Dynamics of a quantum particle constrained to a circle

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Abstract: In this work, we study the tunneling of a quantum particle using the instanton method. As a starting point, we consider the double well potential, then we extend the results to a periodic potential and compare them to a particle constrained to a circle. Lastly, we test the non-perturbative approach of the method, and we discuss the coupling through a specific, parameter-dependent, periodic potential.

I. INTRODUCTION

Quantum physics has allowed us to tackle previously unsolvable problems and has given us an explanation for behaviors considered impossible through classical physics. One of these is Quantum Tunneling [1]. This phenomenon is what allows a particle to surpass a potential barrier when its energy is lower than that of the barrier. We will focus on one of the strongest methods for computing such transitions. It is known as the instanton method, based on Feynman path integrals [2].

This technique is unique because of its non-perturbative approach and because it is easy to generalize for arbitrary dimensions and to retrieve the classical limit [3]. We make use of instantons, finite action solutions that join our tunneling points and, in Euclidean space, are classical solutions to our set of equations.

The double well potential will serve as an introduction to this methodology and, using its results, we will focus on the periodic potential. This potential is one with many applications and present in interesting phenomenons. A particle inside a crystal lattice is described by such potential [4]. It is the one used to constrain a particle to a circle [3, 5] and it is also responsible for the Yang-Mills vacuum [6].

We will analyze the ground state of a particle in such potential and the energy splitting that occurs. We will also discuss the case of a particle in a circle and compare it to the regular periodic potential. Finally, a detailed study for a specific periodic potential with a parameter dependence that represents the coupling will also be done, manifesting the non-perturbative advantage of the instanton method.

II. PATH INTEGRALS

Our goal is to study the propagator operator, also known as transition amplitude, that joins the initial state at time t_i with the final state at time t_f using the path integral method. We will use this to evaluate how likely it is for a particle to tunnel through a potential barrier. This propagator takes the form [2]:

$$\hat{U} = A \int Dx e^{\frac{i}{\hbar} S[x]}, \tag{1}$$

where A is a constant independent of the dynamics of the system and Dx is an integral over all intermediate coordinates while maintaining fixed the beginning and end points. Therefore, Dx represents the sum over all paths. $S[x]$ is the action, namely:

$$S[x] = \int_{t_i}^{t_f} \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) dt, \tag{2}$$

where as usual $\dot{x} = dx/dt$ and $V(x)$ is the potential.

The exponential in Eq. (1) represent the weight of the contribution of a path. The paths that contribute the most are the ones surrounding the classical path [7], for which $\frac{\delta S[x]}{\delta x(t)} = 0$. Thus, we will use the saddle point approximation around such path. Hence, the first step will be to find this classical path that joins our beginning and end points.

III. DOUBLE WELL POTENTIAL

A. One Instanton

Now let us apply this method to the double well potential,

$$V(x) = \frac{m\omega^2}{8a^2}(x^2 - a^2)^2, \tag{3}$$

where m is the mass of the particle, ω is the frequency of an harmonic oscillator and a is a constant. We are assuming that our particle has an energy $E < V_b$, where $V_b = m\omega^2 a^2/8$ is the maximum value of the barrier.

But, as we can see in *Fig. 1*, the potential $V(x)$ does not have any classical paths that join the wells. In order to surpass this inconvenience, we will perform a change of variables so that $t \to -i\tau$. This is what is known as the *Wick Rotation* and consists of going from the Minkowski space to the Euclidean space [8]. With this change, our

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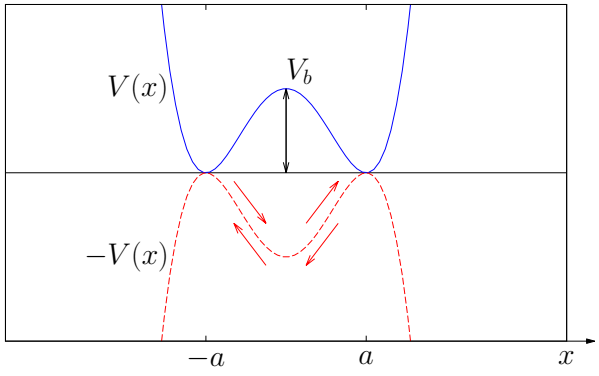

FIG. 1: Double well potential.

Euclidean action can be written as:

$$S_E[x] = \int_{-T/2}^{T/2} \left(\frac{1}{2}m\dot{x}^2 + V(x)\right) d\tau, \tag{4}$$

$$\hat{U}_E = \langle x_f | e^{-\frac{1}{\hbar}HT} | x_f \rangle = A \int Dx\, e^{-\frac{1}{\hbar}S_E[x]}. \tag{5}$$

Notice that now $\dot{x} = dx/d\tau$ and the initial and final time are $-T/2$ and $T/2$ respectively.

We can see that in the transition amplitude instead of an oscillating function we have a decaying exponential. Also, the action has the same expression as in Eq. (2) but with $V(x) \to -V(x)$. This way, as seen in *Fig. 1*, we now have a classically allowed trajectory that joins $-a$ and a and can be calculated using:

$$\frac{\delta S_E[x]}{\delta x(\tau)} = 0 \;\longrightarrow\; m\ddot{x} - V'(x) = 0, \tag{6}$$

where $V'(x) = dV(x)/dx$. Here we obtain three types of solutions, the two stationary $x_{cl}(\tau) = \pm a$, which are of no interest to us, and the non trivial:

$$x_{cl}(\tau) = \pm a \tanh \frac{\omega(\tau - \tau_c)}{2}. \tag{7}$$

The arbitrary constant τ_c is related to a translation symmetry [9]. Let us calculate the action of our classical solution (7):

$$S_0 \equiv S_E[x_{cl}] = \int_{\mp a}^{\pm a} dx \left(\mp\sqrt{2mV(x)}\right) = \frac{2}{3}m\omega a^2. \tag{8}$$

The solutions (7), represented by arrows in *Fig. 1*, which we have shown to have finite action, are known as the instanton (from $-a$ to a) or anti-instanton (from a to $-a$) solutions. They also have a short temporal extension, $\Delta\tau \sim 1/\omega$ [7], that's why they are called instantons, because the solution is localized in time.

As we have stated before, this solution represents the maximum contribution to the transition amplitude, followed by the ones close to it. So let us describe the surrounding trajectories with $x(\tau) \approx x_{cl}(\tau) + \eta(\tau)$, and calculate the contribution to the transition amplitude from one instanton [7, 9, 10].

$$\langle a | e^{-\frac{1}{\hbar}HT} | -a \rangle = \frac{A}{\sqrt{det\left(\frac{1}{\hbar}\left(-m\frac{d^2}{d\tau^2} + V''(x_{cl})\right)\right)}} e^{-\frac{1}{\hbar}S_0}$$
$$= \Lambda e^{-\frac{\omega T}{2}} \frac{1}{2}\omega_s \int_{-T/2}^{T/2} d\tau_c. \tag{9}$$

Here we have defined:

$$\Lambda = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \tag{10}$$

$$\omega_s = 2\omega\sqrt{\frac{6}{\pi}}\sqrt{\frac{S_0}{\hbar}} e^{-\frac{1}{\hbar}S_0}, \tag{11}$$

both constants depend only on the potential. Λ has units of m^{-1} and ω_s has the same units as ω, thus s^{-1}. The expression for the anti-instanton is exactly the same.

B. Multi-instantons contributions

A succession of instantons and anti-instantons can contribute to the transition amplitude as well. We can take advantage of the usually used dilute gas approximation where, considering the short temporal extension of an instanton, we can say that they don't overlap and, thus, there aren't too many instantons in a finite time [9].

If we consider n (anti)instantons, the integration of $d\tau_c$ of Eq. (9) becomes $T^n/n!$ and the factor $\frac{1}{2}\omega_s$ is also elevated to the n^{th} power, thus [7, 10]:

$$\langle a | e^{-\frac{1}{\hbar}HT} | -a \rangle = \frac{\Lambda}{n!}\left(\frac{\omega_s T}{2}\right)^n e^{-\frac{\omega T}{2}}. \tag{12}$$

Let us note that only an even number of (anti)instantons contribute to the transition form a to a or from $-a$ to $-a$. Whereas we need and odd number for the transition from a to $-a$ or vice versa.

Taking the total transition amplitude as a sum over all $n > 0$ and using the appropriate Taylor expressions we get:

$$\langle a | e^{-\frac{1}{\hbar}HT} | a \rangle = \Lambda e^{-\frac{\omega T}{2}} \cosh\left(\frac{\omega_s T}{2}\right), \tag{13}$$

$$\langle a | e^{-\frac{1}{\hbar}HT} | -a \rangle = \Lambda e^{-\frac{\omega T}{2}} \sinh\left(\frac{\omega_s T}{2}\right). \tag{14}$$

C. Energy splitting

The instanton method allows us to retrieve the energy of the system. Let us discuss what we expect the situation to be.

If we neglect tunneling, we would obtain a degenerate ground state with energy $E_0 = \frac{1}{2}\hbar\omega$. This is the lowest energy for a wave function in the bottom of one well and, since we have two, it is two times degenerate. This is the same as if we had the two wells very far apart, with the wave function for the right and left well being ψ_R and ψ_L respectively.

When we start taking tunneling into account, the energy level E_0 will split into two. Following the tight binding approximation, the resulting wave functions are the two linear combinations of the left and right ones, the symmetric and antisymmetric, $\psi_S = \frac{1}{\sqrt{2}}(\psi_R + \psi_L)$ and $\psi_A = \frac{1}{\sqrt{2}}(\psi_R - \psi_L)$. As ψ_S has no nodes, so we can expect it to have the lowest energy E_- and be the true ground state. Therefore, ψ_A will be the first excited state with energy E_+ [9].

To calculate this splitting, we will rewrite the transition amplitude with the corresponding eigenstates ψ_S and ψ_A, and we will identify the two energy levels:

$$\begin{aligned}&\langle a|e^{-\frac{1}{\hbar}HT}|-a\rangle \\ &= \langle a|\psi_S\rangle\langle\psi_S|-a\rangle e^{-\frac{1}{\hbar}E_-T} + \langle a|\psi_A\rangle\langle\psi_A|-a\rangle e^{-\frac{1}{\hbar}E_+T}.\end{aligned} \tag{15}$$

We can rewrite Eq. (13) and Eq. (14) as

$$\langle a|e^{-\frac{1}{\hbar}HT}|a\rangle = \frac{\Lambda}{2}\left(e^{-\frac{1}{2}(\omega-\omega_s)T} + e^{-\frac{1}{2}(\omega+\omega_s)T}\right), \tag{16}$$

$$\langle a|e^{-\frac{1}{\hbar}HT}|-a\rangle = \frac{\Lambda}{2}\left(e^{-\frac{1}{2}(\omega-\omega_s)T} - e^{-\frac{1}{2}(\omega+\omega_s)T}\right), \tag{17}$$

respectively.

Now, from our instanton results, we can clearly see that $E_\pm = \frac{1}{2}\hbar(\omega \pm \omega_s)$. We can also compute the energy splitting $\Delta E = E_+ - E_- = \hbar\omega_s = 2\omega\sqrt{6/\pi}\sqrt{S_0\hbar}\,e^{-\frac{1}{\hbar}S_0}$.

IV. PERIODIC POTENTIAL

In this section we will apply the previous results to a particle with energy E in a periodic potential where we consider $E < V_b$. It can be thought of as a number of double wells joined, thus the discussions and results from section 3 will come in handy.

For now, we will not focus on the exact expression of the potential. We will present our results for a general periodic potential with a period of a, as seen in *Fig. 2*, $V(x) = V(x + na)\ \ \forall n$. Note that in previous sections the distance between wells was $2a$, now it will be a, this will only affect ω_s that now will always be divided by 2. All the results have been expressed with these constants calculated with:

$$m\omega^2 = V''(na) \quad \forall n, \tag{18}$$

$$S_0 = \int_{na}^{(n+1)a} dx\sqrt{2mV(x)} \quad \forall n. \tag{19}$$

A. Particle in a periodic potential

In contrast to the double well, in this potential any number of instantons and anti-instantons contribute to the transition amplitude as long as they start and end in the fixed points, let it be $x_i = na$ and $x_f = ma$. We can quantify this by saying that for q instantons and q' anti-instantons they must satisfy $q - q' = m - n$. Using Eq. (12) and remembering Eqs. (10) and (11), we get [9]:

$$\begin{aligned}&\hat{U}_E(ma, na; T) \\ &\quad = \Lambda\sum_{q=0}^{\infty}\sum_{q'=0}^{\infty}\frac{\delta_{q-q',m-n}}{q!q'!}\left(\frac{\omega_s T}{4}\right)^{q+q'} e^{-\frac{\omega T}{2}}.\end{aligned} \tag{20}$$

By using $\delta_{j,k} = \int_0^{2\pi} d\theta e^{i(j-k)\theta}/2\pi$, it gives [9]:

$$\hat{U}_E(ma, na; T) = \Lambda e^{-\frac{\omega T}{2}}\int_0^{2\pi}\frac{d\theta}{2\pi}e^{-i(n-m)\theta}e^{\frac{\omega_s T}{2}\cos\theta}. \tag{21}$$

B. Energy bands

In the case of the double well we have seen how without tunneling our ground state is two times degenerate. For the infinite number of wells of the periodic potential, it makes sense for it to be infinitely degenerate with the same energy $E_0 = \frac{1}{2}\hbar\omega$. Furthermore, when we consider tunneling effects, we can expect not two but an infinite number of energy levels, namely, a continuous energy band [11]. So with tunneling, our infinitely degenerate ground state will split into an energy band.

Then, similarly to the double well, the corresponding eigenstates will also be a linear combination of the individual wave packets $u_0(x)$:

$$\psi_\theta(x) = \sum_{N=-\infty}^{\infty} e^{iN\theta}u_0(x - Na), \tag{22}$$

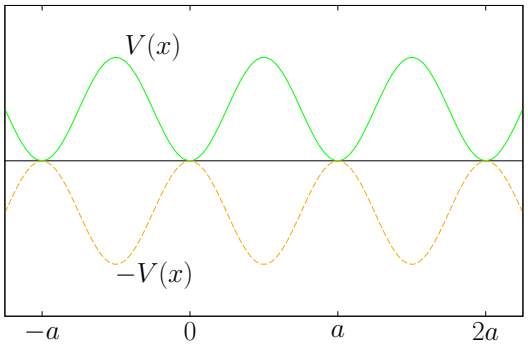

FIG. 2: Periodic potential.

where it is chosen so $\psi_\theta(x+a) = e^{i\theta}\psi_\theta(x)$.

Also as *Bloch's theorem* [11] states, the wave function in a periodic potential must fulfil:

$$\psi_k(x) = e^{ikx}v_k(x), \tag{23}$$

where $k = p/\hbar$ and $v_k(x)$ is periodic under a displacement of $x = a$. So for our case $\psi_k(x+a) = e^{iak}\psi_k(x)$. If we compare this to the expression below Eq. (22), we can identify $ka = \theta$ [3].

If we analyze Eq. (21), we can identify this energy band. So the energy eigenvalues for the lowest band are:

$$E_0(\theta) = \frac{1}{2}\hbar\left(\omega - \omega_s\cos\theta\right). \tag{24}$$

Let us discuss now how we know this band is the lowest energy one. When we express the transition amplitude as exponentials, similarly to what we did in Eq. (15), we now get:

$$\begin{aligned}\langle ma|e^{-\frac{1}{\hbar}HT}|na\rangle &= \sum_i \langle ma|\phi_i\rangle\langle\phi_i|na\rangle e^{-\frac{1}{\hbar}E_iT} \\ &= \sum_k |v_k(0)|^2 e^{ik(n-m)a}e^{-\frac{1}{\hbar}E_pT}.\end{aligned} \tag{25}$$

In the large T limit, the sum of the first result in Eq. (25) will be dominated by the terms with the lowest E_i, namely, the lowest energy band. For this reason, when we made specific calculations beginning Eq. (8), we already had this in mind. It was in order to study the ground state of a particle in this potential or in any other.

If we take a look at the final expression (25), where we have used the Bloch states (23), and we compare it to Eq. (21) we can identify, since k is symmetric, $\theta = ka$, the same as before. Thus, we have given a physical meaning to θ, it is the quasi momentum times the period of the potential [9].

C. Particle constrained to a circle

Let us analyze more carefully this case and compare it to the periodic potential. The only free coordinate is $\varphi(t)$ where $0 < \varphi < 2\pi$ and 0 and 2π are identified. Still, the Lagrangian remains $L = \frac{1}{2}m\dot{\varphi}^2 - V(\varphi)$ and the classical solution will also be the same. The only difference will be in the energy levels because we have reduced considerably the coordinate space, changing the boundary conditions.

We realize that, since $\varphi_i = 0$ and $\varphi_f = 2\pi$ are the same point, they must have the same wave function $\psi(2\pi) = \psi(0)$ and if we look at the expression below Eq. (22), we can see that now $\theta = 0$. Hence, we can use the energy band in Eq. (24) with this in mind, and we get [3]:

$$E_0 = \frac{1}{2}\hbar(\omega - \omega_s), \tag{26}$$

We can also more simply express the transition amplitude using Eq. (21) and we get [3]:

$$\langle 2\pi|e^{-\frac{HT}{\hbar}}|0\rangle = \Lambda e^{-\frac{1}{2}\omega T + \frac{\omega_s}{2}T}. \tag{27}$$

It can be counter-intuitive to talk about instantons and tunneling from the same physical space to itself, but when a particle does one or multiple rotations, it is overcoming potential barriers and those contributions can be viewed as tunneling effects.

If we change the Lagrangian to $L = \frac{1}{2}m\dot{\varphi}^2 - V(\varphi) - \frac{\theta_0}{2\pi}\frac{d\varphi}{dt}$ the physics doesn't change, but the action will have an imaginary part that will become a cosine, and we will eventually recover the same expression (24) of the periodic potential for a particle in a circle with the change $\theta \to \theta_0$ [3]. The difference is that θ_0 is a fixed constant, whereas θ was a continuum of numbers. Thus, we will have one energy level that we can alter with θ_0 instead of the whole band, this is consistent with the reduction of the configuration space.

V. DISCUSSION OF A PARTICULAR CASE

Now let us apply all these results to a specific periodic potential. We will construct this potential with a dependence of two parameters V_0, that represents the height of the barrier the particle has to overcome, and β, that is related to the spacing between wells.

$$V(x) = \frac{1}{2}V_0(1 - \cos\beta x). \tag{28}$$

We will express both parameters using only one, g, that will represent the coupling of the wells. We choose $\frac{1}{2}V_0 = \frac{m^2\omega^4}{g}$ and $\beta = \sqrt{\frac{g}{m\omega^2}}$ so that (18) is satisfied and Λ doesn't change:

$$V(x) = \frac{m^2\omega^4}{g}\left(1 - \cos\left(\sqrt{\frac{g}{m\omega^2}}x\right)\right), \tag{29}$$

with a period of $2\pi\sqrt{m\omega^2/g}$.

If we expand this potential for g small, we get: $V(x) \approx \frac{1}{2}m\omega^2x^2 - \frac{1}{4!}gx^4$. But we will use the instanton method to calculate the splitting and transition amplitude for any value of g, not just the small ones. We can foresee that for g small we will have completely unconnected wells with tall barriers and large separation. For $g \to \infty$, $V(x)$ will be constant, and therefore no tunneling is expected. Let's prove this.

Using Eq. (19) we get $S_0 = 8m^2\omega^3/g$. Substituting this into the expression for ω_s:

$$\omega_s = 2\omega\sqrt{\frac{6}{\pi}}\sqrt{\frac{8m^2\omega^3}{g\hbar}}e^{-\frac{8m^2\omega^3}{g\hbar}}. \tag{30}$$

If we make $g \to \infty$ in this expression, the exponential goes to one, but the square root makes it go to zero. For the limit going to zero, the exponential is the one that dominates, making ω_s go to zero.

If we look at the transition amplitude in Eq. (21) we have seen that in the limit $g \to \infty$, ω_s goes to zero, making the exponential containing it go to one and the

θ integral go to zero for $m \neq n$. So the whole expression is zero for a constant potential, as expected. In the limit $g \to 0$, ω_s goes to zero too, making the transition amplitude zero, as we expected. For the energy band:

$$E_0(\theta) = \frac{1}{2}\hbar\omega\left(1 - 2\sqrt{\frac{6}{\pi}}\sqrt{\frac{g_0}{g}}e^{-\frac{g_0}{g}}\cos\theta\right), \qquad (31)$$

where $g_0 = 8m^2\omega^3/\hbar$. The factor multiplying the cosine is ω_s/ω, and it gives us an idea of the splitting that our potential has. Thus, when g is too small or too big, $\omega_s(g)$ should be zero. Let us plot this factor to see the that our method works for any g. For simplicity, we will plot ω_s/ω against g/g_0, both dimensionless.

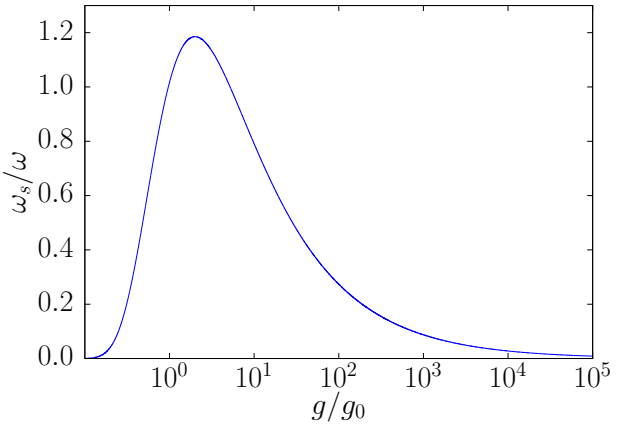

FIG. 3: Factor ω_s/ω as a function of g/g_0.

If we look at *Fig. 3* we can see how we have obtained the expected result. For g small we get no splitting, as our wells are just infinite harmonic potentials, and for $g \to \infty$ our coupling parameter vanishes too. We can see how the instanton method allows us to discuss this situation without imposing any restriction in g. We can also see that the maximum value of $\omega_s/\omega \approx 1,19$ for $g/g_0 = 2$.

VI. CONCLUSIONS

We have seen how useful the instanton method can be to compute the transition amplitude and the energy splitting in a system where tunneling is relevant. To compute the path integral, we started performing a *Wick Rotation* in order to find a classical path to which to make the saddle point approximation from. We used this method for the double well, obtaining expressions for the transition amplitude and energy splitting.

Then, we proceeded with the periodic potential. We used our previous results for the computation of the transition amplitude and the energy splitting of the ground state. We extended the results to a particle in a circle. In the periodic potential, we found that the lowest energy level splits into a continuous energy band dependent on θ. Whereas with a particle in a circle, the energy band takes only one value, $\theta = 0$, due to the reduction of available coordinates. We also saw that we can modify the Lagrangian and obtain a different, but still fixed, value of θ.

Finally, we applied all the above for a specific, parameter-dependent, periodic potential. We parameterized this potential in a way that allowed us to study the coupling, and we proved that the instanton method is suitable for problems where a non-perturbative approach is required. We computed the energy splitting without imposing our parameter to be small, and we obtained the expected results.

VII. ACKNOWLEDGMENTS

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