Quantum Mechanics and Path Integrals: Quadratic Actions

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Abstract: This work aims to calculate the Feynman propagator of several physical systems governed by quadratic actions by means of the Path Integral approach. Consequently, once the propagator is known for the case of a harmonic potential, a system of coupled oscillators will be studied. Finally, it will be possible to determine the time evolution of a Gaussian wave function when its width is initially modified, as well as the effect induced by a periodic external force.

I. INTRODUCTION

This work follows Feynman's program of formulating Quantum Mechanics (QM) in terms of path integrals. According to Feynman [1], the fundamental quantities by which QM is naturally formulated are complex numbers. These numbers, from now on called *Probability Amplitudes* (ϕ_i), contain the whole information of the system such that the probability of finding a particle whose quantum state is described by ϕ, is given by: $P = |\phi|^2$. The probability amplitude can have several contributions in such a way that: $\phi = \sum_{i=1}^{n} \phi_i$. Consequently, the classical rule for adding probabilities is not followed: $P = |\phi_1 + \phi_2|^2 \neq P_1 + P_2$ being $P_i = |\phi_i^2|$.

This rule can be extended to trajectories or paths $x(t)$. In the sense that if you want to calculate the probability amplitude of a particle going from $a = (x_i, t_i)$ to $b = (x_f, t_f)$, i.e., the *propagator* $K(b, a)$, you must calculate it as the sum of the contributions over all possible paths:

$$K(b,a) = \sum_{over\ all\ paths} \phi_i[x(t)] \tag{1}$$

where the probability amplitude of each path is given by: $\phi_i[x(t)] = Ce^{(i/\hbar)S[x(t)]}$, where $S[x(t)]$ is the classical action. Inspired by the principle of least action, Feynman stated [3] that in the quantum case, not only the path with a minimum action but all paths contribute. They contribute with the same amplitude but with different phases.

If we consider a one dimensional non-relativistic particle with mass m subjected to a quadratic potential $V(x)$, we know [1] how its wave function evolves over time by:

$$\Psi(b) = \int_{-\infty}^{\infty} K(b,a)\Psi(a)dx_i \tag{2}$$

In the following sections, the Feynman propagator will be used to determine the time evolution of several physical systems governed by quadratic actions. Only conservative systems are allowed, since otherwise there would be no Lagrangian.

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II. HARMONIC OSCILLATOR PROPAGATOR

Let us imagine we want to compute the probability amplitude for a non-relativistic particle of mass m subjected to a harmonic potential of going from $a = (x_i, t_i)$ to $b = (x_f, t_f)$. This probability amplitude will be given by the propagator:

$$K(b,a) = N \int Dx(t) e^{\frac{i}{\hbar} S[x(t)]} \tag{3}$$

where Dx stands for the sum over all paths between a and b. In the classical limit ($\hbar \to 0$), only the classical path will contribute to the propagator, as the other paths will be canceled out due to destructive interference [4]. For the classical path, i.e. the trajectory that a classical particle obeying the Lagrange equations would follow, the action is [5]:

$$S_{cl}[x(t)] = \int_{t_i}^{t_f} L(\dot{x}, x, t)\, dt = \int_{t_i}^{t_f} (\frac{1}{2} m\dot{x}^2 - \frac{1}{2} m\omega^2 x^2) dt$$
$$= \frac{m\omega}{2\sin\omega(t_f - t_i)} [(x_i^2 + x_f^2)\cos\omega(t_f - t_i) - 2x_i x_f] \tag{4}$$

given that: $x(t_i) = x_i$ and $x(t_f) = x_f$. Now, in an effort to find the expression of the propagator in Eq. (3), the variables can be changed in order to consider the trajectory as the classical one plus a deviation, $y(t)$, (Figure 1):

$$x(t) = x_{cl}(t) + y(t), \tag{5}$$

where y(t) satisfies: $y(t_i) = y(t_f) = 0$. Then, after integrating by parts and using the equation of motion, the cross terms of the action disappear, and it can be rewritten such that:

$$S[x(t)] = S[x_{cl}(t) + y(t)] = S[x_{cl}(t)] + S[y(t)] \tag{6}$$

Thus, the total action is separated into the classical action plus the action of the variation with respect to the classical path. Therefore, the propagator can be now written as:

$$K(b,a) = N \int Dy e^{\frac{i}{\hbar}(S[x_{cl}] + S[y])} = A(t) e^{\frac{i}{\hbar} S[x_{cl}]} \tag{7}$$

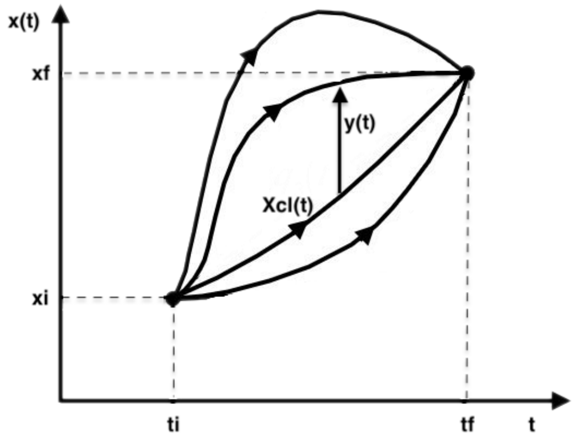

FIG. 1: A change of variables is made in order to consider the trajectory as the classical one plus a deviation, $y(t)$. So, $x(t) = x_{cl}(t) + y(t)$.

where:

$$A(t) = N \int Dy e^{\frac{i}{\hbar} S[y]} \tag{8}$$

Note that the classical term has all the dependence on x whereas A(t) depends only on time, and since the Lagrangian does not depend on time (i.e. it is invariant with respect to time translations), A only depends on the time difference which can be redefined as $A(t_f - t_i) \equiv A(t_f)$.

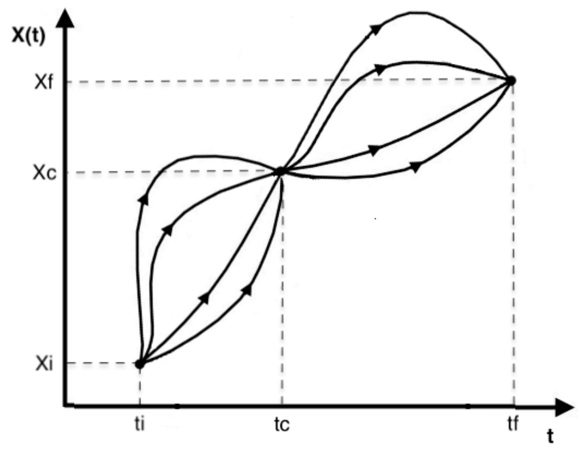

FIG. 2: One can compute the amplitude of going from $a = (x_i, t_i)$ to $b = (x_f, t_f)$ as the product of the amplitude from a to $c = (x_c, t_c)$ and the amplitude from c to b.

According to Feynman [1], the propagator satisfies:

$$K(b,a) = \int_{-\infty}^{\infty} K(c,a) K(b,c) dx_c \tag{9}$$

where $c = (x_c, t_c)$. In other words, the propagator of going from a to b is equal to the product of propagators of going from a to c and from c to b integrated over all possible values of x_c, so that $t_i < t_c < t_f$ (Figure 2). Substituting each propagator in Eq. (9), imposing for convenience that $t_i = 0$ and using the subsequent relation:

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}} \tag{10}$$

the following functional equation is reached:

$$\phi(t_f) = \phi(t_c)\phi(t_f - t_c) \tag{11}$$

where:

$$\phi(t) = A(t)\sqrt{\frac{2\pi i\hbar \sin\omega t}{m\omega}} \tag{12}$$

for every t_c as long as $t_i < t_c < t_f$. The general solution from Eq. (11) is:

$$A(t) = \exp\left[(\alpha + i\beta)t\right]\sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega t}} \tag{13}$$

The real part of the exponential must be zero ($\alpha = 0$) otherwise the solution would not be unitary, and we would have a probability source or drainer. The imaginary part can be neglected ($\beta = 0$) since it is not physical, and it corresponds to a normalization of the energy, i.e., the freedom to choose the zero-point energy. From this result, it follows that:

$$A(t) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega t}} \tag{14}$$

Finally, the expression of the harmonic oscillator propagator is obtained in its full glory:

$$K = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega t}} \exp\frac{im\omega}{2\hbar \sin\omega t}\left[(x_i^2 + x_f^2)\cos\omega t - 2x_i x_f\right] \tag{15}$$

As a check, it can be verified how the harmonic oscillator propagator, Eq. (15), becomes the free particle propagator [2] when ω tends to 0.

$$\lim_{\omega\to 0} K = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\frac{im}{2\hbar t}(x_i - x_f)^2 \tag{16}$$

III. COUPLED OSCILLATORS

In this section, we will study a system of two identical masses coupled to each other by means of a spring of elastic constant k'. In turn, each mass is fixed to the ground by another spring of elastic constant k. The system can be seen in Figure 2. Let our system of coupled oscillators be described by the following Lagrangian:

$$L = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) - \frac{1}{2}k(x_1^2 + x_2^2) - \frac{1}{2}k'(x_2 - x_1)^2 \tag{17}$$

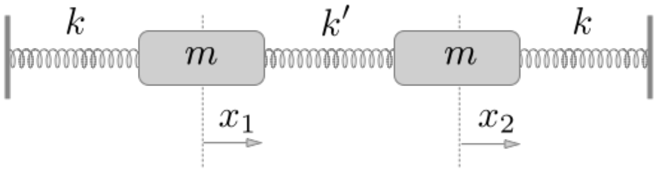

FIG. 3: System of coupled oscillators.

From the Lagrange equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = 0, \tag{18}$$

we can easily obtain the equations of motion for the position of both masses:

$$\begin{aligned} m\ddot{x}_1 &= -kx_1 + k'(x_2 - x_1) \\ m\ddot{x}_2 &= -kx_2 - k'(x_2 - x_1) \end{aligned} \tag{19}$$

Adding and subtracting both expressions, decoupled equations describing single harmonic oscillators are obtained:

$$\begin{aligned} \frac{d^2(x_1+x_2)}{dt^2} + \frac{k}{m}(x_1+x_2) = 0 \\ \frac{d^2(x_1-x_2)}{dt^2} + \frac{k+2k'}{m}(x_1-x_2) = 0 \end{aligned} \tag{20}$$

We can now define the normal coordinates in which the system is totally decoupled and identify its normal frequencies:

$$\begin{aligned} q_1 \equiv \frac{1}{\sqrt{2}}(x_1+x_2) \rightarrow \omega_1 &= \sqrt{\frac{k}{m}} \\ q_2 \equiv \frac{1}{\sqrt{2}}(x_1-x_2) \rightarrow \omega_2 &= \sqrt{\frac{k+2k'}{m}} \end{aligned} \tag{21}$$

The first normal frequency, ω_1, corresponds to a symmetrical motion in which both springs oscillate in phase while maintaining the relative distance between them. On the other hand, the second normal frequency, ω_2, represents an antisymmetric motion in which both springs oscillate in counterphase. Any movement can be expressed as a linear combination of both normal frequencies. If the Lagrangian of the system is expressed as a function of normal coordinates, it is found that:

$$L = \frac{1}{2}m(\dot{q}_1^2 + \dot{q}_2^2) - \frac{1}{2}k(q_1^2 + q_2^2) - k'q_2^2 \tag{22}$$

When expressing it according to the normal frequencies, a decoupled Lagrangian is obtained:

$$L = \left(\frac{1}{2}m\dot{q}_1^2 - \frac{1}{2}m\omega_1^2 q_1^2\right) + \left(\frac{1}{2}m\dot{q}_2^2 - \frac{1}{2}m\omega_2^2 q_2^2\right) \tag{23}$$

Thus,

$$L(\dot{q}_1, \dot{q}_2, q_1, q_2) = L_1(\dot{q}_1, q_1) + L_2(\dot{q}_2, q_2), \tag{24}$$

where L_i is the Lagrangian for a simple harmonic oscillator. Now, the classical action of the whole system can be written as the sum of two independent harmonic oscillators:

$$S_{cl} = \int_{t_i}^{t_f} L(\dot{q}_1, \dot{q}_2, q_1, q_2)\, dt = \int_{t_i}^{t_f} (L_1 + L_2)\, dt$$

$$= S_{cl}(q_1) + S_{cl}(q_2), \tag{25}$$

where $S_{cl}(q_i)$ is the classical action for a simple harmonic oscillator, which is well known and described in Eq. (4). Therefore, in view of this result, one can compute the probability amplitude of going from one point in space-time $a = (q_{1i}, q_{2i}, t_i)$ to another $b = (q_{1f}, q_{2f}, t_f)$ as the product of independent propagators. In other words that is,

$$K(b,a) = K(q_{1f}, t_f; q_{1i}, t_i)K(q_{2f}, t_f; q_{2i}, t_i) \tag{26}$$

where replacing the expressions of the simple harmonic oscillator propagators given by Eq. (15), it turns out that:

$$K(b,a) = \frac{m}{2\pi i\hbar}\sqrt{\frac{\omega_1\omega_2}{\sin\omega_1 t \sin\omega_2 t}}\, e^{\frac{i}{\hbar}[S_{cl}(q_1)+S_{cl}(q_2)]} \tag{27}$$

where it has been defined $t \equiv t_f - t_i$ for simplicity.

IV. TIME EVOLUTION OF A GAUSSIAN WAVE PACKET

This section aims to study the temporal evolution of a Gaussian, in this case corresponding to the wave function of the fundamental level of the harmonic oscillator, when its standard deviation is initially modified. The initial

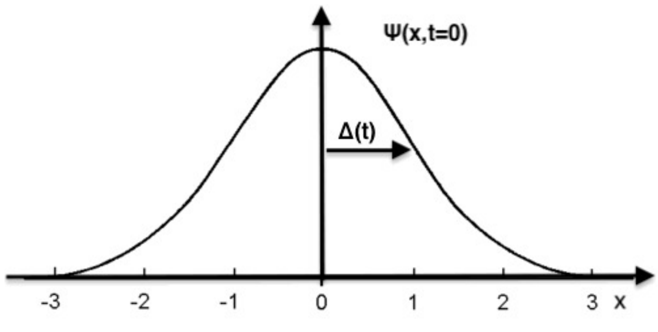

FIG. 4: Wave function of modified width at t=0.

conditions can be seen in Figure 2, where $\Delta_0 \equiv \Delta(t=0)$ is different from x_0, the natural width of the Gaussian. So, at the beginning, we have that:

$$\Psi(x, t=0) = \frac{1}{\sqrt{\Delta_0\sqrt{\pi}}} e^{-\frac{1}{2}\left(\frac{x}{\Delta_0}\right)^2} \tag{28}$$

where $\Delta_0 \neq x_0$, and $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ has units of length. As explained earlier, the propagator gives us the probability amplitude of going from one state (x_i, t_i) to another (x_f, t_f). In Dirac's bra-ket notation this is expressed as:

$$K(x_f, t_f; x_i, t_i) \equiv \langle x_f|\mathcal{U}(t_f, t_i)|x_i\rangle \tag{29}$$

where $\mathcal{U}(t_f, t_i)$ is the time evolution operator. We are now interested in calculating the time evolution of the wave function. That is:

$$\begin{aligned} |\Psi(t_f)\rangle &= \mathcal{U}(t_f, t_i)|\Psi(t_i)\rangle \\ \langle x_f|\Psi(t_f)\rangle &= \langle x_f|\mathcal{U}(t_f, t_i)|\Psi(t_i)\rangle \\ \Psi(x_f, t_f) &= \int dx_i \langle x_f|\mathcal{U}(t_f, t_i)|x_i\rangle\langle x_i|\Psi(t_i)\rangle \end{aligned} \tag{30}$$

where the resolution of the identity has been used, i.e., $Id = \int dx_i|x_i\rangle\langle x_i|$. Now using Eq. (30) and setting $t_i = 0; t_f \equiv t$, we recover:

$$\Psi(x_f, t) = \int dx_i K(x_f, t; x_i, 0)\Psi(x_i, 0) \tag{31}$$

thanks to which the time evolution of the wave function can be determined given the initial conditions and the harmonic oscillator propagator, both known. In order to be able to solve the Gaussian integral from the Eq. (31), it is helpful to use the following relation:

$$\int dx_i e^{-Ax_i^2 - Bx_i} = \sqrt{\frac{\pi}{A}} e^{\frac{B^2}{4A}} \tag{32}$$

In our case, A and B take the following values:

$$A = \frac{1}{2\Delta^2} - \frac{i\cos\omega t}{2x_0^2\sin\omega t} \qquad B = \frac{ix_f}{x_0^2\sin\omega t} \tag{33}$$

Hence, after arranging the Eq. (32) algebraically with the values of Eq. (33), we have that the wave function at an instant t has the following form:

$$\Psi(x, t) = Ce^{D+iE} \tag{34}$$

where $(x_f, t_f) \equiv (x, t)$ has been defined to lighten the notation. C, D, and E take the following values:

$$\begin{aligned} C &= \frac{1}{\sqrt{\frac{1}{\Delta_0}(\Delta_0^2\cos\omega t + ix_0^2\sin\omega t)\sqrt{\pi}}} \\ D &= -\frac{x^2}{\frac{2}{\Delta_0^2}(x_0^4\sin^2\omega t + \Delta_0^4\cos^2\omega t)} \\ E &= \frac{x^2\sin 2\omega t(x_0^4 - \Delta_0^4)}{4x_0^2(x_0^4\sin^2\omega t + \Delta_0^4\cos^2\omega t)} \end{aligned} \tag{35}$$

From Eq. (34) and Eq. (35) we can see how the width of the Gaussian, $\Delta(t)$, oscillates with time according to:

$$\Delta(t) = \frac{\Delta_0}{\sqrt{2}}\sqrt{\left(1 + \left(\frac{x_0}{\Delta_0}\right)^4\right) + \left(1 - \left(\frac{x_0}{\Delta_0}\right)^4\right)\cos 2\omega t} \tag{36}$$

Thus, it has just been demonstrated that when an initial perturbation is applied to the width of the Gaussian wave function corresponding to the ground state of the harmonic oscillator, the wave function oscillates over time widening and thinning with a frequency twice that of the harmonic oscillator, while always keeping the maximum value fixed. Of course, when the initial disturbed width, Δ_0, is stretched to the original width, x_0, the system stays still without oscillating, as it should be.

$$\lim_{\Delta_0 \to x_0} \Delta(t) = x_0 \tag{37}$$

On the other hand, to verify the result of Eq. (34) the following limit for the wave function can be made:

$$\lim_{\Delta_0 \to x_0} \Psi(x, t) = \frac{1}{\sqrt{x_0\sqrt{\pi}}} e^{-\frac{1}{2}(\frac{x}{x_0})^2} e^{-\frac{i}{2}\omega t} \tag{38}$$

Recovering the expression of the original undisturbed wave function, plus a phase introduced by the time evolution operator, as it is expected from a stationary state.

V. PERIODIC EXTERNAL FORCE

In this section, the time evolution of a Gaussian subject to a harmonic potential and a periodic force will be studied. The initial wave function is the same as in the previous section:

$$\Psi(x, t = 0) = \frac{1}{\pi^{1/4}} e^{-\frac{x^2}{2}} \tag{39}$$

(using from now on: $\hbar = m = \omega = 1$ and $x_0 = \sqrt{\frac{\hbar}{m\omega}} = 1$) and the periodic force is: $F(t) = f\sin\alpha t$. Thus, the Lagrangian of the system is:

$$L = \frac{\dot{x}^2}{2} - \frac{x^2}{2} + fx\sin\alpha t \tag{40}$$

There is no temporal homogeneity, as the Lagrangian depends explicitly on time. The classical trajectory for this system is:

$$x_{cl}(t) = A\sin\omega t + B\sin(u - t) + \frac{f}{1 - \alpha^2}\sin\alpha t \tag{41}$$

where $t_i = 0$ and $t_f \equiv u$. By imposing the boundary conditions: $x_{cl}(0) = a$ and $x_{cl}(u) = b$ one get:

$$A = \frac{1}{\sin u}\left(b - \frac{f}{1 - \alpha^2}\sin\alpha u\right) \qquad B = \frac{a}{\sin u} \tag{42}$$

Hence, the propagator is:

$$K(b, t = u; a, t = 0) = \frac{1}{\sqrt{2\pi i\sin u}} e^{iS[x_{cl}]} \tag{43}$$

where $A(t_f = u, t_i = 0) = \frac{1}{\sqrt{2\pi i\sin u}}$ is the same as in the harmonic oscillator since linear terms of the Lagrangian

($fx\sin\alpha t$) do not contribute to $A(t_f,t_i)$. Now, the action has to be calculated using integration by parts:

$$S[x_{cl}]=\int_0^u L(\dot{x}_{cl}(t),x_{cl}(t),t)dt=$$
$$\frac{1}{2}(\dot{x}_{cl}(u)x_{cl}(u)-\dot{x}_{cl}(0)x_{cl}(0))+\frac{1}{2}\int_0^u x_{cl}(t)f\sin\alpha t dt \quad (44)$$

Finally,

$$\Psi(b,u)=\int_{-\infty}^{\infty}K(b,u;a,0)\frac{1}{\pi^{1/4}}e^{-\frac{1}{2}a^2}da \quad (45)$$

In this case, we are only interested in $|\Psi(b,u)|^2$. From S_{cl}, only the terms that depend on a (integration variable) are needed since all the others appear in the imaginary exponential and do not contribute to $|\Psi(b,u)|^2$. Hence:

$$S[x_{cl}]=\frac{a^2}{2}\cot u-\frac{a}{\sin u}(b-x_m(u))+[...] \quad (46)$$

where $x_m(u)=\frac{f}{1-\alpha^2}(\sin(\alpha u)-\alpha\sin u)$. Then, the exponential from Eq. (45) can be separated into:

$$e^{-a^2\tilde{A}+a\tilde{B}+[...]} \quad (47)$$

where:

$$\tilde{A}=\frac{1-i\cot u}{2} \qquad \tilde{B}=\frac{b-x_m(u)}{i\sin u} \quad (48)$$

The result of the Gaussian integral from Eq. (45) is:

$$\Psi(b,u)=\frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2\pi i\sin u}}\sqrt{\frac{\pi}{\tilde{A}}}e^{\frac{\tilde{B}^2}{4\tilde{A}}+i[...]} \quad (49)$$

Since we are only interested in the squared modulus of the wave function, we do not consider the imaginary exponential. Substituting Eq. (48) in Eq. (49), we get:

$$\Psi(b,u)=\frac{1}{\pi^{1/4}}e^{\frac{-1}{2}(b-x_m(u))^2+i[...]} \quad (50)$$

Now, retrieving units and setting $b=x$ and $u=t$, the squared modulus of the wave function is finally obtained:

$$|\Psi(x,t)|^2=\frac{1}{\sqrt{\pi}}e^{(\frac{x-x_m(t)}{x_0})^2} \quad (51)$$

where $x_0=\sqrt{\frac{\hbar}{m\omega}}$ and $x_m(t)=\frac{f}{m(\omega^2-\alpha^2)}(\omega\sin(\alpha t)-\alpha\sin\omega t)$. Notice that it is a coherent state: a Gaussian that does not deform and that moves in block following the trajectory of the maximum point, which is the classical trajectory of a harmonic oscillator subjected to a periodic force with initial conditions: $x(0)=\dot{x}(0)=0$. It should be noted that this motion has been excited, in quantum mechanics, with a classical external force. That is, with a Lagrangian term: $xf\sin\alpha t$. These coherent states exhibit, in quantum mechanics, the quantum behaviors most similar to classical mechanical motions, within the limits imposed by the uncertainty principle. The package has an $x_0=\sqrt{\frac{\hbar}{m\omega}}$ width, it cannot be infinitely narrow or punctual. The resonant case can be retrieved if α tends to ω:

$$\lim_{\alpha\to\omega}x_m(t)=\frac{f}{2m\omega}(\sin\omega t-\omega t\cos\omega t) \quad (52)$$

where L'Hôpital's rule has been used. Indeed, it is a movement where the amplitude grows linearly with time, for large time values.

VI. CONCLUSIONS

Describing Quantum Mechanics by means of the Path Integral approach has allowed us to discover an alternative way of understanding this wonderful theory without the need to abandon certain classical tools. Feynman's approach has proven to be very useful in tackling the problems raised in this work involving quadratic actions. Thus, we have successfully calculated the propagator of the harmonic oscillator, thanks to which we have been able to study a system of coupled oscillators. Finally, it has been possible to determine the time evolution of a Gaussian wave function when its width has been initially modified, as well as the effect induced by a periodic external force in a simple and fun way.

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