

# Quantum optics, a brief introduction

David Zueco<sup>1</sup>

<sup>1</sup>*Instituto de Nanociencia y Materiales de Aragón (INMA) and Departamento de Física de la Materia Condensada,  
CSIC-Universidad de Zaragoza, Zaragoza 50009, Spain*

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## I. QUANTIZATION, A CRASH COURSE

By now, you should know what quantization is. I hope so. In any case, let me write it in a very informal way. Quantization means that you "make quantum, classical stuff". Consider the second Newton law,

$$m\ddot{\mathbf{r}} = -\nabla V(\mathbf{r}, t) \quad (1)$$

In a more formal way, this Newton e.o.m. is obtained from the lagrangian,

$$L = \frac{1}{2}m\dot{\mathbf{r}}^2 - V \quad (2)$$

The Newton equation is indeed obtained by imposing Hamilton's extremal principle stating that the configurations  $x(t)$  that are actually realised are those that extremise the action,  $S = \int dt L$ . This means that for any smooth curve,  $y(t)$ ,

$$\lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} (S(x + \epsilon y) - S(x)) = 0 \quad (3)$$

Applying this condition, one finds that it is fulfilled if and only if  $x(t)$  obeys Lagrange's equation of motion

$$\frac{\partial L}{\partial r_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{r}_i} = 0 \quad (4)$$

In the case discussed here, is just a line to check that using (4) gives the Newton equations (1).

The Lagrangian can be transformed to a Hamiltonian via a Legendre transformation,

$$H = \sum p_i r_i - L \quad (5)$$

with the generalized momentum

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} \quad (6)$$

It is quite easy to work our example giving

$$H = \frac{\mathbf{p}^2}{2m} + V \quad (7)$$

Importantly enough, the Hamiltonian "produces" the dynamical equations via the Poisson brackets. A Poisson bracket is a bilinear operation that given two functions,  $f(\mathbf{r}, \mathbf{p}, t)$  and  $g(\mathbf{r}, \mathbf{p}, t)$  then

$$\{f, g\} = \partial_{\mathbf{r}} f \partial_{\mathbf{p}} g - \partial_{\mathbf{p}} f \partial_{\mathbf{r}} g \quad (8)$$

Notice, as a first consequence that  $\{, \}$  is antisymmetric. Notice, also, that the Poisson bracket provides an operation making (in general) non-commuting two functions  $f$  and  $g$ . This is quite relevant in quantum mechanics.

Within the Poisson brackets, the dynamics is given by

$$\dot{f} = \frac{\partial f}{\partial t} + \{H, f\} \quad (9)$$

Set  $f = \mathbf{r}$  and  $f = \mathbf{p}$  and you will obtain the Newton e.o.m (1).

The final classical equation is the important relation ( $\mathbf{r}$  and  $\mathbf{p}$  are canonical variables)

$$\{r_i, p_j\} = \delta_{ij} . \quad (10)$$

Yep, I needed some extra lines for the Hamiltonian, but they are mandatory. Quantum mechanics (Heisenberg, Dirac) as we know it today is based on these few lines. In fact, one of the postulates tells you how to quantize and the idea is to "update" the canonical variables to operators (matrices, more or less) and that the Poisson brackets are commutators. In equations,

$$H(\mathbf{q}, \mathbf{p}) \rightarrow \hat{H}(\hat{\mathbf{q}}, \hat{\mathbf{p}}) \quad \text{and} \quad \{r_i, p_j\} = \delta_{ij} \rightarrow [\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij} . \quad (11)$$

Here,  $\hat{\cdot}$  emphasizes that they are operators, instead of variables. I hope you can now feel the importance of the noncommutative structure of poisson brackets in making sense of matrix quantum mechanics. In fact, recall that the Heisenberg equations are nothing but

$$\dot{\hat{f}} = \frac{\partial \hat{f}}{\partial t} - \frac{i}{\hbar} [\hat{H}, \hat{f}] , \quad (12)$$

that you must compare to (9).

Summarizing this summary, the quantization itinerary:

classical equation of motion  $\rightarrow$  Lagrangian  $\rightarrow$  Hamiltonian  $\rightarrow$  quantize canonical variables ( $\{, \} \rightarrow [, ]$ )

a. *Example: the harmonic oscillator*

## II. THE DIRAC EQUATION AND SOME OF ITS CONSEQUENCES

Paul Adrien Maurice Dirac (Bristol 1902 -Tallahassee 1984) is one of our physics heroes. An inexhaustible source of anecdotes (his behavior is compatible with having Asperger's <sup>1</sup>). He was one of the fathers of the quantum theory and wrote the most beautiful equation of physics in 1928. The one named after him and which I will try to summarize here. My job is not easy and the only thing I am sure of is that in the following lines I will not do justice to the importance and beauty of the equation and its consequences. Suffice it to quote Weisskopf himself: *A great deal more was hidden in the Dirac equation than the author had expected when he wrote it down in 1928. Dirac himself remarked in one of his talks that his equation was more intelligent than its author. It should be added, however, that it was Dirac who found most of the additional insights.* Given this display of modesty in the face of the equation he himself wrote, what can I do? I do my best following the excellent treatises [2, Chapter 5] and [3, Chapter 2]. Another interesting resource is the excellent review [4].

Before we start and to avoid getting lost, let me list the main consequences of the Dirac equation:

1. It is a relativistic equation for electrons, *i.e.* it combines special relativity and quantum mechanics.
2. Explains the existence of spin.
3. Explains the existence of antimatter.
4. Gives the magnetic momentum of spin.
5. Explains the spin-orbit coupling.
6. Gives the light-matter coupling
7. ...

### A. A Relativistic equation

The energy of a relativistic particle is given by,

$$E^2 = c^2 \mathbf{p}^2 + m^2 c^4 \quad (13)$$

with  $\mathbf{p} = \gamma(v_x, v_y, v_z)$  ( $\gamma = \sqrt{1 - v^2/c^2}$ ). If you take the "Schrödinger correspondence rule":

$$E \rightarrow i\hbar\partial_t \quad \mathbf{p} \rightarrow \frac{\hbar}{i}\nabla , \quad (14)$$

eq. (13) yields

$$\left[ \hbar^2 \frac{\partial^2}{\partial t^2} - c^2 \hbar^2 \nabla^2 + m^2 c^4 \right] |\psi\rangle = 0 \quad (15)$$

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<sup>1</sup> Dirac's biography *The strangest man* written by Graham Farmelo is an excellent book.

This is nothing but the Klein-Gordon (KG) equation.

**PROBLEM.-** The KG equation is a second order differential equation (unlike the Schrödinger equation that it is first order). Thus, the KG need  $|\psi(0)\rangle$  and  $|\dot{\psi}(0)\rangle$  to be solved. Dirac found a relativist, first order wave equation.

**ADVICE.-** Be familiar with the covariant notation, *i.e.*

$$p_\mu \rightarrow i\hbar \partial^\mu \quad \text{with } p_\mu = (E/c, \gamma mv_x, \gamma mv_y, \gamma mv_z) \quad (16)$$

and

$$\partial^\mu = \left( \frac{1}{c} \partial_t, -\nabla \right), \quad (17)$$

The KG can be written as,

$$\hbar^2 c^2 \partial_\mu \partial^\mu \psi + m^2 c^4 \psi = 0 \quad (18)$$

## B. First order relativistic equation

Dirac's idea was to write an Schrödinger-like equation such that

$$i\hbar \frac{\partial}{\partial t} \psi = H_D \psi \quad \text{with, } H_D = c\hat{\alpha} \cdot \mathbf{p} + \hat{\beta} mc^2 \quad (19)$$

such that [Cf. Eq. (13)]

$$H_D^2 = (c\hat{\alpha} \cdot \mathbf{p} + \hat{\beta} mc^2)^2 = E^2 = c^2 \mathbf{p}^2 + m^2 c^4. \quad (20)$$

Obviously to satisfy this equality  $\hat{\alpha}$  and  $\hat{\beta}$  must be matrices. In fact, it is pretty easy to check that, in order to satisfy (20) these matrices must fulfil,

$$\beta^2 = 1 \quad (21a)$$

$$\alpha_i \beta + \beta \alpha_i = 0 \quad (21b)$$

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij} \quad (21c)$$

We will discuss these matrices in detail in a moment. For the time being, it is convenient to introduce the Dirac matrices,

$$\gamma^\mu = (\beta, \beta \alpha) \quad (22)$$

The conditions (21a), (21b) and (21c) can be compactly written in term of the  $\gamma$ -matrices,

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu} 1 \quad (23)$$

with  $\eta^{\mu\nu} = \text{diag}(1, -1, -1, -1)$ . Finally, the Dirac equation can be written in covariant form,

$$(i\hbar \gamma^\mu \partial_\mu - mc) \psi = 0. \quad (24)$$

### 1. Solutions for the Dirac matrices

It turns out that the  $4 \times 4$  matices solve (21a), (21b) and (21c) (thus the equivalent conditions, (23))

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (25)$$

Here,  $\sigma_i$  are the Pauli matrices <sup>2</sup> and the 1 is the  $2 \times 2$  identity matrix.

Why  $4 \times 4$  matrices? Notice that you need 4 matrices and that conditions (21a), (21b) and (21c) remind the anticommutation relations for the Pauli matrices (3 matrices). So with  $2 \times 2$  is not possible. Is it possible with  $3 \times 3$  ones? No. Why? since  $\alpha_i^2 = \beta^2 = 1$ , their eigenvalues are  $\pm 1$ . Besides,

$$\alpha_i = -\beta\alpha_i\beta \rightarrow \text{Tr}(\alpha_i) = 0$$

(doing the same for  $\beta$ ,  $\text{Tr}(\beta) = 0$ ). Hence, the number of positive and negative eigenvalues must be equal; therefore, the dimension is even.  $4 \times 4$  does the work.

### C. Antiparticles

Although not entirely related to what interests us here, which is none other than discussing the theory for the interaction of light and matter, we will not resist outlining one of the most surprising consequences of the Dirac equation. This is none other than the prediction of antimatter. We cannot exaggerate the importance of this result. Although, as we shall see shortly, the Dirac equation explains the existence of spin (introduced to explain earlier experimental results and added by Pauli) and the prediction of the existence of antimatter had no experimental precedent. Indeed, it was in 1932 that Anderson measured it. 5 years after Dirac wrote his equation. He discovered the positron, the antiparticle of the electron. This discovery represents one of the great triumphs of theoretical physics.

Define the two-component spinors  $\phi_A$  and  $\phi_B$ . Then, the eigenvalue problem associated to Eq. (19) can be written,

$$\begin{pmatrix} mc^2 & c\sigma\mathbf{p} \\ c\sigma\mathbf{p} & -mc^2 \end{pmatrix} \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} = E \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} \quad (26)$$

Thus, the solutions to solve are:

$$c\sigma\mathbf{p}\phi_B = (E - mc^2)\phi_A \quad (27a)$$

$$c\sigma\mathbf{p}\phi_A = (E + mc^2)\phi_B \quad (27b)$$

Now, define,

$$\text{and .} \quad (28)$$

For the first couple of solutions, set  $\phi_a^{(s)} = \chi^{(s)}$ . Inserting this in (27b) we obtain that two solutions are:

$$\phi^{(+E,s)} = \begin{pmatrix} \chi^{(s)} \\ \frac{c\sigma\cdot\mathbf{p}}{E+mc^2}\chi^{(s)} \end{pmatrix} \quad (29)$$

For testing, you can check that inserting (29) in (27a) yields the consistency equation:

$$\frac{c^2\mathbf{p}^2}{E+mc^2}\chi^{(s)} = (E - mc^2)\chi^{(s)} \quad (30)$$

Sending the denominator in the l.h.s. to the r.h.s it is easy to see that we recover the relation for the relativistic energy, Eq. (13). On the other hand, this only tell us on the value for  $E^2$ , so positive and negative solutions may be possible. We see that (30) is compatible with positive energy. On the other hand, the other two solutions read,

$$\phi^{(-E,s)} = \begin{pmatrix} \frac{c\sigma\cdot\mathbf{p}}{E-mc^2}\chi^{(s)} \\ \chi^{(s)} \end{pmatrix} \quad (31)$$

In this case, inserting the latter in (27b) yields,

$$\frac{c^2\mathbf{p}^2}{(-E)+mc^2}\chi^{(s)} = ((-E) - mc^2)\chi^{(s)} \quad (32)$$

which is the same as (30) but with  $E \rightarrow -E$ . Therefore, these are solutions with negative energy. The antiparticles.

<sup>2</sup> The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



#### D. Gauge invariance and Light-matter interaction

In the modern viewpoint, *gauge invariance* is promoted to a general principle [5]. A gauge transformation is:

$$A'_\mu(x) = A_\mu(x) - \frac{1}{e} \partial_\mu \lambda(x), \quad (33)$$

for the potential vector,  $A_\mu = (\phi, \mathbf{A})$ . Recall that  $\partial_\mu = (\frac{1}{c} \partial_t, \nabla)$  and  $x_\mu = (ct, -\mathbf{x})$ . Besides, the wave function transforms as,

$$\psi'(x) = \psi(x) \exp[ie\lambda/\hbar c] \quad (34)$$

It turns out that the transformations (33) and (34) fix the interaction between light and matter. In particular, the *Dirac equation* for an electron, of mass  $m$  interacting with the electromagnetic field is

$$(i\hbar \mathcal{D} - m_e c) \psi(x) = 0 \quad (35)$$

Here, we use the field theoretical notation  $\mathcal{D} \equiv \partial_\mu + ieA_\mu(x)$ , which makes explicit the gauge invariance of the Dirac equation.

#### E. The spin explained

##### 1. A little of history (taken from [1, Chapter 9])

In 1886, Pieter Zeeman discovered the splitting of spectral lines in the presence of a static magnetic field. This experimental observation suggests that the interaction of  $\mathbf{B}$  with the angular momentum of the electron is given by the, so called, Zeeman term

$$H = -\frac{e}{2mc} \mathbf{L} \cdot \mathbf{B} = -\mu \cdot \mathbf{B}. \quad (36)$$

Some years later, in 1922, Otto Stern and Walther Gerlach performed the following experiment. They sent an atomic (silver) beam through a region with an inhomogeneous magnetic field (say that the field depends on  $z$ ). Then, the force experienced by the electrons is:

$$\mathbf{F} = \nabla \cdot (\mu \cdot \mathbf{B}) = \mu_z \partial_z B \mathbf{e}_z \quad (37)$$

Thus, depending on the angular momentum, the atoms should split in  $(2l+1)$  beams. However, silver has a spherically symmetric charge distribution plus one  $5s$ -electron. Thus, the total angular momentum of silver is zero, i.e.,  $l = 0$ ; no splitting should occur. However, the experiment gave that atoms split in two beams (!). Thus, the electron should have *internal angular momentum*. In words of Pauli [Z. Phys. (1925)]: *The doublet structure of the alkali spectra, as well as the violation of the Larmor theorem, occur due to a peculiar – and not classically describable – ambiguity of the quantum theoretical properties of the valence electron.* This internal angular momentum is the spin. Now we know that electrons has  $s = 1/2$ , so  $2s + 1 = 2$  possible internal states that produced those two beams in the experiment.

##### 2. The Dirac equation already contains the spin

Remind the Dirac equation solutions, Eqs. (29) and (31). Besides, let us define the, so called, *Dirac spin operator*:

$$\hat{\mathbf{s}} = \frac{\hbar}{2} \hat{\sigma} \quad (38)$$

with,

$$\hat{\sigma} = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}. \quad (39)$$

Notice that

$$\hat{\mathbf{s}} \phi^{\pm E, s} = \pm \frac{\hbar}{2} \phi^{\pm E, s} \quad (40)$$

+ for  $s = 1$  and - for  $s = 2$ . Therefore, apart from the energies  $\pm E$  we have another quantum number  $\pm \hbar/2$ , this is the spin.

Finally, it can be checked that  $\hat{s}$  is an angular momentum. In fact, adding a central potential to  $H_D$ , i.e.

$$H_D = c\hat{\alpha} \cdot \mathbf{p} + \hat{\beta}mc^2 + V(r) \quad (41)$$

we have that

$$[H_D, \mathbf{l} + \hat{\mathbf{s}}] = 0 \quad (42)$$

with  $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ , which is nothing but the angular momentum conservation. We see that we need to add  $\hat{\mathbf{s}}$  to  $\mathbf{l}$  to have such a (desired) conservation.

#### F. Non relativistic limit and the Pauli equation

The Dirac equation presented so far is the fundamental brick for the theory of quantum optics. We have already seen that it incorporates the light-matter interaction. On the other hand, in most cases, we will face nonrelativistic matter so, let's take the nonrelativistic limit of the Dirac equation. But before that, let us be a little more general and add the possibility of an external potential, such that the Eq. (43) is updated to

$$(i\hbar\mathcal{D} - m_e c - eV)\psi(x) = 0 \quad (43)$$

with  $V$  the potential. Now, using the same notation as in (26) we write the Dirac eq. as,

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \tilde{\phi}_A \\ \tilde{\phi}_B \end{pmatrix} = c \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{\pi} \tilde{\phi}_B \\ \boldsymbol{\sigma} \cdot \boldsymbol{\pi} \tilde{\phi}_A \end{pmatrix} + eV \begin{pmatrix} \tilde{\phi}_A \\ \tilde{\phi}_B \end{pmatrix} + mc^2 \begin{pmatrix} \tilde{\phi}_A \\ -\tilde{\phi}_B \end{pmatrix} \quad (44)$$

where,

$$\boldsymbol{\pi} = \mathbf{p} - \frac{e}{c}\mathbf{A} \quad (45)$$

In the nonrelativistic limit, the rest energy  $mc^2$  is the largest energy involved. Thus, to find solutions with positive energy, we write

$$\begin{pmatrix} \tilde{\phi}_A \\ \tilde{\phi}_B \end{pmatrix} = e^{-i\frac{mc^2}{\hbar}t} \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} \quad (46)$$

In doing so, equation (44) is written as,

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} = c \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{\pi} \phi_B \\ \boldsymbol{\sigma} \cdot \boldsymbol{\pi} \phi_A \end{pmatrix} + eV \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} - 2mc^2 \begin{pmatrix} 0 \\ \phi_B \end{pmatrix} \quad (47)$$

In the second equation the terms with  $c$  dominate, thus  $\hbar\dot{\phi}_B$  and  $eV\phi_B$  can be neglected. Then, the second line can be solved yielding

$$\phi_B = \frac{\boldsymbol{\sigma} \cdot \boldsymbol{\pi}}{2mc} \phi_A \quad (48)$$

We see then that  $\phi_B \sim 1/c\phi_A$ , so  $\phi_A$  is referred as large and  $\phi_B$  the small component of the spinor. Inserting (48) in (47) we get,

$$i\hbar \frac{\partial \phi_A}{\partial t} = \left( \frac{1}{2m} (\boldsymbol{\sigma} \cdot \boldsymbol{\pi}) (\boldsymbol{\sigma} \cdot \boldsymbol{\pi}) + eV \right) \phi_A. \quad (49)$$

Using

$$\boldsymbol{\sigma} \cdot \mathbf{a} \boldsymbol{\sigma} \cdot \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}) \quad (50)$$

where we have used  $\sigma_i \sigma_j = \delta_{ij} + I\epsilon^{ijk}\sigma_k$ . It turns out that,

$$\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \boldsymbol{\sigma} \cdot \boldsymbol{\pi} = \boldsymbol{\pi}^2 + i\boldsymbol{\sigma} \cdot \boldsymbol{\pi} \times \boldsymbol{\pi} = \boldsymbol{\pi}^2 - \frac{e\hbar}{c} \boldsymbol{\sigma} \cdot \mathbf{B} \quad (51)$$

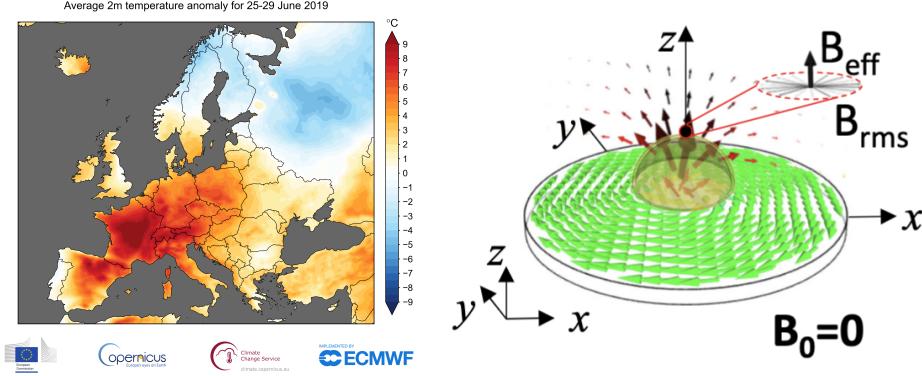


FIG. 1. Temperatute map and magnetic field

Here, we have used

$$\begin{aligned} (\boldsymbol{\pi} \times \boldsymbol{\pi})^i \phi_A &= -i\hbar \left( \frac{-e}{c} \right) \varepsilon^{ijk} (\partial_j A^k - A^k \partial_j) \phi_A \\ &= i \frac{\hbar e}{c} \varepsilon^{ijk} (\partial_j A^k) \phi_A = i \frac{\hbar e}{c} B^i \phi_A \end{aligned} \quad (52)$$

with  $B_i = \epsilon^{ijk} \partial_j A^k$ . This rearrangement can also be very easily carried out by application of the expression:

$$\nabla \times \mathbf{A} \phi_A + \mathbf{A} \times \nabla \phi_A = \nabla \times \mathbf{A} \phi_A - \nabla \phi_A \times \mathbf{A} = (\nabla \times \mathbf{A}) \phi_A \quad (53)$$

Finally, it is obtained,

$$i\hbar \frac{\partial \phi_A}{\partial t} = \left[ \frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 - \frac{e\hbar}{2mc} \boldsymbol{\sigma} \cdot \mathbf{B} + eV \right] \phi_A \quad (54)$$

This is nothing but the Pauli equation (and the Hamiltonian, the Pauli Hamiltonian) which was written in 1927 (by Pauli) to explain the Stern Gerlach experiment introducing the concept of spin (Notice the Zeeman term). Important enough the Dirac equation, in the non relativistic limit, is described naturally by a 2 dimensional spinor and the spin do not need to added adhoc but appears, also, naturally.

For completeness, we write explicitly the *Pauli Hamiltonian*:

$$H = \frac{1}{2m_e} (\mathbf{p} + e\mathbf{A})^2 - e\phi + \frac{\mu_B}{\hbar} \boldsymbol{\sigma} \cdot \mathbf{B} . \quad (55)$$

Here, we have introduced the Bohr magneton  $\mu_B = e\hbar/2m_e$ ,  $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  are the Pauli matrices and  $\mathbf{B} = \nabla \times \mathbf{A}$  is the magnetic field. It is difficult to exaggerate the importance of the Hamiltonian (55). It is the starting point of every quantum optics book. It is *the* light-matter Hamiltonian. Due to its relevance, it deserves to appreciate the way it was found. Notice that only gauge and Lorentz invariance (Dirac equation) and the nonrelativistic limit was used. Grounded in such a general laws, in its validity we trust.

### III. QUANTIZATION OF THE ELECTROMAGNETIC FIELD

#### 1. From particles to fields

So far we have discussed particles and their quantization, both in the relativistic and non-relativistic limit. However, we are interested in the quantization of the electromagnetic field. Yes, field. What is a field? Perhaps, one of the simplest ways to imagine a field is to think of the temperature map like the one in figure 1. There, given a point  $(x, y)$  the map tells you the value of the temperature, *i.e.*  $T(x, y)$  is a scalar field since given a spatial point a scalar (the temperature value) is given. The electromagnetic field is vectorial. In figure 1, one can see the magnetic field

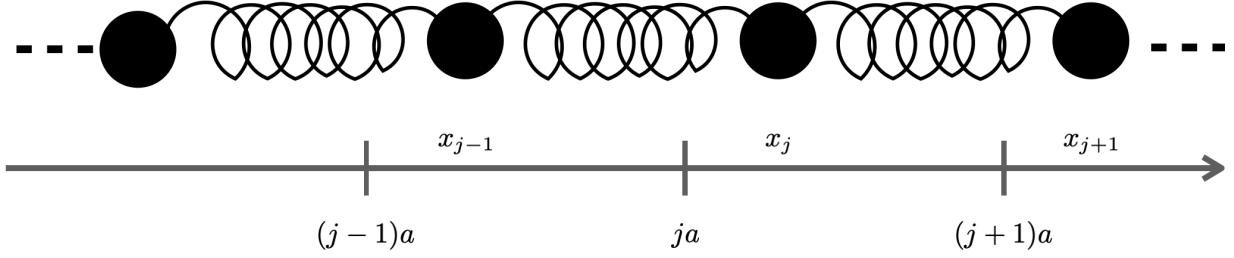


FIG. 2. linear chain

generated by a magnetic vortex. There, at each point in space  $(x, y, z)$  a vector is given, namely  $\mathbf{B}(x, y, z)$ . Thus, a field is nothing more than a function of the spatial coordinates given by a (scalar) number or a (vector) vector.

To make the long history short, consider **the linear chain**. This is a model of particles coupled by springs like in the figure<sup>3</sup>. The lagrangian is,

$$L = \frac{1}{2}m \sum_j \dot{x}_j^2 - \frac{1}{2}k \sum_j (x_j - x_{j+1})^2 \quad (56)$$

$x_j$  are the deviations from the equilibrium positions  $ja$

We are interested in the limit " $a \rightarrow 0$ " which is the continuum limit,

$$x_j = \phi(aj) \rightarrow a^{1/2}\phi(x) \quad (57)$$

The  $\rightarrow$  is the continuum limit where the discreteness  $aj$  is smoothed. Here, you have a field (in this case scalar), given the position  $x$  the field gives you the value of the displacement  $\phi(x)$ . The  $a^{1/2}$  is necessary (be patient!). Finally, remind the definition for the discrete derivative  $(\phi_{j+1} - \phi_j)/a \rightarrow \partial_x\phi(x)$  and that an integral is nothing but a sum  $\sum_j a(\dots) \rightarrow \int dx$ . Putting alltogether the continuum version for (58) is given by

$$L[\phi] = \int_0^L dx \mathcal{L}(\partial_x\phi, \dot{\phi}), \quad \mathcal{L}(\partial_x\phi, \dot{\phi}) = \frac{m}{2}\dot{\phi}^2 - \frac{ka^2}{2}(\partial_x\phi)^2 \quad (58)$$

What are the equations for the fields?

Now, we are interested in fields  $\phi(x, t)$ , but the extremal principle is still valid. Thus, we perform  $\phi(x, t) \rightarrow \phi(x, t) + \epsilon\eta(x, t)$  into Eq. (58) and demand that the contribution first order in  $\epsilon$  vanishes. That's it,

$$S(\phi + \epsilon\eta) = S(\phi) + \epsilon \int dt \int dx m\dot{\phi}\dot{\eta} - ka^2\partial_x\phi\partial_x\eta \quad (59)$$

Integrating by parts and demanding that the contribution linear in  $\epsilon$  ( $\eta(0) = \eta(T) = 0$ ) vanishes, one obtains

$$\int dx \int dt (m\ddot{\phi} - ka^2\partial_x^2\phi)\eta = 0 \quad (60)$$

Therefore the equation of motion for the fields are,

$$(m\partial_t^2 - ka^2\partial_x^2)\phi = 0 \quad (61)$$

which is nothing but the wave equation.

<sup>3</sup> for those used to circuits, the linear chain models an array of LC in series

Notice that we have obtained the e.o.m. for the fields in this very particular case, the linear chain. For the case of the fields, like for the particles, it is possible to find the lagrange equations. However, we are running fast here and we do not have time to develop the full theory. On the other hand, understanding the linear chain is sufficient for the quantization of the EM field.

But in order to quantize we need to go from a Lagrangian to a Hamiltonian description. For that (recall the previous subsection) we introduce the momentum for field. Eq. (6) has the natural generalization

$$\Pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)} \quad (62)$$

The Hamiltonian follows, pretty much like for the particle case [Cf. Eq. (5)], *i.e.*,

$$H[\phi, \pi] = \int dx \mathcal{H}[\phi, \pi], \quad \mathcal{H}[\phi, \pi] = \pi \dot{\phi} - \mathcal{L} \quad (63)$$

In our case, it reads,

$$\mathcal{H}(\phi, \pi) = \frac{1}{2m} \pi^2 + \frac{ka^2}{2} (\partial_x \phi)^2 \quad (64)$$

As we have discussed before, quantization is a recipe that takes us from the Hamiltonian formalism of classical dynamics to the quantum theory. The recipe tells us to take the generalized coordinates and their conjugate momenta and promote them to operators. Notice, that in this case [Cf. Eq. (57)]

$$[\phi_j, \pi_j] = i\hbar \delta_{ij} \implies [\phi_i/\sqrt{a}, \pi_j/\sqrt{a}] = i\hbar \delta_{ij}/a \xrightarrow{a \rightarrow 0} i\hbar \delta(x - x') \quad (65)$$

Therefore, in quantum field theory the position-momentum fields are quantized following,

$$[\phi(x), \pi(x')] = i\hbar \delta(x - x') \quad (66)$$

It turns out that (64) is easy to solve. In fact, it is one of the few solvable QFTs. In order to do so, we introduce the Fourier transform for the field operators (This is quite usual! we have a translational invariant Hamiltonian and moving to "momentum" space is always a good idea).

$$\phi_k \equiv \frac{1}{\sqrt{L}} \int_0^L dx e^{-ikx} \phi(x), \quad \phi(x) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \phi_k \quad (67)$$

$$\pi_k \equiv \frac{1}{\sqrt{L}} \int_0^L dx e^{ikx} \pi(x), \quad \pi(x) = \frac{1}{\sqrt{L}} \sum_k e^{-ikx} \pi_k \quad (68)$$

with  $k = 2\pi m/L$ ,  $m \in \mathbb{Z}$  and  $L$  the lenght. Notice that  $\phi_k^\dagger = \phi_{-k}$  (the same for  $\pi_k$ ).

Notice that

$$[\phi_k, \pi_{k'}] = i\hbar \delta_{kk'}, \quad (69)$$

*i.e.* the transformed operators are (still) canonical ones. The Hamiltonian (64) transforms to

$$H = \sum_k \frac{1}{2m} \pi_k \pi_{-k} + \frac{ka^2}{2} k^2 \phi_k \phi_{-k} \quad (70)$$

Alright! we have reduced the problem to solve independent harmonic oscillators. We know how to do it. Introducing the ladder operators (anhilation /creation),

$$a_k = \sqrt{\frac{m\omega_k}{2\hbar}} \left( \phi_k + \frac{i}{m\omega_k} \pi_{-k} \right), \quad a_k^\dagger = \sqrt{\frac{m\omega_k}{2\hbar}} \left( \phi_{-k} + \frac{i}{m\omega_k} \pi_k \right) \quad (71)$$

The hamiltonian reads,

$$H = \sum_k \hbar \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) \quad (72)$$

Finally, let me write explicitly the expresion for the field  $\phi(x)$  in terms of the creation / annihilation operators. Using (67) and (71),

$$\phi(x) = \frac{1}{\sqrt{L}} \sum_k \sqrt{\frac{2\hbar}{m\omega_k}} (a_k e^{ikx} + a_{-k}^\dagger a_k e^{ikx}) \quad (73)$$

## 2. The Maxwell Equations

In 1865, Maxwell (Edinburgh 1831 - Cambridge 1879) sent his work *A Dynamical Theory of the Electromagnetic Field* to the Philosophical Transactions of the Royal Society. Based on the works of giants such as Thomson, Faraday, Oersted, Ampère, etc., he unified electric field, magnetic field and light, which he encapsulated in dynamical equations for the electromagnetic fields. For more than obvious reasons, these equations are called Maxwell's equations<sup>4</sup>. They are the equations governing the dynamics of the electromagnetic field. Thus, if we want to quantize it, they are our starting point. Maxwell equations are written as,

$$\nabla \cdot \mathbf{E}(\mathbf{r}, t) = \frac{1}{\epsilon_0} \rho(\mathbf{r}, t) \quad (74a)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0 \quad (74b)$$

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{r}, t) \quad (74c)$$

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \frac{1}{c^2} \frac{\partial}{\partial t} \mathbf{E}(\mathbf{r}, t) + \frac{1}{\epsilon_0 c^2} \mathbf{j}(\mathbf{r}, t) \quad (74d)$$

Here  $\mathbf{E}$  ( $\mathbf{B}$ ) are the electric (magnetic) field, while  $\rho$  and  $\mathbf{j}$  are the charge and current density respectively. Associated to the fields, it is convenient to introduce the potentials,

$$\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t) \quad \text{with } \cancel{\nabla \times \mathbf{D}} \cdot \mathbf{D} \quad (75a)$$

$$\mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \cdot \phi(\mathbf{r}, t) \quad (75b)$$

For what we are interested in, potential  $\mathbf{A}$  will be crucial. Notice how easy it is to see the gauge invariance here. Maxwell's equations for the physical fields  $\mathbf{E}$  and  $\mathbf{B}$  are invariant under the following *gauge transformation*

$$\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla \cdot \chi(\mathbf{r}, t) \quad (76a)$$

$$\phi \rightarrow \phi' = \phi - \frac{\partial \chi(\mathbf{r}, t)}{\partial t} \quad (76b)$$

A key gauge (for the quantization) is the coulomb one, defined:

$$\nabla \cdot \mathbf{A} = 0 \quad (77)$$

In this gauge, things are simplified. In particular, and in absence of sources ( $\rho = 0, \mathbf{j} = 0$ ) using the Maxwell equations and the relation between the vector potential and the fields we get,

$$(\partial_t^2 - c^2 \nabla^2) \mathbf{A} = 0 \quad (78)$$

At this point, you must compare this equation with (61). Apart from the vectorial nature of the latter, both are wave equations. And, now, we know that to wave equations a *field Hamiltonian can be associated*. In fact, the analogy can be made even stronger by noticing that the EM energy can be written,

$$E = \frac{\epsilon_0}{2} \int d^3 \mathbf{r} \cdot \mathbf{A}^2 + c^2 (\nabla \times \mathbf{A})^2 \quad (79)$$

Therefore, the Hamiltonian for the free EM reads,

$$H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \quad (80)$$

and the vector potential is

$$\mathbf{A}_\perp(\mathbf{r}) = \frac{1}{\sqrt{L^3}} \sum_k \sqrt{\frac{\hbar}{2\omega_{\mathbf{k}}\epsilon_0}} \mathbf{u}_{\mathbf{k}} (a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} + a_{-\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}}) \quad (81)$$

Notice that we have added the suffix  $\perp$  to the vector potential. This is because we are quantized in the coulomb gauge (you must not forget this! we are in the coulomb gauge) and in this gauge  $\nabla \cdot \mathbf{A}(\mathbf{r}) = 0 \rightarrow \mathbf{k} \cdot \mathbf{A}(\mathbf{k}) = 0$  so the former only has transversal components. In fact  $\mathbf{k} \cdot \mathbf{u} = 0$  in the above formula.

<sup>4</sup> Maxwell equations are very important. No doubts. As a curiosity I write here the report written by William Thomson (Lord Kelvin) on Maxwell's paper: *My dear Stokes I am sorry to have kept Maxwell's paper So long. I read it nearly through with great interest, almost immediately after it came to me, and I think it most decidedly suitable for publication in the Transac toons. If you can allow me to keep it a few days longer I should be glad to have it till Monday, and unless I hear from you I shall post it on that day. Yours very truly W. Thomson*

## IV. QUANTUM PHASE-SPACE DISTRIBUTIONS

The phase-space formulation of quantum mechanics has its roots in the classical work of Wigner<sup>5</sup> (1932), where he introduced the phase space distribution function that now bears his name in the derivation of the quantum correction terms of the Boltzmann formula<sup>6</sup>. Since the phase space formulation provides a framework in which quantum phenomena can be described using as classical a language as possible, it is very attractive. The formulation is naturally intuitive and can often provide useful insights into quantum phenomena. Obviously, its application goes beyond quantum optics but it has been used to describe and visualise quantum states of light. Here, we discuss its main properties.

### A. Motivation

In classical physics, we are used to probability distributions for computing averages. In mechanics, in the single-particle case, the variables are  $(x, p)$  (position and momentum) so,

$$\langle A \rangle = \int_{\mathbb{R}^2} dx dp A(x, p) W_c(x, p; t) \quad (82)$$

The evolution for the distribution  $W_c$  is given by the Liouville equation:

$$\partial_t W_c = \{H, W\} \quad (83)$$

where  $\{\cdot, \cdot\}$  are the Poisson brackets and  $H$  the classical Hamiltonian.

In quantum mechanics, averages are computed following the Von Neuman rule:

$$\langle A \rangle = \text{Tr}(A \varrho) \quad (84)$$

where  $\varrho$  is the density matrix that satisfies the Von Neumann equation

$$\partial_t \varrho = -\frac{i}{\hbar} [H, \varrho] \quad (85)$$

There are obvious similarities looking at Eqs. (82) and (84), (83) and (85). Besides  $\int W_c = 1$  ( $\text{Tr} \varrho = 1$ ) and  $W_c \geq 0$  ( $\varrho > 0$ ). However,  $W_c$  and  $\varrho$  are totally different objects: probability distribution and a hermitean matrix respectively. Therefore, there is not a close connection between the two descriptions. Besides, it is not evident how to reach the classical limit for  $\varrho$  to recover  $W_c$ . To close this relationship, the the phase formulation of quantum mechanics was invented.

### B. Statement of the problem

We follow Ref. [6].

We want to find a distribution for quantum averages (84) but with the classical "way of doing", Eq. (82). Therefore we are searching for the equality:

$$\text{Tr}(A \varrho) = \int dx dp A(q, p) W(q, p, t) \quad (86)$$

where  $A(q, p)$  is a scalar function obtained by replacing the operators  $\hat{x}$  and  $\hat{p}$  by scalar variables  $x$  and  $p$ . However, we are going to see that there is not a unique way of defining  $W$  due to the fact that  $[\hat{x}, \hat{p}] \neq 0$ . This is nice. The

<sup>5</sup> Eugene Wigner (Budapest 1902-Princeton 1995) was one of the biggest mathematical physicists, he won the Nobel prize in Physics for the use of symmetry principles in the theory of atomic nucleous and the elementary particles. He participate in the Manhattan project, in fact (following Wikipedia) *Although he was a professed political amateur, on August 2, 1939, he participated in a meeting with Leó Szilárd and Albert Einstein that resulted in the Einstein-Szilárd letter, which prompted President Franklin D. Roosevelt to initiate the Manhattan Project to develop atomic bombs.*[31] Wigner was afraid that the German nuclear weapon project would develop an atomic bomb first, and even refused to have his fingerprints taken because they could be used to track him down if Germany won.[32] "Thoughts of being murdered," he later recalled, "focus your mind wonderfully." Besides, he and Dirac were brothers-in-law.

<sup>6</sup> In the classical paper, Phys. Rev. 40 749 (1932) Wigner introduces the expression that we derive in these notes without justification, he just writes in a footnote *This expression was found by L.Szilard and the present author some years ago for another purpose.*

difficulties of finding quantum phase space distributions lie at the heart of quantum mechanics:  $[\hat{x}, \hat{p}] = i\hbar$ . In fact, consider

$$\text{Tr}(\varrho e^{i\xi\hat{x}+i\eta\hat{p}}) = \int dx dp e^{i\xi x + \eta p} W(x, p, t) \quad (87)$$

but!

$$\text{Tr}(\varrho e^{i\xi\hat{x}} e^{i\eta\hat{p}}) = \int dx dp e^{i\xi x + \eta p} W(x, p, t) \quad (88)$$

It is obvious that the l.h.s of (87) and (88) are not the same. In fact, using the Bakker-Haussdorf formula,

$$e^{i\xi\hat{x}+i\eta\hat{p}} = e^{i\xi\hat{x}} e^{i\eta\hat{p}} e^{i\hbar\xi\eta/2} \quad (89)$$

which is a consequence of the non commutativity of  $\hat{x}$  and  $\hat{p}$ . We can understand now, that the difficulty arises because there is no unique way of assigning a quantum-mechanical operator to a given classical function of conjugate variables. In short, while for scalar variables  $e^{ix+ip} = e^{ix} e^{ip}$  this is not the case for quantum operators. In the literature different *rules* are used. To understand them, let us define a general class of phase space distribution through the relation:

$$\text{Tr}(\varrho e^{i\xi\hat{x}+i\eta\hat{p}} f(\xi, \eta)) = \int dx dp e^{i\xi q + i\eta p} W^f(q, p; t) \quad (90)$$

Notice that the r.h.s is a Fourier transform, therefore

$$\begin{aligned} W^f &= \frac{1}{4\pi^2} \int d\xi d\eta \text{Tr}(\varrho e^{i\xi\hat{x}+i\eta\hat{p}} f(\xi, \eta)) e^{-i\xi q - i\eta p} \\ &= \frac{1}{4\pi^2} \int d\xi d\eta \int dx' \langle x' + \frac{1}{2}\eta\hbar | \varrho | x' - \frac{1}{2}\eta\hbar \rangle f(\xi, \eta) e^{i\xi(x'-x)} e^{-i\eta p} \end{aligned} \quad (91)$$

In the second line, we have used that

$$\text{Tr}(\varrho A) = \int dx dx' \langle x | \varrho | x' \rangle \langle x' | A | x \rangle \quad (92)$$

the identity,

$$e^{i\xi\hat{x}+i\eta\hat{p}} = e^{i\eta\hat{p}/2} e^{i\xi\hat{q}} e^{i\eta\hat{p}/2} \quad (93)$$

and,

$$e^{i\eta\hat{p}} |q\rangle = |x - \eta\hbar\rangle. \quad (94)$$

It is important to notice that in the case of pure states:  $\varrho = |\psi\rangle\langle\psi|$ , Eq. (91) reduces to,

$$W^f = \frac{1}{4\pi^2} \int d\xi d\eta \int dx' \psi^*(x' - \frac{1}{2}\eta\hbar) \psi(x' + \frac{1}{2}\eta\hbar) f(\xi, \eta) e^{i\xi(x'-x)} e^{-i\eta p}. \quad (95)$$

### C. The Wigner function

The Wigner function follows from the simplest choice  $f(\xi, \eta) = 1$  in (91) and (95). This corresponds to the Weyl rule  $e^{i\xi\hat{x}+i\eta\hat{p}} \leftrightarrow e^{i\xi x+i\eta p}$ . Using this prescription we obtain that,

$$W(x, p; t) = \frac{1}{2\pi} \int d\eta \langle x + \frac{1}{2}\eta\hbar | \varrho | x - \frac{1}{2}\eta\hbar \rangle e^{-i\eta p} \quad (96)$$

which is the celebrated equation written by Wigner in 1932 (in fact, it seems to have been written before this date, see footnote 6).

For pure states,

$$W(x, p; t) = \frac{1}{2\pi} \int d\eta e^{-i\eta p} \psi^*(x - \frac{1}{2}\eta\hbar) \psi(x + \frac{1}{2}\eta\hbar). \quad (97)$$

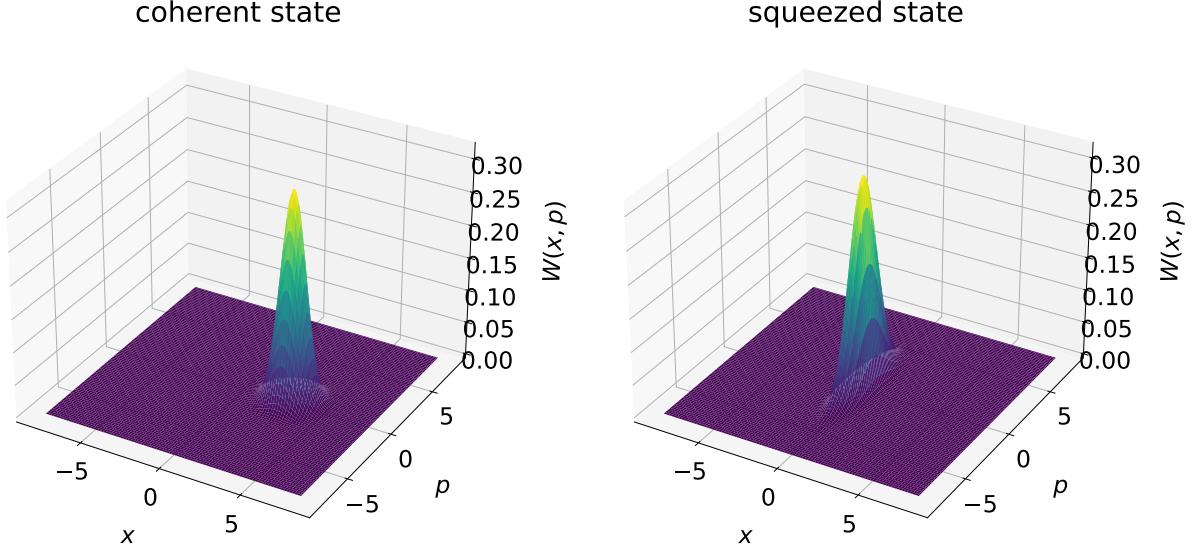


FIG. 3. Wigner functions

#### D. Examples

First, let us consider the Wigner function for a coherent state. You know already that

$$\psi_{\text{coh}}(x) = \langle x | \alpha \rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-|\alpha|^2/2} e^{z^2/2} e^{-(z-\alpha/\sqrt{2})^2} \quad (98)$$

with  $z = \sqrt{\frac{m\omega}{\hbar}}x$ . This expression can be used to obtain the integrand in (97). Then, the integral can be computed explicitly (they are gaussian integrals!). Finally,

$$W(x, p) = \frac{1}{\pi\hbar} e^{-\frac{m\omega}{\hbar}(x-\tilde{\alpha})^2} e^{-p^2/m\omega\hbar} \quad (99)$$

with  $\tilde{\alpha} = \sqrt{\frac{2\hbar}{m\omega}}\alpha$ . You can see a plot for the Wigner function for a coherent state in the Fig. 3. Well, from the formula it is clear that we will obtain a gaussian distribution (i.e. positive) which can be considered a classical probability distribution (normalized and positive). This is another way of understanding the mantra saying that "coherent states are the more classical states". Besides, from the Wigner function you can also check the fact that they are "minimum uncertainty" Gaussian wavepackets. In fact, you know that in Gaussian distributions you can define the variance, that from (99)

$$\Delta x = \frac{1}{m\omega} \Delta p \sim \hbar / \sqrt{m\omega} \quad (100)$$

With everything you know about squeezed states, it should not be difficult to calculate their Wigner function. In fact, the squeezing operator  $S$  rescales the position. Thus knowing the  $W_{\text{coh}}$  we obtain that

$$W_{\text{sq}} = W_{\text{coh}}(e^\xi x, e^{-\xi} p) \quad (101)$$

such that,

$$\Delta x \rightarrow e^{-\xi} \Delta x \quad \Delta p \rightarrow e^\xi \Delta p \quad (102)$$

See figure 3 for an example.

So far, the Wigner functions discussed were gaussian functions (positive ones). Classical, let us say. In order to feel the quantumness of states we can compute the Wigner function for Fock states. The explicit calculation is done in [7, Sect. 4.1.3] and we do not repeat here. The final expression is given by,

$$W_n(x, p) = \frac{(-1)^n}{\pi\hbar} e^{-2\eta(x, p)} L_n[4\eta(x, p)] \quad (103)$$

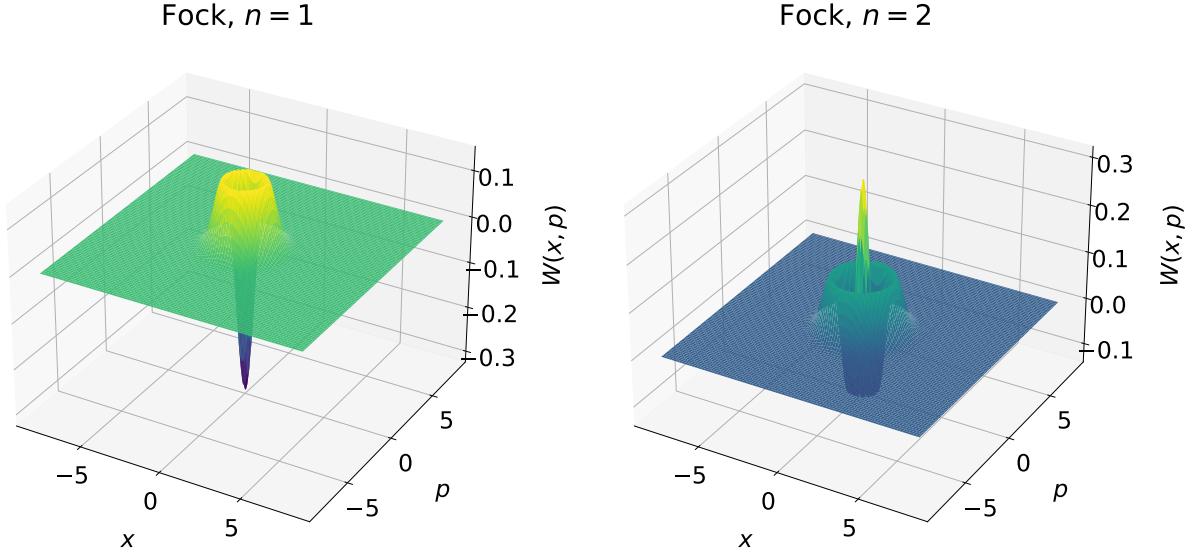


FIG. 4. Wigner functions

Here,  $\eta(x, p) = 1/\hbar\Omega(p^2/2m + \frac{1}{2}m\omega^2x^2)$  (the normalized energy functional) and  $L_n$  is the Laguerre polynomial. Examples for the  $n = 1$  and  $n = 2$  are plotted in Fig. 4. As you can see, they are non positive, which is typically linked to "quantumness".

Finally, let us compute the Wigner function for a cat state,

$$|\pm\rangle = \frac{1}{\sqrt{1 \pm e^{-2\alpha^2}}}(|\alpha\rangle \pm |-\alpha\rangle) \quad (104)$$

In this case, the Wigner function is given by (not normalized)

$$W_{\text{cat}} \sim W_{\text{coh}, \alpha} + W_{\text{coh}, -\alpha} + 2e^{-\frac{m\omega}{\hbar}(x)^2} e^{-p^2/m\omega\hbar} \cos(2\tilde{\alpha}p) \quad (105)$$

The last term  $\sim \cos$  is non positive and gives the interference term. This is a way of visualizing the coherences in a quantum superposition. Figure 5 shows this Wigner function. We can see that between the two Gaussian distributions centered at  $\pm\tilde{\alpha}$  there are the interference terms.

### E. Other distributions

## V. SPONTANEOUS EMISSION

We have found the light-matter Hamiltonian. We have discussed the quantization of light. Therefore, both matter and light are quantum now!. Now, we are going to solve the light-matter interaction Hamiltonian in a very particular (but paradigmatic) situation. We want to estimate the spontaneous emission, *i.e.* the process by which an excited atom emits light (photons). This process, together with absorption, are basic processes, see figure 6.

For this, we will think of the atom (or molecule) as a dipole in free space. This is a typical situation, a dipole coupled to the EM field. Although simple, we need to manipulate the Hamiltonian (55) a bit. We remind that (55) is written in the Coulomb gauge and that we can work in a different one. Why? In this example, we are dealing with dipoles, and dipoles interact with the electric field,  $\mathbf{d} \cdot \mathbf{E}$ . Therefore, what we want is for the electric field to appear explicitly. But before going to the actual calculations, being that what we are dealing with is an atom, we can think that the vector potential will be constant along the atom, thus  $\mathbf{A}(\mathbf{r}) \cong \mathbf{A}$ . A Gauge transformation,

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla\chi \quad (106a)$$

$$\phi \rightarrow \phi - \partial_t\chi \quad (106b)$$

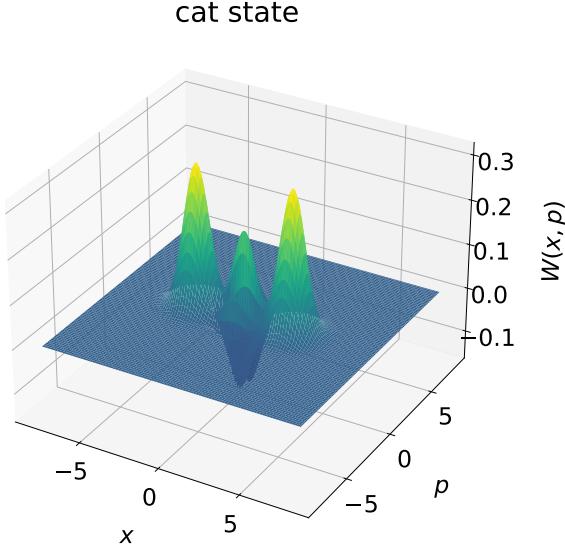


FIG. 5. Wigner functions

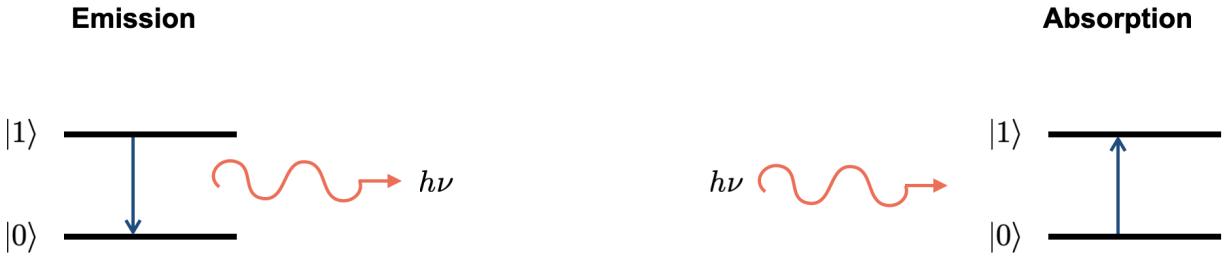


FIG. 6. Emission and Absorption processes

If we choose,  $\chi = -\mathbf{r}\mathbf{A}$ , thus [See. EQ. (75b)]

$$A \rightarrow 0 \quad (107a)$$

$$\phi \rightarrow \phi - \mathbf{r}\mathbf{E} \quad (107b)$$

Then, the light matter Hamiltonian can be written as,

$$H = H_0 - \mathbf{d} \cdot \mathbf{E} \quad (108)$$

with  $H_0$  the atomic Hamiltonian. Using, (81) and (75b) we have the quantized version for the electric field:

$$\mathbf{E} = \frac{-i}{\sqrt{L^3}} \sum_k \sqrt{\frac{\hbar\omega_k}{2\epsilon_0}} \mathbf{u}_k (a_k e^{i\mathbf{k}\mathbf{r}} + a_{-k} e^{-i\mathbf{k}\mathbf{r}}) \quad (109)$$

Now, we need to discuss the "atomic part" of the Hamiltonian. As you can expect, we are going to make some simplifications. First, the atom will be described by two levels, say the ground state and the first excited state,

$$H_0|\phi_j\rangle = \epsilon_j |\phi_j\rangle \quad (110)$$

The level splitting is  $\Delta = \epsilon_1 - \epsilon_0$ . You can write  $|0\rangle \equiv |\phi_0\rangle$  and  $|1\rangle \equiv |\phi_1\rangle$ , i.e. the atom is a qubit! Typically, the atomic potential is a central one and invariant under  $\mathbf{r} \rightarrow -\mathbf{r}$ . Therefore, the wave functions have a well-defined parity. Since  $\mathbf{r}$  is an odd function of  $\mathbf{r}$  we will have  $\langle \phi_j | \mathbf{r} | \phi_j \rangle = 0$  and  $|d| \equiv e \langle 0 | \mathbf{r} | 1 \rangle$ . Therefore, within this two-level

description (110) can be written (by inserting (75b)),

$$H = -\hbar \frac{\Delta}{2} \sigma^z + \hbar \sum_k \omega_k a_k^\dagger a_k + \hbar \sum_k \lambda_k \sigma^x (a_k + a_k^\dagger) \quad (111)$$

with,

$$\hbar \lambda_k = |d| \frac{-i}{\sqrt{L^3}} \sqrt{\frac{\hbar \omega_k}{2\epsilon_0}} \hat{z} \cdot \mathbf{u}_k \quad (112)$$

Here, w.l.o.g. we have assumed that  $\mathbf{d} \sim \hat{z}$ : we are in free space, so we can fix the axes at convenience.

Now, another simplification will be made, and it won't be the last! Disclaimer: Physics is the art of doing (good) approximations. At the end of this chapter, we will see that light-matter coupling is "weak". Thus, in some sense, the last term above can be considered in a perturbative fashion. Besides, the interaction is more important at resonance, *i.e.* for those photons fulfilling  $\omega_k \cong \Delta$ . Therefore, terms like  $\sigma^+ a_k^\dagger$  contribute in higher perturbation order than  $\sigma^- a_k^\dagger$ . This is the so-called Rotating Wave Approximation (RWA). Within it, the Hamiltonian is approximated by,

$$H = -\hbar \frac{\Delta}{2} \sigma^z + \hbar \sum_k \omega_k a_k^\dagger a_k + \hbar \sum_k \lambda_k (\sigma^+ a_k + \sigma^- a_k^\dagger) \quad (113)$$

This is a crucial simplification, since (now) the Hamiltonian is number conserving. *I.e.* the sum of excitations in the EM field and atom are conserved. Obviously, the first two terms conserve the number of excitations while (now) the third term also conserves the total number since one term creates a photon but annihilates one atomic excitation  $\sigma^- a_k^\dagger$  (emission), the other,  $\sigma^+ a_k$ , does the opposite. These two terms are represented graphically in Fig. (6). Moreover, it can be solved. Since the total number of excitations is conserved we can write an *ansatz* for the wave function in the case of a single excitation,

$$|\psi(t)\rangle = \beta |1; 0_k\rangle + \sum_k \beta_k |0; 1_k\rangle. \quad (114)$$

Here,  $0_k$  means zero photons and  $1_k$  is one  $k$ -photon. Notice that  $|\psi(t)\rangle$  is indeed in the subspace of one excitation. In the first term, the excitation is in the atom, while in the second term the excitation is in the photon  $k$  (each of the summands). With this ansatz, we can solve the Schrödinger equation. The time evolution for the  $\beta$  and  $\beta_k$  coefficients is,

$$\dot{\beta} = -i\Delta\beta - i \sum_k \lambda_k \beta_k \quad (115a)$$

$$\dot{\beta}_k = -i\omega_k \beta_k - i\lambda_k \beta \quad (115b)$$

It is a good idea to move to the rotating frame,

$$\beta \rightarrow \bar{\beta} = \beta e^{i\Delta t} \quad \beta_k \rightarrow \bar{\beta}_k = \beta_k e^{i\Delta t} \quad (116)$$

In this frame, the equations read (I eliminate the  $^-$  in the new variables, to alleviate the notation),

$$\dot{\beta} = -i \sum_k \lambda_k \beta_k \quad (117a)$$

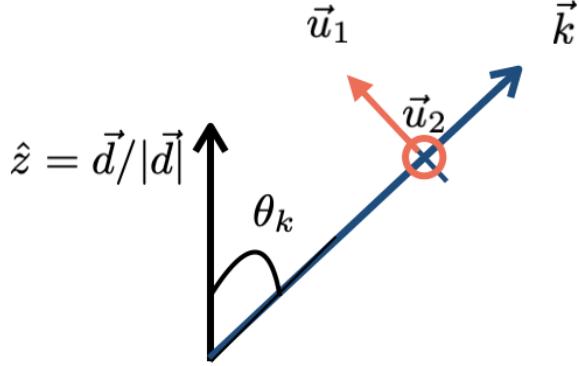
$$\dot{\beta}_k = -i(\omega_k - \Delta) \beta_k - i\lambda_k \beta \quad (117b)$$

This is a set of coupled linear equations, that can be solved (in principle and with the corresponding discretization for the field modes) in a computer. However, we are going to develop a series of tricks to find an analytical solutions for it. The idea is to integrate the solution for the  $\beta_k$  in the equation for  $\dot{\beta}$  and solve it. The solution for (117b) is

$$\beta_k(t) = \beta_k(0) e^{i(\omega_k - \Delta)t} - i\lambda_k \int_0^t d\tau e^{i(\omega_k - \Delta)(t-\tau)} \beta(\tau) \quad (118)$$

We are discussing spontaneous emission, therefore (at the beginning) the excitation is in the atom, *i.e.*

$$|\psi(0)\rangle = |1; 0_k\rangle \quad (119)$$

FIG. 7. graphical representation for  $\hat{z} \cdot \mathbf{u}_k$ .

i.e.  $\beta(0) = 1$  and  $\beta_k(0) = 0$ . Thus,

$$\dot{\beta} = - \sum_k \lambda_k^2 \int_0^t d\tau e^{i(\omega_k - \Delta)(t-\tau)} \beta(\tau) \quad (120)$$

Let's take a break and discuss what we have achieved. After our simplifications (RWA and TLS) we have obtained a simple enough Hamiltonian to solve it. In particular, we have been able to write the form of the wave function (single excitation subspace) and thus we have obtained a set of linear equations. In order to solve it analytically we have transformed it into a single equation for  $\beta$ , the price we have paid for this "reduction" is that the equation is now integrodifferential.

Now, we are going to develop several tricks to solve (120). First, it is convenient to write the  $k$ -sum as an integral with the help of the density of states,

$$\sum_k \rightarrow \int d^3k D(k) = \frac{V}{(2\pi)^3} \int dk d\Omega k^2 = \frac{V}{(2\pi)^3} \frac{1}{c^3} \int d\omega d\Omega \omega^2 \quad (121)$$

Here, we have used that for 3D  $D(k) = V/(2\pi)^3$  and  $d^3k = dk d\Omega k^2$ ,  $d\Omega = d\phi \sin(\theta) d\theta$  is the solid angle. Looking at (112), the term  $\hat{z} \cdot \mathbf{u}_k$  depends on the solid angle, see figure 7. In fact,

$$\hat{z} \cdot \mathbf{u}_k = \sin(\theta_k) . \quad (122)$$

Therefore,

$$\sum_k \lambda_k^2 \frac{1}{\hbar^2} \frac{V}{(2\pi)^3} \frac{1}{c^3} |d|^2 \frac{1}{L^3} \frac{\hbar}{2\epsilon_0} \int d\omega \omega^2 \int d\phi d\theta \sin^3 \theta \quad (123)$$

Notice that  $\int d\omega \omega^2 \int d\phi d\theta \sin^3 \theta = 8\pi/3$ .

Now, we perform the, so-called, Markovian approximation. This means that we are going to eliminate the memory

$$\int_0^t d\tau e^{i(\omega_k - \Delta)(t-\tau)} \beta(\tau) = \int_0^t d\tau e^{i(\omega_k - \Delta)(\tau)} \beta(t - \tau) \cong \int_0^\infty d\tau e^{i(\omega_k - \Delta)(\tau)} \beta(t) \quad (124)$$

It turns out that,

$$\int_0^\infty d\tau e^{i(\omega_k - \Delta)(\tau)} = \pi\delta(\omega - \Delta) - iP\left(\frac{1}{\omega - \Delta}\right) \quad (125)$$

wit  $P()$  means principal part. Here, we will no comment on the contribution of the principal part (it goes with the imaginary part and contributes to a shift in the frequency, *i.e.* the Lamb shift). In this case, we are interested in the real contribution. Therefore the equation for  $\beta$  (120) yields,

$$\dot{\beta} = -\frac{\Gamma}{2}\beta \rightarrow P_e = \langle \psi(t)|1\rangle\langle 1|\psi(t)\rangle = |\beta(t)|^2 = e^{-\Gamma t} \quad (126)$$

with,

$$\Gamma = 2 \frac{8}{3} \alpha \frac{\Delta^2 |\mathbf{r}|^2}{c^2} \Delta \quad (127)$$

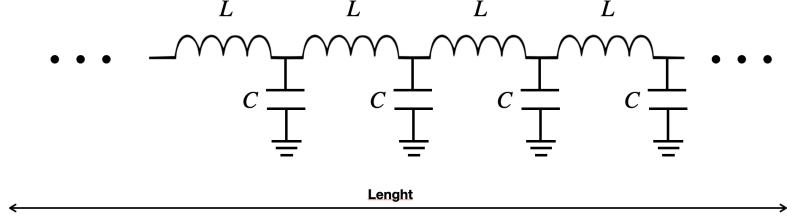
Here,

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \quad (128)$$

is the Fine-structure constant,  $\alpha \cong 1/137$  is a small number. This explains that  $\Gamma$  is "small", so it is the light-matter coupling, typically. Some numbers. As always to tell if something is small, we need to make it dimensionless. To do this, let's consider  $\Gamma/\Delta$  *i.e.*, the rate compared to the frequency of the atom. Thus,  $\Gamma/\Delta \sim \alpha \frac{\Delta^2 |\mathbf{r}|^2}{c^2}$ . Therefore, the rate is nothing more than the ratio between the emission frequency and the "associated frequency" of the dipole  $\omega_{dipole} \equiv |\mathbf{r}|/c$ . Take the hydrogen atom,  $|\mathbf{r}| \sim \text{\AA}$ , while  $\Delta/c \sim 10^3$  nm. Also, this is weighted by the small number,  $\alpha$ . So it is small, yes.

## VI. EXERCISES

1. Consider the circuit "LC-chain": write the Kirchoff equations for the flux variables. Find the associated La-



grangian and Hamiltonian.

2. Make a plot of your favorite Wigner function.
3. Using the Maxwell equations write the quantum expression for the magnetic and electric fields (for the electric field we have already given the expression in Eq. (109), you must justify it).
4. Rabi oscillations. For simplicity, let us consider a spin  $s = 1/2$  in a (classical and time-dependent) magnetic field. The Pauli Hamiltonian and its Zeeman term, Eq. (55) says that the Hamiltonian dictating the dynamics is given by ( $\hbar = 1$  below),

$$H = -\frac{\Delta}{2}\sigma_z - \lambda \cos(\omega t)\sigma_x \quad (129)$$

In matrix form

$$H = - \begin{pmatrix} \Delta/2 & \lambda \cos(\omega t) \\ \lambda \cos(\omega t) & -\Delta/2 \end{pmatrix} \longrightarrow H = - \begin{pmatrix} 0 & \lambda \cos(\omega t) \\ \lambda \cos(\omega t) & -\Delta \end{pmatrix} \quad (130)$$

In the second expression we shift the zero of energy (without physical consequences) Write the wave function as,

$$|\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \quad (131)$$

Write the e.o.m for  $c_0$  and  $c_1$ . Moving to a rotating frame  $\hat{c}_1 = c_1 e^{i\Delta t}$  and using the Rotating Wave approximation show that ,

$$\dot{c}_0 = -i \frac{\lambda}{2} e^{i(\omega-\Delta)t} \hat{c}_1 \quad (132a)$$

$$\dot{\hat{c}}_1 = -i \frac{\lambda}{2} e^{-i(\omega-\Delta)t} c_0 \quad (132b)$$

Take the time derivative in the second equation and write the equation in terms of  $\hat{c}_1$ . Find that,

$$\ddot{\hat{c}}_1 + i\delta \dot{\hat{c}}_1 + \frac{\lambda^2}{4} c_1 = 0 \quad (133)$$

with  $\delta = \omega - \Delta$ . Solve it and find that if  $c_0(0) = 1$ ,  $c_1(0) = 0$ , i.e. the atom starts at the ground state the probability for the excited state is given by,

$$|P_1|^2 = |c_1|^2 = \frac{\lambda^2}{2\Omega_R} \sin^2(\Omega_R t) \quad (134)$$

with

$$\Omega_R = \frac{1}{2} \sqrt{\delta^2 + \lambda^2} \quad (135)$$

This is the Rabi frequency. Finally, plot  $|P_1|^2$  as a function of  $\delta$  and  $\lambda$ .

5. Solve numerically (129). Compare the numerical simulations with the analytical treatment done in the previous example (do it at resonance,  $\delta = 0$ , and out of resonance  $\delta \neq 0$ ).
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