Quantum diffusion on a cyclic one dimensional lattice

A. C. de la Torre, H. O. Martín, D. Goyeneche
Departamento de Física, Universidad Nacional de Mar del Plata
Funes 3350, 7600 Mar del Plata, Argentina
dltorre@mdp.edu.ar
(April 1, 2022)

Abstract

The quantum diffusion of a particle in an initially localized state on a cyclic lattice with $N$ sites is studied. Diffusion and reconstruction time are calculated. Strong differences are found for even or odd number of sites and the limit $N \to \infty$ is studied. The predictions of the model could be tested with micro- and nanotechnology devices.

I. INTRODUCTION

The problem of a classical particle performing a random walk in various geometrical spaces\textsuperscript{1} and the quantum random walk\textsuperscript{2} have been thoroughly studied and compared. The classical and quantum cases have striking differences. One of these differences is that, whereas the classical spread increases with time as $\sqrt{T}$, in the quantum case we have a stronger linear time dependence of the width of the distribution. In the quantum mechanical case, we can identify two different causes for the spreading of the probability distribution describing the position of a particle. There is a spreading of the distribution caused by the random walk itself, also present in the classical case, and superposed to it, there is the quantum mechanical spreading of the probability distribution due to the time evolution of a particle in a localized state. This second type of spreading is the main interest of this contribution. For this study, we will consider a quantum mechanical particle initially localized in one site of a one dimensional cyclic lattice with $N$ points. In most treatments of quantum random walks in a lattice it is assumed that the number of sites, $N$, is large compared with the number of jumps of the time evolution and therefore the system does not notice whether the lattice is infinite or cyclic, that is, finite with periodic boundary conditions. In our analysis we will not assume that $N$ is large and we will find some peculiar
and interesting features like, for instance, a very different behaviour for even or odd values of $N$. There are several motivations, besides the general academic interest, for allowing low values of $N$. For instance, cyclic lattices with a few sites have been built (quantum corrals) with nanofabrication techniques and in quantum computers we deal with systems with $N = 2$ (qubits) or $N = 3$ (quptrits). In all these cases we may be interested in the quantum diffusion time of an initially localized state. The quantum behaviour in the continuous case $N \to \infty$ is also interesting because it can be experimentally tested building small conducting rings with microfabrication techniques.

II. DEFINITION OF THE MODEL

In this work we will consider a particle moving in a one dimensional periodic lattice with $N$ sites and lattice constant $a$ represented in Figure 1. The quantum mechanical treatment\(^3\) of this system requires an $N$ dimensional Hilbert space $\mathcal{H}$. The lattice sites will be labelled by an index $x$ running through the values $0, 1, \ldots, N - 1$. We will adopt a very useful notation for the principal $N^{th}$ root of the identity defined by

$$\omega = e^{i \frac{2\pi}{N}}. \quad (1)$$

Integer powers of this quantity build a cyclic group with the important property

$$1 = \omega^{Nn}, \forall n = 0, \pm 1, \pm 2, \cdots. \quad (2)$$

The position of the particle in the lattice can take any value (eigenvalue) $a(x - j)$ where $a$ has units of length, $j = (N - 1)/2$ and the integer number $x$ can take any value in the set $\{0, 1, \cdots, N - 1\}$. The eigenvalues have been chosen in a way that position can take positive or negative values in the interval $[-aj, aj]$. Notice that $j$ is integer for odd $N$ and half-odd-integer if $N$ is even. The state of the particle in each position is represented by a Hilbert space element $\varphi_x$ and the set $\{\varphi_x\}$ is a basis in $\mathcal{H}$. In the spectral decomposition, we can write the position operator $X$ as

$$X = \sum_{x=0}^{N-1} a(x - j) \varphi_x \langle \varphi_x, \cdot \rangle, \quad (3)$$

that clearly satisfies $X \varphi_x = a(x - j) \varphi_x$. Momentum is formalized in the Hilbert space by means of a basis $\{\phi_p\}$, unbiased to the position basis, where $p$ is an integer number that can take any value in the set $\{0, 1, \cdots, N - 1\}$. The momentum operator is given in terms of its spectral decomposition as
\[ P = \sum_{p=0}^{N-1} g(p-j) \langle \phi_p, \cdot \rangle \phi_p \]  

where \( g \) is a constant with units of momentum. The eigenvalues of \( P \) have been defined in a way to allow for movement of the particle in both directions, anti-clockwise (positive eigenvalues) and clockwise (negative eigenvalues) along the circular lattice. Notice however that the state of zero momentum is only possible when \( N \) is odd. We will find in this work that there are several important differences in the system when \( N \) is even or odd.

The position and momentum bases are related by a unitary transformation similar to the Discrete Fourier Transform

\[ \varphi_x = \frac{1}{\sqrt{N}} \sum_{p=0}^{N-1} \omega^{-(p-j)(x-j)-\alpha(x-p)} \phi_p \]  

and

\[ \phi_p = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \omega^{(p-j)(x-j)+\alpha(x-p)} \varphi_x \]  

with

\[ \langle \varphi_x, \phi_p \rangle = \frac{1}{\sqrt{N}} \omega^{(p-j)(x-j)+\alpha(x-p)} \]  

where \( \alpha \) is a parameter such that

\[ \alpha = \begin{cases} 0 & \text{for } N \text{ odd,} \\ \frac{1}{2} & \text{for } N \text{ even.} \end{cases} \]  

The constants \( a \) and \( g \) are not independent but are related by

\[ agN = 2\pi \]  

This condition follows from the requirement that in the limit \( N \to \infty \) the commutation relation of position and momentum should be \([X, P] \to i\) (we adopt units such that \( \hbar = 1 \)). Notice that for finite \( N \), the commutation relation \([X, P] = i\) is impossible.

All these definitions are compatible with the physical requirement that momentum is the generator of translation and position generates increase in momentum. That is,

\[ e^{-iaP} \varphi_x = \omega^\alpha \varphi_{[x+1]} \]
\[ e^{igX} \phi_p = \omega^\alpha \phi_{[p+1]} \]  

where the symbol \([\cdot]\) denotes modulo \( N \), that is, \([N] = 0\). Notice that an \( N \)-fold application of these translation operators is equal to the identity 1 if \( N \) is odd but is equal to \(-1\) if \( N \) is even. This is reminiscent of a \( 2\pi \) rotation of a spin 1/2 system.
In equations (5), (6) and (7) we could absorb the phases $\alpha x$ and $\alpha p$ in the bases $\{\varphi_x\}$ and $\{\phi_p\}$ by an appropriate phase transformation (this is only relevant for even $N$ because $\alpha \neq 0$). However this option would result in a complication of Eqs. (10) where the phase $\omega^\alpha$ would not appear but a sign change would appear in the translation from site $x = N - 1$ to site $x = 0$ and also from $p = N - 1$ to $p = 0$ loosing thereby the homogeneity of the lattice because not all lattice sites would be equivalent. Later in this work it will be convenient to take this option.

**III. SPREADING OF A LOCALIZED STATE AND DIFFUSION TIME**

At any instant of time, the state of the particle will be determined by a Hilbert space element $\Psi(t)$ that in the position representation is given by the coefficients $c_x(t)$ such that

$$\Psi(t) = \sum_{x=0}^{N-1} c_x(t) \varphi_x .$$

A given state $\Psi(0)$ at an initial time $t = 0$ will evolve according to the time evolution unitary operator given in terms of the hamiltonian $H$ as

$$U_t = \exp(-iHt) .$$

In this work we are interested in the time evolution of a state corresponding to a particle initially localized in a lattice site, say at $x = 0$, at rest, that is, with $\langle P \rangle = 0$. Such a state is given by $\Psi(0) = \varphi_0$, that is, $c_x(0) = \delta_{x,0}$. Let us assume a free particle with hamiltonian $H = P^2/2m$. With this hamiltonian we can easily find that the state for any time will be given by

$$c_x(T) = \frac{1}{N} \sum_{p=0}^{N-1} \omega^{(x(p-j+\alpha)-(p-j)^2T)},$$

where we have introduced a dimensionless time parameter $T = t/\tau$ with a time scale $\tau$ defined by

$$\tau = \frac{2ma}{g} ,$$

that, as we will see later, corresponds essentially to the diffusion time. We have chosen the free particle hamiltonian, however many of the following results do not depend on the specific form of this hamiltonian and are also valid for any hamiltonian invariant under the transformation $P \rightarrow -P$. During the time evolution of a particle, initially in the site $x = 0$,
the expectation value of the position and momentum will remain zero, \( \langle X \rangle = \langle P \rangle = 0 \) but, due to the quantum spreading of the state, the probability distribution of the occupation of other lattice sites will grow. We will study some features of this quantum diffusion. The probability of occupation of the lattice site \( x \) at time \( T \) is given by

\[
|c_x(T)|^2 = \frac{1}{N^2} \sum_{p=0}^{N-1} \sum_{q=0}^{N-1} \omega^{(p-q)x-(p-q)(p+q-2)T}.
\] (15)

One of the sums can be analytically performed after a change of the summation indices but it is not really convenient to do it.

Due to the periodicity of the lattice, we expect that the amplitudes and probabilities of Eqs.(13) and (15) will be periodic in time. This is indeed the case but with different periodicity for \( N \) even or odd. That is, for the amplitude we have

\[
c_x(T) = \begin{cases} 
c_x(T + N) & \text{for } N \text{ odd} \\
c_x(T + 4N) & \text{for } N \text{ even} \end{cases},
\] (16)

and for the probability we get

\[
|c_x(T)|^2 = \begin{cases} 
|c_x(T + N)|^2 & \text{for } N \text{ odd} \\
|c_x(T + N/2)|^2 & \text{for } N \text{ even} \end{cases}.
\] (17)

It is remarkable that the period of the amplitude is equal to the period of the probability for \( N \) odd, but it is eight times longer if \( N \) is even. The periodicity shown in Eqs.(16) and (17) correspond to our particular initial state but it follows essentially from the hamiltonian and the cyclic relation (2) and therefore this periodicity is also valid for arbitrary states and probabilities.

From the symmetry of the lattice and of the initial state we expect that the particle will diffuse with equal probability clockwise or anti-clockwise, that is, \( |c_{N-x}(T)| = |c_x(T)| \) but for the amplitude we may have a different phase on both sides of the initial position. We will now show that the amplitude on lattice points symmetric with respect to the initial position \( x = 0 \) are related by

\[
c_{N-x}(T) = \omega^{-2\alpha x}c_x(T).
\] (18)

In order to prove this, consider

\[
c_{N-x}(T) = \frac{1}{N} \sum_{p=0}^{N-1} \omega^{N(p-j+\alpha)-x(p-j+\alpha)-(p-j)^2T}.
\] (19)

Using (2) we eliminate \( N(p - j + \alpha) \) in the exponent and we add \( Nx \). Therefore
\[ c_{N-x}(T) = \frac{1}{N} \sum_{p=0}^{N-1} \omega^{(x(N-p+j+\alpha)-(p-j)^2T)} . \] (20)

Now we define another summation index \( q = N - p \) with values in \( \{N, N-1, \ldots, 1\} \).

\[ c_{N-x}(T) = \frac{1}{N} \sum_{q=1}^{N} \omega^{(x(q+j+\alpha)-(N-q-j)^2T)} . \] (21)

Since \( N = 2j + 1 \), the squared parenthesis in the exponent becomes \( (q - 1 - j)^2 \). Then

\[ c_{N-x}(T) = \frac{\omega^{x(1+2j-2\alpha)}}{N} \sum_{q=1}^{N} \omega^{(x(q-1-j+\alpha)-(q-1-j)^2T)} . \] (22)

Finally, redefining the summation index \( p = q - 1 \) and using again (2), we find that the right hand side of this equation is \( \omega^{-2\alpha c_{x}(T)} \). A remarkable consequence of relation (18) is that, for even \( N \), a quantum particle in a localized state will never diffuse to the antipode location. The antipode location, \( x = N/2 \), exists only for even \( N \). The proof follows from Eq.(18) since we have \( c_{N-N/2} = \omega^{-N/2}c_{N/2}, \) but \( \omega^{-N/2} = -1 \) therefore \( c_{N/2} = -c_{N/2} \). That is,

\[ c_{N/2}(T) = 0 \ \forall \ T . \] (23)

This is a remarkable result that can be checked by explicit evaluation from Eq.(13) redefining the summation index \( q = p - j \) running from \(-j\) to \( j \). Doing this we obtain a sum whose terms are anti-symmetric under \( q \to -q \); therefore they add to zero. Another physically appealing proof of this result is provided by Feynman’s “sum over paths” method.\(^4\) In this case, a path contributing to the probability amplitude for the transition from \( x = 0 \) at \( t_i \) to \( x = N/2 \) at \( t_f \) is defined by a set \( \{x_k; t_k\} \) for each partition of the time interval \( t_i < t_k < t_f \). It turns out that for each path \( \{x_k; t_k\} \) going from \( x = 0 \) to \( x = N/2 \) there is another path \( \{z_k; t_k\} \), symmetric with respect to \( x = 0 \), that is, \( z_k = N - x_k \) but with the same values of \( \{t_k\} \), that cancels its contribution to the probability amplitude, simply because \( dz_k = -dx_k \).

In the case \( N = 2 \), besides the initial location, there is only one remaining location, the antipode. Therefore, for all time, the particle will remain in its initial position. Clearly, for \( N = 2 \) the states \( \varphi_0 \) and \( \varphi_1 \) are not only position eigenvectors but also eigenstates of the hamiltonian and therefore they are stationary states. For odd values of \( N \) the antipode does not exists but we can study the transition probability to diffuse to the “farthest” locations \( x = (N \pm 1)/2 \). We will later see a remarkable difference in the odd-\( N \) case. We will see that, contrary to what happens in the even case in which the antipodes are never reached, if \( N \) is odd a sharp distribution will build up in an environment of the antipode at the time
$T = N/2$. This is precisely the time when the state is reconstructed in the $N$-even case but at the original site.

We will now calculate the **diffusion time**, that is, the time that is required for a particle, initially localized in one lattice site, to “diffuse” to the whole cyclic lattice. Since the state is periodic in time, with period proportional to $N$, we expect that the state reconstruction happens after the whole lattice is visited and therefore the diffusion time should be, at most, proportional to $N$. In order to calculate the diffusion time we must find the time dependence of the width of the probability distribution of position. It turns out that for finite $N$, or for periodic distributions, the quantities $\langle \Psi(t), X\Psi(t) \rangle$ and $\langle \Psi(t), X^2\Psi(t) \rangle - \langle \Psi(t), X\Psi(t) \rangle^2$ are not appropriate estimates for the center $\overline{X}$ and width $\Delta$ of the distribution along a cyclic lattice or ring. The main reason why they are not appropriate is that any physical quantity in a cyclic lattice should be periodic, that is, invariant under $x \to x + Na$ and clearly the quantity $\langle \Psi(t), X\Psi(t) \rangle$ does not complies to this. Two simple examples: first, let us suppose a distribution given by $|c_{N-1}|^2 = |c_0|^2 = |c_1|^2 = 1/3$. Clearly the center of the distribution is at the location corresponding to the label $x = 0$, that is, at the position $-aj = -a(N-1)/2$, but the quantity $\langle \Psi(t), X\Psi(t) \rangle$ is $\sum_{x=0}^{N-1} a(x-j)|c_x|^2 = -a(N-3)/6$. For another example, consider a uniform distribution that fills completely a ring. In our case of a cyclic lattice we have $|c_x|^2 = 1/N, \forall x$. Clearly, this distribution **does not have a center**; it should be undefined on the ring because all points are equivalent, but the quantity $\langle \Psi(t), X\Psi(t) \rangle$ is $\sum_{x=0}^{N-1} a(x-j)|c_x|^2 = 0$.

The problem of defining the center $\overline{X}$ and width $\Delta$ of a distribution in a ring or cyclic lattice has been solved using the concept of the **centroid** of a distribution on a ring. Let us build a map of the ring into a unit circle in the complex plane. In order to define the centroid $Z$ for a probability distribution $|c_x|^2$ on the sites $x = 0, 1, \cdots, N-1$ of a cyclic lattice, let us consider the unit circle in the complex plane with $N$ points located at $\omega^x$. The centroid of the distribution is a complex number $Z = \rho e^{i\theta}$ given by

$$Z = \rho e^{i\theta} = \sum_{x=0}^{N-1} \omega^x|c_x|^2. \quad (24)$$

The radial projection of the centroid on the unit circle maps the center of the distribution on the ring. Therefore,

$$\overline{X} = a\left(\frac{\theta}{2\pi}N - j\right), \quad \text{ (25)}$$

and the width $\Delta$ of the distribution is given by

$$\Delta^2 = (aN)^2(1 - |Z|^2), \quad \text{(26)}$$
where the factor $aN$ has been chosen such that for a uniform distribution covering the whole lattice ($Z = 0$) the width of the distribution is equal to the size of the lattice. Notice that when only one site is occupied, the width is zero. These definitions are clarified in an example shown in Figure 2.

We can now study the time dependence of the width for our initial condition of a particle at rest, localized in $x = 0$. Let us calculate first the centroid. From Eqs.(24) and (15) we obtain

$$Z = \frac{1}{N^2} \sum_{p=0}^{N-1} \sum_{q=0}^{N-1} \sum_{x=0}^{N-1} \omega^x \omega^{(p-q)x-(p-q)(p+q-2j)T}.$$  \hspace{1cm} (27)

The sum over $x$ can be performed:

$$\sum_{x=0}^{N-1} \omega^{(p-q+1)x} = N(\delta_{q,p+1} + \delta_{q,0}\delta_{p,N-1}).$$  \hspace{1cm} (28)

The first term of the parenthesis corresponds to the vanishing of the exponent of $\omega$ and the second term is for the case when the exponent is equal to $Nx$. With the Kronecker deltas we perform the sum over $q$, and the remaining sum over $p$ has a known result. We get then,

$$Z = \frac{1}{N} \left( \frac{\sin \left( \frac{2\pi}{N} (N - 1)T \right)}{\sin \left( \frac{2\pi}{N} T \right)} + 1 \right).$$  \hspace{1cm} (29)

As expected, the centroid has the same time periodicity as the probability distribution, that is, $N$ for odd number of lattice sites and $N/2$ for an even number of sites. Due to the initial condition of a particle in the site $x = 0$ and to the symmetric diffusion, the centroid is real at all times. The study of the time dependence of the centroid, shown in Figs. 3a and 3b for $N = 16$ and 17, allows a simple qualitative description of the time evolution of the distribution. In the figures we notice that the centroid oscillates most of the time with values close to zero, corresponding to distributions close to (but not necessarily equal to) uniform distributions covering the whole lattice. At time $T = N/2$ the centroid assumes the value of $Z = 1$ in the $N$-even case, as expected because at this time the initial state is reconstructed, and for odd $N$ it takes the value $-(N - 2)/N$, close to $Z = -1$ for large $N$, implying that at the time $T = N/2$ the distribution is concentrated at the antipodes of the initial location; however, precisely at the antipode there is no lattice site for odd $N$ and the state can not be reconstructed in one location. We see here a sharp distinction in the behaviour of diffusion in the even and odd case: the antipode is never reached in the $N$-even case but the distribution peaks in the neighbourhood of the antipode (at time $T = N/2$) in the $N$-odd case.
With the knowledge of the centroid, we can now calculate the time dependence of the width of the distribution. In particular we want to find the diffusion time $T_D$, that we define as the time when the width assumes its maximal value $aN$ for the first time. Notice that when the centroid vanishes, the width assumes its maximal value. From Eq.(29) we see that the centroid vanishes for $T = 1$ for all $N$, therefore the width is maximal ($aN$) at $T = 1$. However Eq.(29) has another root for a time $T$ smaller than 1 when $N > 4$. Of course, when $N = 2$ the diffusion time is infinite because the particle never diffuses out of the initial site. Summarizing we have

$$T_D = \begin{cases} 
\infty, & \text{for } N = 2 \\
1, & \text{for } N = 3 \\
\frac{N}{2(N-2)}, & \text{for } N \geq 4
\end{cases}$$  \hspace{1cm} (30)$$

It might at first seem strange that the defined diffusion time decreases towards a constant value $T_D = 1/2$ with an increasing number of sites $N$, but we can see that this is to be expected as a consequence of indeterminacy principle. Increasing the number of sites $N$ with the same initial condition of a particle in one site, is equivalent to a sharper localization of the initial state. This implies a wider momentum spread, responsible for a faster diffusion that decreases the diffusion time. The explicit time dependence of the width of the distribution is then given by

$$\Delta = a\sqrt{N^2 - \left(\frac{\sin\left(\frac{2\pi}{N}(N-1)T\right)}{\sin\left(\frac{2\pi}{N}T\right)} + 1\right)^2}.$$  \hspace{1cm} (31)$$

This quantity is zero at $T = 0$, grows with time, and takes the maximal value $aN$ at $T = T_D$; then it oscillates with values close to the maximal value except at time $T = N/2$ when the width becomes zero for $N$-even or decreases to $a2\sqrt{N-1}$ for odd $N$. At this time, that we call first reconstruction time $T_R = N/2$, the particle is reconstructed at the original site ($N$ even) or is concentrated near the antipode ($N$ odd). Notice that at this reconstruction time $T_R$ the state is reconstructed only if $N$ is even whereas for odd $N$ the probability distribution for the location of the particle peaks but there is no exact reconstruction of the particle in one location of the antipode. For very short times $T \ll T_D$ the system does not notices the geometry of the cyclic lattice and the width grows linearly with time with a diffusion speed increasing with the lattice size $N$. Indeed, the first term in the Taylor expansion of $\Delta$ is

$$\Delta = a2\pi\sqrt{\frac{1}{3}(N-1)(N-2)} \ T \ for \ T \ll T_D.$$  \hspace{1cm} (32)$$

We can now investigate whether the reconstruction of a localized state for the particle at time $T_R = N/2$ at the original site ($N$ even) or the concentration of the particle near the
antipodes ($N$ odd) is affected by the parity of the initial state. The initial state considered above, a particle in one site, has necessarily even parity. In order to be able to study also the effect of an odd parity initial state we will consider an initial state of a particle at rest, $\langle P \rangle = 0$, in an even or odd superposition of two neighbouring position eigenstates corresponding to the sites $x = 0$ and $x = 1$: 

$$ \Psi_\pm(0) = \frac{1}{\sqrt{2}} (\varphi_0 \pm \omega^a \varphi_1) $$

(33)

With this initial state, we can calculate the time evolution of the centroid. However, the centroid will no longer be a real number. It is therefore convenient to make a rotation of the centroid in the complex plane by an angle $\omega^{-1/2}$ in order to obtain the real quantity $\tilde{Z}_\pm(T) = \omega^{-1/2} Z_\pm(T)$, where $Z_\pm(T)$ is the centroid corresponding to the two initial states $\Psi_\pm(0)$. This results in

$$ \tilde{Z}_\pm(T) = \frac{1}{N} \left( \cos \left( \frac{\pi}{N} \right) \frac{\sin \left( \frac{\pi}{N}(N-1)2T \right)}{\sin \left( \frac{\pi}{N}2T \right)} \pm \frac{\sin \left( \frac{\pi}{N}(N-1)(2T-1) \right)}{2 \sin \left( \frac{\pi}{N}(2T-1) \right)} \right. $$

$$ + \left. \frac{\sin \left( \frac{\pi}{N}(N-1)(2T+1) \right)}{2 \sin \left( \frac{\pi}{N}(2T+1) \right)} + \cos \left( \frac{\pi}{N} \mp 1 \right) \right) . $$

(34)

In Figures 4a and 4b we see the time evolution of the (rotated) centroid $\tilde{Z}_+ (T)$ for an even initial state $\Psi_+(0)$ for even and odd $N$. For a qualitative comparison with Figure 1, we have taken $N = 33$ and $N = 34$ in order to have similar relation between the size of the lattice and the number of sites of the initial state. From this comparison it is clear that the behaviour is similar. At time $T = N/2$, a localized even state is reconstructed at the original locations if $N$ is even or the particle is localized at the antipodes if $N$ is odd. In Figures 5a and 5b we can see that this is also true when the initial state $\Psi_-(0)$ is odd, but the effect is much blurred by rapid oscillations of the centroid. Shortly before and after every reconstruction of the particle, it is almost reconstructed but on the opposite side of the lattice. For both, even and odd parity states, the initial value of the centroid, $\tilde{Z}_\pm(0) = \cos(\pi/N)$, is exactly recovered for even $N$ at time $T = N/2$ (this must be so because the state is periodic) and for odd $N$ the centroid reaches the minimum value $\tilde{Z}_\pm(N/2) = -((N-2) \cos(\pi/N) \pm 2)/N$. For large $N$ this minimum value approaches $-\cos(\pi/N)$, corresponding to the occupation of two neighbouring sites at the antipodes.

IV. THE CONTINUOUS LIMIT

We have found that there are very strong differences in the behaviour of the system when $N$ takes even or odd values. Of course, all these differences must be compatible with the
continuous limit when $N \to \infty$ where we can not differentiate between even or odd $N$. In this section we will investigate this limit. First we must redefine the indices of summation in a symmetric way such that they can take positive and negative values. Let then

$$y = a(x - j) \in [-aj, aj]$$
$$q = g(p - j) \in [-gj, gj].$$

(35)

Anticipating that in the limit $N \to \infty$ the position and momentum eigenfunctions will not be normalizable, we define these eigenfunctions in terms of the symmetric indices as

$$\varphi_y = \frac{1}{\sqrt{a}} \varphi_x \quad \text{and} \quad \phi_q = \frac{1}{\sqrt{g}} \phi_p.$$  

(36)

If in the limit $N \to \infty$ we also take $a \to 0$ or $g \to 0$ then the summations become integrals according to the scheme

$$\sum_{y=-aj}^{aj} a \to \int_{-\infty}^{\infty} dy \quad \text{or} \quad \sum_{q=-gj}^{gj} g \to \int_{-\infty}^{\infty} dq.$$  

(37)

The limit $N \to \infty$ is constrained by the condition $Nag = 2\pi$ and therefore we will consider three different limits $L_1, L_2, L_3$, that will correspond to three different physical systems:

$$L_1 : \begin{cases} N \to \infty, a \to 0, g \to 0, \\ y \in [-\infty, \infty], q \in [-\infty, \infty]. \end{cases}$$  

(38)

$$L_2 : \begin{cases} N \to \infty, a \to 0, Na = L, g = \frac{2\pi}{L}, \\ y \in [-L/2, L/2], q = \frac{2\pi}{L} n, n = \begin{cases} \pm1/2, \pm3/2, \cdots & \text{Neven}, \\ 0, \pm1, \pm2, \cdots & \text{Nodd}. \end{cases} \end{cases}$$  

(39)

$$L_3 : \begin{cases} N \to \infty, g \to 0, Ng = G, a = \frac{2\pi}{G}, \\ q \in [-G/2, G/2], y = \frac{2\pi}{G} n, n = \begin{cases} \pm1/2, \pm3/2, \cdots & \text{Neven}, \\ 0, \pm1, \pm2, \cdots & \text{Nodd}. \end{cases} \end{cases}$$  

(40)

In the limit $L_1$ both variables $y$ and $q$ are continuous and unbound whereas in $L_2$ the variable $y$ is bounded and continuous but $q$ is unbound and discrete; these properties are exchanged in $L_3$.

In the limit $L_1$, the physical system becomes a free particle moving in a one dimensional infinite space where position and momentum observable can take continuous values. In the limit $L_2$, the physical system is a free particle moving in a ring of perimeter $L$. Position is
continuous and takes values from $-L/2$ to $L/2$ whereas momentum is a discrete variable. We will later see that among the two choices for the number $n$, only the values $0, \pm 1, \pm 2, \cdots$ are physically meaningful. This system also corresponds to a particle in a box with periodic boundary conditions. Finally, in the limit $L3$, the physical system is a particle moving in a one dimensional infinite lattice with lattice constant $a = 2\pi/G$ and continuous momentum restricted to the Brillouin zone $[-G/2, G/2]$.

The striking differences in the behaviour of the system between even and odd $N$ appear in the time periodicity of the state and probability, and in the first reconstruction time for the probability distribution. These differences involve a time scale $t = N\tau \propto Na/g = 2\pi/g^2$. In both limits, $L1$ and $L3$, this time scale is infinite and therefore we should not worry about whether $N$ is even or odd when taking the limit $N \to \infty$; however in the limit $L2$ the time scale is finite and proportional to $L^2$. In this last case we will see that the even $N$ case is mathematically sound but does not correspond to any reasonable physical system.

It is convenient, in order to analyse the $L1$ and $L2$ limits, to adopt the position representation of the eigenfunctions where the momentum eigenvectors are given by Eqs.(7,36) as

$$
\psi_q(y) = \langle \psi_y, \phi_q \rangle = \frac{1}{\sqrt{2\pi}} e^{iqy+ig(y-aq)} .
$$

In the limit $L1$, where $a \to 0$ and $g \to 0$, this eigenfunction becomes

$$
\phi_q(y) = \frac{1}{\sqrt{2\pi}} e^{iqy} ,
$$

provided that, in the even $N$ case ($\alpha = 1/2$), The values of $y$ and $q$ remain finite (otherwise a minus sign can appear). Expanding the position eigenfunctions in the momentum basis we obtain

$$
\varphi_{q'}(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dq \ e^{iq(y-y')} = \delta(y-y') .
$$

We obtain therefore the usual position and momentum eigenfunctions for a free particle moving in a line.

Let us now consider the $L2$ limit where we have two possibilities: $\alpha = 0, n = 0, \pm 1, \pm 2, \cdots$ and $\alpha = 1/2, n = \pm 1/2, \pm 3/2, \cdots$. In the first case Eq.(41) results in

$$
\phi_q(y) = \frac{1}{\sqrt{2\pi}} e^{iyq/2n} , \quad n = 0, \pm 1, \pm 2, \cdots ,
$$

and in the second case, assuming $m = \pm 1/2, \pm 3/2, \cdots$, we have

$$
\phi_q(y) = \frac{1}{\sqrt{2\pi}} e^{iyq/2n + \frac{1}{2} x + \frac{1}{2} y} = \frac{1}{\sqrt{2\pi}} e^{iyq/2(n+\frac{1}{2})} = \frac{1}{\sqrt{2\pi}} e^{iyq/2n} , \quad n = 0, \pm 1, \pm 2, \cdots .
$$
Therefore both cases lead to the same position representation of the momentum eigenfunction. So far it would seem that the even and odd $N$ cases are identical in the limit $N \to \infty$ however this is not so as we will see next. It turns out that in the even $N$ case, when $\alpha = 1/2$, the momentum operator in the position representation is not given by the derivative operator as usual. In order to prove this, consider the first equation in (10) written in terms of the symmetric variables, that is,

$$e^{-iaP} \varphi_y = e^{i\frac{2\pi}{N} \alpha} \varphi_{y+a} = e^{i\frac{2\pi}{N} \alpha} \varphi_{y+a}.$$  \hfill (46)

Applying the limit $L^2$ we get,

$$(1 - iaP) \varphi_y = (1 + i \frac{2\pi}{L} a \alpha) \varphi_{y+a}.$$  \hfill (47)

Therefore

$$P \varphi_y = i \lim_{a \to 0} \frac{\varphi_{y+a} - \varphi_y}{a} - \frac{2\pi}{L} \alpha \varphi_{y+a},$$  \hfill (48)

where we see that only in the odd $N$ case, when $\alpha = 0$, is the momentum operator given by the derivative operator.

The inadequacy of even $N$ in the limit is more conveniently seen if we absorb the phase $e^{i\alpha(y-aq)}$ in the eigenfunctions as was mentioned at the end of section II. In this case the $\alpha$-dependent phase in Eq.(41) would not appear and we would have two different position representations of the momentum eigenfunctions given by

$$\phi^1_q(y) = \frac{1}{\sqrt{2\pi}} e^{iy\frac{2\pi}{L} (0, \pm 1, \pm 2, \ldots)} \text{ for odd } N$$

$$\phi^2_q(y) = \frac{1}{\sqrt{2\pi}} e^{iy\frac{2\pi}{L} (\pm 1/2, \pm 3/2, \ldots)} \text{ for even } N.$$  \hfill \text{for even } N.

The momentum eigenfunctions $\phi^1_q(y)$ are the same as the ones obtained before in Eq.(44) and the other ones, $\phi^2_q(y)$, are mathematically sound but are inadequate for physical systems because they are anti-symmetric, $\phi^2_q(-L/2) = -\phi^2_q(L/2)$ and have period $2L$, whereas all reasonable physical states for a particle in a ring are symmetric and have space periodicity $L$.

As a further confirmation that the $L^2$ limit corresponds with the odd $N$ case, we will show that an initial state in a ring is reconstructed at the antipodes at the reconstruction time $t_R = T_R T = N \pi/2 = mL^2/(2\pi)$ as it happens in the case of finite but odd $N$. In order to prove this we assume an arbitrary initial state expanded in terms of the momentum base

$$\psi(y, 0) = \sum_q c_q \phi_q(y).$$  \hfill (49)
We apply the time evolution operator to this state, considering that

\[ e^{-i\frac{\phi^2}{2m}t} \phi_q(y) = e^{-i\frac{\phi^2}{2m}t} \phi_q(y) , \]  

(50)

and using Eq.(44) we get

\[ \psi(y, t) = \frac{1}{\sqrt{2\pi}} \sum_{n=0, \pm 1, \pm 2, \ldots} c_n e^{-i\frac{\phi^2}{2m}2\pi n^2 t + iy \frac{2\pi n}{L}} . \]  

(51)

Consider now this state at the reconstruction time \( t_R = mL^2/(2\pi) \),

\[ \psi(y, t_R) = \frac{1}{\sqrt{2\pi}} \sum_{n=0, \pm 1, \pm 2, \ldots} c_n e^{-i\pi n^2} e^{iy \frac{2\pi n}{L}} . \]  

(52)

Now, since \( n^2 \) and \( n \) have the same parity, it is \( e^{-i\pi n^2} = e^{-i\pi n} \), and we get,

\[ \psi(y, t_R) = \frac{1}{\sqrt{2\pi}} \sum_{n=0, \pm 1, \pm 2, \ldots} c_n e^{i(y - \frac{L}{2}) \frac{2\pi n}{L}} . \]  

(53)

Therefore

\[ \psi(y, t_R) = \psi(y - \frac{L}{2}, 0) . \]  

(54)

with the meaning that the state at the reconstruction time \( t_R \) is equal to the initial state, but shifted to the antipode \( y - L/2 \).

A particle in a localized state in a continuous ring will flip back and forth between the original position and its antipode. If the particle is electrically charged, the system will radiate electromagnetic energy and decay to a nonlocalized stationary state (not necessarily the ground state) and a small fluctuation away of a nonlocalized state will grow, absorbing electromagnetic energy of the appropriate frequency (for an electron in a ring of 10\( \mu \) to 100\( \mu \) of perimeter, the radiation will be in the radio frequencies). This radiation, or the corresponding absorption, could be experimentally detected, in particular if one builds a material with a large number of conducting rings. Such a material, whose dielectric properties follow from a fundamental quantum mechanical effect, could find technological applications.

Finally, the \( L^3 \) limit is treated equal to the \( L^2 \) case but in terms of the momentum representation of the eigenfunctions. Similar arguments show that the even \( N \) case leads, in the limit, to unphysical situations.

V. CONCLUSION

In this work we have studied the diffusion of a quantum mechanical particle, initially localized, in a ring with \( N \) sites. This diffusion has qualitative features quite different from
the diffusion of a particle performing a classical random walk. It is well known that in a classical random walk, the width of the distribution grows like $\sqrt{T}$ whereas quantum mechanical diffusion grows initially proportional to $T$. Furthermore, we see in Eq. (32) that the speed of quantum diffusion, for large $N$, increases linearly with the size of the lattice $aN$. This non local effect is contrary to the classical behaviour and can be understood qualitatively as a consequence of Heisenberg’s indeterminacy principle: if the initial state is a particle in one site of the lattice, increasing the number of sites is equivalent to a sharper localization relative to the lattice size, and this results in a wider momentum spread, responsible for the increase in diffusion speed. Since the diffusion speed increases with the number of sites $N$ it is reasonable to expect that the time necessary to diffuse to the whole lattice will be constant independent of the lattice size. This is indeed the result shown in Eq.(30) where we see that, for large $N$, the diffusion time $T_D$ is constant. This is again in contradiction with the behaviour of the classical random walk where the covering time (the time it takes for a random walk to visit all the lattice sites) for a cyclic lattice increases quadratically with $N$ (precisely, $N(N - 1)/2$).

ACKNOWLEDGMENTS

This work received partial support from “Consejo Nacional de Investigaciones Científicas y Técnicas” (CONICET) and from ADPCyT (Picto 03-08431), Argentina.
REFERENCES

1 J. W. Haus, K. W. Kehr. “Diffusion in regular and disordered lattices” Phys. Rep. 150, 263-416, (1987).

2 See for instance a recent review by J. Kempe. “Quantum random walks - an introductory overview” arXiv:quant-ph/0303081 to appear in Contemporary Physics.

3 A. C. de la Torre, D. Goyeneche “Quantum mechanics in finite dimensional Hilbert space” Am. J. Phys. 71, 49-54, (2003).

4 R. P. Feynman, A. R. Hibbs Quantum Mechanics and Path integrals. McGraw-Hill, New York, 1965.

5 G. W. Forbes, M. A. Alonso “Measures of spread for periodic distributions and the associated uncertainty relations” Am. J. Phys. 69, 340-347, (2001).

6 G. W. Forbes, M. A. Alonso “Consistent analogs of the Fourier uncertainty relations” Am. J. Phys. 69, 1091-1095, (2001).

7 A. M. Nemirovsky, H. O. Márton, and M. D. Coutinho-Filho “Universality in lattice-covering time problem” Phys. Rev. A 41, 861-767 (1990).
FIGURE CAPTIONS

FIGURE 1. Cyclic lattice with $N$ sites characterized by a label $x$ running from $x = 0$ to $x = N - 1$ and lattice constant $a$. The position observable corresponding to site $x$ has the eigenvalue $a(x - j)$ where $j = (N - 1)/2$ and can take positive and negative values.

FIGURE 2. An example for the centroid of a distribution. The symbol $\oplus$ shows the position of the centroid $Z = \rho e^{i\theta}$ for a distribution where the filled dots have a constant occupation probability and all other sites are empty. The center $\overline{X}$ of the distribution is shown and the width $\Delta$ is proportional to the chord $C$ shown.

FIGURE 3. Time dependence of the centroid for even (a) and odd (b) number of sites. At time $N/2$ the state is reconstructed at the original site for even $N$ and is concentrated at the antipodes for odd $N$.

FIGURE 4. Time dependence of the (rotated) centroid for even (a) and odd (b) number of sites for an initial even state occupying two neighbouring sites. At time $N/2$ the state is reconstructed at the original sites for even $N$ and is concentrated at the antipodes for odd $N$.

FIGURE 5. Time dependence of the (rotated) centroid for even (a) and odd (b) number of sites for an initial odd state occupying two neighbouring sites. At time $N/2$ the state is reconstructed at the original sites for even $N$ and is concentrated at the antipodes for odd $N$. 
(a) $N=16$

(b) $N=17$
$N=34$. EVEN STATE $\psi_+$

$N=33$. EVEN STATE $\psi_+$
\( \hat{N} = 34. \) ODD STATE \( \psi_+ \)

\( \hat{N} = 33. \) ODD STATE \( \psi_- \)