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# The Feynman path integral, from the harmonic oscillator to quantum electrodynamics

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## ABSTRACT

The Feynman path-integral formulation of quantum mechanics is developed. The mathematical framework is worked out from Schrödinger's equation, illustrating the compatibility of the two formulations. We introduce the sum over all paths, known as the kernel $K$, and discuss its implications for events occurring in succession. We compute the kernel for quadratic Lagrangians. Then, making use of imaginary time, we consider the discrete version of the kernel, known as the Euclidean path integral, and use it to solve the (quantum) harmonic and anharmonic oscillators through numerical Monte Carlo simulations. Lastly, we use the framework to quantize the electromagnetic field, as a motivation to discuss perturbation theory via Feynman diagrams.



**Keywords**: Feynman's integral. Quantum mechanics. Numerical simulations. Monte Carlo methods. Quantum electrodynamics

## CONTENTS

# 1 INTRODUCTION

In the usual formulation of non-relativistic quantum mechanics, the state of a system is described by a complex wave function $\Psi(\boldsymbol{r}_b, t_b)$. It is a postulate that the probability density to find the particle in position $\boldsymbol{r}_b$ at a time $t_b$ is given by $|\Psi(\boldsymbol{r}_b, t_b)|^2$. (1) These wave functions are elements of the Hilbert space, a complete vector space with an inner product, which we define as $\int \Phi^*(\boldsymbol{r}_b, t_b)\, \Psi(\boldsymbol{r}_b, t_b)\, d^3\boldsymbol{r}_b$. Since $\Psi$ is associated with a probability we also demand that it be normalized, $\int |\Psi|^2\, d^3\boldsymbol{r}_b = 1$. In this formulation the observable quantities are represented by Hermitian operators (i.e., let $\hat{\mathbf{O}}$ represent an observable, then $\hat{\mathbf{O}}^\dagger \equiv (\hat{\mathbf{O}}^T)^* = \hat{\mathbf{O}}$). These operators have a set of real eigenvalues $\lambda_n$ that correspond to the possible values that a measurement of $\hat{\mathbf{O}}$ can take. Each $\lambda_n$ correspond to an eigenfunction $u_n(\boldsymbol{r})$ of $\hat{\mathbf{O}}$, with these forming a complete set of orthonormal functions, that is $\int u_n\, u_{n'}\, d^3\boldsymbol{r}_b = \delta_{nn'}$, where $\delta_{nn'}$ is the Kronecker delta. The probability of occurrence of an eigenvalue $\lambda_n$ is given by the absolute value of the coefficient $c_n$, the projection of the state $\Psi$ onto the corresponding eigenfunction $c_n = \int u_n^*\, \Psi\, d^3\boldsymbol{r}_b$. Time evolution of the system is given by Schrödinger's wave equation

$$\hat{\boldsymbol{\mathcal{H}}}\, \Psi(\boldsymbol{r}_b, t) = -\frac{\hbar^2}{2m}\, \nabla^2 \Psi(\boldsymbol{r}_b, t) \,+\, V(\boldsymbol{r}_b, t)\, \Psi(\boldsymbol{r}_b, t) = i\hbar\, \frac{\partial \Psi(\boldsymbol{r}_b, t)}{\partial t}, \tag{1.1}$$

where $\hbar$ is the Planck constant and $\hat{\boldsymbol{\mathcal{H}}}$ is the Hamiltonian operator for the system. When the potential is time-independent we can separate the solution of this equation in a temporal part given by $\exp(-i\, E_n\, t_b/\hbar)$, where $E_n$ is identified as the constant energy of the system, and a corresponding spatial part, which is a solution of Schrödinger's time independent equation

$$\hat{\boldsymbol{\mathcal{H}}}\, u_n(\boldsymbol{r}_b) = -\frac{\hbar^2}{2m}\, \nabla^2 u_n(\boldsymbol{r}_b) \,+\, V(\boldsymbol{r}_b)\, u_n(\boldsymbol{r}_b) = E_n\, u_n(\boldsymbol{r}_b), \tag{1.2}$$

where the stationary states $u_n$ are the eigenfunctions of $\hat{\boldsymbol{\mathcal{H}}}$. From the properties of the eigenfunctions discussed above, we know that any linear combination of the product $u_n(\boldsymbol{r})\, \exp(-i\, E_n\, t_b/\hbar)$ is also a solution of Eq. (1.1). So, the general form of $\Psi$ can be written as

$$\Psi(\boldsymbol{r}_b, t) = \sum_n c_n\, u_n(\boldsymbol{r}_b)\, \exp\left(-i\, E_n\, t_b/\hbar\right), \tag{1.3}$$

where the coefficients $c_n$ can be obtained from the initial state $\Psi(\boldsymbol{r}_a, t_a)$, by projecting it onto each $u_n$

$$c_n = \int_{-\infty}^{+\infty} u_n^*(\boldsymbol{r}_a)\, \Psi(\boldsymbol{r}_a, t_a)\, d^3\boldsymbol{r}_a. \tag{1.4}$$

We can associate each function $\Psi$ to a vector $|\Psi\rangle$ called *ket*. In the same way, we define a *bra* $\langle\Psi|$ associated with $\Psi^*$ in such a way that its action on $|\Psi\rangle$ is the inner product $\langle\Psi|\Phi\rangle$

as was defined above. Using the fact that the eigenstates of the space operator $\hat{\boldsymbol{r}}$ are Dirac delta functions,* we see that the wave function is the projection of the state $|\Psi\rangle$ on the basis of coordinates $u_{\boldsymbol{r}_b}$, i.e., $\langle u_{\boldsymbol{r}_b}|\Psi\rangle = \int \delta^3(\boldsymbol{r}_b)\,\Psi(\boldsymbol{r},t_b)\,d^3\boldsymbol{r} = \Psi(\boldsymbol{r}_b,t_b)$, as expected.†.

The path-integral formulation offers an alternative way to obtain expectation values of measurements, and a more general framework to interpret the statistical nature of the evolution of a quantum system. This formulation was worked out by Richard Feynman in 1948, using the Lagrangian function $L$ of the system instead of its Hamiltonian. In Feynman's formulation, we deal with all the possible paths that a system can take to evolve from an initial configuration $(\boldsymbol{r}_a,t_a)$ to a final one $(\boldsymbol{r}_b,t_b)$. To each path $i$ we associate an amplitude $\phi_i$, with the total amplitude for the evolution, $K$, being the sum of the amplitudes for all the , paths(2)

$$K(\boldsymbol{r}_b,t_b,\boldsymbol{r}_a,t_a) = \sum_{\text{all paths}} \phi_i, \tag{1.5}$$

referred to as the *path integral*. With this in mind, we present the Feynman formulation of quantum mechanics, with this monograph being divided in the following way: in Chapter 2 we develop, from the Schrödinger picture, Feynman's theory of quantum mechanics, showing how to formulate the sum over all paths in Eq. (1.5). We also present a theorem concerning quadratic Lagrangians and show how to compute path integrals numerically. In Chapter 3, we make use of the theory and present results for the harmonic and anharmonic oscillators. We use numerical Monte Carlo simulations, for which we developed our own computer codes. In Chapter 4 we describe the method to study the quantum electrodynamics of non-relativistic electrons, using it as a motivation to present the perturbation theory in the path-integral formulation. Finally, we present some conclusions in Chapter 5.

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* That is, $\hat{\boldsymbol{r}}\,u_{\boldsymbol{r}} = \boldsymbol{r}u_{\boldsymbol{r}} \rightarrow u_{\boldsymbol{r}} = \delta^3(\boldsymbol{r})$. These space eigenstates cannot be normalized in the same way as done before. Instead, they are *Dirac normalized*, i.e., $\langle u_{\boldsymbol{r}}|u_{\boldsymbol{r}'}\rangle = \delta^3(\boldsymbol{r}-\boldsymbol{r}')$. The momentum eigenfunctions, defined by $\hat{\mathbf{p}}\,u_{\mathbf{p}'} = \mathbf{p}'u_{\mathbf{p}'}$ also follow this same rule. Note that eigenvalues of these two operators are contained in the continuum.

† In fact, as said, each operator $\hat{\mathbf{O}}$ has a complete set of eigenstates, defined by $\hat{\mathbf{O}}\,u_n = \lambda_n\,u_n$. Being this set complete we can also represent $|\Psi\rangle$ in this basis. This is done by the projection operation $|\Psi\rangle = \sum_n |u_n\rangle\langle u_n|\Psi\rangle$. The two sides of the last equation are equal only if $\sum_n |u_n\rangle\langle u_n| = 1$. We call this the completeness relation. To eigenstates with a continuum spectrum of eigenvalues, as momentum and position, the sum must be replaced by an integral.

# 2 THE FEYNMAN FORMULATION FOR THE KERNEL

The evolution of a quantum system is obtained from the solution of Eq. (1.1). At this stage, we will restrict ourselves to one particle in one spatial dimension. As we shall see, the generalization of the results will be immediate. For time-independent potentials we know that the state evolves as given in Eq. (1.3). Replacing the coefficients $c_n$ in Eq. (1.3) using Eq. (1.4) we have that the state is

$$\begin{aligned}\Psi(x_b,t_b) &= \int_{-\infty}^{+\infty}\left\{\sum_{n=0}^{\infty} u_n^*(x_a)u_n(x_b)\exp\left[-i\frac{E_n}{\hbar}(t_b-t_a)\right]\right\}\Psi(x_a,t_a)\,dx_a \\ &= \int_{-\infty}^{+\infty} K(x_b,t_b,x_a,t_a)\Psi(x_a,t_a)dx_a,\end{aligned} \tag{2.1}$$

where we have defined

$$K(x_b,t_b,x_a,t_a) = \begin{cases}\sum\limits_{n=0}^{\infty} u_n^*(x_a)u_n(x_b)\exp\left[-iE_n(t_b-t_a)/\hbar\right] & \text{if } t_b > t_a, \\ 0 & \text{if } t_b < t_a.\end{cases} \tag{2.2}$$

We shall refer to the term $K(x_b,t_b,x_a,t_a)$ as the kernel. From Eq. (2.1) it is clear that this term is responsible for the propagation of the system state from the initial configuration at $\Psi(x_a,t_a)$ to the final one, $\Psi(x_b,t_b)$. We can identify a completeness relation in the expression of Eq. (2.2) (assuming $t_b > t_a$)

$$K(x_b,t_b,x_a,t_a) = \langle u_{x_b}|\sum_{n=0}^{\infty}|u_n\rangle\langle u_n|\exp\left[-i\frac{\hat{\boldsymbol{\mathcal{H}}}}{\hbar}(t_b-t_a)\right]|u_{x_a}\rangle, \tag{2.3}$$

so

$$K(x_b,t_b,x_a,t_a) = \langle u_{x_b}|\exp\left[-i\frac{\hat{\boldsymbol{\mathcal{H}}}}{\hbar}(t_b-t_a)\right]|u_{x_a}\rangle. \tag{2.4}$$

Therefore, the function $|K(x_b,t_b,x_a,t_a)|^2$ gives us the probability of transition between the final and initial configuration, being this the fundamental interpretation for $K$ in Chapter 1. For this reason we will use this term to construct Feynman's formulation from the usual operator one.

### 2.0.1 The sum over all paths

The exponential of Eq. (2.4) has the composition property, so we can divide the time interval $T = (t_b - t_a)$ in $N$ steps. So we discretize our time variable in equally spaced $t_j$'s, i.e., $t_j = j\Delta t$, with $j \in \mathbb{Z}$ and $\Delta t = T/N$. In the limit of a large number of partitions we have, at each time step, the amplitude $\exp(-i\,\Delta t\,\hat{\mathbf{p}}_j^2/2m\hbar)\exp(-i\,\Delta t\,V(\hat{\mathbf{x}}_j)/\hbar)$, where $\hat{\mathbf{x}}_j$ and $\hat{\mathbf{p}}_j$ are the position and momentum operators at this instant of time. Including

the completeness relations for these operators at each time step we have

$$K(x_b,t_b,x_a,t_a)=\langle u_{x_b}|\left[\int\prod_{j=0}^{N}e^{-\frac{i\Delta t\,p_j^2}{2m\hbar}}e^{-\frac{i\Delta t\,V(x_j)}{\hbar}}|u_{x_j}\rangle\langle u_{x_j}|u_{p_j}\rangle\langle u_{p_j}|\,dx_j\frac{dp_j}{2\pi\hbar}\right]|u_{x_a}\rangle. \quad (2.5)$$

In the above expression, the operators have already acted on the states, living us with numbers to work with. This is one of the great advantages of Feynman's formulation. Note that the terms inside the brackets repeat $N+1$ times, so we call the individual cell at a specific $j$ as $T_j$ and deal with it. Inserting the position representation of the momentum eigenstates $\langle u_{x_j}|u_{p_j}\rangle=\exp\left(ip_jx_j/\hbar\right)$ (1) we have

$$T_j=\int_{-\infty}^{+\infty}\exp\left[-i\frac{\Delta t}{\hbar}\frac{p_j^2}{2m}-i\frac{\Delta t}{\hbar}V(x_{j-1})+i\frac{p_j(x_j-x_{j-1})}{\hbar}\right]dx_j\,\frac{dp_j}{2\pi\hbar}. \quad (2.6)$$

Now we want to isolate the coordinate variables by computing the momentum integrals. To do this, we shall do an analytic continuation by taking the complex-time $\tau_j=it_j$. This change of variable reduces the complex integral in Eq. (2.6) to a Gaussian one. However, $\tau$ is a complex variable so, by this change of coordinate, we have abandoned the physical time. Now we can calculate the momentum integral

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\exp\left\{\frac{-\Delta\tau}{\hbar}\left[\frac{p_j^2}{2m}-ip_j\left(\frac{x_j-x_{j-1}}{\Delta\tau}\right)\right]\right\}dp_j=\sqrt{\frac{m}{2\pi\hbar\Delta\tau}}\exp\left[-\frac{m\Delta\tau}{2\hbar}\left(\frac{x_j-x_{j-1}}{\Delta\tau}\right)^2\right]. \quad (2.7)$$

Replacing this result in Eq. (2.6) and returning to real-time, we have that the cell $T_j$ is

$$T_j=\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{1/2}\int_{-\infty}^{+\infty}\exp\left\{\frac{-i\Delta t}{\hbar}\left[\frac{m}{2}\left(\frac{x_j-x_{j-1}}{i\Delta t}\right)^2+V(x_{j-1})\right]\right\}dx_j. \quad (2.8)$$

Now we can use the obtained value for each cell and write Eq. (2.5) as

$$K=\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2}\int_{-\infty}^{+\infty}\exp\left\{\frac{i\Delta t}{\hbar}\sum_{j=1}^{N}\left[\frac{m}{2}\left(\frac{x_j-x_{j-1}}{\Delta t}\right)^2-V(x_{j-1})\right]\right\}dx_{N-1}dx_{N-2}\ldots dx_1. \quad (2.9)$$

Note that our time discretization has created a natural space discretization, with the system evolution being described on a space-time lattice. Furthermore, we can recognize a discrete Lagrangian function being calculated in the lattice sites and being multiplied by a temporal increment, which characterizes a discrete version of the action integral

$$S[x(t)]=\int_{t_a}^{t_b}L(\dot{x},x;t)\,dt\approx\sum_{j=1}^{N}\left[\frac{m}{2}\left(\frac{x_j-x_{j-1}}{\Delta t}\right)^2-\frac{V(x_j)+V(x_{j-1})}{2}\right]\Delta t. \quad (2.10)$$

So, the trajectory of the particle is described by a collection of space-time points on this lattice. To reconstruct the continuum trajectory one can connect these points by straight lines, as shown in Figure 1. It is good to remember that this path is an arbitrary one, not necessarily the classical path, which is fixed by the condition $\delta S/\delta x(t)=0$. (3)

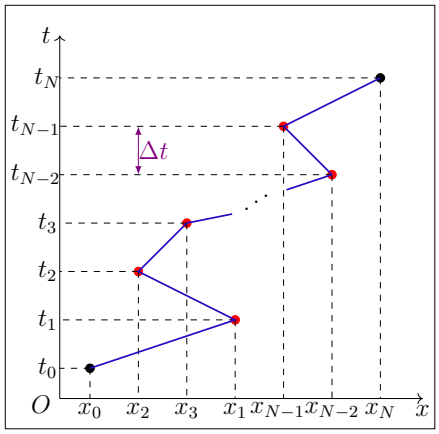


Figure 1 – Construction of a possible path on the space-time lattice.

Source: By the author.

So, we have found that the amplitude $\phi_i$ for the occurrence of a path $i$ is given by the complex exponential of the associated action in units of $\hbar$. (2) We consider all the possible paths by taking all the possible values that the $x_j$'s can assume, which is done by the integrals in Eq. (2.9). So we have found a way to calculate the sum over all the paths of Eq. (1.5). Of course, in a formal sense, the paths defined above cannot be real, due to the edges in the connections of the lattice points, as shown in Figure 1. This problem arises from the fact that we are trying to describe a continuous function (a possible path for the particle) with a finite number of points. This can be solved if we take the limit of an infinity number of partitions.

Then, we can define the kernel, or path integral, as (2)

$$\boxed{K(x_b,t_b,x_a,t_a)=\lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{N/2}\int_{-\infty}^{+\infty}\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}L(\dot{x}(t),x(t);t)\,dt\right)\,dx_{N-1}dx_{N-2}\ldots dx_1}. \tag{2.11}$$

We shall define the symbols

$$\frac{1}{A}\equiv\sqrt{\frac{m}{2\pi\hbar i\Delta t}},\quad\text{and}\quad\mathcal{D}x(t)=\lim_{N\to\infty}\frac{1}{A^N}dx_{N-1}dx_{N-2}\ldots dx_1. \tag{2.12}$$

With these definitions, we say that the amplitude for a system to evolve from an initial condition $(x_a,t_a)$, which we shall refer to as point $a$ on our lattice, to a final one $(x_b,t_b)$, point $b$, is given by the kernel $K(b,a)$, and computed by the sum over all paths, with each path being weighed by its associated action in units of $\hbar$. (2) We represent this as

$$\boxed{K(b,a)=\int_a^b\exp\left[\frac{iS[x(t)]}{\hbar}\right]\mathcal{D}x(t).} \tag{2.13}$$

Eq. (2.11) was obtained for time-independent potentials. However we shall extend this definition to the class of time-dependent potentials, $V(\boldsymbol{r},t)$, with the difference that, in

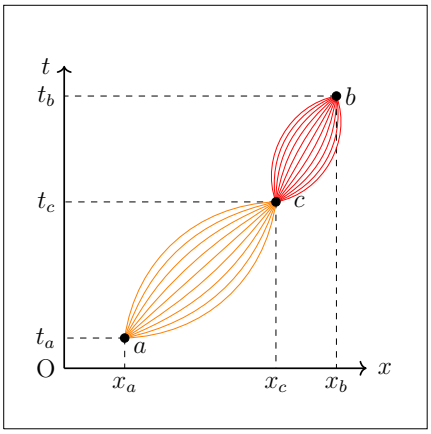


Figure 2 – Example of a transition between points $a$ and $b$ passing through point $c$.

Source: By the author.

this case, a global factor $1/A$ does not exist. Being the one responsible for the convergence of the Eq. (2.11), one must find an equivalent to it when dealing with path integrals of time-dependent potentials. Furthermore, as we saw, to describe the paths we only need to create a lattice in time and then integrate over all the possible values of the space coordinates at the lattice sites. This directs us to a natural generalization for three-dimensional systems, where the path $\boldsymbol{r}$ shall be described by its coordinates $t, x, y, z$. We keep all the process the same, but now our path differential is given by $\mathcal{D}x(t)\mathcal{D}y(t)\mathcal{D}z(t)$. (2)

Undoubtedly the formulation of Eq. (2.13) seems more complicated to work with than Schrödinger's one. However, the kernel formulation, besides its computation issues, has many positive points, with the most striking one being the intuition about the system that it is capable of providing. To illustrate this let us take an intermediary time $t_c$ in the evolution from an initial state $a$ to a final one $b$. Let the position of the particle at this instant be $x_c$. An algebraic manipulation of the terms shows that

$$K(b,a) = \int_{-\infty}^{+\infty} K(b,c)\, K(c,a)\, dx_c. \tag{2.14}$$

This important result shows that amplitudes for events occurring in succession in time must multiply. So, the amplitude to go from $a$ to $b$ is equal to the amplitude to go from $a$ to $c$, times the one to go from $c$ to $b$, in a very similar association rule as that for simple probabilities of two independently events.

We conclude, therefore, that the transitions are not associated, being discorrelationated events. Note that this result does not assume any particular property for the paths, since it was obtained passing through a particular space point $x_c$, but then we integrated over all the possibilities for $x_c$.

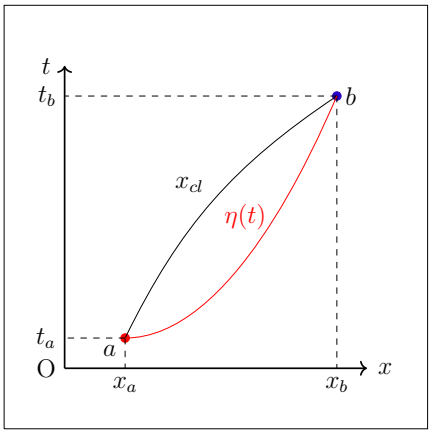


Figure 3 – Construction of an arbitrary path from the classical one and a virtual displacement from it.

Source: By the author.

### 2.0.2 A theorem concerning quadratic actions

Up to this point our results, although essential, are not useful for a concrete computation of the sum over all paths of Eq. (2.11). In fact, for the majority of the systems there is not a simple way to calculate the path integral. However, for the very important class of quadratic Lagrangians, there is a useful result providing us a systematic way to compute the kernel. Let us consider Lagrangians of the form

$$L(\dot{x}, x; t) = a(t)\dot{x}^2 + b(t)x^2 + c(t)x\dot{x} + d(t)\dot{x} + e(t)x + f(t), \tag{2.15}$$

where $a, b, c, d, e$ and $f$ are all well behaved functions of time. Now we describe the arbitrary path $x(t)$ as a combination of the classical one, $x_{cl}$ (which satisfies $\delta S/\delta x(t) = 0$), and a virtual displacement from it $\eta(t)$, (2) as shown in Figure 3. So, we have

$$x(t) = x_{cl}(t) + \eta(t) \quad \text{and} \quad \dot{x}(t) = \dot{x}_{cl}(t) + \dot{\eta}(t), \tag{2.16}$$

with the boundary conditions $\eta(t_a) = \eta(t_b) = 0$. By definition, the classical path is the one that, when shifted by an arbitrary function $\eta(t)$, keeps the action constant to first order in $\eta$. (3) Therefore, when we vary the path, we expect to see $\eta$ contributing in the action integral with only terms of order 2 and higher.

Moreover, the fact that the classical path is a fixed one implies that $\mathcal{D}x_{cl} = 0$. Then, when describing an arbitrary path $x$ by a sum of $x_{cl}$ and a virtual displacement $\eta$, we have that $\mathcal{D}x(t) = \mathcal{D}\eta(t)$. So we can describe all the paths by taking all the possible virtual displacements. We compute now the kernel for the Lagrangian of Eq. (2.15), splitting the path as in Eq. (2.16). Keeping terms to order 2 in $\eta$ we can write the total action as a sum of the action of the classical path, $S_{cl} = S[x_{cl}(t)]$, and a term that depends only on the square of $\eta$ (remembering that terms of first order in $\eta$ cause no changes in the action),

so

$$S[x(t)] = S_{cl} + \int_{t_a}^{t_b} \left[a(t)\dot{\eta}^2(t) + b(t)\eta^2(t) + c(t)\dot{\eta}(t)\eta(t)\right]\, dt, \tag{2.17}$$

which allows us to write the path integral in terms of the virtual displacement $\eta$ as

$$K(x_b, t_b, x_a, t_a) = e^{\frac{i}{\hbar}S_{cl}} \int_0^0 \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}\left(a(t)\dot{\eta}^2(t) + b(t)\eta^2(t) + c(t)\dot{\eta}(t)\eta(t)\right)\, dt\right] \mathcal{D}\eta(t), \tag{2.18}$$

where the term $\exp[iS_{cl}/\hbar]$ is a constant one. The limits of integration in the path integral for $\eta$ are remainders of the boundary conditions (the virtual displacement must vanish at the ends of the interval). Note that these conditions forbid any dependence on $\eta$ itself. So, the second path integral must be a function of only the times at the limits. (2) Calling this function of $F(t_b, t_a)$, we can write the path integral for quadratic Lagrangians as

$$K(x_b, t_b, x_a, t_b) = F(t_b, t_a) \exp\left[\frac{iS_{cl}}{\hbar}\right], \tag{2.19}$$

where

$$F(t_b, t_a) = \int_0^0 \mathcal{D}\eta(t) \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\left[a(t)\dot{\eta}^2(t) + b(t)\eta^2(t) + c(t)\dot{\eta}(t)\eta(t)\right]\, dt\right\}. \tag{2.20}$$

The result expressed in Eq. (2.19) says that, for quadratic Lagrangians, the amplitude for the evolution of the system between two points is dominated by the classical path between these points, with the non-classical paths contributing with a fluctuation term $F(t_b, t_a)$. (2) To work out the classical action one must solve the Euler-Lagrange equations of motion and obtain $x_{cl}$, then use this function to compute the action integral of Eq. (2.10). In other words, the exponential term in Eq. (2.19) can be completely known from classical mechanics. So, to determine the kernel we just need to carry out the computation of $F(t_b, t_a)$. Since $F$ is also given by a path integral, one could think that this work was done in vain. However, the fact that $\eta$ must vanish at the limits of the path makes this integral very special, allowing us to expand the virtual displacement function in a Fourier series in sines

$$\eta(t) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi t}{T}\right). \tag{2.21}$$

Each particular function $\eta$ would return us a particular set of coefficients $b_n$'s, so we can describe the paths by changing the variable of integration to these coefficients. We need to find the increase in the integration volume that is caused by this change. This can be done in a simple way by going to our space-time lattice. With time being a discrete variable that grows in equally spaced steps of $\Delta t$, we can write Eq. (2.21) in matrix form

$$\begin{pmatrix} \eta(t_1) \\ \vdots \\ \eta(t_N) \end{pmatrix} = \begin{pmatrix} \sin\left(\frac{\pi t_1}{T}\right) & \dots & \sin\left(\frac{N\pi t_1}{T}\right) \\ \vdots & \ddots & \vdots \\ \sin\left(\frac{\pi t_N}{T}\right) & \dots & \sin\left(\frac{N\pi t_N}{T}\right) \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix}. \tag{2.22}$$

The change in the volume of integration will be given by the absolute value of the determinant of the transformation matrix. However, note that this matrix is orthogonal, so its determinant is, in module, equal to 1. This fact allows us to calculate the fluctuation term of Eq. (2.20) with the Fourier coefficients of the series expansion. To illustrate the method we show the computation of the kernel for the free particle and the harmonic oscillator.

#### 2.0.2.1 Free particle

We start our examples with the free particle in one dimension. We need to calculate the path integral for the associated Lagrangian, which is quadratic. We make use of Eq. (2.19). The Lagrangian function and the associated action between the points $a$ and $b$ are

$$L(\dot{x}(t);t) = \frac{m\dot{x}^2(t)}{2} \quad \text{and} \quad S_{cl} = \frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a}. \tag{2.23}$$

Describing the virtual displacements by the Fourier expansion of Eq. (2.21) allows us to write $F$ as

$$\begin{aligned} F(t_b,t_a) &= \int_{-\infty}^{+\infty} \prod_{n=1}^{N-1} \exp\left[\frac{im}{2\hbar}\sum_{n,n'=1}^{N-1}\left(\frac{\pi}{T}\right)^2 nn' \int_{t_a}^{t_b} \sin\left(\frac{n\pi t}{T}\right)\sin\left(\frac{n'\pi t}{T}\right)dt\right] db_n, \\ &= \prod_{n=1}^{N-1}\int_{-\infty}^{+\infty} \exp\left[\frac{im}{2\hbar}\frac{T}{2}\left(\frac{\pi n}{T}\right)^2 b_n^2\right] db_n, \end{aligned} \tag{2.24}$$

which is just a product of Gaussian integrals. By computing the integrals and taking the limit of $N \to \infty$ we find that the kernel for the free particle in the evolution from a point $a$ to a point $b$, which we shall refer to as $K_F(b,a)$, is (2)

$$K_F(b,a) = K_F(x_b,t_b,x_a,t_a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}\exp\left[\frac{mi}{2\hbar}\frac{(x_b - x_a)^2}{t_b - t_a}\right]. \tag{2.25}$$

#### 2.0.2.2 Harmonic oscillator

Our second example is the harmonic oscillator. Its Lagrangian is

$$L(\dot{x}(t),x(t);t) = \frac{m\dot{x}^2(t)}{2} - \frac{m\omega^2 x^2(t)}{2}, \tag{2.26}$$

where $\omega$ is the frequence of the oscillator. Once more, this is a quadratic Lagrangian, so we can apply the method of Section 2.0.2. The procedure in this calculation is essentially the same as that of Section 2.0.2.1, with the final result being

$$F(t_b,t_a) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}, \tag{2.27}$$

where $T = t_b - t_a$. To completely determine the kernel we need also to know the classical action. This is done by solving the Euler-Lagrange equations and using the resulting

function to compute the action integral. After this calculation one finds that the kernel for the harmonic oscillator is

$$K(x_b,t_b,x_a,t_a)=\sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}\exp\left\{\frac{im\omega}{2\hbar\sin(\omega T)}\left[(x_b^2+x_a^2)\cos(\omega T)-2x_bx_a\right]\right\}. \tag{2.28}$$

In our work in Chapter 4, we are going to deal with harmonic oscillators that interact with an external field, that is, there exists a driving force $f(t)$. The Lagrangian for the system under the external force is

$$L(\dot{x}(t),x(t);t)=\frac{m\dot{x}^2(t)}{2}-\frac{m\omega^2x^2(t)}{2}+xf(t). \tag{2.29}$$

To know the quantum mechanics of this system we need to find its kernel. However, note that the driven term appears only in the first order in $x$, so it is effectless in the function $F$ of Eq. (2.27). For the kernel to be completely determined we only need to know the action of the classical driven harmonic oscillator. Once more this is a completely classical calculation (a much longer one in this case) and the final result is

$$\begin{aligned}K=&\sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}\exp\left\{\frac{im\omega}{2\hbar\sin(\omega T)}\left[(x_b^2+x_a^2)\cos(\omega T)-2x_bx_a+\frac{2x_b}{m\omega}\int_{t_a}^{t_b}f(t)\sin\omega(t-t_a)dt\right.\right.\\&\left.\left.+\frac{2x_a}{m\omega}\int_{t_a}^{t_b}f(t)\sin\omega(t_b-t)dt-\frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t}f(t)f(t')\sin\omega(t_b-t)\sin\omega(t'-t_a)dtdt'\right]\right\}.\end{aligned} \tag{2.30}$$

Result of Eq. (2.30) returns us the quantum mechanical evolution of the system for any driving force $f(t)$. It also shows us the utility of quadratic actions: once the driven term appeared just in order 1 in $x$ we already knew the function $F$ and all the computation was restriced to the action.

### 2.0.3 Euclidean path integrals

Analytical solutions are not always available in quantum mechanics in either of its formulations. This fact forces us to resort to numerical simulations. Feynman's formulation offers us an interesting way to deal with the problem numerically, based on the definition of Eq. (2.9). Let us rewrite this equation, making use of the complex time* $\tau_j=it_j$

$$K=\left(\frac{m}{2\pi\Delta\tau}\right)^{N/2}\int_{-\infty}^{+\infty}\exp\left\{\sum_{j=1}^{N}\left[\frac{m}{2\Delta\tau}\left(x_j-x_{j-1}\right)^2+\Delta\tau V(x_{j-1})\right]\right\}dx_{N-1}dx_{N-2}\ldots dx_1. \tag{2.31}$$

Analytical issues emerge when we take the limit of an infinite number of partitions. Note, however, that by staying with a finite number of divisions of the interval we find a discrete version of the kernel. In it, the path $x(t)$ is represented by a set of real numbers $x(t)=$

* As is common in numerical work, we adopt dimensionless variables, making $\hbar=1$. The dimensions can be recovered in the end

$\{x(t_0), x(t_1), \ldots, x(t_N)\}$ in the same sense of that of Figure 1. Nevertheless, it should be noted that the use of the complex-time is no longer just a trick for the calculation, it is now used to define the kernel. This use has some consequences, e.g., the change in the definition of the Lagrangian function† and the fact that time is no longer a physical variable, since that $\tau_j = it_j$ means that $\tau_j$ is a complex variable. We shall refer to the path integral of Eq. (2.31) as an Euclidean path integral. (4) Euclidean path integrals are very useful in numerical work, since they reduce quantum mechanics to a problem of numerical integration in $N-1$ dimensions, which can be done by Monte Carlo methods of integration. (5)

With the numerical approach, we can find the kernel. We can use this obtained kernel to compute other properties of the system. Lets us exemplify this by showing how to find the ground state. Returning to Eq. (2.4), now in the complex-time formalism, and inserting the completeness relation of the energy eigenstates ($\sum |u_n\rangle\langle u_n| = 1$) we find

$$K(x_b, \tau_b, x_a, \tau_a) = \langle u_{x_b}| \exp\left(-\tau \hat{\boldsymbol{\mathcal{H}}}\right) \sum_n |u_n\rangle\langle u_n|u_{x_a}\rangle, \tag{2.32}$$

where $\tau_a = i\,t_a$, $\tau_b = i\,t_b$ and $\tau = i\,T$. If we compute the kernel with the final and initial points of the interval being the same, $x_b = x_a$, the previous relation becomes

$$K(x_b, \tau_b, x_b, \tau_a) = \sum_n |u_n(x_b)|^2 \exp(-\tau E_n) \xrightarrow{\tau \text{ large}} |u_0(x_b)|^2 \exp(-\tau E_0). \tag{2.33}$$

For long times the exponentials of the large $E_n$'s shall vanish, with only the smallest energy surviving. As said in Chapter 1, the eigenfunctions must be normalized, so if we integrate over $x_b$ we can determine the energy and the ground state eigenfunction by

$$E_0 = -\frac{1}{\tau} \log\left(\int_{-\infty}^{+\infty} K(x_b, \tau_b, x_b, \tau_b) dx_b\right) \quad \text{and} \quad |u_0(x_b)|^2 = K(x_b, \tau_b, x_b, \tau_a) \exp\left(\tau E_0\right). \tag{2.34}$$

Eq. (2.34) returns us the ground-state for the system. Some applications of these results will be shown in the next section. There is also a useful way to compute observables with numerical path integrals, (4) but we shall not discuss it here, since it is not our goal.

† A direct substitution of the complex time in Eq. (2.9) can show that the Lagrangian is now defined as $L = K.E. + V$, where $K.E.$ is the kinetic energy for the system and $V$ its potential energy.

# 3 RESULTS FOR HARMONIC AND ANHARMONIC OSCILLATORS

We start by approaching the one-dimensional harmonic oscillator by the method of the last section and finding its ground state. We start with it, although its solution is completely known, because it shall give us a way to compare our results with the theory. We know the ground state eigenfunction and its energy from the Schrödinger theory* (in units of $\hbar = \omega = m = 1$)

$$u_0(x) = \left(\frac{1}{\pi}\right)^{1/4} \exp\left(-\frac{x^2}{2}\right), \quad E_0 = \frac{1}{2}. \tag{3.1}$$

To determine the ground state numerically we must follow the method of Section 2.0.3. So, we have to discretize the complex-time on a lattice with $N+1$ points (indexed by 0 and $N$ are the boundaries) and then calculate the integral of Eq. (2.31). To compute this integral we apply the Monte Carlo method. (5) In this method, we draw a number $n_s$ of random points inside a volume of integration† $V$. Then, we replace the integral with the mean value of the function times the volume of integration. That is, for the integral of a function $g(x)$ we have

$$\int_V g(x)\, dV = \frac{V}{n_s} \sum_{i=1}^{n_s} g(x_i). \tag{3.2}$$

The equality holds only for $n_s \to \infty$. In our computations, we will be using a finite $n_s$, so our results will contain an error bar. More than that, our paths are randomly generated, so if we run the code twice we shall not get the same result. To deal with that, we will compute the desired values (kernel at a point and energy) $n_r$ times, and use the mean value of the set as our estimate for the quantities. With this, we can also find the standard deviation from the mean, which gives us the error that is being made. With the method well established, we could solve the problem of the harmonic oscillator. For this, we replaced the simple harmonic potential, that in our units is written as $x^2/2$, in Eq. (2.31), and then integrated it as described above. We used $N = 6$ and $\tau = 4$, and computed the kernel in 50 equally spaced $x$ points, with $x$ in the interval $-2.5 \leq x \leq 2.5$.

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* The eigenstates for the harmonic oscillator could be found completely from Feynman's theory, once we know the kernel for the system. To do this, we should rewrite Eq. (2.28) not in terms of sines and co-sines, but in $\exp(\pm i\omega T)$, and then expand the exponential. Then a direct correspondence between this expansion and Eq. (2.2) give us the eigenfunctions and energies. Since this is just an algebraic work we shall not develop it here.

† When the integration region goes to infinity, one must be careful in the application of Monte Carlo methods. To our goals, the desired integral vanishes at the infinity, so we can replace the limits of integration by a cutoff point, $x_{\text{cut}}$. In the examples of this Chapter we used $x_{\text{cut}} = 5$.

We used $n_s = 100000$ samples, and $n_r = 100$. The energy value obtained was[‡]

$$E_{MC}^{HO} = (0.486 \pm 0.006). \tag{3.3}$$

The eigenstate found is shown in Figure 4, where we compare it with the analytical solution. Note that both, energy and eigenstate, are in good accordance with the theoretical values. We could get a better result by increasing the number of partitions of the path. But this also increases the dimension of our integral, requiring more computation time. This is a symptom of the Monte Carlo slow convergence, which goes as $1/\sqrt{n_s}$. We can also apply the method to a Lagrangian of the type

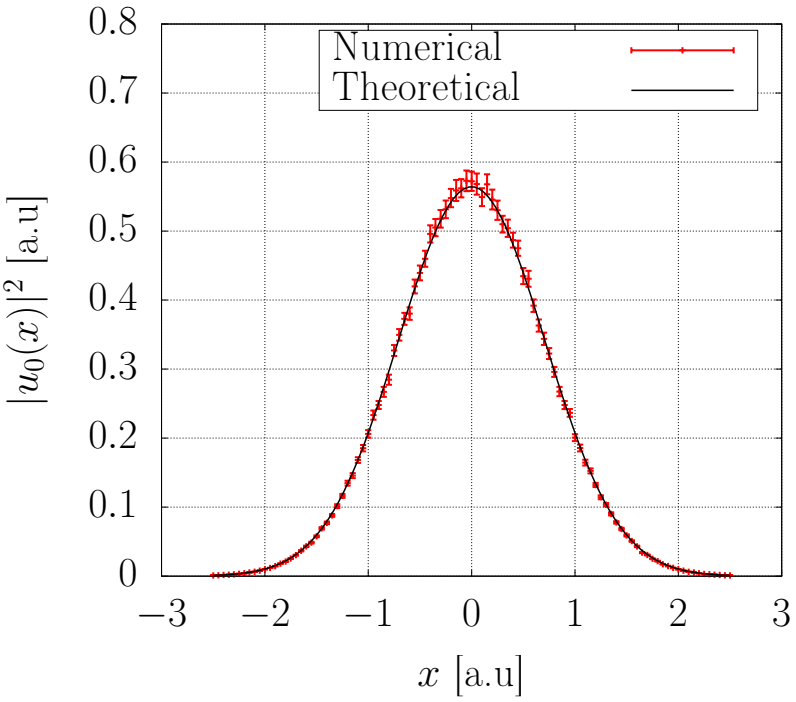


Figure 4 – Numerical solution for the harmonic oscillator eigenstate and the comparison with the analytical result.

$$L = \frac{m\,\dot{x}^2}{2} + \frac{1}{2} m\,\omega^2\,x^2 + \kappa\,x^4, \tag{3.4}$$

with is known as the anharmonic oscillator. Note that the term $x^4$ does not allow the application of the preceding results, and in fact, no analytical solution for this system is available. However, we can use the numerical approach to find the ground state. As an example let us solve the case where $\kappa = 0.1$, for which we expect that the behavior is close to the harmonic oscillator, since the $\kappa$ term is small compared to $\omega$ ($= 1$ in these units). Using the same conditions as before, we found for the ground state the energy of Eq. (3.5) and the eigenfunction of Figure 5, where we compare it with the ground state of the

[‡] All the results shown in this section were obtained by a code written by the author in FORTRAN 90, following. (4)

harmonic oscillator. In both results, we verify that the solutions are close to the harmonic oscillator, with the quartic term being just a small perturbation of it. This perturbation causes a small shift in the energy of the state and increases the probability of the particle being found around the origin.

$$E_{MC}^{ANO} = (0.518 \pm 0.006) \tag{3.5}$$

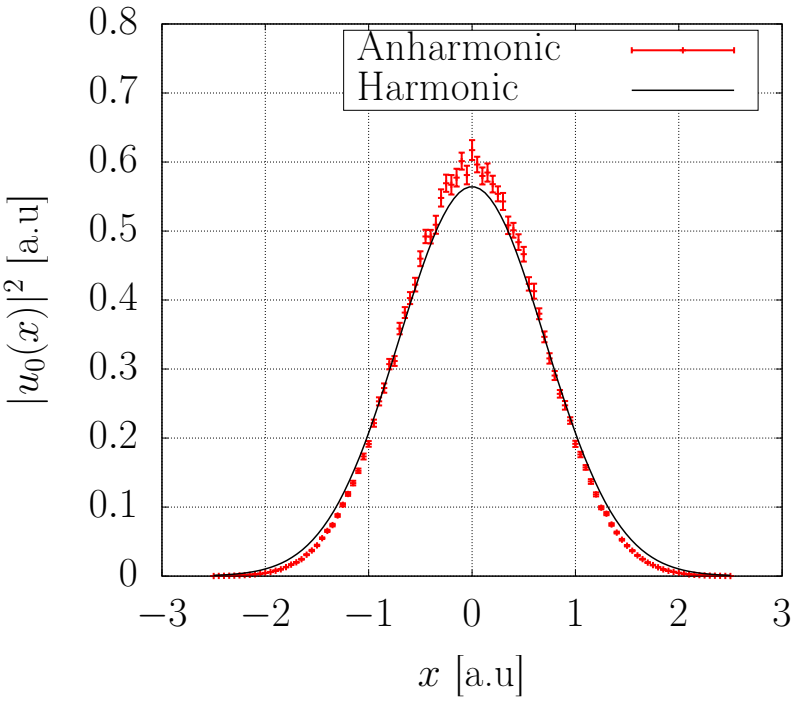


Figure 5 – Numerical solution for the anharmonic oscillator eigenstate and comparison to the ground state of the harmonic oscillator.

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# 4 QUANTUM ELECTRODYNAMICS (QED)

In the preceding sections, we have been dealing with the quantum mechanics of point particles. We showed that, if we know the classical action $S[x(t)]$ for the system, then the quantum mechanical amplitude to evolve from an initial to a final state is given by the sum of $\exp\{iS[x(t)]/\hbar\}$ over all the possible paths that connect the two boundaries. This procedure yields the quantization of the theory. Our goal now is to study the quantum phenomena associated with the electromagnetic field, which is known as quantum electrodynamics (QED). To do this we shall use the same procedure as before, but now for the *fields* that determine the system. This is an extension of the initial postulate (which encompassed only actual paths $x(t)$) to functions of the paths through the space. To start, we need an action that returns the correct equations of motion for the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$, that is, the Maxwell equations. (6) We know that $\mathbf{B}$ is the curl of a field $\mathbf{A}$, known as the vector potential, so $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$. The electric field $\mathbf{E}$ depends on $\mathbf{A}$ and the gradient of a potential $V$, so $\mathbf{E} = -\boldsymbol{\nabla} V - (1/c)\,\partial\mathbf{A}/\partial t$, where $c$ is the speed of light in vacuum. To completely determine the field $\mathbf{A}$ we still have to give its divergence. We will use $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$. With this, manipulation of Maxwell's equations returns the equations of motion in terms of the potential fields

$$\nabla^2 V = -4\pi\,\rho(\boldsymbol{r},t) \quad \text{and} \quad \nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} = -\frac{4\pi}{c}\,\mathbf{j}(\boldsymbol{r},t) + \frac{1}{c}\,\boldsymbol{\nabla}\frac{\partial V}{\partial t}. \tag{4.1}$$

It will be useful to write the action for the system in terms of Fourier components*. So, we take the Fourier transform of the potentials $\mathbf{A}$ and $V$, and the charge and current densities $\rho$ and $\mathbf{j}$, and rewrite Eq. (4.1) in terms of these. We shall refer to components of $V(\boldsymbol{r},t)$ as $\tilde{V}(\boldsymbol{k},t)$, of $\mathbf{A}(\boldsymbol{r},t)$ as $\tilde{\mathbf{A}}(\boldsymbol{k},t)$, of $\rho(\boldsymbol{r},t)$ as $\tilde{\rho}(\boldsymbol{k},t)$ and of $\mathbf{j}(\boldsymbol{r},t)$ as $\tilde{\mathbf{j}}(\boldsymbol{k},t)$. In terms of these, components the equations of motion are written as

$$\tilde{V} = \frac{4\pi\,\tilde{\rho}}{k^2}, \quad \text{and} \quad \ddot{\tilde{\mathbf{A}}} + (kc)^2\,\tilde{\mathbf{A}} = -\sqrt{4\pi}\left(\tilde{\mathbf{j}} + \frac{\boldsymbol{k}\,(\boldsymbol{k}\cdot\tilde{\mathbf{j}})}{k^2}\right). \tag{4.2}$$

These equations show us that, if we know the charge density we also know $\tilde{V}$. This means that $V$ does not contain any retarded effect, with it all relying on $\mathbf{A}$. This is an effect of our choice for $\boldsymbol{\nabla} \cdot \mathbf{A}$. The important fact is that Eq. (4.2) shows that field $\mathbf{A}$ can be seen as a collection of driven harmonic oscillators propagating throughout the space. Each oscillator has an individual frequency $\omega_k = kc$ and the oscillators associated with

* The convention used for the direct Fourier transform $\tilde{f}$ of some function $f$ was

$$\tilde{f}(\boldsymbol{k}) = \int_{-\infty}^{+\infty} f(\boldsymbol{r})\exp(-i\boldsymbol{k}\cdot\boldsymbol{r})d^3\boldsymbol{r}, \quad f(\boldsymbol{r}) = \int_{-\infty}^{+\infty} \tilde{f}(\boldsymbol{k})\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\frac{d^3\boldsymbol{k}}{(2\pi)^3}.$$

two distinct wave numbers $k$ and $k'$ do not interact. This means that we have decomposed field $\mathbf{A}$ into its normal coordinates. This is an important fact, since the problem of the driven harmonic oscillator was completely solved in Eq. (2.30).

Now we are ready to write an action for the electromagnetic field. We are interested in the situation where we have matter and fields present, so we must also consider their interaction. The Lagrangian that describes the field and its interaction with matter is (2)

$$L = \int \left\{ -\rho\, V + \frac{1}{c}\,\mathbf{j}\cdot\mathbf{A} + \frac{1}{8\pi}\,\left[ \left( -\boldsymbol{\nabla} V - \frac{1}{c}\,\frac{\partial \mathbf{A}}{\partial t} \right)^2 - (\boldsymbol{\nabla}\times\mathbf{A})^2 \right] \right\} d^3\boldsymbol{r}. \tag{4.3}$$

Replacing the expressions for the fields and densities in terms of the Fourier components, we find that the Lagrangian function for the complete system (including the motion of the matter) is

$$\begin{aligned} L = \int \Bigg[ & \frac{1}{2}\,\dot{\tilde{\sigma}}^2 + \frac{1}{2}\left( |\tilde{V}|^2\,\frac{k^2}{4\pi} + \dot{\tilde{\mathbf{A}}}^*\cdot\dot{\tilde{\mathbf{A}}} - \omega_k^2\,\tilde{\mathbf{A}}^*\cdot\tilde{\mathbf{A}} \right) - \\ & \left( \tilde{\rho}(-\boldsymbol{k},t)\,\tilde{V} - \sqrt{4\pi}\,\tilde{\mathbf{j}}(-\boldsymbol{k},t)\cdot\tilde{\mathbf{A}} \right) \frac{d^3\boldsymbol{k}}{(2\pi)^3}, \end{aligned} \tag{4.4}$$

where $\sigma$ is the matter density in the region and $\tilde{\sigma}$ is its Fourier transform. Quantum electrodynamics arises when we compute the sum over all the paths for the action associated with this Lagrangian. Note that the boundary conditions are now the initial and final displacement of the matter $\tilde{\sigma}$ and configurations of the fields $\tilde{V}$ and $\tilde{\mathbf{A}}$. So our path integral is carried over all the possible configurations for these functions[†]. The fact that the action for the system contains a term of interaction means that not only the field interferes in the matter evolution, but also the matter interferes in the dynamics of the field.

For a better understanding of the quantum behavior of the field, we take a situation where there is no matter present. In this case, the field oscillators are free, since they do not interact with each other, the final solution is just a product of the solutions for each mode of frequency $\omega_k$. We also know, from Schrödinger's theory, that the energy levels for an oscillator are $\hbar\omega(n+1/2)$, where $n = 0, 1, 2\ldots$, and so on. The total energy for our field will be a sum of the energies from each oscillator in each polarization[‡]. Once we have

[†] The fact the $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$ implies that $\boldsymbol{k}\cdot\tilde{\mathbf{A}} = 0$, so the Fourier components of the vector potential do not vanish only in two directions orthogonal to $\boldsymbol{k}$. We shall refer to these directions as $\tilde{A}_1$ and $\tilde{A}_2$.

[‡] In the continuous approach that was being taken until this point, this would mean an integral over $d^3\boldsymbol{k}$. Is easier to deal with the system inside a box of volume Vol and use periodic boundary conditions. With this the integrals became simple sums, $\int_{-\infty}^{+\infty} () \, d^3\boldsymbol{k}/(2\pi)^3 \to \sum_{\boldsymbol{k}} ()/\mathrm{Vol}$, with the values of $\boldsymbol{k}$ being now equally spaced. With this change we must normalize our functions, multiplying each one by $1/\sqrt{\mathrm{Vol}}$. Once this change affects only the boundaries of the problem in the limit of a huge box, where we would not be interested in what goes on next to the walls, our results are not changed.

an infinite number of oscillators, this sum diverges. To solve this we make a change the zero point energy, assigning the zero energy for the states with $n = 0$. Then, the energy for any state of the field is

$$E = \sum_{n_{\boldsymbol{k}}} (n_{1,\boldsymbol{k}} + n_{2,\boldsymbol{k}})\hbar kc, \tag{4.5}$$

where $n_{1,\boldsymbol{k}}$ and $n_{2,\boldsymbol{k}}$ are the quantum numbers for the oscillators in each polarization direction. The change in the zero of energy does not affect the physics, since this depends only on energy differences. The excitation energies are multiples of $\hbar kc$. In the field theory, we can see these excited states as the presence of a particle, which in the case of the electromagnetic field, is named a *photon*. (2) So, if the energy associated with a mode is $n_{p,\boldsymbol{k}}\hbar kc$, this means that we have $n_{p,\boldsymbol{k}}$ photons present, with polarization in the direction $p$ and with momentum $\hbar\boldsymbol{k}$. This means that when all the modes are in the ground state we have no photons present. This is known as the vacuum of the field.

This interpretation for the excited states is really useful and holds for more complicated theories (such as quantum field theory). It still holds even when matter is present, but, in this case, photons can be emitted or absorbed in the evolution of the system. So, when matter is present our boundary conditions are the matter displacement and the initial and final number of photons in each mode. So, given an initial state $|\Psi(\mathbf{x}_a, \mathbf{A}_a, V_a, t_a)\rangle$ the probability amplitude that the system will evolve to a final state $|\Psi(\mathbf{x}_b, \mathbf{A}_b, V_b, t_b)\rangle$ is given by $\langle\Psi(\mathbf{x}_b, \mathbf{A}_b, V_b, t_b)|K(\mathbf{x}_b, \mathbf{A}_b, V_b, t_b, \mathbf{x}_a, \mathbf{A}_a, V_a, t_a)|\Psi(\mathbf{x}_a, \mathbf{A}_a, V_a, t_a)\rangle$, where $K$ is the kernel for the action of Eq. (4.4), computed between the states for field and matter that determine $\Psi$ at $t_b$ and $t_a$. The fact is that the path integral for the system is complicated, and we do not know how to compute it analytically in most situations. This is a recurrent problem in quantum mechanics.

However, in situations where we can split the original Lagrangian in $L = L_0 + v$, where $L_0$ is a Lagrangian function for which we know the analytical result, and $v$ is a small term compared to it, we can apply what is known as *perturbation theory*. Once $v$ is small compared to $L_0$, its integral over time also is it. So, we can expand the kernel in a power series of $\int iv/\hbar\, dt$. Calling $K_0$ the kernel associated with Lagrangian $L_0$, we find, after the expansion and some algebraic manipulation, that the kernel is given by

$$K(b,a) = K_0(b,a) - \frac{i}{\hbar}\int K_0(b,c)v(c)K_0(c,a)dx_c\, dt_c + \dots, \tag{4.6}$$

where the second term in the right-hand side of the above equation is called the *first-order perturbation term*, the next one would be the order 2 term, and so on. The order 1 term represents the evolution of the system under the action of only $L_0$ between the state $a$ and a state $c$, where this last one is arbitrary. In this state $c$ the potential acts, which is represented by the term $v(c)$. Then, the system evolves to the final state under the influence of only $L_0$ again. We integrate over all possible positions and times for that occurrence of $v(c)$, so this is just an auxiliary state. We call $c$ a virtual state where there

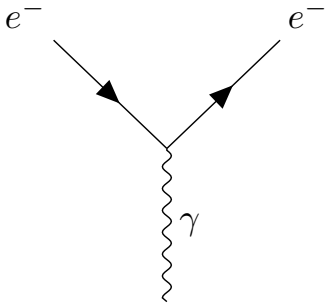
is an interaction between the unperturbed system, $L_0$, and the perturbation potential $v$. The first-order term represents only one interaction. The same development for the second-order therm would show (2) that it corresponds to two interactions, the third-order term to three, and so on. This interpretation for the perturbation expansion is one of the main advantages of Feynman's formulation, with no close physical interpretation being available in Schrödinger's picture.

A manipulation of the action for the Lagrangian of Eq. (4.4) shows (2) that the terms of the driven harmonic oscillators ($\tilde{\mathbf{A}}$ and $\tilde{\mathbf{j}}$) are proportional to $\alpha = e^2/\hbar c \approx 1/137$, known as the fine structure constant. This implies that the electromagnetic terms are, generally, small compared to the matter ones. So, perturbation theory plays a key role in QED. It is so fundamental, that there exists a special tool, known as ***Feynman diagrams***, used to construct and understand each of the perturbation expansion terms. In these diagrams, we represent the time running to the right, charged particles[§] by arrows, and photons by wavy lines (and the symbol $\gamma$). With it, the fundamental process of QED is represented by the *vertex* (7) of Figure 6(a). By connecting replicas of this primitive vertex, we can construct physical phenomena. However, observable particles are represented only by the particles that came in and out of the diagram. Particles that are contained inside it, that is, that begin at one vertex and end at another, are virtual particles.

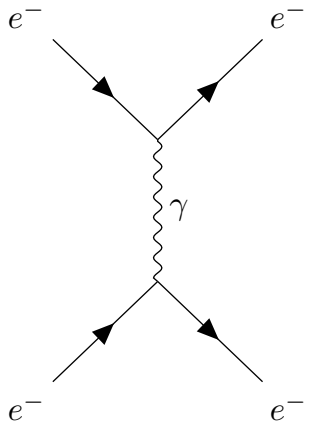
We can take as an example the case of two electrons. The evolution of the system would be given by the associated kernel for the system. If we apply perturbation theory to it, a first-order term would represent the interaction of the electrons with the vacuum field and can be represented by the diagram of Figure 6(b). Note that we do not have any photons at the beginning or the end of the process. The emitted photon is virtual, and represents one interaction of the matter and the field (it is the term $v(c)$ of Eq. (4.6)). We can also take cases where we have one photon and one electron initially. A first-order term would be represented by the diagram of Figure 6(c), where the electron absorbed the photon and later scattered it, which is Compton's scattering. Again, note that we have one electron and one photon at the beginning and the end of the process.

Second-order terms would mean two interactions of the unperturbated system with the potential. This is represented with more vertices in our diagrams. For example, in the two electrons case, a second-order interaction means that two virtual photons were emitted and absorbed, which can be represented by the diagram of Figure 6(d).

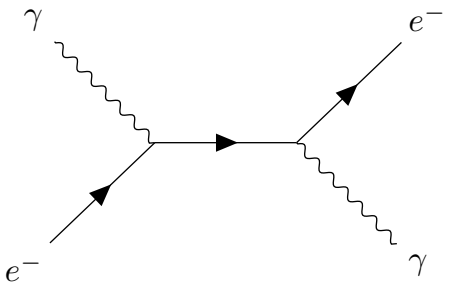
§ For us, these particles are non-relativistic electrons. We restrict to this case because relativistic electrons must be described not by Schrödinger's equation, as done here, but by Dirac's.



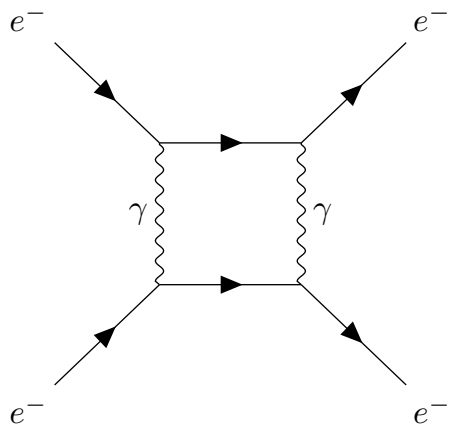

(a) Primitive vertex




(b) One photon exchange between two electrons




(c) Compton's scattering




(d) Two photons exchange between two electrons

Figure 6 – Examples of Feynman diagrams for first and second order phenomenas.

Source: By the author.

# 5 CONCLUSION

We developed Feynman's formulation for quantum mechanics. The initial postulate was that the amplitude for the evolution from an initial state $a$ to a final one $b$ is given by a kernel $K(b, a)$ that is the sum over all the paths that connect these two boundary states, Eq. (1.5). In Chapter 2 we developed the mathematical formulation of the theory starting by the Schrödinger equation. So, we have that these two formations do match. We saw that in the kernel formulation the operators are replaced by numbers, with this simplification being one of the advantages of the theory. Furthermore, we also showed that the probability interpretation is natural, with events in succession being unrelated, Eq. (2.14), and that for quadratic Lagrangians we have a well established method for the kernel computation, Eq. (2.19).

Otherwise, the kernel computation is not a simple task. For this reason, we developed a numerical approach to the problem in Section 2.0.3 and Chapter 3. We called this version the Euclidean path integral and showed that it is obtained by keeping the complex-time $\tau$. Then,we solved the harmonic and anharmonic oscillators by the Euclidean path integral method showing that the results do match with what was expected. This is a striking result, since it was obtained using a non-physical time. In fact, when we use the complex time there is a direct identification of the kernel with a partition function, (2) being this another advantage of the theory.

Lastly, in Chapter 4 we extend the quantization of the action for the electromagnetic field. As we saw, we cannot write an action in which the field and matter are not coupled. This means that not only the field interferes in the matter dynamics, but the matter also interferes in the field evolution, being this is a new result. Otherwise, the kernel for the system is complicated, which creates the need of an expansion in a power series, know as perturbation theory. The expansion done is valid not only in QED but in theory as a whole. We saw that Feynman's formulation for the perturbative series gives us a really useful interpretation for each of the terms, e.g., the order 1 term means one interaction of the system with the perturbation potential, the order 2 two interactions, etc. This interpretation is so important that in QED we have a special tool for the understanding of each of them, the *Feynman diagrams*, exemplified in Figure 6.

So, as we saw, besides the intricate computation of the kernel, Feynman's formulation has many advantages, among which the quantization being simple and perturbation theory very intuitive. More than that, the quantization of the fields, as done in Chapter 4, can be extended to more complicated systems with this formulation being useful, for example, also in quantum field theory.

# REFERENCES

1 SAKURAI, J.; NAPOLITANO, J. **Modern quantum mechanics**. 2nd ed. Boston: Addison-Wesley, 2014.

2 FEYNMAN, R. P.; HIBBS, A. R.; STYER, D. F. **Quantum mechanics and path integrals**. Massachusetts: Courier Corporation, 2010.

3 LEMOS, N. A. **Mecânica analítica**. São Paulo: Editora Livraria da Física, 2007.

4 LEPAGE, G. P. Lattice QCD for novices. In: GOITY, J.L.(ed.). **Strong Interactions at Low and Intermediate Energies**, Singapure: World Scientific, 1998. p. 49–90.

5 PRESS, W. *et al.* **Numerical recipes in FORTRAN 77:** the art of scientific computing. Cambridge: Cambridge University Press, 1992.

6 GRIFFITHS, D. **Introduction to electrodynamics**. 4th. ed. Cambridge: Cambridge University Press, 2017.

7 GRIFFITHS, D. **Introduction to elementary particles**. Weinheim: John Wiley & Sons, 2020.