+1}(t)|0, m+1\rangle + c_{1,m}(t)|1, m\rangle \tag{123}$$

whose Schödinger equation in the matrix representation:

$$\begin{cases} i\hbar\dfrac{dc_{0,m+1}(t)}{dt} = c_{0,m+1}(t)(E_{0,e} + E_{1,p}) + c_{1,m}(t)\omega_{R,m} \\ i\hbar\dfrac{dc_{1,m}(t)}{dt} = c_{1,m}(t)(E_{1,e} + E_{0,p}) + c_{0,m+1}(t)\omega_{R,m} \end{cases} \implies i\hbar\begin{pmatrix} \frac{dc_{0,m+1}(t)}{dt} \\ \frac{c_{1,m}(t)}{dt} \end{pmatrix} = \begin{pmatrix} E_{0,e} + E_{m+1,p} & \hbar\omega_{R,m} \\ \hbar\omega_{R,m} & E_{1,e} + E_{m,p} \end{pmatrix}\begin{pmatrix} c_{0,m+1}(t) \\ c_{1,m}(t) \end{pmatrix} \tag{124}$$

We have defined the new frequency $\omega_{R,m}$ as:

$$\omega_{R,m} = \omega_{I,m}\sqrt{m+1} \tag{125}$$

Using the change $c_{n,m}(t) = \tilde{c}_{n,m}(t)e^{-(E_{n,e}+E_{m,p})t/\hbar}$ we get:

$$\begin{cases} i\dfrac{d\tilde{c}_{0,m+1}(t)}{dt} = \tilde{c}_{1,m}(t)\omega_{R,m}e^{-i2\Delta_m t} \\ i\dfrac{d\tilde{c}_{1,m}(t)}{dt} = \tilde{c}_{0,m+1}(t)\omega_{R,m}e^{+i2\Delta_m t} \end{cases} \tag{126}$$

where Δ_m is defined as the **quantum detuning parameter**:

$$\Delta_m = \frac{E_{0,e} - E_{1,e} - (E_{m+1,p} - E_{m,p})}{2\hbar} \tag{127}$$

The solution of the system is done in the exercise below:

Exercise 3.6.2 — Evaluation of $c_{0,m+1}(t)$ and $c_{1,m}(t)$

If we set the initial conditions to be $c_0 = 1, c_1 = 0$, we get:

$$|\langle 0|\Psi(t)\rangle|^2 = |c_0(t)|^2 = \frac{\omega_{R,m}^2}{\omega_{R,m}^2 + \Delta_m^2}\sin^2(\Omega_{R,m}t) \tag{128}$$

See the detailed solution of this exercise in 5.23 at page 56

where $\omega_{R,m}$ is defiend in Eq. (125) and $\Omega_{R,m}$ is the **quantum Rabi angular frequency** defined as:

$$\Omega_{R,m} = \sqrt{\omega_{R,m}^2 + \Delta_m^2} \tag{129}$$

In the semi-classical case, when the electromagnetic field is absent (zero photons) and the system starts in the electron's excited state $|1\rangle$, there is no evolution because it is an eigenstate of the Hamiltonian. Consequently, the system remains in this state indefinitely. However, in the quantum case, if we remove the radiation field—i.e., there are no photons ($m = 0$)—the solution becomes [8]. So we see that in the quantum case, even without an electromagnetic field, the system has transitions from the ground to the excited states due to spontaneous photon emission.

Exercise 3.6.3 — Computation of quantum Rabi angular frequency $\Omega_{R,0}$

For a system with one electron with a mass of 0.042 times the free electron mass, oscillating between the ground and excited state of a quantum well with a length $L_x = 16$ nm, and light oscillating between ground and excited state of the harmonic oscillator inside an optical cavity of length $L_c = 5930$ nm, with an interaction parameter given by $\alpha = 0.01$

eV/nm, show that **quantum Rabi angular frequency** in Eq. (129) gives:

$$\Omega_{R,0} = \sqrt{\omega_{R,0}^2 + \Delta_m^2} = \omega_{R,m} = \frac{\alpha \langle 0| \hat{x} |1\rangle \langle 0| \hat{q} |1\rangle}{\hbar} = 30 \text{ rad/ps}. \tag{130}$$

The angular frequency can be translated into a linear frequency, giving ≈ 4.7 THz. This computation of the frequency is used in simulation 4.8.1 at page 37.

See the detailed solution of this exercise in 5.15 at page 51

3.7 Matter as quantum trajectory and light as quantum trajectory

Identically to what we have done in sections 3.3 and 3.5, according to the hydrodynamic (or Bohmian) formulation of quantum mechanics, the time evolution of $|\Psi(x,q,t)|^2$ mentioned in section 3.6 can be described in terms of quantum trajectories [8]. The description of the time-evolution of $\rho(x,q,t) = |\Psi(x,q,t)|^2$ is given as a sum of quantum trajectories by:

$$\rho(x,q,t) = |\Psi(x,q,t)|^2 = \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} \delta(x - x_j(t))\delta(q - q_j(t)) \tag{131}$$

Exercise 3.7.1 — Continuity equation in quantum mechanics

Show that there is a *local* continuity equation associated with the Hamiltonian Eq. (109) given by:

$$\frac{\partial \rho(x,q,t)}{\partial t} + \frac{\partial}{\partial x} J_x(x,q,t) + \frac{\partial}{\partial q} J_q(x,q,t) = 0 \tag{132}$$

with

$$J_x(x,q,t) = i\frac{\hbar}{2m_e}\left(\psi(x,q,t)\frac{\partial \psi^*(x,q,t)}{\partial x} - \psi^*(x,t)\frac{\partial \psi(x,q,t)}{\partial x}\right) = \frac{\hbar}{m_e} Im\left(\frac{\Psi(x,q,t)}{dx}\Psi^*(x,q,t)\right) \tag{133}$$

and

$$J_q(x,q,t) = i\frac{\omega}{2}\left(\Psi(x,q,t)\frac{\partial \Psi^*(x,q,t)}{\partial q} - \Psi^*(x,q,t)\frac{\partial \Psi(x,q,t)}{\partial q}\right) = \omega Im\left(\frac{\Psi(x,q,t)}{dq}\Psi^*(x,q,t)\right) \tag{134}$$

See the detailed solution of this exercise in 5.25 at page 56

From these results, Eq. (132), Eq. (133) and Eq. (134), we can compute the velocity of the quantum trajectories as

$$v_x(x,q,t) = \frac{J_x(x,q,t)}{|\Psi(x,q,t)|^2} = \frac{\hbar}{m_e} Im\left(\frac{\frac{\Psi(x,q,t)}{dx}}{\Psi(x,q,t)}\right) \tag{135}$$

and

$$v_q(x,q,t) = \frac{J_q(x,q,t)}{|\Psi(x,q,t)|^2} = \omega Im\left(\frac{\frac{\Psi(x,q,t)}{dq}}{\Psi(x,q,t)}\right) \tag{136}$$

Such velocities, when time-integrated, leads to the x-trajectory:

$$x_j(t) = x_j(t_0) + \int_{t_0}^{t} v_x(x_j(t'), q_j(t'), t')dt' \tag{137}$$

and q-trajectory

$$q_j(t) = q_j(t_0) + \int_{t_0}^{t} v_q(x_j(t'), q_j(t'), t')dt' \tag{138}$$

Notice that the two trajectories are coupled because the computation of $x_j(t)$ needs $v_x(x_j(t'), q_j(t'), t')$ which depends on $q_j(t')$, and the computation of $q_j(t)$ needs $v_q(x_j(t'), q_j(t'), t')$ which depends on $x_j(t')$. See Ref. [8].

4 Simulated experiments

Hereafter, there is a list of examples where you can visualize through animations the theoretical concepts mentioned in the previous section. To run the examples, you need to install the QCslim.exe on your computer.

4.1 Classical simulation

In the following simulated experiments, the light is modeled by a classical trajectory $q_{cl}(t)$ (plotted in the right top plot in the QCslim) and the electron by a classical trajectory $x_{cl}(t)$ (plotted in the left bottom plot in the QCslim) as explained in section 3.1.

Simulation 4.1.1 — Classical electron and classical light with no light-matter interaction

Simulate a classical electron and a classical light with no light-matter interaction ($\alpha = 0$) in a single experiment

Goals and description of the simulation 4.1.1 at page 24

Goals of the simulation:

- Check that an electron, without interaction, follows a Newton law with a velocity fixed by the initial data of the simulation and the electromagnetic field is just a sinusoidal signal with a frequency computed in the initial data, as indicated in Exercise 3.1.1 at page 9
- Check that the $q(t)$ is proportional to the time-dependence of the amplitude of the electromagnetic field as seen in Eq. (26). The parameter q(t) has no units as discussed in the note of section 2.4.

Description of the simulation:

- Open the file *example1.json* in the QCslim and check the parameters (in particular, $\alpha = 0$).
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 3. The trajectory of the electron $x_{cl}(t)$ follows a free flight inside the quantum well until it suffers a specular reflection when reaching the barriers of the quantum well. The velocity of the electron can be evaluated as $v_{x0} = \frac{5L_x}{90\text{fs}-10\text{fs}} = 1$ nm/fs with the length of the well $L_x = 16$ nm. The amplitude of the light $q_{cl}(t)$ is sinusoidal as determined by Eq. (35). From the cavity length $L_c = 5930$ nm, , using Eq. (26), we get $\omega = 158$ Trad/s or 25.30 THz.

Simulation 4.1.2 — Classical electron and classical light with light-matter interaction

Simulate the interaction ($\alpha \neq 0$) of a classical electron and a classical light.

Goals and description of the simulation 4.1.2 at page 24

Goals of the simulation:

- Analyze how the classical electron and classical light interact in the system described in section 3.1.
- Check that the larger the values of $q_{cl}(t)$ and $x_{cl}(t)$, the larger the interaction. Check that a small α provides almost no distortion on the trajectories. Such trajectories become comparable to the non-interacting trajectories described in simulation 4.1.1 at page 24.

Description of the simulation:

- Open the file *example2.json* in the QCslim and check the parameters. The final plot in the QCslim for this particular animation is seen in Figure 4.
- Run a simulation with ten times smaller interaction, i.e., $\alpha = 0.001$ eV/nm.

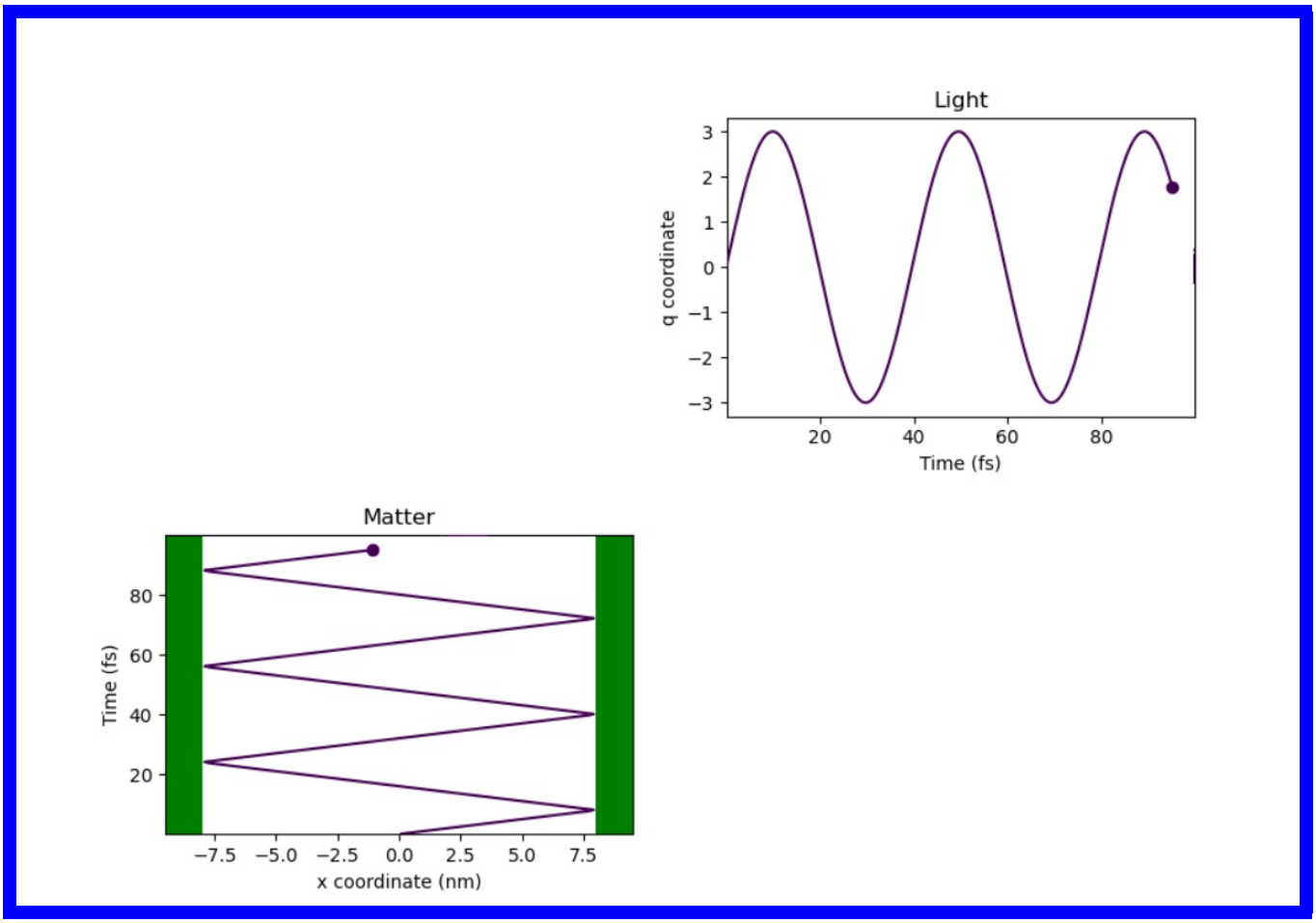

Figure 3: This is the result of the simulation of the file *example1.json* for the simulation 4.1.1 at page 24.

- Run a simulation with the initial $\alpha = 0.01$ eV/nm and fix $x_0 = 0$ nm and $v_0 = 0$ nm/fs, for the electron, and $q_0 = 0$ and $s_0 = 0$, for the light, in the "particle positions" box. The amplitude of the light is zero and the oscillation of the electron is also zero. However, if we allow an electron to move (put $v_0 = 0.1$ nm/fs) then the oscillations of the light $s_{cl}(t)$ and $q_{cl}(t)$ are generated by variations of $x_{cl}(t)$, as seen in $\frac{ds_{cl}}{dt} = -\omega q_{cl} - \frac{\alpha}{\hbar} x_{cl}$ and $\frac{dq_{cl}}{dt} = \omega s_{cl}$ in Eq. (33).

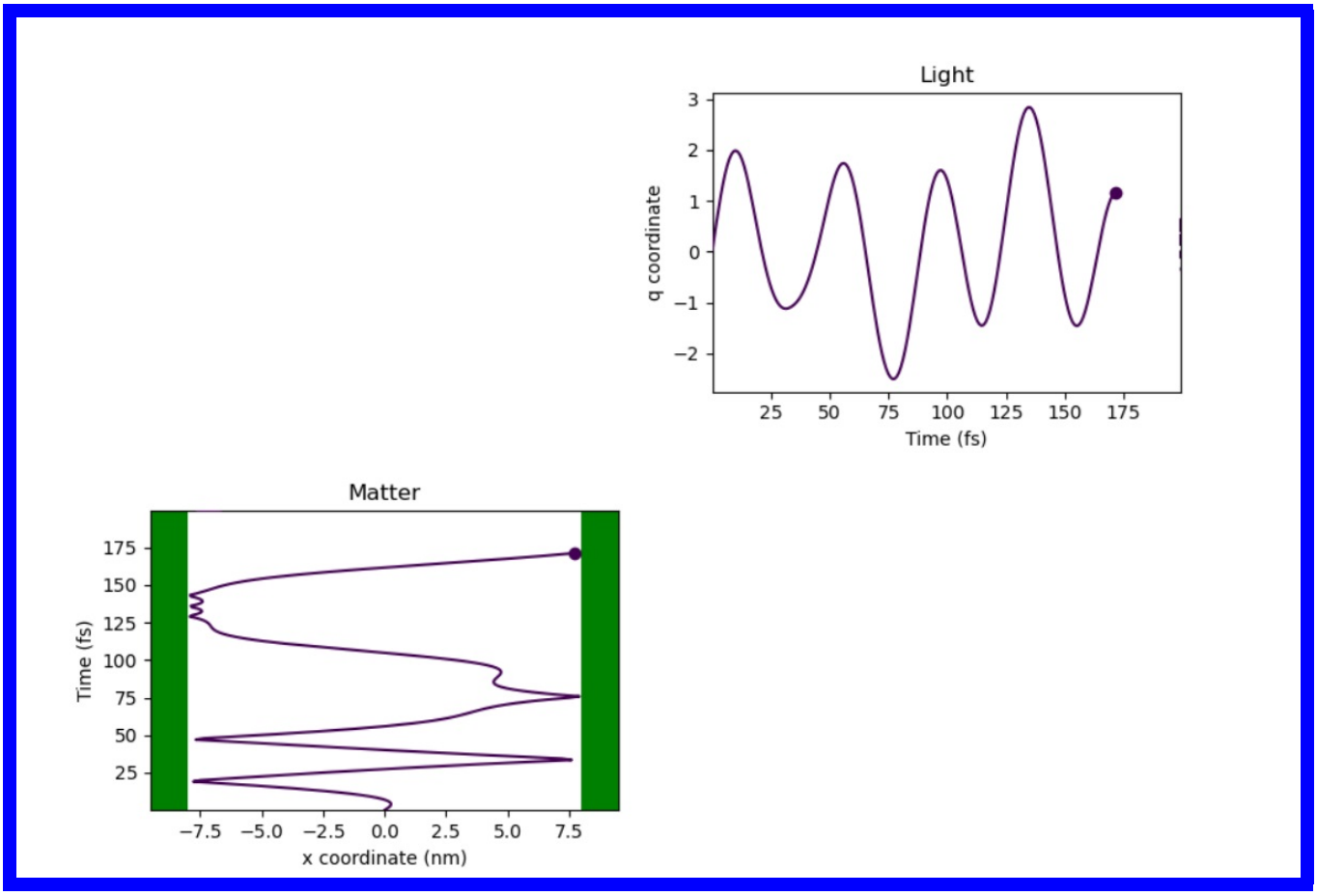

Figure 4: This is the result of the simulation of the file *example2.json* for the simulation 4.1.2 at page 24.

4.2 Classical probability distributions

In the following simulated experiments, the light is modeled by a classical trajectory $q_{cl}(t)$ (plotted in the right top plot in the QCslim) and the electron by a classical trajectory $x_{cl}(t)$ (plotted in the left bottom plot in the QCslim) as explained in section 3.1.

Simulation 4.2.1 — A classical probability distribution from an ensemble of experiments

Simulate the probability distribution of a classical electron and a classical light for an ensemble of $N = 10$ "identical" experiments, with and without light-matter interaction.

Goals and description of the simulation 4.2.1 at page 26

Goals of the simulation:

- Check how to construct a classical probability distribution $\rho_{cl}(x,t)$ on the position x of the electron for a (large) ensemble of "identical" experiments as discussed in section 3.3.
- Identically, check how to construct a classical probability distribution $\rho_{cl}(q,t)$ for the amplitude (without units) q of the light for an ensemble of "identical" experiments as discussed in section 3.5. Here "identical" means, the same quantum well and optical cavity, but different initial conditions for the electrons and the light. All experiments involve only one electron and only one mode of the electromagnetic field. In each experiment, the initial conditions of the electron are different (**all experiments are plotted together in the same to represent an ensemble of experiments, but this plot do not have to be confused with a N-body system**).

Description of the simulation:

- Open the file *example3.json* in the QCslim and check the parameters. There is no interaction ($\alpha = 0$ eV/nm) and the selected distribution of the initial positions $x_{j,cl}(0)$ and $p_{j,cl}(0)$, and $q_{j,cl}(0)$ and $s_{j,cl}(0)$, is Gaussian for light and matter.
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 5. Repeat the simulation several times. The results will change in each simulation because, each time, the initial values are selected randomly from the Gaussian distribution. If needed, the initial values can be fixed by hand in the "particle position" box of the QCslim. The probability distributions $\rho_{cl}(x,t)$ and $\rho_{cl}(q,t)$ can be constructed by counting trajectories (see Eq. (81) and Eq. (100)).
- Repeat the simulation with light matter interaction activated ($\alpha = 0.01$ eV/nm) to visualize how the probability distributions $\rho_{cl}(x,t)$ and $\rho_{cl}(q,t)$ change because of the interaction. The construction of the exact probability distribution will require a large number of "identical" experiments ($N \to \infty$). If required, a probability distribution $\rho(x,q,t)$ can also be constructed by properly combining $\rho_{cl}(x,t)$ and $\rho_{cl}(q,t)$.

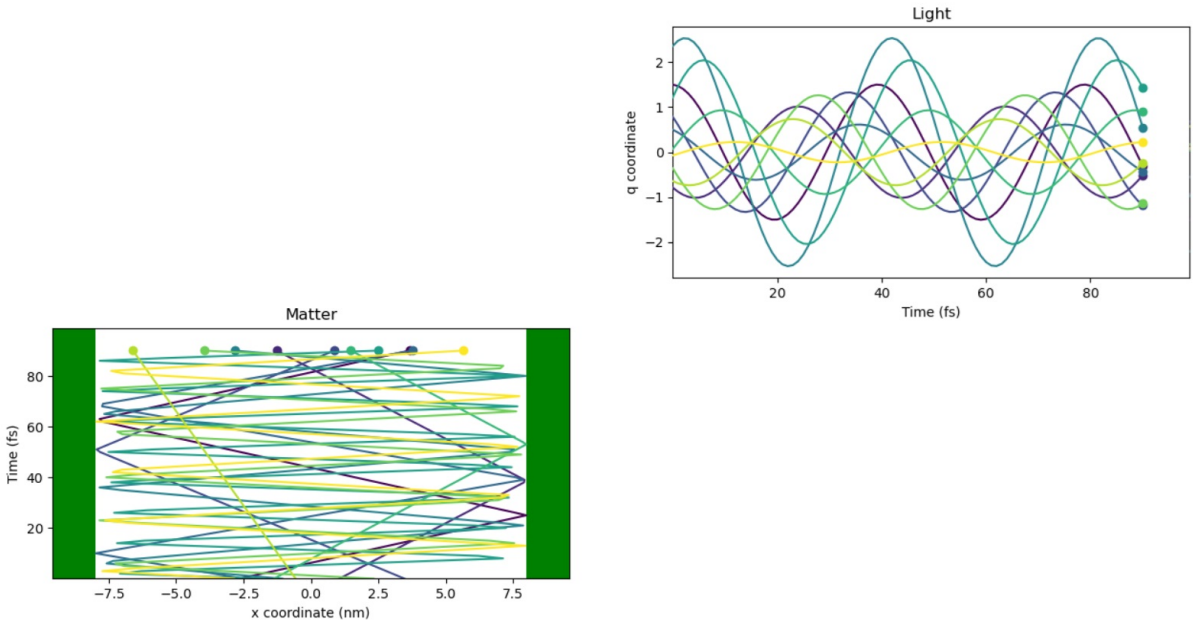

Figure 5: This is the result of the simulation of the file *example3.json* for the simulation 4.2.1 at page 26. The results will change in each simulation because the initial values are selected randomly from the Gaussian distribution. If needed, the initial values can be fixed by hand in the QCslim.

4.3 Electrons in an infinite well interacting with a classical light: A semiclassical simulation

In the following simulated experiment, the light is considered as a classical field described by $q_{cl}(t)$, and the electron as a quantum wave function as explained in section 3.2. Here, the eigenstates and the wave function of the electron will be plotted in the left bottom plot. A plot in the bottom left will indicate the evolution of the different eigenstates that define the electron wave function.

Simulation 4.3.1 — Electrons in an infinite well interacting with a classical light: A semiclassical simulation

Simulate a quantum electron and a classical light in a single experiment. In this particular type of simulation explained in 3.2, the electron is described by the wave function $\Psi(x,t)$ as a superposition of the energy eigenstates $\phi_n(x)$ of an infinite quantum well as described in Eq. (42)). The light is modeled, as an external parameter, by the classical trajectory $q_{cl}(t)$ defined as a sinusoidal signal solution of Eq. (35).

Goals and description of the simulation 4.3.1 at page 28

Goals of the simulation:

- The energy eigenstates $\phi_n(x)$ of an electron in an infinite quantum well are the energy eigenstates of the electron Hamiltonian (see Exercise 3.2.1 at page 10). Thus, check that an initial electron at one eigenstate of the quantum well $\Psi(x,0) = \phi_n(x)$, does not remain in such eigenstate as time goes by.
- Check that the energy is not conserved. The energy of the electron can change although the energy of the (external) light does not change.

Description of the simulation:

- Open the file *example4.json* in the QCslim and check the parameters. In this particular example, the wave function of the electron $\Psi(x,t)$ in Eq. (42) is a superposition of two eigenstates $\phi_0(x)$ and $\phi_1(x)$ of an electron in the quantum well. Initially, the electron is at $\Psi(x,0) = \phi_1(x)$ (with $c_0(0) = 0$ and $c_1(0) = 0$). For the length of the well, $L_x = 16$ nm, we get the energies $E_0 = 0.035$ eV and $E_1 = 0.1401$ eV for the electron from Eq. (40), giving $\omega = \frac{E_1 - E_0}{\hbar} = 159 Trad/s$ or 25 THz. See Exercise 3.2.7 at page 15.
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 6. The probability of each eigenstate $|c_n(t)|^2$ defined in Eq. (43) is plotted in the bottom right subplot. See the change form a state defined by the eigenstate with energy $E_1 = 0.1401$ eV to another with energy given by $E_0 = 0.0350$ eV, as indicated by Eq. (40).
- Change the parameters $\alpha = 0$ to check that the electron remains in its initial eigenstate all the time.
- For the initial parameter $\alpha = 0.01$ check that the electron remains in its initial eigenstate all the time when there is no light (or the light has zero amplitude by fixing $q_0 = 0$ and $s_0 = 0$ in the "particle positions" box of the QCslim).
- For the initial parameter $\alpha = 0.01$ check that the perturbation on the electron's wave function is proportional to how large the is $q(t)$. Use $s_0 = 5$ and $s_0 = 0.1$. Now, there is no restriction on the conservation of the electron energy as seen in Eq. (46). The energy of the electron can change despite the energy of the (external) light does not change.

4.4 Absorption and stimulated emission: exact, perturbative and rotating wave approximation

In the following simulated experiment, the light is considered as a classical field described by $q_{cl}(t)$, and the electron as a quantum wave function as explained in section 3.2. Here, the eigenstates and the wave function of the electron will be plotted in the left bottom plot. A plot in the bottom left will indicate the evolution of the different eigenstates that define the electron wave function. In the top left panel, we will plot the exact solution of the QC-SLIM, the perturbative approximation (see Sec. 3.2.3), and the approximation obtained with the rotating wave approximation (see Sec. 3.2.2).

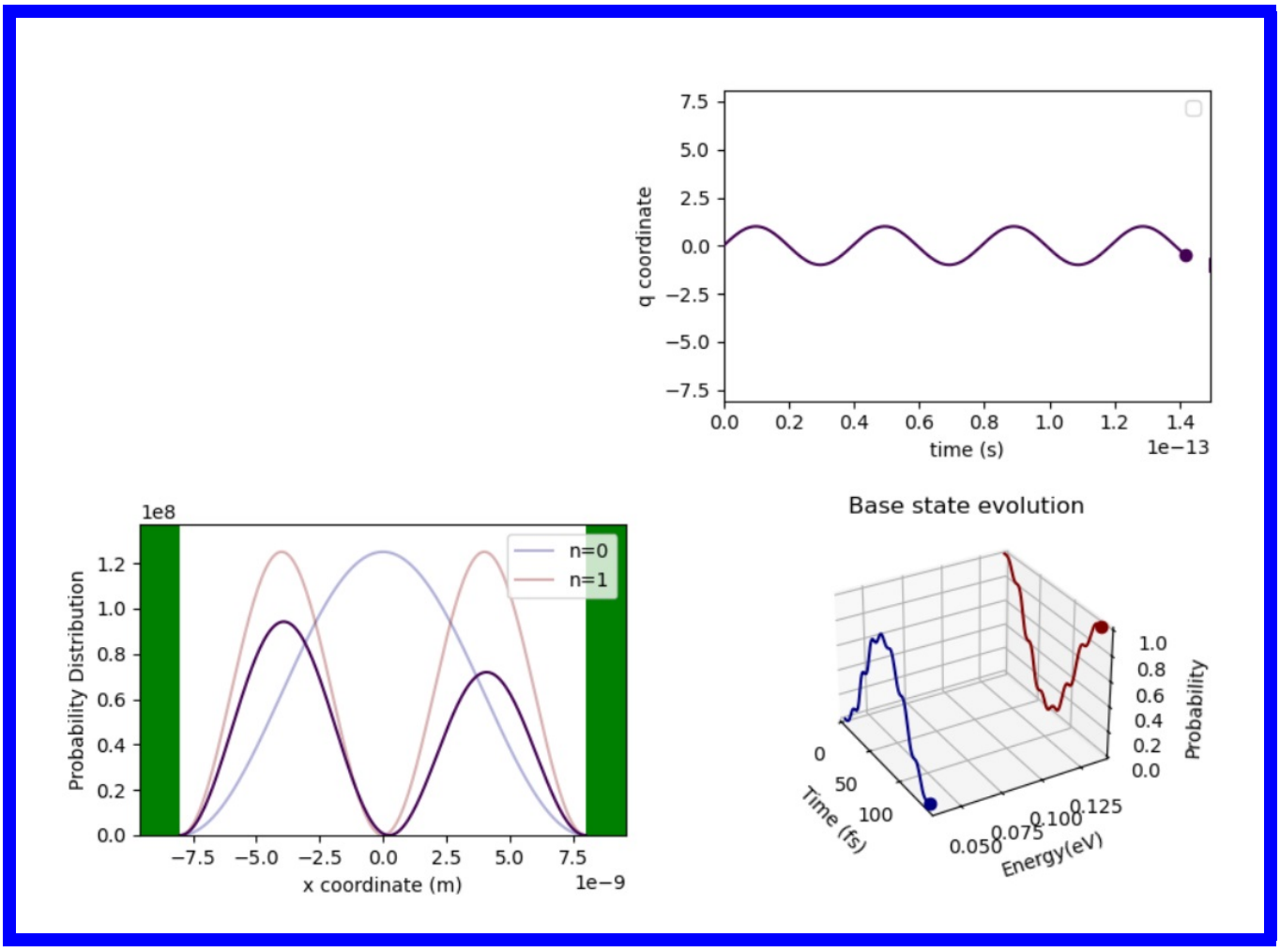

Figure 6: This is the result of the simulation of the file *example4.json* for the simulation 4.3.1 at page 28.

Within the semiclassical simulation described in simulation 4.3.1 at page 28, it is possible to get a first understanding of the process of absorption and stimulated emission. However, as we will see here, it is not possible to simulate the spontaneous emission when we consider $q_{cl}(t) = 0$ for all times.

Simulation 4.4.1 — Absorption and stimulated emission: exact, perturbative and rotating wave approximation

Simulate the transition of an electron in a quantum well from $\phi_1(x)$ to $\phi_0(x)$, and vice versa, when the light is understood as an external (classical) time-dependent parameter. Check the exact solution of the QC-SLIM, the perturbative approximation (see Sec. 3.2.3), and the approximation obtained with the rotating wave approximation (see Sec. 3.2.2).

Goals and description of the simulation 4.4.1 at page 30

Goals of the simulation:

- Check the simulation of stimulated emission and absorption with classical light. Check the exact solution of the QC-SLIM, the perturbative approximation (see Sec. 3.2.3), and the approximation obtained with the rotating wave approximation (see Sec. 3.2.2).

Description of the simulation:

- Open the file *example5.json* in the QCslim and check the parameters. Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 7. See how the electron starting at the eigenstate $\phi_1(x)$ of an electron in the quantum well with $|c_1(t)|^2 = 1$ becomes, after some time, an eigenstate $\phi_0(x)$ of an electron in the quantum well with $|c_0(t)|^2 = 1$. This process can be understood as stimulated emission. Stimulated emission is a key concept in the operation of lasers. It occurs when an incoming photon interacts with an excited atom or molecule, causing it to drop to a lower energy state and emit light. Here, we do not see an increment of the energy of the light because in this semi classical simulation, the light is an external parameter. See simulation 4.9.1 at page 41.

- In the top left panel, we will plot the exact solution of the QC-SLIM in black, the perturbative approximation in blue (see Sec. 3.2.3), and the approximation obtained with the rotating wave approximation in red (see Sec. 3.2.2). In blue $c_0(t)$ is plotted according to the final result Eq. (80) includes both the rapid and the slow oscillating terms, without the rotating wave approximation, thus being much more precise than Eq. (71), but only as long as but only as long the initial non-zero state $c_n(t)$ remains similar to $c_n(0) = 1$ (for larger time this approximation gives unphysical probabilities greater than 1). In particular, for the conditions simulated here, with $c_1(0) = 1$, we get $t \ll \hbar/E_1 = 5$ fs with $E_1 = 0.14$ eV.

- Consider new a scenario involving also $\phi_0(x)$, $\phi_1(x)$ but changing the initial conditions. Fix the "Electron coefs." to 1 and 0 (instead of its initial values 0 and 1) in the "Semiclassical parameters box" of the QCslim (as indicated in the file *example5b.json*). Now the electron initially at $\phi_0(x)$ changes to $\phi_1(x)$ because of the light interaction. This process can be understood as the absorption of light. An electron increases its energy by absorbing light and transitions to a higher energy state. This phenomenon is key to understanding various physical processes and technologies, such as lasers, LEDs, and certain types of spectroscopy. Again, we do not see an decrement of the energy of the light because in this semi classical simulation because the light is an external parameter that is not explicitly simulated. See simulation 4.9.1 at page 41.

- In the top left panel, we will plot the exact solution of the QC-SLIM in black, the perturbative approximation in blue (see Sec. 3.2.3), and the approximation obtained with the rotating wave approximation in red (see Sec. 3.2.2). In blue $c_1(t)$ is plotted according to the final result Eq. (79) includes both the rapid and the slow oscillating terms, without the rotating wave approximation, thus being much more precise than Eq. (71), but only as long as but only as long the initial non-zero state $c_n(t)$ remains similar to $c_n(0) = 1$ (for larger time this approximation gives unphysical probabilities greater than 1). In particular, for the conditions simulated here, with $c_0(0) = 1$, we get $t \ll \hbar/E_0 \approx 20$ fs with $E_0 = 0.035$ eV.

- Check that the electron remains in its initial eigenstate all the time when $\alpha \neq 0$ and there is no light (or the light has zero amplitude by fixing $q_0 = 0$ and $s_0 = 0$ in the simulation). This result is compatible with expressions Eq. (45) where we see that the "effective" interaction is the product of α and $q_{cl}(t)$, i.e., $\alpha\, q_{cl}(t) \sum_{n'=0}^{N} c_{n'}(t) \int dx\, \phi_n^*(x)\, x\, \phi_{n'}(x)$. Thus, assuming $q_{cl}(t) = 0$ (and $\alpha \neq 0$) is mathematically equivalent

to assume $\alpha = 0$ ($q_{cl}(t) \neq 0$). This result has been used in the literature to argue that spontaneous emission cannot be simulated with a classical (or semi-classical) picture of the light because the minimum value of the light energy is zero. However, we have seen in simulation 4.1.2 at page 24 that spontaneous emission is possible with classical system when we only impose $q_{cl}(0) = 0$ at the initial time (not at all times) and allow for the electron to generate the light. A full quantum treatment of the spontaneous emission will be done in simulation 4.9.1 at page 41.

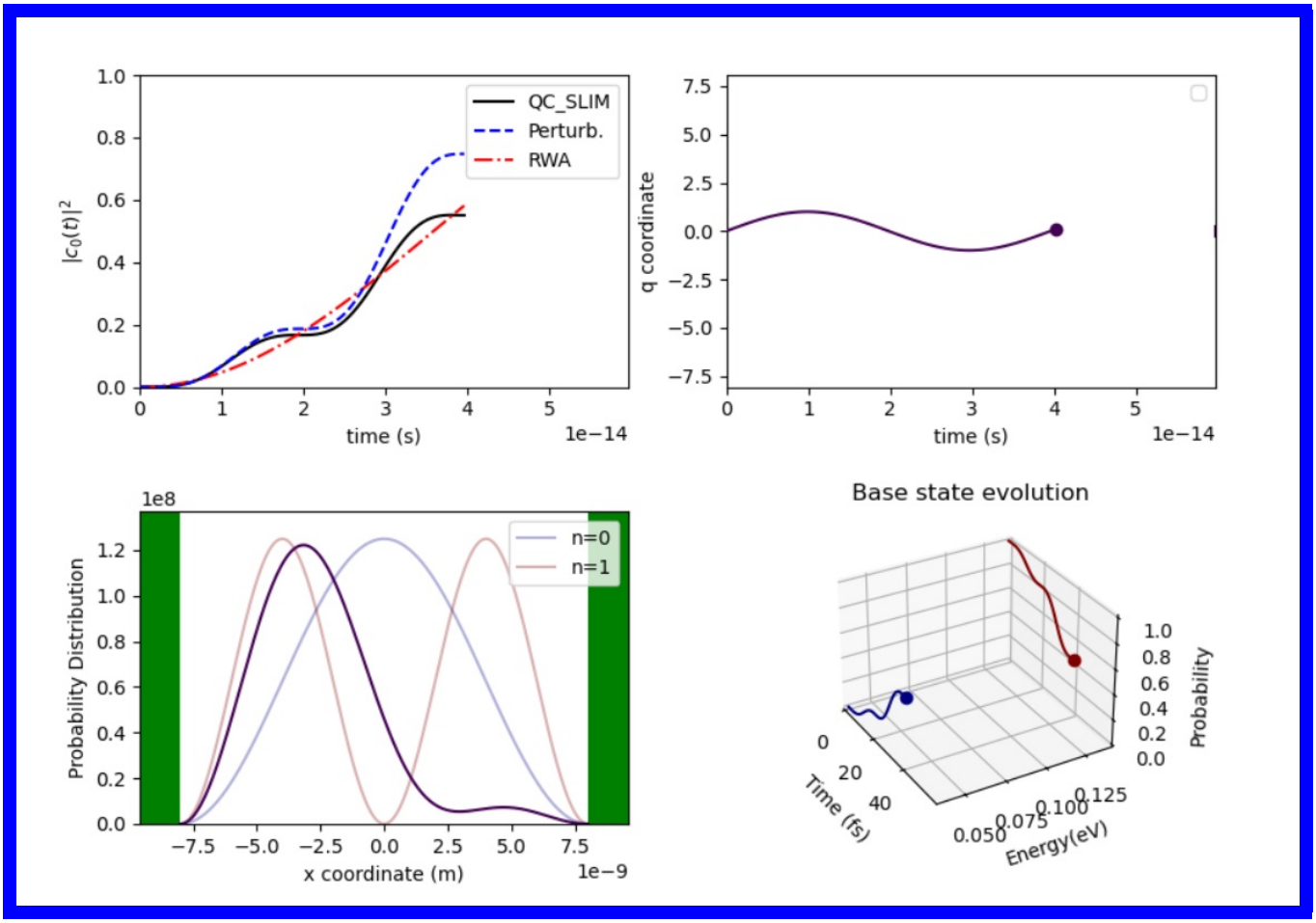

Figure 7: This is the result of the simulation of the file *example5.json* for the simulation 4.4.1 at page 30.

4.5 Semiclassical Rabi oscillations

In the semiclassical simulation, we have seen in the previous section that an electron in the ground state "jumps" to an electron in the excited state because of its interaction with the light. Thus, it si possible to observe a continuous oscillation from the ground to the excited state, and to the ground state again. This oscillation is known as semiclassical Rabi oscillation as explained in Sec. 3.2.2.

Simulation 4.5.1 — Semiclassical Rabi oscillations

Simulate the semiclassical Rabi oscillations and check the results presented in Sec. 3.2.2.

Goals and description of the simulation 4.5.1 at page 31

Goals of the simulation:

- Check the semiclassical Rabi frequency presented in Eq. (26).
- Check the Rabi frequency with and without energy resonance.

Description of the simulation:

- Open the file *example5c.json* in the QCslim and check the parameters. In particular, notice that $c_0(t) = 0$, $c_1(0) = 1$, $q_0 = 0$ and $s_0 = 1$. Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 8. See the top left figure to compute the oscillations of $|c_0(t)|^2$. It takes $T = 0.15$ ps for one period. Notice that the electron frequency $f_e = 25$ THz is equal to light frequency $f = 25$ THz so that, under this resonance conditions, we can use the results of Exercise 3.2.6 at page 14 to compute the Rabi frequency in Eq. (26). he results of $\Omega/(2\pi) = 7$ THz is roughly equal to the $1/T = 6.7$ THz. In the comparison between simulated and analytical results, notice that $\sin^2(\Omega/2t) = 0.5(1 - \cos(\Omega t))$ meaning that $\sin^2(\Omega/2t)$ oscillates at the double of Ω, i.e., $2\Omega/2 = \Omega$.
- Open the file *example5d.json*. Now, we consider a system outside of resonance. Change the lenght of the cavity to $L_c = 8000$ nm. Now, the frequency of the light is $f = 18.74$ THz according to Eq. (26). Now, the detuning paramter in Eq. (68) becomes $\Delta = 2\omega_r - \omega = (E_1 - E_0)/\hbar - 2\pi f = 41$ rad/ps. Then, the amplitude of the oscillation, following Eq. (63) and using the results $\omega_I = 43$ rad/ps from 14, the amplitude of the oscillation becomes $43^2/(43^2 + 41^2) \approx 0.5$ and the new oscillation frequency is $\sqrt{\Delta + \omega_I} = \sqrt{41^2 + 43^2} = 60$ rad/ps or 9.5 THz which coincide with the new simulated results (perdiod of $T = 01.$ ps). These results are in agreement with Figure1.

4.6 A quantum probability distribution

In the following simulated experiment, the light is considered a classical field, and the electron as a quantum electron, involving a wave function and a trajectory, as explained in section 3.3. Using quantum trajectories will allow us to easily connect the classical and quantum results through the concept of probability distributions.

Simulation 4.6.1 — A quantum probability distribution for the electron

Building a quantum probability distribution for the electron from an ensemble of $N = 10$ quantum trajectories.

Goals and description of the simulation 4.6.1 at page 32

Goals of the simulation:

- Check that all the results in simulation 4.3.1 at page 28 and simulation 4.4.1 at page 30 can be understood from an ensemble of quantum trajectories.
- Check the similarities and differences between an ensemble of classical trajectories in simulation 4.1.2 at page 24 and an ensemble of quantum trajectories.

Description of the simulation:

- Open the file *example6.json* in the QCSslim and check the parameters. Now, we consider $n = 10$ experiments. Each experiment is described by a wave function and by a quantum trajectory for the electron. All quantum trajectories are affected by the same parameters of the (external) light. Still, they are different because they are defined from different initial positions $x_j(t_0 = 0)$ as described by Eq. (86) and Eq. (87).
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 9. See how the quantum trajectories oscillate to reproduce the oscillations of the modulus of the wave function $|\Psi(x,t)|^2$ to satisfy Eq. (83). Compare these results with the simulation 4.1.2 at page 24 for

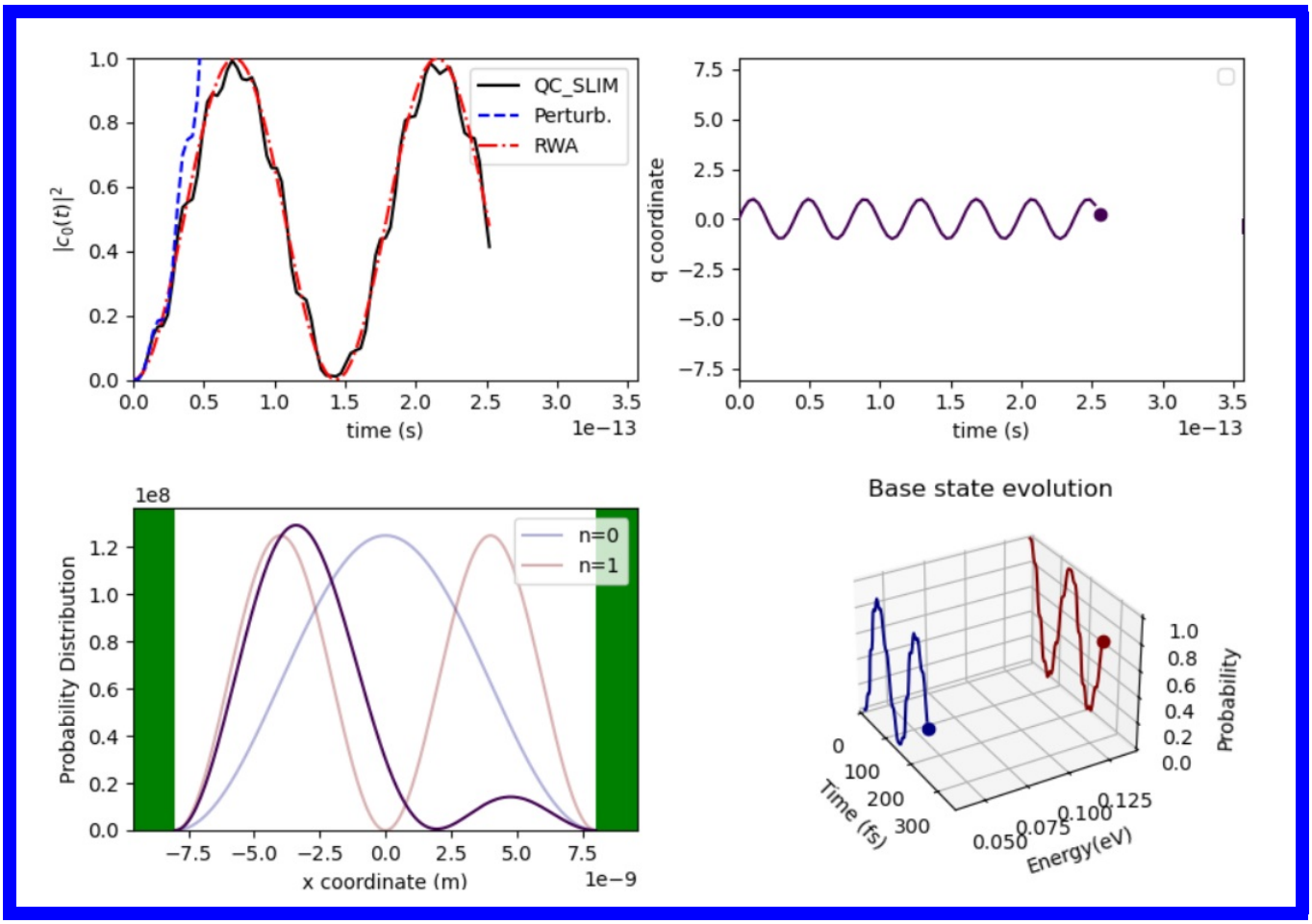

Figure 8: This is the result of the simulation of the file *example5c.json* for the simulation 4.5.1 at page 31.

building $\rho_{cl}(x,t)$ with a classical ensemble of trajectories. We recover the meaning of $\rho(x,t) = |\Psi(x,t)|^2$ as the probability distribution of finding the electron at different positions at different experiments.

- Fix the number of particles to $N = 1$ (press "Set"). The quantum trajectories oscillate as the classical trajectories of the simulation 4.1.2 at page 24 and simulation 4.2.1 at page 26 but, contrary to what happens in the classical systems, these quantum trajectories never reach the limits of the quantum well because the wave function is zero at such positions, $\Psi(x = \pm L_x/2, t) = 0$ to satisfy Eq. (83). Repeat the simulation by changing the initial conditions x_0 of the electrons in the "Particle positions" box. It is evident now that $\rho(x,t) = |\Psi(x,t)|^2$ is a description of an ensemble of experiments. The ensemble results like $\langle x \rangle$ can be computed directly from $\rho(x,t) = |\Psi(x,t)|^2$, but the fluctuations (quantum uncertainty) in different experiments are clearly appreciated by the use of these quantum trajectories.

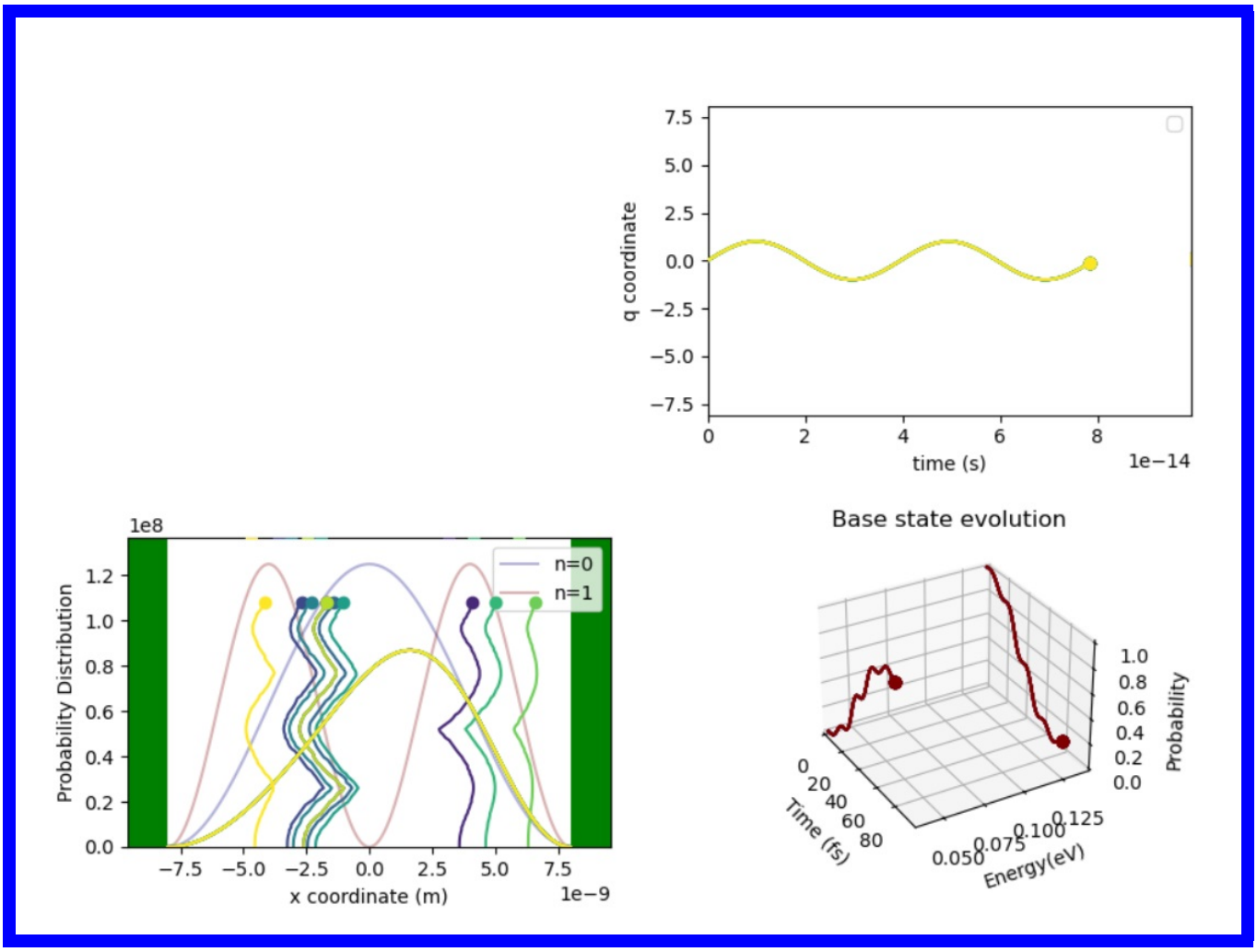

Figure 9: This is the result of the simulation of the file *example6.json* for the simulation 4.6.1 at page 32. The results will change in each run of the simulation because, each time, the initial values are selected randomly according to the probability distribution given by the initial wave function modulus.

4.7 The photon as a quantized amount of light energy

In the following simulated experiment, the light is described by a quantum wave function and the electron by a classical trajectory. This particular type of simulation is explained in 3.4. These simulations will help to understand the meaning of photon and its description $\Psi(q,t)$.

Simulation 4.7.1 — Description of quantum light from eigenstates of a parabolic well

The light is described by the wave function $\Psi(q,t)$ as a superposition of the energy eigenstates $\psi_n(x)$ of the light in a harmonic oscillator (see Exercise 3.4.2 at page 18 and in Eq. (96)). The electron, modeled as an external parameter, is defined by $x_{cl}(t)$ as a sinusoidal trajectory.

Goals and description of the simulation 4.7.1 at page 35

Goals of the simulation:

- Understand the quantum description of light by $\Psi(q,t)$ and the concept of photon as a way of describing the quantization of the energy of the light.
- Check that the description of the light by the wave function $\Psi(q,t)$ provides a probability distribution $\rho(q,t) = |\Psi(q,t)|^2$ that can be understood as the quantum version of the classical distribution $\rho_{cl}(q,t)$ discussed in Eq. (100).
- Check that the energy eigenstates $\psi_n(q)$ of the light in a parabolic well are not energy eigenstates of the Hamiltonian Eq. (38). Thus, the light described by an initial eigenstate of the harmonic oscillator $\Psi(q,0) = \psi_n(q)$, does not remain in such eigenstate as time goes by due to the interaction with the matter.
- Check the minimum energy of the light. From the simulation 4.3.1 at page 28, check analogy between the labeling:

light	matter
$\psi_0(q) \rightarrow$ zero photons	$\phi_0(x) \rightarrow$ ground state
$\psi_1(q) \rightarrow$ one photons	$\phi_1(x) \rightarrow$ first excited state
$\psi_2(q) \rightarrow$ two photons	$\phi_2(x) \rightarrow$ second excited state

  In particular, the minimum energy of the light corresponds to $\psi_0(q)$ (zero photons) as the minimum energy of the electron corresponds to $\phi_0(x)$ (ground state).

Description of the simulation:

- Open the file *example7.json* in the QCslim and check the parameters. In this particular example, the wave function of the light $\Psi_0(q,t)$ in Eq. (96) is a superposition of two eigenstates $\psi_0(q)$ and $\psi_1(q)$ of the light in the harmonic oscillator. Initially, the light is described by $\Psi(q,0) = \psi_1(q)$.
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 10. The time evolution of the probability of each eigenstate $|c_n(t)|^2$ defined in Eq. (97) is plotted in the bottom right subplot.
- Change the parameters $\alpha = 0$ to check that the light remains in its initial eigenstate all the time. Describe the initial light by $\Psi(q,0) = \psi_0(q)$ by changing "photon coefs." from the initial values 0 1 to 1 0 in the "semiclassical parameters" box (as indicated in the file *example7b.json*). Now, the light remains all the time in its lowest value of energy equal to $E_0 = 0.0517$ eV as described by Eq. (94). We have $\omega = 159 Trad/s$ or 25 THz. Thus, $E_0 = \hbar\omega/2 = 0.0517$ eV and $E_1 = 3\hbar\omega/2 = 0.1552$ eV.
- For the initial parameter $\alpha = 0.01$ check that the light remains in its initial eigenstate all the time when classical electron does not oscillate (fix $x_0 = 0$ and $p_0 = 0$ in the simulation). This result is analog to the results obtained in simulation 4.4.1 at page 30 when the classical light had zero energy.

Simulation 4.7.2 — A quantum probability distribution for the light

In the following simulated experiment, the light is considered as a quantum object, involving a wave function and a trajectory, and the electron as a classical trajectory as explained in section 3.5.

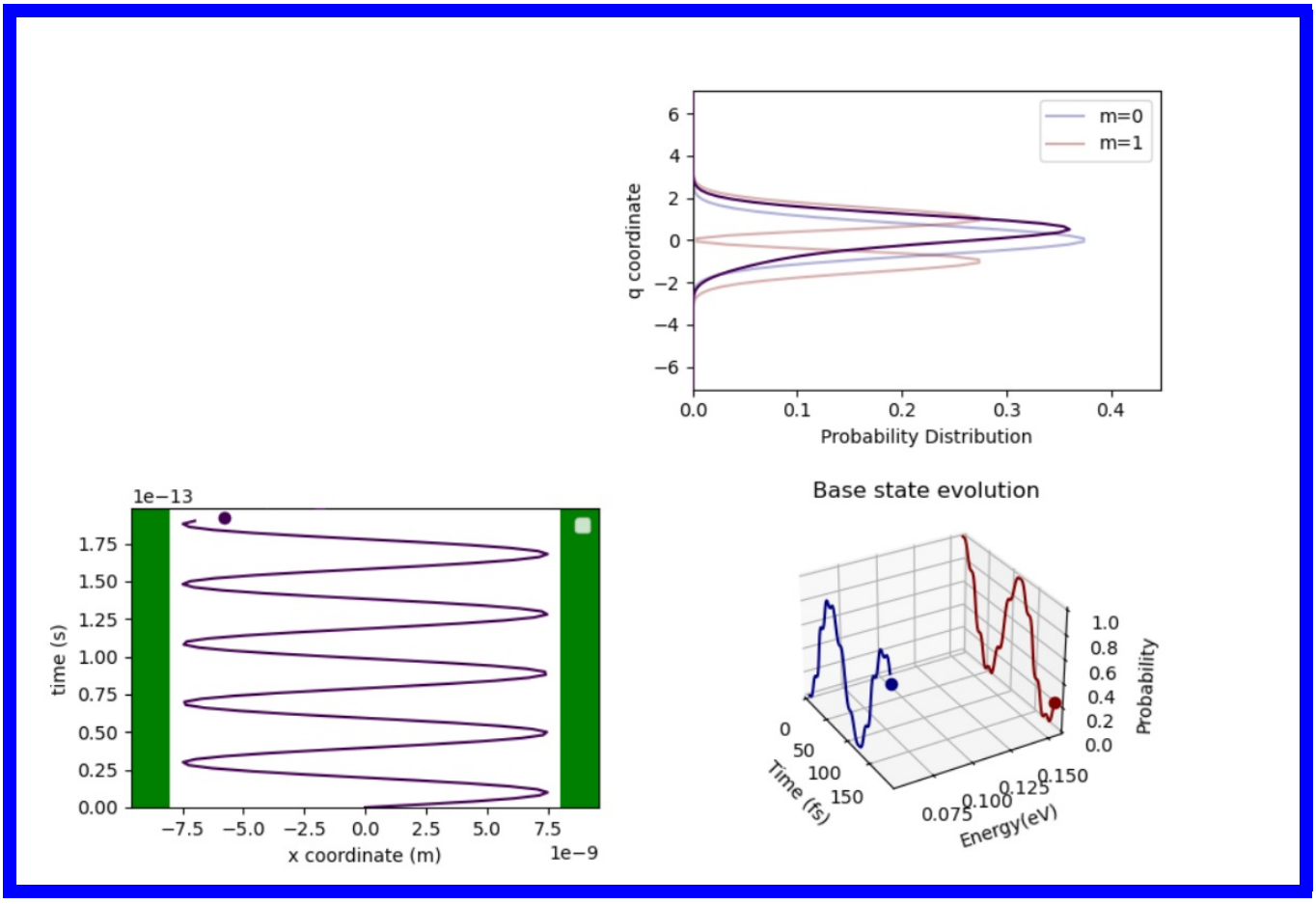

Figure 10: This is the result of the simulation of the file *example7.json* for the simulation 4.7.1 at page 35.

Goals and description of the simulation 4.7.2 at page 35

Goals of the simulation:

- To better understand the meaning of $\Psi(q,t)$ we construct the quantum probability distribution for the light from an ensemble of $N = 10$ identical experiments and compare the results with the classical distribution of q build by an ensemble of classical trajectories for the light in simulation 4.1.2 at page 24. Check the differences between the ensemble of classical trajectories for the light in simulation 4.1.2 at page 24 and an ensemble of quantum trajectories for the light.
- Check that all the results in simulation 4.7.1 at page 35 can be understood from an ensemble of quantum trajectories.

Description of the simulation:

- Open the file *example8.json* in the QCslim and check the parameters. In addition to the wave functions for the light, in the top right plot, an ensemble of $M = 10$ quantum trajectories for the light $q_j(t)$ are plotted. They are affected by the same parameters of the (external) electron trajectory $x_c l(t)$ seen in the bottom left plot. Still, quantum trajectories of the light are different because they are defined from different initial positions $q_j(t_0 = 0)$ as described by Eq. (105) and Eq. (106). We use the name "trajectories" for $q_j(t)$ by analogy with $x_j(t)$, but here the name can be misunderstood. The parameter $q_j(t)$ does not describe how the light moves in physical space, but only how the amplitude of the electric filed changes with time in the q-space (such q space is much more arbitrary than the physical space and we have adopted here a q space without units as described at the end of section 2.4). Thus, the wave function $\Psi(q,t)$ describes the different values of q available at each time in an ensemble of experiments.
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 11. See how the quantum trajectories of the light oscillate to reproduce the oscillations of the modulus of the wave function $|\Psi(q,t)|^2$ to satisfy Eq. (102). Compare these results with the simulation 4.1.2 at page 24 for a classical ensemble of quantum trajectories. We recover the meaning of $|\Psi(q,t)|^2$ as the probability distribution of finding different amplitudes $q(t)$ at different experiments.
- Fix the number of particles to $N = 1$ (press "Set"). At first sight, the quantum trajectory oscillates as the classical trajectory of the light in the simulation 4.1.2 at page 24 and simulation 4.2.1 at page 26 but their behavior is different as their equations of motion are different (the classical $q_{cl}(t)$ is determined by Eq. (33), while the quantum $q(t)$ is determined by Eq. (105)).

4.8 Quantum Rabi oscillations

Rabi oscillations describe the periodic oscillation of a quantum system between two energy states due to the coupling between light and matter. This phenomenon is named after the physicist Isidor Isaac Rabi, who first described it in the context of nuclear magnetic resonance. In the following simulated experiment, the light and the matter are described by a common Hamiltonian in Eq. (109) ensuring global conservation of energy. There is a unique wave function $\Psi(x,q,t)$ to described simultaneously their quantum nature.

This particular type of simulation is explained in section 3.6. In the top right plot of the QCslim the time-evolution of the probability distribution $|\Psi(x,q,t)|^2$ is depicted in the configuration space (q-x space).

Simulation 4.8.1 — Rabi oscillations

Rabi oscillation for an electron in an infinite quantum well interacting with light in an optical cavity.

Goals and description of the simulation 4.8.1 at page 37

Goals of the simulation:

- Show the quantum Rabi oscillation are because two different quantum states with are not eiegnstates of the whole system (of the light-matter system) have similar/identical energies.

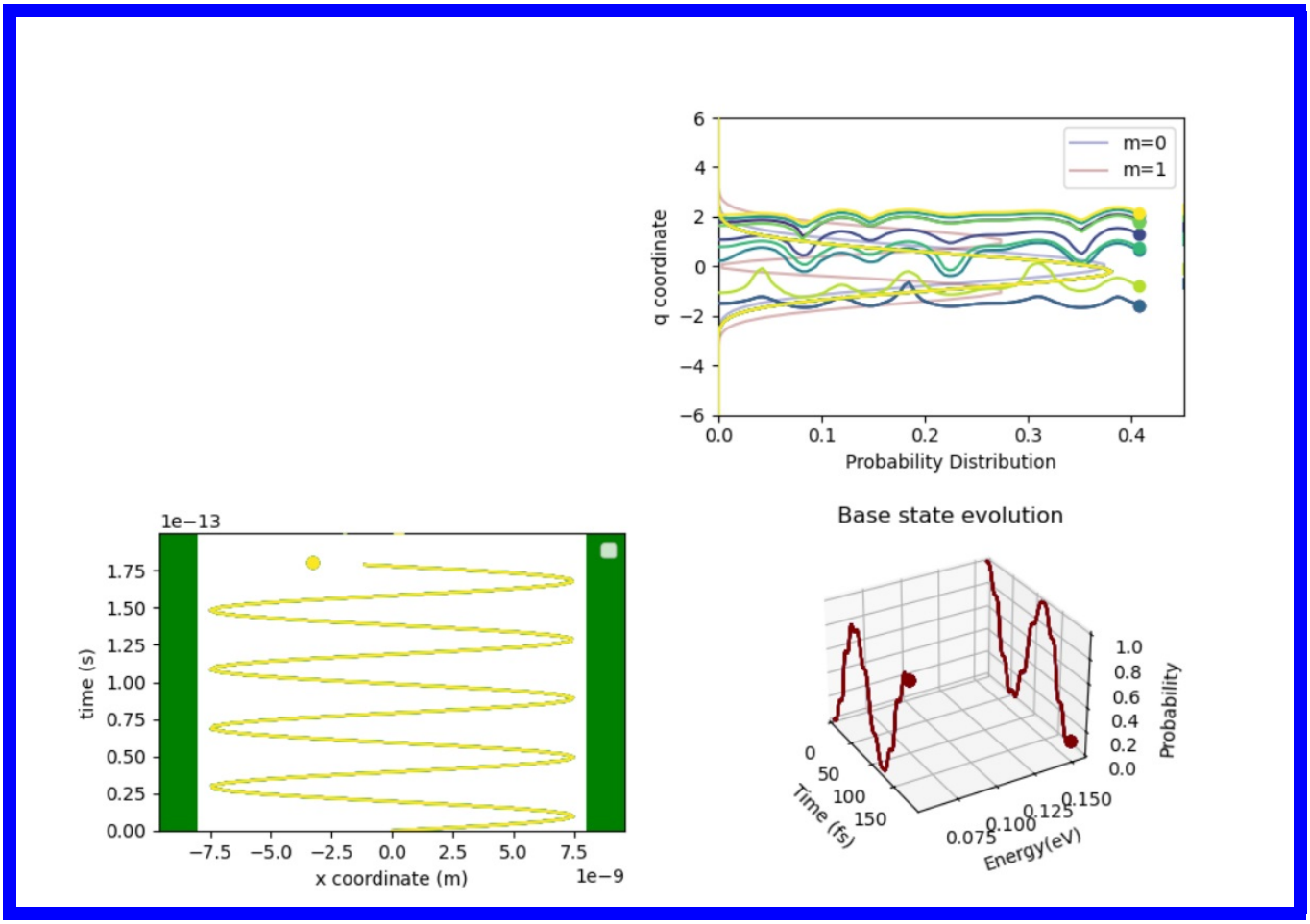

Figure 11: This is the result of the simulation of the file *example8.json* for the simulation 4.7.2 at page 35.

- Check how the quantum Rabi frequency depends on the parameter α and others in Eq. (129).
- Check that the quantum Rabi oscillation is maximum at resonance and check its dependence with the number of photons indicated by the index of the phtoon m .

Description of the simulation:

- Open the file *example9.json* in the QCslim and check the parameters. Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 12. See how the electron changes from $\phi_1(x)$ (eigenenergy $E_{1,e} = 0.14$ eV) to $\phi_0(q)$ (eigenenergy $E_{0,e} = 0.035$ eV), while the light changes from $\phi_0(q)$ (eigenenergy $E_{1,p} = 0.052$ eV) to $\phi_1(q)$ (eigenenergy $E_{1,p} = 0.157$ eV). The energy of the light-matter eigenstate $\phi_1(x)\phi_0(q)$ is roughly $E_{1,e} + E_{0,p} = 0.14 + 0.052 = 0.192$ eV). Identically, the energy of the light-matter eigenstate $\phi_0(x)\phi_1(q)$ is roughly $E_{0,e} + E_{1,p} = 0.035 + 0.157 = 0.192$ eV). See the energies of these two eigenstates in the bottom right plot. The Rabi oscillation is a periodic transition between these two light-matter eigenstates that keeps the total energy constant (i.e. an oscillation between an electron in the excited state and zero photon, and an electron in the ground state and one photon).
- The number of oscillations is 2 in a perdiod of $T = 200$ fs. Thus, the Rabi oscillation frequency of the simulation is 10 THz. Notice that in these particular conditions, we are in resonance, so that $\Delta_m = \frac{E_{0,e} - E_{1,e} - (E_{m+1,p} - E_{m,p})}{2\hbar} = 0$ in Eq. (127). Then, the quantum Rabi frequency can be computed as from from Exercise 3.2.7 at page 15 where $\Omega_{R,0} = 30 rad/ps$ or 4.7 THz are obtained. Notice that $\sin^2(\Omega_{R,0}t) = 0.5(1 - \cos(2\Omega_{R,0}t))$ in Eq. (128) so that the theorethical oscillation of the square of the sinus happens at $2(4.7) = 9.4$ THz which coincides with value obtained in the simulation.
- Consider the case with 3 photons by introducing the number of photons levels as 3 in the box "Quantum parameters". Now, assume that the system starts in the state $\phi_0(x)$ for the electron and $\phi_1(q)$ for the light, so that the index m that specifies $\omega_{R,m}$ in Eq. (125) is $m = 1$ with $\sqrt{1+1} = 1.41$. See the file *example9b.json*. Check that, under these new conditions, $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$, we get a Rabi frequency 1.41 times larger than before, now ≈ 14 THz, under the same resonant conditions as before. Change the parameter $\alpha = 0.02$ eV/nm and compare to the results with $\alpha = 0$ eV/nm to check how the frequency of the Rabi oscillation depends on α.
- Modify the length of the optical cavity to $L_c = 2000$ nm so that electron and light are no longer in resonance. See how the light and matter evolve independent because conservation of energy forbids the transition. Now, the states $|c_{1,0}(t)|^2 = 1$ (electron in the excited state and zero photon) and $|c_{0,1}(t)|^2 = 1$ (electron in the ground state and one photon) have quite different energies. The transition from one state to the other is forbidden because it would violate the conservation of the energy imposed by Eq. (115).

4.9 A full quantum treatment of absorption, spontaneous and stimulated emissions

In the simulation 4.4.1 at page 30 we have studied absorption and stimulated emission from a semi-classical view where the electron is considered as a quantum wave, while the light is treated as an (external) classical parameter. Such type of semi classical simulation had some important drawbacks: There was no rule for the conservation of the total light-matter energy and the minimum energy of the light was assumed as zero. Because of this last semi classical assumption, the matter has no spontaneous emission was not predicted because there was no light-matter interaction when the energy of the light was zero.

In this full quantum scenario studied here, the light and the matter are described by a common Hamiltonian in Eq. (109) ensuring global conservation of energy. In particular, the light is treated as a wave and its minimum energy is no longer zero (see Eq. (94)). Then, the spontaneous emission can be predicted. Such spontaneous emission is a fundamental process in quantum optics where an excited atom, molecule, or nucleus loses energy by emitting a photon and transitions to a lower energy state without external provocation. This phenomenon is key to understanding various physical processes and technologies, such as lasers, LEDs, and certain types of spectroscopy.

This particular type of simulation is explained in section 3.6. In the top right plot of the QCslim, the time-evolution of the probability distribution $|\Psi(x, q, t)|^2$ is depicted in the configuration space (q-x space).

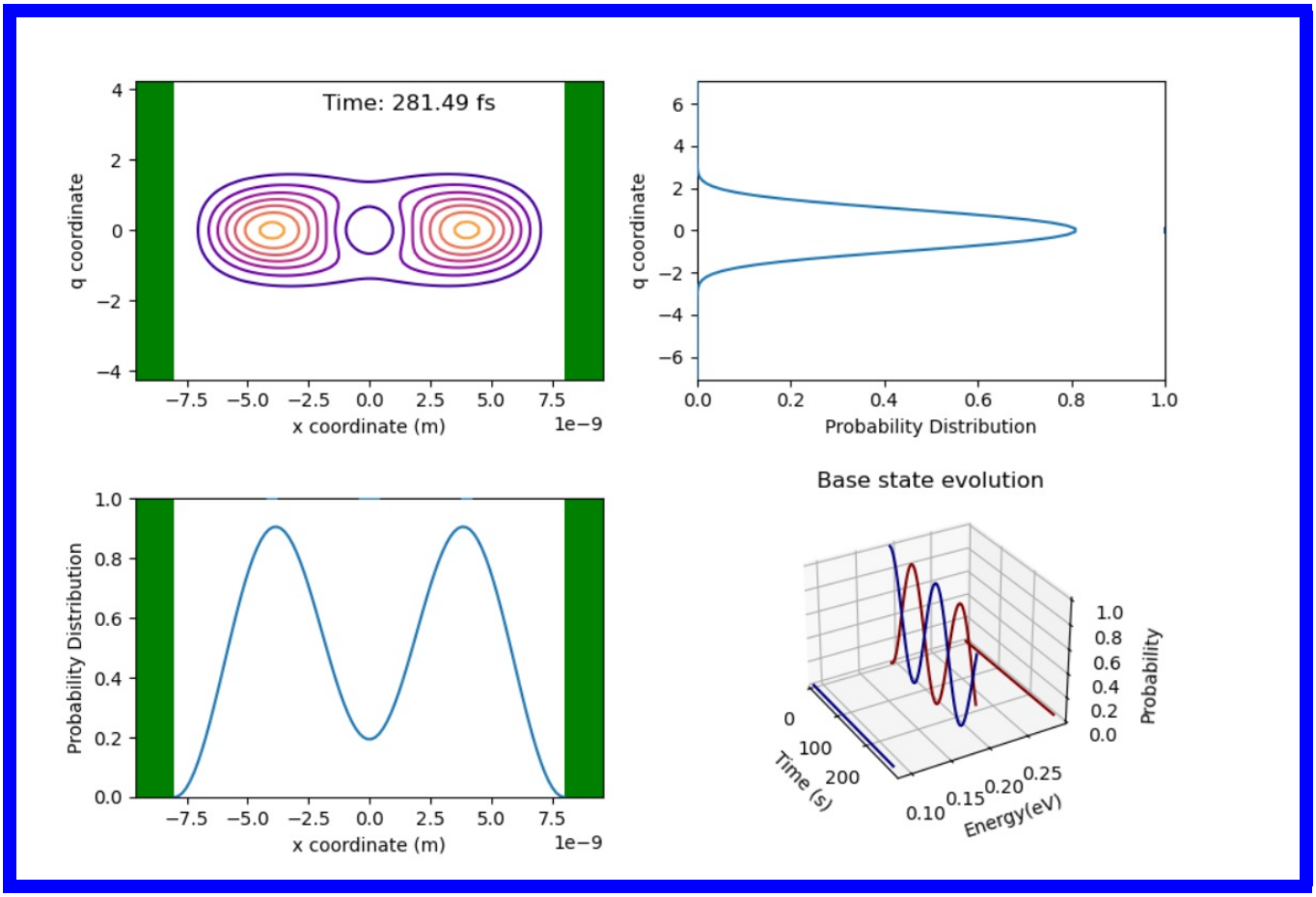

Figure 12: This is the result of the simulation of the file *example9.json* for the simulation 4.8.1 at page 37.

Simulation 4.9.1 — A full quantum simulation of absorption, spontaneous and stimulated emissions

Simulate the absorption, spontaneous and stimulated emission for a full quantum treatment of light and matter, with emphasis on the requirement of conservation of the total energy.

Goals and description of the simulation 4.9.1 at page 41

Goals of the simulation:

- Check how spontaneous emission can be produced with zero photons.
- Check how absorption, spontaneous and stimulated emission satisfy energy conservation discussed in Eq. (115).

Description of the simulation:

- Open the file *example10.json* in the QCslim and check the parameters.
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 13. See how the common wave function of the electron and light described initially by the eigenstate $\phi_1(x)\psi_0(q)$ (electron in the excited state and zero photons) with $|c_{1,0}(t)|^2 = 1$, transits to the eigenstate $\phi_0(x)\phi_1(q)$ (electron in the ground state and one photon) with $|c_{0,1}(t)|^2 = 1$. As shown in the bottom right plot, the energy of both states is the same because the difference of the energy levels of the electrons $E_{1,e} - E_{0,e} = 0.105$ eV defined in Eq. (40) is identical to the difference of the energy levels of the light $E_{1,p} - E_{0,p} = 0.105$ eV defined in Eq. (94). This process corresponds to a spontaneous emission of a photon.

  Notice that the initial energy of the light was the minimum energy that an harmonic oscillator can has $E_{0,p} = \frac{1}{2}\hbar\omega = 0.0523$ eV. This spontaneous emission is not possible to be simulated with classical light as discussed in simulation 4.4.1 at page 30.
- Notice that the frequency ω is related to the optical cavity length through Eq. (26). Modify the length of the optical cavity to $L_c = 2000$ nm so that the electron and the light are no longer in resonance. See how the light and matter evolve independently (no interaction). Now, the states $|c_{1,0}(t)|^2 = 1$ (electron in the excited state and zero photon) and $|c_{0,1}(t)|^2 = 1$ (electron in the ground state and one photon) have quite different energies. $E_{1,e} - E_{0,e} = 0.31$ eV defined in Eq. (40) is very different from the difference of the energy levels of the light $E_{1,p} - E_{0,p} = 0.105$ eV defined in Eq. (94). The transition from one state to the other is now forbidden because it would imply no conservation of the total energy.
- Put again the initial value of the optical cavity to $L_c = 5930$ nm to ensure that the electron and light are again in resonance. In the "quantum parameters" box, modify the initial matrix $\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ to $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$. Now, the initial state is $\phi_0(x)\phi_1(q)$ (electron in the ground state and one photon) with $|c_{0,1}(t)|^2 = 1$ and the final state will be $\phi_1(x)\psi_0(q)$ (electron in the excited state and zero photons) with $|c_{1,0}(t)|^2 = 1$. This modifications are present in the simulation file *example10b.json*. This process corresponds to absorption.
- In the "quantum parameters" box, set the "number of photon levels" to 3 and modify the initial matrix $\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ to $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$. Now, the initial state is $\phi_1(x)\phi_1(q)$ (electron excited state and light in the one photon state) and the final state will be $\phi_0(x)\psi_2(q)$ (electron in the ground state and the light in the two-photon state). These modifications are present in the simulation file *example10c.json*. This corresponds to the stimulated emission where one photon interacting with the electron creates an additional identical photon, at the price of reducing the energy of the electron. This modifications are present in the simulation file *example10b.json*

4.10 Weak values

Weak values arise in the context of weak measurements, which are a type of quantum measurement that minimally disturbs the system being measured [10,11]. This allows certain properties of a quantum system to be probed in a way that avoids the strong perturbations associated with conventional (or "strong") measurements. In particular, it is possible to measure simultaneously

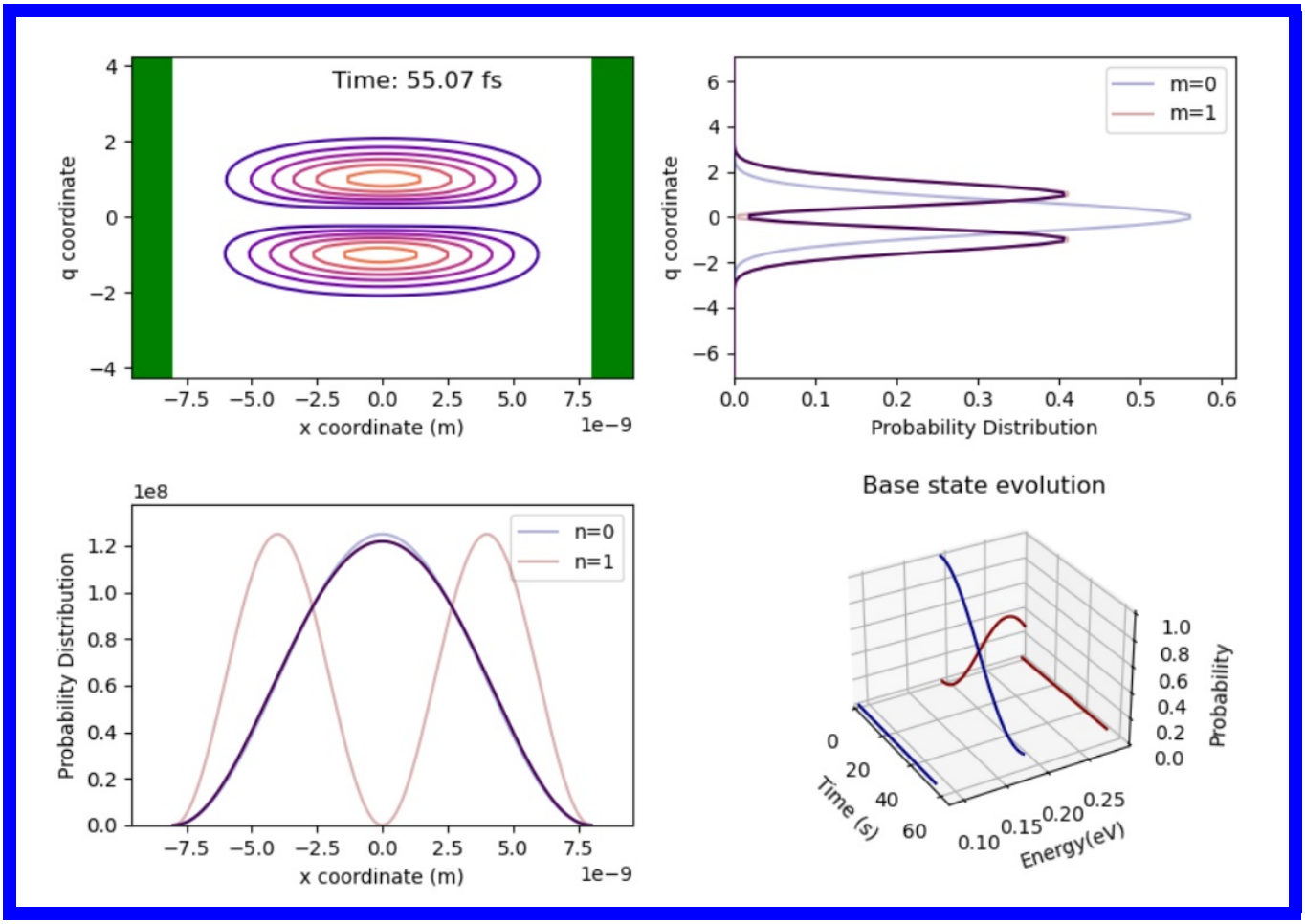

Figure 13: This is the result of the simulation of the file *example10.json* for the simulation 4.9.1 at page 41.

the position and the momentum of a particle.

In particular, we describe here a weak value of the momentum post-selected in position. It involves two consecutive measurements:

- a weak measurement of the momentum of the quantum system (with a small perturbation on it) giving p_w.
- a strong measurement of the position of the quantum system giving x_s.

When such two consecutive measurements are repeated many times in an ensemble of identically prepared quantum systems, we can build the probability $P(p_w, x_s)$ by just counting the number of times that the couple $\{p_w, x_s\}$ occurs in the experiments. The weak value can be constructed in the laboratory as the mean value of the momentum p_w conditioned to the fact the second measurement of the position gives the value $x_s = x$. For an electron described by the wave function $\Psi(x,t)$, such conditional probability can be shown to be given by the Bohmian velocity described in Eq. (86):

$$\frac{\int dp_w\ p_w\ P(p_w, x_s = x)}{\int dp_w P(p_w, x_s = x)} = \frac{J_x(x,t)}{|\Psi(x,t)|^2} = v_x(x,t) \tag{139}$$

Thus, the velocity (and the quantum trajectories) in Eq. (86) can be measured in the laboratory for an ensemble of identical experiments (not from a single experiment!) through Eq. (139)showing the ability of the quantum trajectory $x(t)$ as an additional way of characterizing quantum systems [10, 11].

In the following simulated experiment, the light and the electron are described by quantum object, including a wave function and a trajectory for both, as explained in section 3.7. The type of simulation in explained in section 3.3 will also be used.

Simulation 4.10.1 — Weak values

Building a quantum probability distribution for the electron and from the light from an ensemble of $N = 5$ quantum trajectories.

Goals and description of the simulation 4.10.1 at page 43

Goals of the simulation:

- Check that all the results in simulation 4.8.1 at page 37 and simulation 4.9.1 at page 41 can be understood from an ensemble of quantum trajectories.
- Check the utility of weak values showing how the velocity (or other predictions of quantum trajectories) can be measured in the laboratory.
- Check the similitudes and differences between an ensemble of classical trajectories in simulation 4.1.2 at page 24 and an ensemble of quantum trajectories.

Description of the simulation:

- Open the file *example11.json* in the QCslim and check the parameters. Quantum trajectories are defined from different initial positions $x_j(t_0 = 0)$ and $q_j(t_0 = 0)$ as described by Eq. (135), Eq. (137), Eq. (136) and Eq. (138).
- Run the simulation and check the graphical results. The final plot in the QCslim for this particular animation is seen in Figure 14. See how the quantum trajectories oscillate to reproduce the oscillations of the modulus square of the wave function $|\Psi(x,q,t)|^2$ to satisfy Eq. (131). Notice the representation of the trajectories in three different plot. The trajectories $x(t)$ anmd $q(t)$ tend to concentrate in regions with a large modulus square of the wave function $|\Psi(x,q,t)|^2$ and avoid such regions where it is negligible.
- Put $\alpha = 0$ and in the "quantum parameters" box, and see how the quantum trajectories reproduce the no time-evolution modulus evolution of the wave function through a velocity zero. modify the initial matrix $\begin{matrix} 0 & 0 \\ 1 & 0 \end{matrix}$ to $\begin{matrix} 1 & 0 \\ 1 & 0 \end{matrix}$. Now, the light and the matter evolve independently and the electron's wave function is described by a superposition of $\phi_0(x)$ and $\phi_1(x)$ so that the Bohmian trajectories will oscillate to reproduce the oscillation of the modulus of the wave function. The velocity of such quantum trajectories at each position x and time t can

be measured in the laboratory following the protocol mentioned in Eq. (139). These measurement can be used, for example, to discuss the presence or not of superposition of states.

- Fix the number of particles to $N = 1$ (press "Set") and put $\alpha = 0.01$ eV. Repeat the simulation several times. Each time the wave function evolution $|\Psi(x, q, t)|^2$ depicted in the top left plot will be the same, but the quantum trajectories are different because in each run of the simulation the initial values of the trajectories are selected randomly according to the probability distribution given by the initial wave function modulus square. From these results, we see that will the ensemble results over and ensemble of experiments can be computed from $|\Psi(x, q, t)|^2$ (or from an ensemble of trajectories), each run of the trajectory shows that each experiment is different (because of the quantum uncertainty). Check the similarities and differences between an ensemble of classical trajectories in simulation 4.1.2 at page 24 and an ensemble of quantum trajectories.

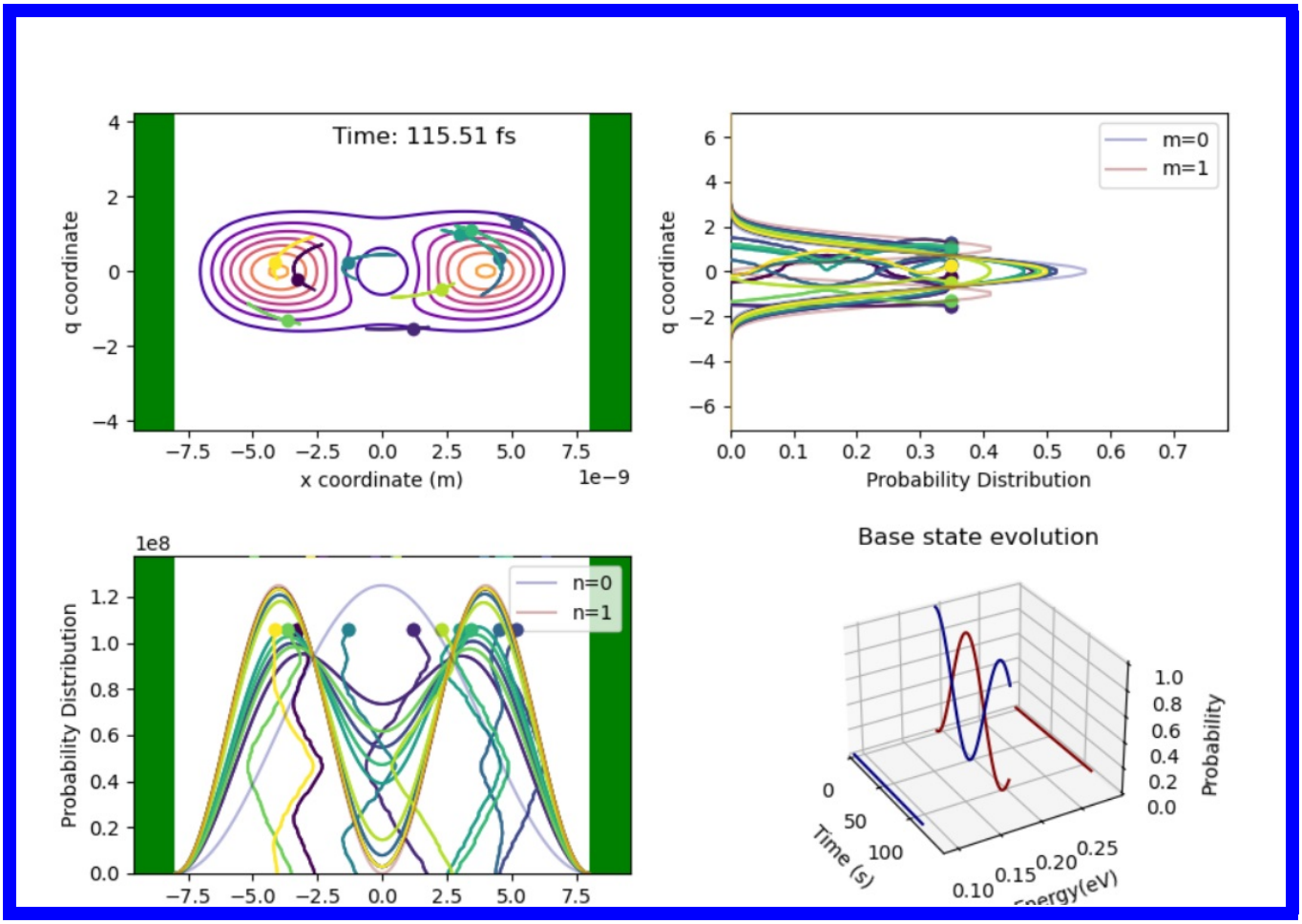

Figure 14: This is the result of the simulation of the file *example11.json* for the simulation 4.10.1 at page 43. The results will change in each run of the simulation because, each time, the initial values are selected randomly according to the probability distribution given by the initial wave function modulus square.

5 Solutions to the proposed exercises

5.1 — Solution of Exercise 2.1.1 at page 5

Using Eq. (3), the the electric field in Eq. (1) is defined in the new gauge as:

$$\mathbf{E}^g = -\nabla A_0^g - \frac{\partial \mathbf{A}^g}{\partial t} = -\nabla A_0 + \cancel{\frac{\partial \nabla g(\mathbf{r},t)}{\partial t}} - \frac{\partial \mathbf{A}}{\partial t} - \cancel{\frac{\partial \nabla g(\mathbf{r},t)}{\partial t}} = -\nabla A_0 - \frac{\partial \mathbf{A}}{\partial t} = \mathbf{E}$$

and the magnetic field in Eq. (2) :

$$\mathbf{B}^g = \nabla \times \mathbf{A}\mathbf{g}^g = \nabla \times \mathbf{A} + \cancel{\nabla \times \nabla g(\mathbf{r},t)} = \nabla \times \mathbf{A} = \mathbf{B}$$

where $\nabla \times \nabla g(\mathbf{r},t) = 0$, by construction.

5.2 — Solution of Exercise 2.2.1 at page 6

The Helmholtz decomposition allows to express any vector as a sum of a transversal component (zero divergence) and a longitudinal component (zero rotational). A longitudinal electric field is defined by $\nabla \times \mathbf{E}_L = 0$. From Eq. (1), knowing that the rotational of the gradient is zero, we see that $\mathbf{E}_L = -\nabla A_0$ satisfies $\nabla \times \mathbf{E}_L = 0$. Identically, by knowing that transversal electromagnetic field has divergence equal to zero, we see that $\mathbf{E}_T = -\frac{\partial \mathbf{A}}{\partial t}$ because $\nabla \cdot \mathbf{A} = 0$ in the Coulomb gauge. The electromagnetic vector potential is a transversal vector in the Coulomb gauge.
Notice that Gauss law can now be written as $\nabla \cdot \mathbf{E}_L = \frac{\rho}{\epsilon_0}$ and $\nabla \cdot \mathbf{E}_T = 0$ with ρ the instantaneous charge. Finally, we reach the Laplace kaw $\nabla^2 A_0 = -\frac{\rho}{\epsilon_0}$ that justifies why the radiation energy depends solely on $\mathbf{E}_T$, while $\mathbf{E}_L$ takes into account the Coulomb energy among electrons.

5.3 — Solution of Exercise 2.2.2 at page 6

The Maxwell's equation $\nabla \times \mathbf{E}_T(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t}$, using Eq. (6) and Eq. (7), means $\frac{\partial \tilde{B}_\gamma(t)}{\partial t} = -i|\mathbf{k}_\gamma|\tilde{E}_\gamma(t)$. We have used $\nabla \times \mathbf{e}_\gamma e^{i\mathbf{k}_\gamma \mathbf{r}} = i\mathbf{k}_\gamma \times \mathbf{e}_\gamma e^{i\mathbf{k}_\gamma \mathbf{r}} = i|\mathbf{k}_\gamma|\mathbf{e'}_\gamma e^{i\mathbf{k}_\gamma \mathbf{r}}$ where the definition $\mathbf{e'}_\gamma = \frac{\mathbf{k}_\gamma}{|\mathbf{k}_\gamma|} \times \mathbf{e}_\gamma$ is used.

The Maxwell's equation $\nabla \times \mathbf{B}(\mathbf{r},t) = \mu_0 \left(\mathbf{J} + \epsilon \frac{\partial \mathbf{E}_T(\mathbf{r},t)}{\partial t} \right)$, using Eq. (6) and Eq. (7), means $\frac{\partial \tilde{E}_\gamma(t)}{\partial t} = -ic\omega_\gamma \tilde{B}_\gamma(t) - \frac{1}{\epsilon_0}\tilde{J}_{T,\gamma}$. We have used $\nabla \times \mathbf{e'}_\gamma e^{i\mathbf{k}_\gamma \mathbf{r}} = i\mathbf{k}_\gamma \times \mathbf{e'}_\gamma e^{i\mathbf{k}_\gamma \mathbf{r}} = i\mathbf{k}_\gamma \times \left(\frac{\mathbf{k}_\gamma}{|\mathbf{k}_\gamma|} \times \mathbf{e}_\gamma \right) e^{i\mathbf{k}_\gamma \mathbf{r}} = -i|\mathbf{k}_\gamma|\mathbf{e}_\gamma e^{i\mathbf{k}_\gamma \mathbf{r}}$, where we have used $\mathbf{v}_1 \times (\mathbf{v}_2 \times \mathbf{v}_3) = \mathbf{v}_2(\mathbf{v}_1\mathbf{v}_3) - \mathbf{v}_3(\mathbf{v}_1\mathbf{v}_2)$. The (transversal) component of the current density $\mathbf{J}_T(\mathbf{r},t)$ is decomposed into:

$$\mathbf{J}_T(\mathbf{r},t) = \sum_\gamma \mathbf{e}_\gamma \tilde{J}_\gamma(t) e^{i\mathbf{k}_\gamma \mathbf{r}}$$

5.4 — Solution of Exercise 2.2.3 at page 6

By multiplying Eq. (8) by $-ic$ and Eq. (9) by i, we get $\frac{\partial -ic\tilde{B}_\gamma(t)}{\partial t} = -i\omega_\gamma(-i\tilde{E}_\gamma(t))$ plus $i\frac{\partial \tilde{E}_\gamma(t)}{\partial t} = i\omega_\gamma(-ic\tilde{B}_\gamma(t)) - i\frac{1}{\epsilon_0}\tilde{J}_{p,T}$. When added, using α in Eq. (11), we get:

$$\frac{\partial \alpha_\gamma(t)}{\partial t} = i\omega_\gamma(\alpha_\gamma(t)) - i\frac{1}{2Z_\gamma \epsilon_0}\tilde{J}_{p,T}$$

By multiplying Eq. (8) by $-ic$ and Eq. (9) by $-i$, we get $\frac{\partial -ic\tilde{B}_\gamma(t)}{\partial t} = i\omega_\gamma(i\tilde{E}_\gamma(t))$ plus $-i\frac{\partial \tilde{E}_\gamma(t)}{\partial t} = -i\omega_\gamma(-ic\tilde{B}_\gamma(t)) + i\frac{1}{\epsilon_0}\tilde{J}_{p,T}$. When added, using β in Eq. (11), we get:

$$\frac{\partial \beta_\gamma(t)}{\partial t} = -i\omega_\gamma(\beta_\gamma(t)) + i\frac{1}{2Z_\gamma \epsilon_0}\tilde{J}_{p,T}$$

5.5 — Solution of Exercise 2.2.4 at page 7

By inverting Eq. (11) we get: $\tilde{E}_\gamma(t) = Z_\gamma(-i\alpha_\gamma + i\beta_\gamma)$ and $\tilde{B}_\gamma(t) = \frac{Z_\gamma}{c}(i\alpha_\gamma + i\beta_\gamma)$. Then:

$$\mathbf{E}_T(\mathbf{r},t) = i\sum_{\gamma>0}\mathbf{e}_\gamma Z_\gamma[(-i\alpha_\gamma + i\beta_\gamma)e^{i\mathbf{k}_\gamma\mathbf{r}} + (-i\alpha_{-\gamma} + i\beta_{-\gamma})e^{-i\mathbf{k}_\gamma\mathbf{r}}]$$

where we have used that $\mathbf{e}_\gamma = \mathbf{e}_{-\gamma}$. Identically, using $\mathbf{e'}_\gamma = -\mathbf{e'}_{-\gamma}$ we get

$$\mathbf{B}(\mathbf{r},t) = i\sum_{\gamma>0}\mathbf{e'}_\gamma\frac{Z_\gamma}{c}[(i\alpha_\gamma + i\beta_\gamma)e^{i\mathbf{k}_\gamma\mathbf{r}} + (-i\alpha_{-\gamma} - i\beta_{-\gamma})e^{-i\mathbf{k}_{-\gamma}\mathbf{r}}]$$

Knowing that $\tilde{E}_\gamma(t) = \tilde{E}^*_{-\gamma}(t)$ and $\tilde{B}_\gamma(t) = \tilde{B}^*_{-\gamma}(t)$ because the electric field $\mathbf{E}_T(\mathbf{r},t)$ and magentic field $\mathbf{B}(\mathbf{r},t)$ must be real, we get:

$$\alpha_{-\gamma}(t) = \beta^*_\gamma$$

so that $\tilde{E}_\gamma(t) = iZ_\gamma[-\alpha_\gamma(t) + \alpha^*_{-\gamma}(t)]$ and $\tilde{B}_\gamma(t) = i\frac{Z_\gamma}{c}[\alpha_\gamma(t) + \alpha^*_{-\gamma}(t)]$. Finally, we can rewrite:

$$\mathbf{E}_T(\mathbf{r},t) = i\sum_\gamma\mathbf{e}_\gamma Z_\gamma[-\alpha_\gamma(t)e^{i\mathbf{k}_\gamma\mathbf{r}} + \alpha^*_{-\gamma}(t)e^{i\mathbf{k}_\gamma\mathbf{r}}] = i\sum_\gamma\mathbf{e}_\gamma Z_\gamma[-\alpha_\gamma(t)e^{i\mathbf{k}_\gamma\mathbf{r}} + \alpha^*_\gamma(t)e^{-i\mathbf{k}_\gamma\mathbf{r}}]$$

In the summation of $\alpha^*_{-\gamma}(t)$, the variable γ is a dummy index that can be substituted by $-\gamma$ to reach the final expression. Identically, for the magnetic field, we get:

$$\mathbf{B}(\mathbf{r},t) = i\sum_\gamma\mathbf{e'}_\gamma\frac{Z_\gamma}{c}[\alpha_\gamma(t)e^{i\mathbf{k}_\gamma\mathbf{r}} + \alpha^*_{-\gamma}(t)e^{i\mathbf{k}_\gamma}] = i\sum_\gamma\mathbf{e'}_\gamma\frac{Z_\gamma}{c}[\alpha_\gamma(t)e^{i\mathbf{k}_\gamma\mathbf{r}} + \alpha^*_\gamma(t)e^{-i\mathbf{k}_\gamma\mathbf{r}}]$$

5.6 — Solution of Exercise 2.4.1 at page 8

We use Eq. (13) for a single mode, neglecting the spatial dependence (because of the long wavelength approximation), as:

$$\mathbf{E}_T(\mathbf{r},t) = i\mathbf{e}Z[-\alpha(t)e^{i\mathbf{kr}} + \alpha^*(t)e^{-i\mathbf{kr}}] \approx i\mathbf{e}Z[-\alpha(t) + \alpha^*(t)]$$

For a single mode, we avoid the subscript γ. We rewrite Eq. (16) as

$$\tilde{q}(t) = -2Z\sqrt{\frac{\epsilon_0 V}{\omega}}Im(\alpha(t)) = Z\sqrt{\frac{\epsilon_0 V}{\omega}}\frac{(-\alpha(t) + \alpha^*(t))}{i}$$

Combining both expressions, we get:

$$\mathbf{E}_T(\mathbf{r},t) = \mathbf{e}\sqrt{\frac{\omega}{\epsilon_0 V}}\tilde{q}(t)$$

5.7 — Solution of Exercise 3.1.1 at page 9

For $\alpha = 0$, there is no difference in the equations of motion for $\{\tilde{q}_{cl}, \tilde{s}_{cl}\}$ and $\{q_{cl}, s_{cl}\}$. By evaluating $\frac{d}{dt}\frac{dx_{cl}}{dt}$ in Eq. (32), with $\alpha = 0$, we get:

$$m_e\frac{d^2x_{cl}}{dt^2} = -\frac{\partial V(x_{cl})}{\partial x_{cl}}$$

By evaluating $\frac{d}{dt}\frac{dq}{dt}$ in Eq. (33), with $\alpha = 0$, we get:

$$\frac{d^2q_{cl}}{dt^2} = -\omega^2 q_{cl}$$

Then,

$$q_{cl}(t) = A_q\sin\left(\omega t + \theta_q\right)$$

is a solution where A_q and θ_q have to be defined from the initial conditions. We can evaluate s_{cl} from Eq. (33) getting:

$$s_{cl}(t) = \frac{1}{\omega}\frac{dq_{cl}}{dt} = A_q \cos\left(\omega t + \theta_q\right)$$

Notice that Eq. (33) is compatible with Eq. (12) when $\tilde{J}_\gamma = 0$. Then, we can write:

$$\frac{\partial \alpha_\gamma}{\partial t} = i\omega_\gamma \alpha_\gamma$$

giving

$$\frac{\partial Re(\alpha_\gamma)}{\partial t} + i\frac{\partial Im(\alpha_\gamma)}{\partial t} = i\omega_\gamma \left(Re(\alpha_\gamma) + i\ Im(\alpha_\gamma)\right) = \omega_\gamma i Re(\alpha_\gamma) - \omega_\gamma Im(\alpha_\gamma)$$

From Eq. (16) and Eq. (17) for a single-mode, we recover Eq. (31) as follows:

$$\frac{\partial \tilde{s}_{cl}}{\partial t} = -\omega_\gamma \tilde{q}_{cl} \qquad \text{and} \qquad \frac{\partial \tilde{q}_{cl}}{\partial t} = \omega_\gamma \tilde{s}_{cl}$$

5.8 — Solution of Exercise 3.1.2 at page 9

From the Hamiltonian in Eq. (30), we compute:

$$\frac{dH}{dt} = \frac{p_{cl}}{m_e}\frac{dp_{cl}}{dt} + \frac{\partial V(x_{cl})}{\partial x_{cl}}\frac{dx_{cl}}{dt} + \hbar\omega s_{cl}\frac{ds_{cl}}{dt} + \hbar\omega q_{cl}\frac{dq_{cl}}{dt} + \alpha\frac{dx_{cl}}{dt}q_{cl} + \alpha x_{cl}\frac{dq_{cl}}{dt},$$

By using Eq. (32) and Eq. (33), we get:

$$\frac{dH}{dt} = \frac{p_{cl}}{m_e}\left(-\frac{\partial V(x_{cl})}{\partial x_{cl}} - \alpha q_{cl}\right) + \frac{\partial V(x_{cl})}{\partial x_{cl}}\frac{p_{cl}}{m_e} + \hbar\omega s_{cl}\left(-\omega q_{cl} - \frac{\alpha}{\hbar}x_{cl}\right) + \hbar\omega q_{cl}\omega s_{cl} + \alpha\frac{p_{cl}}{m_e}q_{cl} + \alpha x_{cl}\omega s_{cl} = 0,$$

Notice that the variation of energy of the matter system that depends on fields $-\alpha\frac{p_{cl}}{m_e}q_{cl}$ is compensated by part of the energy of the interaction $\alpha\frac{p_{cl}}{m_e}q$. Identically, the variation of energy of the light that depends on matter $-\alpha x\omega s_{cl}$ is compensated by part of the energy of the interaction $\alpha x_{cl}\omega s_{cl}$.
Notice that a positive (negative) product $p_{cl}q_{cl}$ means decrement (increment) of the energy of the electron, while a positive (negative) product $x_{cl}s_{cl}$ means decrement (increment) of the energy of the field.

5.9 — Solution of Exercise 3.2.1 at page 10

If we eliminate the dependence on the light in the Hamiltonian Eq. (91), we reach a typical Hamiltonian of an electron alone in an infinite well, whose associated Schrödinger equation, inside the well ($V(x) = 0$), is:

$$i\hbar\frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_e}\frac{\partial^2 \Psi(x,t)}{\partial x^2},$$

If we assume that the state $\Psi(x,t)$ is an energy eigenstate of the infinite well, we get $\Psi(x,t) = e^{-iE_n t/\hbar}\phi_n(x)$ so that the state $\phi_n(x)$ has to satisfy the equation:

$$E_n\phi_n(x) = -\frac{\hbar^2}{2m_e}\frac{\partial^2 \phi_n(x)}{\partial x^2}, \tag{140}$$

By imposing the additional information that $\phi_n\left(x = \pm\frac{L_x}{2}\right) = 0$, it can be straightforwardly checked that the following

wave functions (normalized to unity):

$$\phi_n(x) = \langle x|\phi_n\rangle = \sqrt{\frac{2}{L_x}}\cos\left(\frac{(n+1)\pi x}{L_x}\right) \quad \text{n=0,2,4,...}$$

$$\phi_n(x) = \langle x|\phi_n\rangle = \sqrt{\frac{2}{L_x}}\sin\left(\frac{(n+1)\pi x}{L_x}\right) \quad \text{n=1,3,5,,...}$$

satisfy Eq. (140) when the energy of each eigenstate is given by:

$$E_n = \frac{\hbar^2\pi^2(n+1)^2}{2\,m_e\,L_x^2}$$

Notice that such states are not eigenstates of the Eq. (38) because of the additional term $\alpha x q(t)$. In any case, the eigenstates $\phi_n(x)$ can be considered a complete and orthonormal base of the system.

5.10 — Solution of Exercise 3.2.2 at page 11

From the Hamiltonian in Eq. (38),written as $i\hbar\frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle$ we compute the time derivative of the expectation value $\langle\Psi|\hat{H}|\Psi\rangle$ as

$$\frac{d\langle\Psi|\hat{H}|\Psi\rangle}{dt} = \frac{d\langle\Psi|}{dt}\hat{H}|\Psi\rangle + \langle\Psi|\frac{d\hat{H}}{dt}|\Psi\rangle + \langle\Psi|\hat{H}\frac{d|\Psi\rangle}{dt}$$

By using $\frac{d|\Psi\rangle}{dt} = \frac{-i}{\hbar}\hat{H}|\Psi\rangle$ and $\frac{d\langle\Psi|}{dt} = \frac{i}{\hbar}\hat{H}\langle\Psi|$, we get:

$$\frac{d\langle\Psi|\hat{H}|\Psi\rangle}{dt} = \langle\Psi|\frac{d\hat{H}}{dt}|\Psi\rangle = \alpha\frac{dq_{cl}(t)}{dt}\int dx\Psi^*(x,t)x\Psi(x,t) = \omega\alpha\langle x(t)\rangle s(t)$$

Notice we have used Eq. (33) and defined the time-dependent ensemble value $\int dx\Psi^*(x,t)x\Psi(x,t) = \langle x(t)\rangle$. A positive (negative) product $\langle x(t)\rangle s(t)$ means increment (decrement) of the energy of the electron, which can be understood as decrement (increment) of the energy of the field as discussed in Exercise 3.2.2 at page 11.

5.11 — Solution of Exercise 3.2.3 at page 11

If we assume $E_1 = E_0 = E$, the system in Eq. (50) can be solved with the change of variables $c_a(t) = e^{-iE/\hbar t}\tilde{c}_a(t)$, for $a = 0, 1$, as:

$$\begin{cases} i\hbar\dfrac{d\tilde{c}_0(t)}{dt} = \tilde{c}_1(t)\hbar\omega_I \\ i\hbar\dfrac{d\tilde{c}_1(t)}{dt} = \tilde{c}_0(t)\hbar\omega_I \end{cases} \tag{141}$$

Now, we can make the time derivative on the first equation and substitute the second one on the frist one to obtain:

$$-\hbar^2\frac{d^2\tilde{c}_0(t)}{dt^2} = (\hbar\omega_I)^2\tilde{c}_0(t) \tag{142}$$

A similar equation can be found for $\tilde{c}_1(t)$. The general solution to this equation is a combination of a cosine and a sine $\tilde{c}_0(t) = A\cos(\omega_I t) + B\sin(\omega_I t)$. The same solution can be found for $\hat{c}_1(t)$. Using the initial conditions $c_0(0) = 1, c_1(0) = 0$, we set $A = 1, B = 0$ for $\hat{c}_0$ and $A = 0, B = 1$ for $\hat{c}_1$. Finally, we can write the final solution to the problem as:

$$|\psi(t)\rangle = e^{-i\frac{E_0}{\hbar}t}\cos(\omega_I t)\,|0\rangle + e^{-i\frac{E_1}{\hbar}t}\sin(\omega_I t)\,|1\rangle \tag{143}$$

which is Eq. (52) leading to the semi-classical Rabi oscillations. Note that if we now set the interaction to zero $\hbar\omega_I = 0$, we recover that the original states $|0\rangle, |1\rangle$ are eigenstates of the system. The result shows a periodic oscillation between the $|0\rangle$ state and the $|1\rangle$ state, with frequency ω_I in Eq. (49). See Fig. 1 for the case $\Delta E = E_1 - E_0 = 0$.

5.12 — Solution of Exercise 3.2.4 at page 12

Let us consider a general matrix $\hat{H}$ defined as $\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$ that will be useful in further computations. In particular, we consider H_{11} and H_{22} as real elements. We aslo consider H_{12} and H_{21} as complex elements satisfying $H_{12} = H_{21}^*$. The matrix H can be rewritten as:

$$\begin{aligned} \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} &= \begin{pmatrix} \frac{H_{11}+H_{22}}{2} & 0 \\ 0 & \frac{H_{11}+H_{22}}{2} \end{pmatrix} + \begin{pmatrix} \frac{H_{22}-H_{11}}{2} & H_{12} \\ H_{21} & \frac{H_{22}-H_{11}}{2} \end{pmatrix} \\ &= \frac{H_{11}+H_{22}}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{H_{22}-H_{11}}{2} \begin{pmatrix} 1 & \frac{2H_{12}}{H_{22}-H_{11}} \\ \frac{2H_{21}}{H_{22}-H_{11}} & -1 \end{pmatrix} \end{aligned} \tag{144}$$

We rewrite the second matrix as:

$$\hat{K} = \begin{pmatrix} 1 & \frac{2H_{12}}{H_{22}-H_{11}} \\ \frac{2H_{21}}{H_{22}-H_{11}} & -1 \end{pmatrix} = \begin{pmatrix} 1 & \tan(\theta')e^{-i\gamma} \\ \tan(\theta')e^{i\gamma} & -1 \end{pmatrix} \tag{145}$$

with $\tan(\theta') = \frac{2|H_{21}|}{H_{22}-H_{11}}$, with $0 \leq \theta' \leq \pi$, and $H_{21} = |H_{21}|e^{i\gamma}$, with $0 \leq \gamma \leq 2\pi$. Then, the eigenvalues $k_\pm$ of such matrix $\hat{K}$ are:

$$det(\hat{K} - k_\pm I) = 0 \tag{146}$$

The equation to solve is $(k_\pm)^2 = 1 + \tan^2(\theta') = \frac{\cos^2(\theta')+\sin^2(\theta')}{\cos^2(\theta')} = \frac{1}{\cos^2(\theta')}$. Thus, the eigenvalues of $\hat{K}$ are $k_\pm = \pm\frac{1}{\cos(\theta')}$. Notice that $\tan^2(\theta') = \frac{4|H_{21}|^2}{(H_{22}-H_{11})^2}$ implies that:

$$k_\pm = \pm\frac{1}{\cos(\theta')} = \pm\sqrt{1+\tan^2(\theta')} = \pm\frac{\sqrt{4|H_{21}|^2 + (H_{22}-H_{11})^2}}{H_{22}-H_{11}}. \tag{147}$$

It is clear from Eq. (144) that $\hat{H}$ and $\hat{K}$ has the same eiegn vectors that we define as $|\phi_+\rangle$ and $|\phi_-\rangle$. Then, the eiegnvalues $E_\pm$ of the operator $\hat{H}$ and the eiegnvalues $k_\pm$ of the oeprator $\hat{K}$ satisfy $E_\pm = \frac{H_{11}+H_{22}}{2} + \frac{H_{22}-H_{11}}{2}k_\pm$. So finally, we get:

$$E_\pm = \frac{H_{11}+H_{22}}{2} \pm \frac{1}{2}\sqrt{4|H_{21}|^2 + (H_{22}-H_{11})^2} \tag{148}$$

Since the eigenstates of $\hat{H}$ have to be eigenstates $\hat{K}$, the eigenstate of $\hat{K}$ satisfy:

$$\begin{pmatrix} 1 & \tan(\theta')e^{-i\gamma} \\ \tan(\theta')e^{i\gamma} & -1 \end{pmatrix} \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = \pm\frac{1}{\cos(\theta')} \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} \tag{149}$$

Then, we get: $a_\pm + \tan(\theta')b_\pm e^{-i\gamma} = \pm\frac{1}{\cos(\theta')}a_\pm$, which can be rewritten as: $a_\pm\left(\cos(\theta') \mp 1\right) = -\sin(\theta')e^{-i\gamma}b_\pm$. Now, we use the following trigonometric relation relating θ' and $\theta'/2$, as $\sin(\theta') = 2\sin(\theta'/2)\cos(\theta'/2)$ and $2\sin^2(\theta'/2) = 1 - \cos(\theta')$ and $2\cos^2(\theta'/2) = 1 + \cos(\theta')$, we get:

$$\begin{aligned} a_+\left(\cos(\theta') - 1\right) = \sin(\theta')e^{-i\gamma}b_+ &\Longrightarrow a_+\sin(\theta'/2)e^{i\gamma/2} = \cos(\theta'/2)b_+e^{-i\gamma/2} \\ a_-\left(\cos(\theta') + 1\right) = -\sin(\theta')e^{-i\gamma}b_- &\Longrightarrow a_-\cos(\theta'/2)e^{i\gamma/2} = -\sin(\theta'/2)b_-e^{-i\gamma/2} \end{aligned} \tag{150}$$

Finally, we get:

$$\begin{cases} |\phi_+\rangle = \cos(\theta'/2)e^{-i\gamma/2}|0\rangle + \sin(\theta'/2)e^{i\gamma/2}|1\rangle \\ |\phi_-\rangle = -\sin(\theta'/2)e^{-i\gamma/2}|0\rangle + \cos(\theta'/2)e^{i\gamma/2}|1\rangle \end{cases} \tag{151}$$

The final results are obtained by re-defining $\theta' = 2\theta$.

5.13 — Solution of Exercise 3.2.5 at page 13

From the initial conditions and Eq. (56), we get:

$$|\Psi(0)\rangle = |0\rangle = \cos\theta \left|\phi_+\right\rangle - \sin\theta \left|\phi_-\right\rangle \tag{152}$$

comparing Eq. (62) with Eq. (152), we see that $c_+ = \cos\theta$ and $c_- = -\sin\theta$, giving:

$$|\Psi(t)\rangle = \cos\theta e^{-iE_+/\hbar t} \left|\phi_+\right\rangle - \sin\theta e^{-iE_-/\hbar t} \left|\phi_-\right\rangle \tag{153}$$

so we can now compute the probaiblity transition to $|1\rangle$ at time t:

$$\langle 1|\Psi(t)\rangle = \cos(\theta)e^{-iE_+/\hbar} \overbrace{\left\langle 1\middle|\phi_+\right\rangle}^{\sin(\theta)} - \sin\theta e^{-iE_-/\hbar} \overbrace{\langle 1\left|\phi_-\right\rangle}^{\cos\theta} = \tag{154}$$

$$= \frac{1}{2}\sin(2\theta)\left(e^{-iE_+/\hbar} - e^{-iE_-/\hbar}\right) = \tag{155}$$

$$= i\sin(2\theta)e^{-i\frac{(E_+ + E_-)}{2\hbar}t} \sin\left(\frac{E_+ - E_-}{2\hbar}t\right) \tag{156}$$

Finally,

$$|\langle 1|\Psi(t)\rangle|^2 = \sin^2(2\theta)\sin^2\left(\frac{E_+ - E_-}{2\hbar}t\right) \tag{157}$$

Notice that $\tan^2(2\theta) = \frac{\omega_I^2}{\omega_r^2}$ in the definition Eq. (60) implies that $\sin(2\theta) = \frac{\omega_I}{\sqrt{\omega_r^2+\omega_I^2}}$. So, using the eigenenergies expressions Eq. (55) with $\hbar\omega_r = \frac{H_{22}-H_{11}}{2} = \frac{E_1-E_0}{2}$ and $H_{12} = H_{21} = \hbar\omega_I$, we get $E_+ - E_- = \sqrt{4|H_{21}|^2 + (H_{22}-H_{11})^2} = 2\hbar\sqrt{\omega_I^2+\omega_r^2}$. Finally:

$$\begin{aligned} |\langle 1|\Psi(t)\rangle|^2 &= \frac{(\hbar\omega_I)^2}{(E_0-E_1)^2 + (\hbar\omega_I)^2} \sin^2\left(\frac{1}{2\hbar}\sqrt{(E_0-E_1)^2 + 4(\hbar\omega_I)^2}t\right) \\ &= \frac{\omega_I^2}{\omega_r^2+\omega_I^2}\sin^2\left(\sqrt{\omega_r^2+\omega_I^2}t\right) \end{aligned} \tag{158}$$

5.14 — Solution of Exercise 3.2.6 at page 14

From Eq. (70), we make the follwing change of variables $\tilde{c}_0 = \tilde{\tilde{c}}_0 e^{-i\frac{\Delta}{2}t}$ and $\tilde{c}_1 = \tilde{\tilde{c}}_1 e^{i\frac{\Delta}{2}t}$:

$$\begin{cases} i\hbar\dfrac{d\tilde{\tilde{c}}_0}{dt} = \hbar\dfrac{\Delta}{2}\tilde{\tilde{c}}_0 + \hbar\dfrac{\omega_I}{2}\tilde{\tilde{c}}_1 e^{i\frac{3\pi}{2}} \\ i\hbar\dfrac{d\tilde{\tilde{c}}_1}{dt} = \hbar\dfrac{\Delta}{2}\tilde{\tilde{c}}_1 + \hbar\dfrac{\omega_I}{2}\tilde{\tilde{c}}_0 e^{-i\frac{3\pi}{2}} \end{cases} \implies i\hbar\frac{d}{dt}\begin{pmatrix}\tilde{\tilde{c}}_0(t)\\ \tilde{\tilde{c}}_1(t)\end{pmatrix} = \begin{pmatrix} -\hbar\frac{\Delta}{2} & \hbar\frac{\omega_I}{2}e^{i\frac{3\pi}{2}} \\ \hbar\frac{\omega_I}{2}e^{-i\frac{3\pi}{2}} & \hbar\frac{\Delta}{2}\end{pmatrix}\begin{pmatrix}\tilde{\tilde{c}}_0(t)\\ \tilde{\tilde{c}}_1(t)\end{pmatrix} \tag{159}$$

This Hamiltonian in Eq. (159) becomes time independent and it correspons to Eq. (145): where

$$\begin{pmatrix} -\hbar\frac{\Delta}{2} & \hbar\frac{\omega_I}{2}e^{i\frac{3\pi}{2}} \\ \hbar\frac{\omega_I}{2}e^{-i\frac{3\pi}{2}} & \hbar\frac{\Delta}{2}\end{pmatrix} = -\hbar\frac{\Delta}{2}\begin{pmatrix} 1 & \frac{\omega_I}{\Delta}e^{i\frac{3\pi}{2}} \\ \frac{\omega_I}{\Delta}e^{-i\frac{3\pi}{2}} & -1\end{pmatrix} = -\hbar\frac{\Delta}{2}\begin{pmatrix} 1 & \tan(\theta')e^{-i\gamma} \\ \tan(\theta')e^{i\gamma} & -1\end{pmatrix} = -\hbar\frac{\Delta}{2}\hat{K} \tag{160}$$

with $\gamma = -\frac{3\pi}{2}$ and $\tan(\theta') = \tan(2\theta) = \frac{\omega_I}{\Delta}$. If we consider now that our inital state is $|\Psi(0)\rangle = |0\rangle$, inverting the relations 56, we can rewrite:

$$|\Psi(0)\rangle = |0\rangle = \cos(\theta)e^{i\gamma/2}\left|\phi_+\right\rangle - \sin(\theta)e^{i\gamma/2}\left|\phi_-\right\rangle \tag{161}$$

comparing Eq. (62) with Eq. (152), we see that $c_+ = \cos(\theta)e^{i\gamma/2}$ and $c_+ = -\sin(\theta)e^{i\gamma/2}$, giving:

$$|\Psi(t)\rangle = \cos(\theta)e^{i\gamma/2}e^{-iE_+/\hbar t}\left|\phi_+\right\rangle - \sin(\theta)e^{i\gamma/2}e^{-iE_-/\hbar t}\left|\phi_-\right\rangle \tag{162}$$

so we can now compute the probability transition to $|1\rangle$ at time t:

$$\langle 1|\Psi(t)\rangle = \cos(\theta)e^{i\gamma/2}e^{-iE_+/\hbar t}\overbrace{\left\langle 1\middle|\phi_+\right\rangle}^{\sin(\theta)e^{i\gamma/2}} - \sin(\theta)e^{i\gamma/2}e^{-iE_-/\hbar t}\overbrace{\langle 1|\phi_-\rangle}^{\cos(\theta)e^{i\gamma/2}} = \tag{163}$$

$$= \frac{1}{2}\sin(2\theta)e^{i\gamma}\left(e^{-iE_+/\hbar t} - e^{-iE_-/\hbar t}\right) = \tag{164}$$

$$= i\sin(2\theta)e^{i\gamma}e^{-i\frac{(E_+ + E_-)}{2\hbar}t}\sin\left(\frac{E_+ - E_-}{2\hbar}t\right) \tag{165}$$

Finally, noticing that $\tan^2(2\theta) = \frac{\omega_I^2}{\Delta^2}$ in the definition Eq. (160), we get $\sin^2(2\theta) = \frac{\omega_I^2}{\Delta^2+\omega_I^2}$. Using the eigen-energies expressions Eq. (55) with $\hbar\Delta = H_{22} - H_{11}$ and $|H_{12}| = |H_{21}| = \hbar\frac{\omega_I}{2}$, we get $E_+ - E_- = \sqrt{4|H_{21}|^2 + (H_{22} - H_{11})^2} = \hbar\sqrt{\omega_I^2 + \Delta^2}$. Finally:

$$|\langle 1|\Psi(t)\rangle|^2 = \sin^2(2\theta)\sin^2\left(\frac{E_+ - E_-}{2\hbar}t\right) = \frac{\omega_I^2}{\Delta^2+\omega_I^2}\sin^2\left(\frac{\sqrt{\Delta^2+\omega_I^2}}{2}t\right) \tag{166}$$

Alternatively, if we are considering now that the inital state is $|\Psi(0)\rangle = |1\rangle$, inverting the relations 56, we can rewrite:

$$|\Psi(0)\rangle = |1\rangle = \cos(\theta)e^{-i\gamma/2}\left|\phi_-\right\rangle + \sin(\theta)e^{-i\gamma/2}\left|\phi_+\right\rangle \tag{167}$$

comparing Eq. (62) with Eq. (167), we see that $c_+ = \sin(\theta)e^{-i\gamma/2}$ and $c_- = \cos(\theta)e^{-i\gamma/2}$, giving:

$$|\Psi(t)\rangle = \sin(\theta)e^{-i\gamma/2}e^{-iE_+/\hbar t}\left|\phi_+\right\rangle + \cos(\theta)e^{-i\gamma/2}e^{-iE_-/\hbar t}\left|\phi_-\right\rangle \tag{168}$$

so we can now compute the probability transition to $|0\rangle$ at time t:

$$\langle 0|\Psi(t)\rangle = \sin(\theta)e^{-i\gamma/2}e^{-iE_+/\hbar t}\overbrace{\left\langle 0\middle|\phi_+\right\rangle}^{\cos(\theta)e^{i\gamma/2}} + \cos(\theta)e^{-i\gamma/2}e^{-iE_-/\hbar t}\overbrace{\langle 0|\phi_-\rangle}^{-\sin(\theta)e^{-i\gamma/2}} = \tag{169}$$

$$= \frac{1}{2}\sin(2\theta)e^{-i\gamma}\left(e^{-iE_+/\hbar t} - e^{-iE_-/\hbar t}\right) = \tag{170}$$

$$= i\sin(2\theta)e^{-i\gamma}e^{-i\frac{(E_+ + E_-)}{2\hbar}t}\sin\left(\frac{E_+ - E_-}{2\hbar}t\right) \tag{171}$$

Finally, using again $\sin^2(2\theta) = \frac{\omega_I^2}{\Delta^2+\omega_I^2}$, we get:

$$|\langle 0|\Psi(t)\rangle|^2 = \sin^2(2\theta)\sin^2\left(\frac{E_+ - E_-}{2\hbar}t\right) = \frac{\omega_I^2}{\Delta^2+\omega_I^2}\sin^2\left(\frac{\sqrt{\Delta^2+\omega_I^2}}{2}t\right) \tag{172}$$

5.15 — Solution of Exercise 3.2.7 at page 15

We have to compute $\Omega = \sqrt{\Delta^2 + \omega_I^2}$ from Eq. (72). From the cavity length, $L_c = 5930$ nm, we get $\omega = 158$ Trad/s or 25.30 THz for the light from Eq. (26). For the length of the well, $L_x = 16$ nm, we get the energies $E_1 = 0.035$ eV

and $E_2 = 0.1401$ eV from Eq. (40), giving $\omega = \frac{E_1 - E_0}{\hbar} = 159 T rad/s$ of 25 THz. Thus, the system is in resonance. In the case of resonance, we get $\Omega = \omega_I$. From Eq. (41), we can compute:

$$\begin{aligned}
\langle 0|\, x\, |1\rangle &= \int_{-L_x/2}^{L_x/2} dx\ \phi_0^*(x)\ x\ \phi_1(x) = \int_{-L_x/2}^{L_x/2} dx \sqrt{\frac{2}{L_x}} \cos\left(\frac{\pi x}{L_x}\right) x \sqrt{\frac{2}{L_x}} \sin\left(\frac{2\pi x}{L_x}\right) \\
&= 2L_x \int_{-0.5}^{0.5} dx' \cos(\pi x') x' \sin(2\pi x') \\
&= 2L_x \left[\frac{9\sin(\pi x') + \sin(3\pi x') - 9\pi x' \cos(\pi x') - 3\pi x' \cos(3\pi x')}{18\pi^2} \right]_{x'=-0.5}^{x'=0.5} \\
&= 2(0.0901) L_x
\end{aligned} \tag{173}$$

where we have done the change of variable $x' = \frac{x}{L_x}$. Finally, using the values mentioned in the problem (and noticing that α is expressed in eV/nm), we get:

$$\Omega = \sqrt{\Delta^2 + \omega_I^2} = \omega_I \equiv \frac{\alpha A_{cl} \langle 0|\, \hat{x}\, |1\rangle}{\hbar} = 43 \text{ rad/ps}. \tag{174}$$

The angular frequency can be translated into a linear frequency giving ≈ 7 THz.

5.16 — Solution of Exercise 3.2.8 at page 16

So, if we set the initial conditions to be as usual $c_0 = 1, c_1 = 0$, which implies $c_0^0(t) = 1$ because we have seen in Eq. (77) to be constant, then, the solution for $\tilde{c}_1^1(t)$ from Eq. (78) is simply:

$$a_1^1(t) = \frac{1}{i\hbar} \hbar\omega_I \int_0^t \sin(\omega t') e^{i2\omega_r t'} dt' \tag{175}$$

Using $\sin(\omega t) = \frac{e^{i\omega t} - e^{-i\omega t}}{2i}$, and looking for the modulus square, the transition probability from state $|0\rangle$ to state $|1\rangle$ at time t is:

$$|\langle 1|\psi(t)\rangle|^2 = \omega_I^2 \left| \int_0^t e^{i2\omega_r t'} \sin(\omega t') dt' \right|^2 = \frac{\omega_I^2}{4} \left| \int_0^t \left(e^{i(\omega + 2\omega_r)t'} - e^{-i(\omega - 2\omega_r)t'} \right) dt' \right|^2 \tag{176}$$

This last integral can be easily computed, finally giving:

$$|\langle 1|\psi(t)\rangle|^2 = |c_1(t)|^2 = \frac{\omega_I^2}{4} \left| \frac{1 - e^{i(\omega + 2\omega_r)t}}{\omega + 2\omega_r} - \frac{1 - e^{-i(\omega - 2\omega_r)t}}{2\omega_r - \omega} \right|^2 \tag{177}$$

On the other hand, starting from the excited state, the transition probability to the ground state is:

$$|\langle 0|\psi(t)\rangle|^2 = |c_0(t)|^2 = \frac{\omega_I^2}{4} \left| \frac{1 - e^{i(\omega + 2\omega_r)t}}{\omega + 2\omega_r} + \frac{1 - e^{-i(\omega - 2\omega_r)t}}{2\omega_r - \omega} \right|^2 \tag{178}$$

5.17 — Solution of Exercise 3.3.1 at page 17

In order to find a local continuity equation, let us work with $\psi(x,t)$ and its complex conjugate $\psi^*(x,t)$. In particular, we can rewrite Eq. (38) as:

$$\psi^*(x,t) i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\psi^*(x,t) \frac{\hbar^2}{2m_e} \frac{\partial^2 \psi(x,t)}{\partial x^2} + \psi^*(x,t)(V(x,t) + \alpha\ q_{cl}(t) x) \psi(x,t) \tag{179}$$

and the complex conjugate of Eq. (38) as:

$$-\psi(x,t)i\hbar\frac{\partial\psi^*(x,t)}{\partial t} = -\psi(x,t)\frac{\hbar^2}{2m_e}\frac{\partial^2\psi^*(x,t)}{\partial x^2} + \psi(x,t)(V(x,t)+\alpha\, q_{cl}(t)x)\psi^*(x,t) \quad (180)$$

From Eq. (179) and Eq. (180), we obtain:

$$\frac{\partial|\psi(x,t)|^2}{\partial t} = i\frac{\hbar}{2m_e}\frac{\partial}{\partial x}\left(\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}\right)$$

which can easily be identified with a local conservation of particles discussed where $\rho(x,t) = |\psi(x,t)|^2$ and the current density, $J(x,t)$, is defined as:

$$J_x(x,t) = i\frac{\hbar}{2m_e}\left(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x} - \psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right) = \frac{\hbar}{m_e}Im\left(\frac{\Psi(x,t)}{dx}\Psi^*(x,t)\right)$$

5.18 — Solution of Exercise 3.4.1 at page 18

The Hamiltonian of the electromagnetic energy in Eq. (91) involves the operators in Eq. (90). We define the creation operator $\hat{a}^\dagger$ and the annihilation operators $\hat{a}$, whose relationship with the previous operators is given by

$$\hat{a} = \frac{1}{\sqrt{2}}\left(q + \frac{\partial}{\partial q}\right) \quad , \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(q - \frac{\partial}{\partial q}\right).$$

Then, the evaluation of $\hat{a}^\dagger\hat{a}$ gives

$$\hat{a}^\dagger\hat{a} = \frac{1}{2}\left(q - \frac{\partial}{\partial q}\right)\left(q + \frac{\partial}{\partial q}\right) = \frac{1}{2}\left(q^2 - \frac{\partial}{\partial q}q + q\frac{\partial}{\partial q} - \frac{\partial^2}{\partial q^2}\right)$$

By developing $\frac{\partial}{\partial q}q = 1 + \frac{\partial}{\partial q}$, we get: $\hat{a}^\dagger\hat{a} = -\frac{1}{2}\frac{\partial^2}{\partial q^2} - \frac{1}{2} + \frac{1}{2}q^2$. Thus, we can write $\frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial q^2} + q^2\right) = \hbar\omega(\hat{a}^\dagger\hat{a}) + \frac{\hbar\omega}{2}$. Somehow, the use of the operators q and $-i\frac{\partial}{\partial q}$, instead of $\hat{a}$ and $\hat{a}^\dagger$, allows us to re-use all the machinery of the Schrodinger equation used to describe matter (with x and $-i\hbar\frac{\partial}{\partial x}$) to describe light too.

5.19 — Solution of Exercise 3.4.2 at page 18

The eigenstates of a parabolic well is straightforwardly elaborated in most textbooks of quantum mechanics. Here we will just see how the typical solution for a massive particle can be equivalently used to light. The typical Hamiltonian is:

$$H(q') = \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial q'^2} + \frac{1}{2}m_e\omega^2 q'^2$$

with the eigenenergy $E_m = \hbar\omega\left(m + \frac{1}{2}\right)$ for $m = 0, 1, 2, 3, ,,$. The general m eigenstate is given by

$$\psi_m(q') = \left(\frac{m_e\omega}{\pi\hbar}\right)^{1/4}\frac{1}{2^m m!}H_m(y)e^{-y^2/2}$$

with

$$y = \sqrt{\frac{m_e\omega}{\hbar}}q'$$

Some useful properties for the Hermite polynomials $H_m(y)$ are:

$$\begin{aligned}
H_0(y) &= 1 \\
H_1(y) &= 2y \\
H_2(y) &= 4y^2 - 2 \\
H_3(y) &= 8y^3 - 12y \\
H_4(y) &= 16y^4 - 48y^2 + 12 \\
H_5(y) &= 32y^5 - 160y^3 + 120y \\
H_6(y) &= 64y^6 - 480y^4 + 720y^2 - 120 \\
H_7(y) &= 128y^7 - 1344y^5 + 3360y^3 - 1680y \\
H_8(y) &= 256y^8 - 3584y^6 + 13440y^4 - 13440y^2 + 1680 \\
H_9(y) &= 512y^9 - 9216y^7 + 48384y^5 - 80640y^3 + 30240y
\end{aligned}$$

with the condition:

$$H_{m+1}(y) = 2yH_m(y) - 2mH_{m-1}(y)$$

In particular, we have:

$$\psi_0(q') = \left(\frac{m_e\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m_e\omega}{2\hbar}q'^2}$$

and

$$\psi_1(q') = \left(\frac{m_e\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} 2\left(\sqrt{\frac{m_e\omega}{\hbar}}q'\right) e^{-\frac{m_e\omega}{2\hbar}q'^2}$$

If we consider the change of variables $q' = \sqrt{\frac{\hbar}{m_e\omega}}q$, we reach the Hamiltonian:

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

Then, $y = \sqrt{\frac{m_e\omega}{\hbar}}q' = \sqrt{\frac{m_e\omega}{\hbar}}\sqrt{\frac{\hbar}{m_e\omega}}q = q$ and

$$\psi_m(q) = \left(\frac{1}{\pi}\right)^{1/4} \frac{H_m(q)}{\sqrt{2^m m!}} e^{-q^2/2}$$

5.20 — Solution of Exercise 3.4.3 at page 19

From the Hamiltonian in Eq. (91),written as $i\hbar\frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle$ we compute the time derivative of the expectation value $\langle\Psi|\hat{H}|\Psi\rangle$ as

$$\frac{d\langle\Psi|\hat{H}|\Psi\rangle}{dt} = \frac{d\langle\Psi|}{dt}\hat{H}|\Psi\rangle + \langle\Psi|\frac{d\hat{H}}{dt}|\Psi\rangle + \langle\Psi|\hat{H}\frac{d|\Psi\rangle}{dt}$$

By using $\frac{d|\Psi\rangle}{dt} = \frac{-i}{\hbar}\hat{H}|\Psi\rangle$ and $\frac{d\langle\Psi|}{dt} = \frac{i}{\hbar}\hat{H}\langle\Psi|$, we get:

$$\frac{d\langle\Psi|\hat{H}|\Psi\rangle}{dt} = \langle\Psi|\frac{d\hat{H}}{dt}|\Psi\rangle = \alpha\frac{dx(t)}{dt}\int dq\Psi^*(q,t)q\Psi(q,t) = \frac{\alpha}{m}\langle q(t)\rangle p(t)$$

Notice we have used Eq. (32) and defined the time-dependent ensemble value $\int dq\Psi^*(q,t)q\Psi(q,t) = \langle q(t)\rangle$. A positive (negative) product $\langle q(t)\rangle p(t)$ means increment (decrement) of the energy of the electron, which can be understood as a decrement (increment) of the energy of the field as discussed in Exercise 3.2.2 at page 11.

5.21 — Solution of Exercise 3.5.1 at page 19

In order to find a local continuity equation, let us work with $\psi(q,t)$ and its complex conjugate $\psi^*(q,t)$. In particular, we can rewrite Eq. (93) as:

$$\psi^*(q,t)i\hbar\frac{\partial\psi(q,t)}{\partial t} = -\psi^*(q,t)\frac{\hbar\omega}{2}\frac{\partial^2\psi(q,t)}{\partial q^2} + \psi^*(q,t)\left(\frac{\hbar\omega}{2}q^2 + \alpha x(t)q\right)\psi(x,t) \tag{181}$$

and the complex conjugate of Eq. (38) as:

$$-\psi(q,t)i\hbar\frac{\partial\psi^*(q,t)}{\partial t} = -\psi(q,t)\frac{\hbar\omega}{2}\frac{\partial^2\psi^*(q,t)}{\partial q^2} + \psi(q,t)\left(\frac{\hbar\omega}{2}q^2 + \alpha x(t)q\right)\psi^*(q,t) \tag{182}$$

From Eq. (181) and Eq. (182), we obtain:

$$\frac{\partial|\psi(q,t)|^2}{\partial t} = i\frac{\omega}{2}\frac{\partial}{\partial q}\left(\psi^*(q,t)\frac{\partial\psi(q,t)}{\partial q} - \psi(q,t)\frac{\partial\psi^*(q,t)}{\partial q}\right)$$

which can easily be identified with a local conservation of particles discussed where $\rho(q,t) = |\psi(q,t)|^2$ and the current density, $J(q,t)$, is defined as:

$$J_q(q,t) = i\frac{\omega}{2}\left(\psi(q,t)\frac{\partial\psi^*(q,t)}{\partial q} - \psi^*(q,t)\frac{\partial\psi(q,t)}{\partial q}\right) = \hbar\omega Im\left(\frac{\Psi(q,t)}{dq}\Psi^*(q,t)\right)$$

5.22 — Solution of Exercise 3.6.1 at page 20

From the Hamiltonian in Eq. (91),written as $i\hbar\frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle$ we compute the time derivative of the expectation value $\langle\Psi|\hat{H}|\Psi\rangle$ as

$$\frac{d\langle\Psi|\hat{H}|\Psi\rangle}{dt} = \frac{d\langle\Psi|}{dt}\hat{H}|\Psi\rangle + \langle\Psi|\frac{d\hat{H}}{dt}|\Psi\rangle + \langle\Psi|\hat{H}\frac{d|\Psi\rangle}{dt}$$

By using $\frac{d|\Psi\rangle}{dt} = \frac{-i}{\hbar}\hat{H}|\Psi\rangle$ and $\frac{d\langle\Psi|}{dt} = \frac{i}{\hbar}\hat{H}\langle\Psi|$, we get $\frac{d\langle\Psi|\hat{H}|\Psi\rangle}{dt} = 0$ because Tha Hamiltonian has no (external) time-dependent potential.

We also want to check that the norm of the state is equal to 1 (as far as it was properly well-normalized at the initial time): $\int dx\int dq\Psi(x,q,t)\Psi^*(x,q,t) = 1$ so that $\int dx\int dq\left(\frac{\partial\Psi(x,q,t)}{\partial t}\Psi^*(x,q,t) + \Psi(x,q,t)\frac{\partial\Psi^*(x,q,t)}{\partial t}\right) = 0$. Thus, we have to find:

$$\int dx\int dq\frac{\partial\Psi(x,q,t)}{\partial t}\Psi^*(x,q,t) + \Psi(x,q,t)\frac{\partial\Psi^*(x,q,t)}{\partial t} = \sum_{n=0}^{N}\sum_{m=0}^{M}\frac{dc_{n,m}(t)}{dt}c^*_{n,m}(t) + \frac{dc^*_{n,m}(t)}{dt}c_{n,m}(t)$$

$$= \sum_{n=0}^{N}\sum_{m=0}^{M}\frac{-i}{\hbar}(E_{n,e}+E_{m,p})c_{n,m}(t)c^*_{n,m}(t) + \frac{-i\alpha}{\hbar}\sum_{n',n=0}^{N}\sum_{m',m=0}^{M}c_{n',m'}(t)c^*_{n,m}(t)\int dx\phi^*_n(x)x\phi_{n'}(x)\int dq\psi^*_m(q)q\psi_{m'}(q)$$

$$+ \sum_{n=0}^{N}\sum_{m=0}^{M}\frac{i}{\hbar}(E_{n,e}+E_{m,p})c^*_{n,m}(t)c_{n,m}(t) + \frac{i\alpha}{\hbar}\sum_{n',n=0}^{N}\sum_{m',m=0}^{M}c^*_{n',m'}(t)c_{n,m}(t)\int dx\phi_n(x)x\phi^*_{n'}(x)\int dq\psi_m(q)q\psi^*_{m'}(q)$$

which is zero by construction.

5.23 — Solution of Exercise 3.6.2 at page 22

From Eq. (126), we make the follwing change of variables $\tilde{c}_{0,m+1} = \tilde{\tilde{c}}_{0,m+1} e^{-i\Delta_m t}$ and $\tilde{c}_{1,m} = \tilde{\tilde{c}}_{1,m} e^{i\Delta_m t}$:

$$\begin{cases} i\dfrac{d\tilde{\tilde{c}}_{0,m+1}}{dt} = -\Delta_m \tilde{\tilde{c}}_{0,m} + \omega_{R,m}\tilde{\tilde{c}}_{1,m} \\ i\dfrac{d\tilde{\tilde{c}}_{1,m}}{dt} = \Delta_m \tilde{\tilde{c}}_{1,m} + \omega_{R,m}\tilde{\tilde{c}}_{0,m+1} \end{cases} \tag{183}$$

This Hamiltonian in Eq. (183) becomes time independent and it correspons to Eq. (145): where

$$\begin{pmatrix} -\hbar\Delta_m & \hbar\omega_{R,m} \\ \hbar\omega_{R,m} & \hbar\Delta_m \end{pmatrix} = -\hbar\Delta_m \begin{pmatrix} 1 & \frac{\omega_{R,m}}{\Delta_m} \\ \frac{\omega_{R,m}}{\Delta_m} & -1 \end{pmatrix} = -\hbar\Delta_m \begin{pmatrix} 1 & \tan(\theta')e^{-i\gamma} \\ \tan(\theta')e^{i\gamma} & -1 \end{pmatrix} = -\hbar\Delta_m \hat{K} \tag{184}$$

with $\gamma = 0$ and $\tan(\theta') = \tan(2\theta) = \frac{\omega_{R,m}}{\Delta_m}$. The solution to this system is the same of Eq. (166). We use now, $\sin^2(2\theta) = \frac{\omega_m^2}{\Delta_m^2+\omega_m^2}$ and the eigen-energies expressions Eq. (55) with $\hbar 2\Delta_m = H_{22} - H_{11}$ and $|H_{12}| = |H_{21}| = \hbar\omega_{R,m}$, we get $E_+ - E_- = \sqrt{4|H_{21}|^2 + (H_{22}-H_{11})^2} = 2\hbar\sqrt{\omega_{R,m}^2 + \Delta_m}$. If we set the initial conditions to be $c_0 = 1, c_1 = 0$, following the same development done in Exercise 3.2.5 at page 13, we get:

$$|\langle 0|\Psi(t)\rangle|^2 = |c_0(t)|^2 = \frac{\omega_{R,m}^2}{\omega_{R,m}^2 + \Delta_m^2}\sin^2\left(\Delta_m t\right) \tag{185}$$

with $\omega_{R,m}$ defined in Eq. (125) and Δ_m in Eq. (129).

5.24 — Solution of Exercise 3.6.3 at page 22

From the cavity length, $L_c = 5930$ nm, we get $\omega = 158$ Trad/s or 25.30 THz for the light from Eq. (26). For the length of the well, $L_x = 16$ nm, we get the energies $E_1 = 0.035$ eV and $E_2 = 0.1401$ eV from Eq. (40), giving $\frac{E_1-E_0}{\hbar}) = 159 Trad/s = \omega$. Thus, the system is in resonance. We have already computed $\langle 0|\, x\, |1\rangle = 2(0.0901)L_x$ in Exercise 3.2.7 at page 15. Now, we compute:

$$\int_{-\infty}^{\infty} dq\ \psi_0^*(q)\ q\ \psi_1(q) = \int_{-\infty}^{\infty} dq \frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{2}} e^{-q^2/2} q e^{-q^2/2} 2q = \frac{4}{\sqrt{2\pi}}\int_0^{\infty} dq e^{-q^2} q^2 = \frac{1}{\sqrt{2}} \tag{186}$$

where we have used Exercise 3.4.2 at page 18 and the definite integral $\int_0^{\infty} dq e^{-q^2} q^2 = \sqrt{\pi}/4$. Since we are dealing with transitions $0 \to 1$ that means $m \to m+1$, we have $m = 0$ so that, from Eq. (125), we get $\omega_{R,0} = \omega_{I,0}\sqrt{0+1}\omega_{I,0}$. Finally, using the values mentioned in the problem (and noticing that α is expressed in eV/nm), we get:

$$\omega_{I,0} \equiv \frac{2(0.0901)L_x}{\hbar}\frac{1}{\sqrt{2}} = \frac{43}{\sqrt{2}} = 30 \text{ rad/ps}. \tag{187}$$

The angular frequency can be translated into a linear frequency giving ≈ 4.7 THz. Finally, since we have already demonstrated that the system is in resonance, $\Delta_m = 0$ in Eq. (127) and the final value is: $\Omega_{R,0} = \sqrt{\omega_{R,0}^2 + \Delta_m^2} = \omega_{R,0} = \omega_{I,0} = 30$ rad/ps or ≈ 4.7 THz

5.25 — Solution of Exercise 3.7.1 at page 23

In order to find a local continuity equation, let us work with $\Psi(x,q,t)$ and its complex conjugate $\Psi^*(x,q,t)$. By repeating Exercise 3.3.1 and Exercise 3.5.1 in the schrodinger equation Eq. (110), we reach the requested continuity equation.

6 Bibliography

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