Quantum diffusion on a cyclic one-dimensional lattice

A. C. de la Torre,* H. O. Mártin, and D. Goyeneche
Departamento de Física, Universidad Nacional de Mar del Plata, Funes 3350, 7600 Mar del Plata, Argentina

(Received 28 March 2003; published 19 September 2003)

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 $N\rightarrow\infty$ is studied. The predictions of the model could be tested with microtechnology and nanotechnology devices.

DOI: 10.1103/PhysRevE.68.031103 PACS number(s): 05.40.Fb, 03.65.Ca, 05.60.Gg

I. INTRODUCTION

The problem of a classical particle performing a random walk in various geometrical spaces [1] and the quantum random walk [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. This faster diffusion of the quantum random walk has arisen interest in quantum computation because of the possibility to develop algorithms more efficient than those based on the classical random walk. 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, for instance, a very different behavior for even or odd values of N. These even-odd differences also appear in quantum random walk in circles, although they are based on a dynamics completely different from the one that we consider here. 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 with nanofabrication techniques and in quantum computers we deal with systems with $N=2$ (qubits) or $N=3$ (qutrits). In all these cases we may be interested in the quantum diffusion time of an initially localized state. The quantum behavior in the continuous case $N\rightarrow\infty$ is also interesting because it could be experimentally tested building small conducting rings with microfabrication techniques.

*Email address: dltorre@mdp.edu.ar

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 Fig. 1. The quantum mechanical treatment [3] of this system requires an N-dimensional Hilbert space $\mathcal{H}$. The lattice sites will be labeled by an index x running through the values $0,1,\ldots,N-1$. We will adopt a very useful notation for the principal Nth root of the identity defined by

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

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

$$1=\omega^{Nn},\forall n=0,\pm1,\pm2,\ldots. \tag{2}$$

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 $\{0,1,\ldots,N-1\}$. 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 φ_x and the

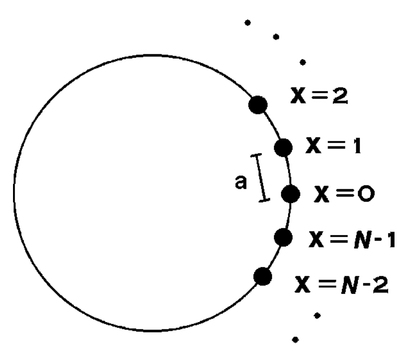

FIG. 1. Cyclic lattice with N sites characterized by a label x running from $x=0$ to $x=N-1$ and lattice constant a. The position observable corresponding to site x has the eigenvalue $a(x-j)$, where $j=(N-1)/2$ and can take positive and negative values.

set $\{\varphi_x\}$ is a basis in $\mathcal{H}$. In the spectral decomposition, we can write the position operator X as

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

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 $\{0,1,\ldots,N-1\}$. The momentum operator is given in terms of its spectral decomposition as

$$P=\sum_{p=0}^{N-1} g(p-j)\phi_p\langle\phi_p,\cdot\rangle, \tag{4}$$

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, counter 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,

$$\varphi_x=\frac{1}{\sqrt{N}}\sum_{p=0}^{N-1} \omega^{-(p-j)(x-j)-\alpha(x-p)}\phi_p \tag{5}$$

and

$$\phi_p=\frac{1}{\sqrt{N}}\sum_{x=0}^{N-1} \omega^{(p-j)(x-j)+\alpha(x-p)}\varphi_x, \tag{6}$$

with

$$\langle\varphi_x,\phi_p\rangle=\frac{1}{\sqrt{N}}\omega^{(p-j)(x-j)+\alpha(x-p)}, \tag{7}$$

where α is a parameter such that

$$\alpha=\begin{cases}0 & \text{for}\quad N\ \text{odd}\\ \dfrac{1}{2} & \text{for}\quad N\ \text{even.}\end{cases} \tag{8}$$

The constants a and g are not independent but are related by

$$agN=2\pi. \tag{9}$$

This condition follows [3] 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,

$$e^{-iaP}\varphi_x=\omega^{\alpha}\varphi_{[x+1]},$$
$$e^{igX}\phi_p=\omega^{\alpha}\phi_{[p+1]}, \tag{10}$$

where the symbol $[\cdot]$ denotes mod N, that is, $[N]=0$. Note that an N-fold application of these translation operators is equal to the identity **1** if N is odd but is equal to $-\mathbf{1}$ if N is even. This is reminiscent of a 2π rotation of a spin 1/2 system.

In Eqs. (5)–(7) we could absorb the phases αx and αp 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 ω^{α} 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 $p=0$, losing 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

$$\Psi(t)=\sum_{x=0}^{N-1} c_x(t)\varphi_x. \tag{11}$$

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

$$U_t=\exp(-iHt). \tag{12}$$

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

$$c_x(T)=\frac{1}{N}\sum_{p=0}^{N-1} \omega^{x(p-j+\alpha)-(p-j)^2T}, \tag{13}$$

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

$$\tau=\frac{2ma}{g}, \tag{14}$$

which, 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 $P\to -P$. 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

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

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

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

and for the probability we get

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

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 counterclockwise, 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 $x=0$ is related by

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

In order to prove this, consider

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

Using Eq. (2) we eliminate $N(p-j+\alpha)$ in the exponent and add Nx. Therefore

$$c_{N-x}(T)=\frac{1}{N}\sum_{p=0}^{N-1}\omega^{x(N-p+j-\alpha)-(p-j)^2T}. \quad (20)$$

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

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

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

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

Finally, redefining the summation index $p=q-1$ and using again Eq. (2), we find that the right-hand side of this equation is $\omega^{-2\alpha x}c_x(T)$. 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,

$$c_{N/2}(T)=0, \quad \forall \quad T. \quad (23)$$

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 antisymmetric 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 φ_0 and φ_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 exist 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 Δ 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 comply 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 $\Sigma_{x=0}^{N-1}a(x-j)|c_x|^2=-a(N-3)/6$. For another example, consider a uniform distribution that fills a ring completely. 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 $\Sigma_{x=0}^{N-1}a(x-j)|c_x|^2=0$.

The problem of defining the center $\overline{X}$ and width Δ of a distribution in a ring or cyclic lattice has been solved [5,6] 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 $x=0,1,\dots,N-1$ of a cyclic lattice, let us consider the unit circle in the complex plane with N points located at ω^x. The centroid of the distribution is a complex number $Z=\rho e^{i\theta}$ given by

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

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

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

and the width Δ of the distribution is given by

$$\Delta^2=(aN)^2(1-|Z|^2), \tag{26}$$

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. Note that when only one site is occupied, the width is zero. These definitions are clarified in an example shown in Fig. 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

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

The sum over x can be performed:

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

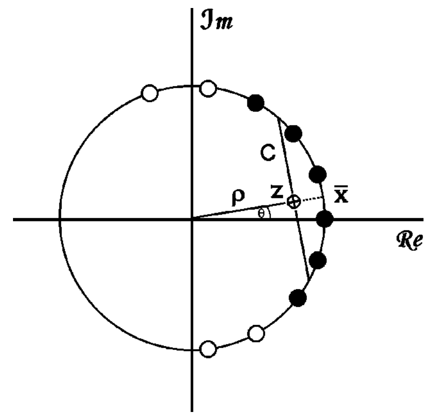

FIG. 2. An example for the centroid of a distribution. The symbol $\oplus$ shows the position of the centroid $Z=\rho e^{i\theta}$ for a distribution where the filled dots have a constant occupation probability and all other sites are empty. The center $\overline{X}$ of the distribution is shown and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

The first term inside the parentheses corresponds to the vanishing of the exponent of ω and the second term is for the case where the exponent is equal to Nx. With the Kronecker δ's we perform the sum over q, and the remaining sum over p has a known result. We then get

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

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. 3(a) and 3(b) 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 cannot be reconstructed in one location. We see here a sharp distinction in the behavior of diffusion in the even and odd case: the antipode is never reached in the N-even case but the distribution peaks in the neighborhood 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, which we define as the time when the width assumes its maximal value

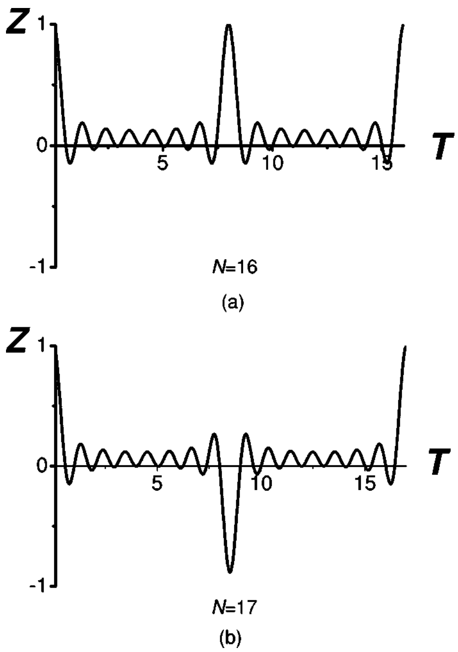

FIG. 3. Time dependence of the centroid for even (a) and odd (b) number of sites. At time $N/2$ the state is reconstructed at the original site for even N and is concentrated at the antipodes for odd N.

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

$$T_D=\begin{cases}\infty & \text{for } N=2\\ 1 & \text{for } N=3\\ \dfrac{N}{2(N-2)} & \text{for } N\geqslant 4.\end{cases} \tag{30}$$

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

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

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 $a(2\sqrt{N-1})$ for odd N. At this time, which 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). Note 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 notice 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 Δ is

$$\Delta=a2\pi\sqrt{\tfrac{1}{3}(N-1)(N-2)}T \quad \text{for} \quad T\ll T_D. \tag{32}$$

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 neighboring position eigenstates corresponding to the sites $x=0$ and $x=1$:

$$\Psi_\pm(0)=(1/\sqrt{2})(\varphi_0\pm\omega^\alpha\varphi_1). \tag{33}$$

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

$$\tilde{Z}_\pm(T)=\frac{1}{N}\left[\cos\left(\frac{\pi}{N}\right)\frac{\sin\left(\frac{\pi}{N}(N-1)2T\right)}{\sin\left(\frac{\pi}{N}2T\right)}\pm\frac{\sin\left(\frac{\pi}{N}(N-1)(2T-1)\right)}{2\sin\left(\frac{\pi}{N}(2T-1)\right)}\pm\frac{\sin\left(\frac{\pi}{N}(N-1)(2T+1)\right)}{2\sin\left(\frac{\pi}{N}(2T+1)\right)}+\cos\left(\frac{\pi}{N}\right)\mp 1\right]. \tag{34}$$

In Figs. 4(a) and 4(b) 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 Fig. 1, we

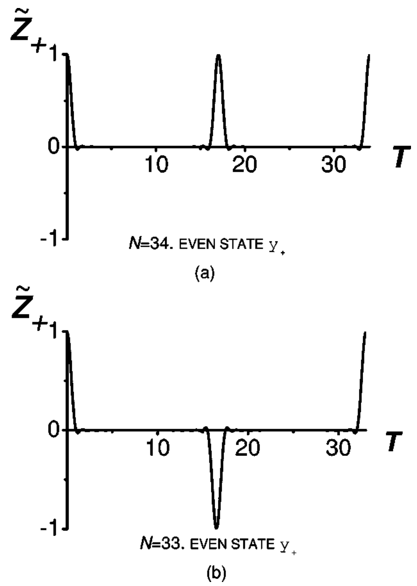

FIG. 4. Time dependence of the (rotated) centroid for even (a) and odd (b) number of sites for an initial even state occupying two neighboring sites. At time $N/2$ the state is reconstructed at the original sites for even N and is concentrated at the antipodes for odd N.

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 behavior 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 Figs. 5(a) and 5(b) we can see that this is also true when the initial state

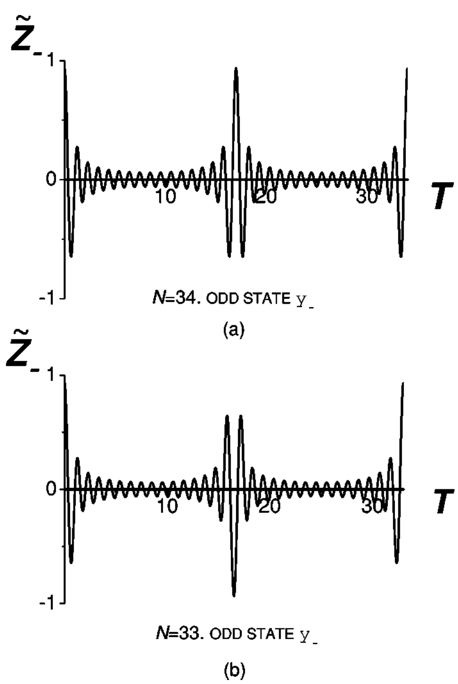

FIG. 5. Time dependence of the (rotated) centroid for even (a) and odd (b) number of sites for an initial odd state occupying two neighboring sites. At time $N/2$ the state is reconstructed at the original sites for even N and is concentrated at the antipodes for odd N.

$\Psi_-(0)$ 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 neighboring sites at the antipodes.

IV. THE CONTINUOUS LIMIT

We have found that there are very strong differences in the behavior 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 cannot 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

$$y=a(x-j)\in[-aj,aj],$$

$$q=g(p-j)\in[-gj,gj]. \tag{35}$$

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

$$\varphi_y=\frac{1}{\sqrt{a}}\varphi_x \text{ and } \phi_q=\frac{1}{\sqrt{g}}\phi_p . \tag{36}$$

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

$$\sum_{y=-aj}^{aj} a\to\int_{-\infty}^{\infty}dy \text{ or } \sum_{q=-gj}^{gj} g\to\int_{-\infty}^{\infty}dq. \tag{37}$$

The limit $N\to\infty$ is constrained by the condition $Nag=2\pi$, and therefore we will consider three different limits $L1$, $L2$, $L3$, which will correspond to three different physical systems:

For $L1$

$$N\to\infty,\ \ a\to 0,\ \ g\to 0,$$

$$y\in[-\infty,\infty],\ \ q\in[-\infty,\infty]. \tag{38}$$

For $L2$

$$N\to\infty,\ \ a\to 0,\ \ Na=L,\ \ g=\frac{2\pi}{L},$$

$$y\in[-L/2,L/2],\ \ q=\frac{2\pi}{L}n,$$

$$n=\begin{cases}\pm 1/2,\pm 3/2,\ldots, & N \text{ even}\\ 0,\pm 1,\pm 2,\ldots, & N \text{ odd.}\end{cases} \tag{39}$$

For $L3$

$$N\to\infty,\;\; g\to 0,\;\; Ng=G,\;\; a=\frac{2\pi}{G},$$

$$q\in[-G/2,G/2],\;\; y=\frac{2\pi}{G}n,$$

$$n=\begin{cases}\pm 1/2,\pm 3/2,\ldots, & N \text{ even}\\ 0,\pm 1,\pm 2,\ldots, & N \text{ odd.}\end{cases} \tag{40}$$

In the limit $L1$ both variables y and q are continuous and unbound whereas in $L2$ the variable y is bounded and continuous but q is unbound and discrete; these properties are exchanged in $L3$.

In the limit $L1$, 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 $L2$, 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 $0,\pm 1,\pm 2,\ldots$ 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 behavior 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 analyze the $L1$ and $L2$ limits, to adopt the position representation of the eigenfunctions where the momentum eigenvectors are given by Eqs. (7) and (36) as

$$\phi_q(y)=\langle\varphi_y,\phi_q\rangle=\frac{1}{\sqrt{2\pi}}e^{iqy+i\alpha(gy-aq)}. \tag{41}$$

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

$$\phi_q(y)=\frac{1}{\sqrt{2\pi}}e^{iqy}, \tag{42}$$

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

$$\varphi_{y'}(y)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dq\,e^{iq(y-y')}=\delta(y-y'). \tag{43}$$

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: $\alpha=0$, $n=0,\pm 1,\pm 2,\ldots$ and $\alpha=1/2$, $n=\pm 1/2,\pm 3/2,\ldots$. In the first case Eq. (41) results in

$$\phi_q(y)=\frac{1}{\sqrt{2\pi}}e^{iy(2\pi/L)n},\;\; n=0,\pm 1,\pm 2,\ldots, \tag{44}$$

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

$$\phi_q(y)=\frac{1}{\sqrt{2\pi}}e^{iy(2\pi/L)m+i(1/2)(2\pi/L)y}=\frac{1}{\sqrt{2\pi}}e^{iy(2\pi/L)[m+1/2]}$$
$$=\frac{1}{\sqrt{2\pi}}e^{iy(2\pi/L)n},\;\; n=0,\pm 1,\pm 2,\ldots. \tag{45}$$

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 Eq. (10) written in terms of the symmetric variables, that is,

$$e^{-iaP}\,\varphi_y=e^{i(2\pi/N)\alpha}\varphi_{[y+a]}=e^{i(2\pi/Na)a\alpha}\,\varphi_{[y+a]}. \tag{46}$$

Applying the limit $L2$ we get,

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

Therefore

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

where we see that only in the odd-N case, where $\alpha=0$, 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 $e^{i\alpha(gy-aq)}$ in the eigenfunctions as was mentioned at the end of Sec. II. In this case the α-dependent phase in Eq. (41) would not appear and we would have two different position representations of the momentum eigenfunctions given by

$$\phi_q^1(y) = \frac{1}{\sqrt{2\pi}} e^{iy(2\pi/L)(0,\pm 1,\pm 2,\dots)} \quad \text{for odd } N,$$

$$\phi_q^2(y) = \frac{1}{\sqrt{2\pi}} e^{iy\frac{2\pi}{L}(\pm 1/2,\pm 3/2,\dots)} \quad \text{for even } N.$$

The momentum eigenfunctions $\phi_q^1(y)$ are the same as the ones obtained before in Eq. (44) and the other ones, $\phi_q^2(y)$, are mathematically sound but are inadequate for physical systems because they are antisymmetric, $\phi_q^2(-L/2) = -\phi_q^2(L/2)$, 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 $L2$ 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 $t_R = T_R\tau = N\tau/2 = mL^2/(2\pi)$, 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

$$\psi(y,0) = \sum_q c_q\, \phi_q(y). \tag{49}$$

We apply the time evolution operator to this state, considering that

$$e^{-i(P^2/2m)t}\, \phi_q(y) = e^{-i(q^2/2m)t}\, \phi_q(y), \tag{50}$$

and using Eq. (44) we get

$$\psi(y,t) = \frac{1}{\sqrt{2\pi}} \sum_{n=0,\pm 1,\pm 2,\dots} c_n e^{-(i/2m)(2\pi/L)^2 n^2 t + iy(2\pi/L)n}. \tag{51}$$

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

$$\psi(y,t_R) = \frac{1}{\sqrt{2\pi}} \sum_{n=0,\pm 1,\pm 2,\dots} c_n\, e^{-i\pi n^2} e^{iy(2\pi/L)n}. \tag{52}$$

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

$$\psi(y,t_R) = \frac{1}{\sqrt{2\pi}} \sum_{n=0,\pm 1,\pm 2,\dots} c_n\, e^{i[y-(L/2)](2\pi/L)n}. \tag{53}$$

Therefore

$$\psi(y,t_R) = \psi\left(y - \frac{L}{2}, 0\right), \tag{54}$$

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

Finally, the $L3$ limit is treated equal to the $L2$ 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. ABSORPTION AND RADIATION IN A RING

In the preceding section we have seen that the state of an initially localized particle in a continuous ring will flip back and forth between the original position and its antipode. We can then imagine that the particle is oscillating in the ring with a frequency given by $f_0 = 1/(2t_R) = \pi/(mL^2)$. However, this oscillation does not correspond to a smooth rotation along the ring because, between every reconstruction event, the state is strongly distorted and therefore higher Fourier components will also be present. Now if the particle is electrically charged, there will be a charge transfer from the original position to the antipode and back, and therefore we can expect an emission of electromagnetic radiation with the fundamental frequency f_0 and the higher harmonics $2f_0, 3f_0, \dots$. An electron in a localized state is then expected to decay to a nonlocalized state with lower energy by emission of electromagnetic radiation.

For an electron in a conducting ring of $(10\text{–}100)\mu$ of perimeter, the radiation will be in the radio frequency region, and therefore there are chances to observe experimentally this quantum effect at temperatures low enough such that the coherence length of the electron should be comparable with the size of the ring. With an heuristic argument based on the uncertainty principle (a dangerous thing to do), we can estimate that the number of photons of frequency f_0 emitted in the transition from an initial state localized within a region λ and a decayed state occupying the whole ring L is proportional to $(L/\lambda)^2$. This number follows from the ratio between the energy difference of the initial and final state and the energy of the photons.

It may be quite difficult to put an electron in a localized state in order to detect the radiation but it could be much easier to observe the opposite effect, that is, absorption. In this case an electron in a state spread on the ring will get localized by the absorption of electromagnetic radiation. In order to observe this effect one could try to deposit on a plane, or perhaps immerse in a fluid, a large number of conducting rings. Such a material, whose dielectric properties follow from a fundamental quantum mechanical effect, could find technological applications. Another possibility to observe this quantum effect could be presented by some ring shaped molecules if their electronic structures could be reasonably modeled by a conducting ring. For molecules with 10–100 Å diameter, the radiation falls in the infrared region of the spectrum.

VI. 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 nonlocal effect is contrary to the classical behavior 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 behavior of the classical random walk where the covering time [7] (the time it takes for a random walk to visit all the lattice sites) for a cyclic lattice increases quadratically with N [precisely, $N(N-1)/2$].

Finally, we would like to relate our results with interesting recent work on quantum random walk. It is remarkable that even though these two studies are based on a completely different dynamics, a free particle in our case and a quantum stochastic process in the other, there are striking qualitative similarities among them. Quantum random walks on general graphs do not converge to a stationary distribution but a limiting time-average distribution can be found and several criteria for the speed of convergence, called mixing time, sampling time, or filling time can be defined [8]. In all cases, it turns out that the quantum random walk achieves a faster covering of the space compared with the classical random walk, and this can be advantageous in the development of more efficient algorithms for quantum computing. In the particular case of a quantum random walk on a circular lattice with N sites, controlled by a Hadamard dynamics, there are striking differences in the limiting distribution for even or odd number of sites [9,10], and this difference remains if decoherence is included in the quantum system [11]. In our work we have found that these two main features of the quantum random walk, faster covering and even-odd differences, are also present in our system although we have a completely different dynamics. Apparently, these two features respond to two essential features of all quantum systems. The faster quantum covering appears to be a consequence of the inherent nonlocality of quantum mechanics whereas the even-odd effect may be due to different interference arrangements.

ACKNOWLEDGMENTS

This work received partial support from the ''Consejo Nacional de Investigaciones Científicas y Técnicas'' (CONICET) and from the ANPCyT (Grant No. 03-08431), Argentina.

[1] J.W. Haus and K.W. Kehr Phys. Rep. **150**, 263 (1987).
[2] See, for instance, a recent review by J. Kempe, Contemp. Phys. (to be published), e-print quant-ph/0303081.
[3] A.C. de la Torre and D. Goyeneche Am. J. Phys. **71**, 49 (2003).
[4] R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[5] G.W. Forbes and M.A. Alonso, Am. J. Phys. **69**, 340 (2001).
[6] G.W. Forbes and M.A. Alonso, Am. J. Phys. **69**, 1091 (2001).
[7] A.M. Nemirovsky, H.O. Mártin, and M.D. Coutinho-Filho, Phys. Rev. A **41**, 761 (1990).
[8] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, in *Proceedings of the 33rd Annual ACM Symposium on Theory of Computation*, edited by M. Yannakakis (ACM Press, New York, 2001), pp. 50–59; D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, e-print quant-ph/0012090.
[9] B. Tregenna, W. Flanagan, R. Maile, and V. Kendon, New J. Phys. **5**, 83 (2003).
[10] M. Bednarska *et al.*, e-print quant-ph/0304113
[11] V. Kendon and B. Tregenna, Phys. Rev. A **67**, 042315 (2003).