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Spread of highly localized wave-packet in the tight-binding lattice: Entropic and information-theoretical characterization

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A R T I C L E I N F O

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The spread of a wave-packet (or its deformation) is a very important topic in quantum mechanics. Understanding this phenomenon is relevant in connection with the study of diverse physical systems. In this paper we apply various "spreading measures" to characterize the evolution of an initially localized wave-packet in a tight-binding lattice, with special emphasis on information-theoretical measures. We investigate the behavior of both the probability distribution associated with the wave packet and the concomitant probability current. Complexity measures based upon Rényi entropies appear to be particularly good descriptors of the details of the delocalization process.

0. Introduction

The study of the evolution of wave-packets from different initial conditions is essential to the goal of typifying some interesting physical effects related to the internal and structural properties of diverse systems. In some cases it is possible to characterize the spread of the wave-packet using standard techniques that generally proceed through complicated analytical developments that do not always provide direct, intuitively clear answers. Alternatively, it is often necessary to apply numerical procedures. The understanding of the evolution of wave-packets is motivated by problems in various fields of physics, such as quantum information theory and solid state physics, among others.

There are fundamental quantum models that successfully capture some of the essential features exhibited by real physical systems encountered in Nature. For instance, deep insights on the dynamics

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of particles in a one-dimensional lattice can be obtained through the celebrated tight-binding model. This model, characterized by nearest-neighbor couplings, is described by a Hamiltonian whose eigenvalues and eigenvectors are well-known [1]. According to this model an electron in an atomic lattice can jump from one atom to its neighbor in either direction with a certain amplitude.

Until now, the tight-binding model has been one of the most useful models to describe many physical systems [2–6]. As examples we can mention the electronic structures in solid systems such as heterostructures, lattices, superlattices and crystals. In recent years the tight-binding model has been applied to the study of basic properties of nanostructures, such as the local density of states of semiconductor–metal double-well carbon nanotubes [7]. The tight-binding model provides a valuable framework for the analysis of many physical problems, such as the role of boundaries, diffusion in discrete lattices, quantum random walks, etc.

The relationship between the tight-binding model and quantum random walks is particularly interesting because of the relevance of the latter in the field of quantum information. The quantum counterpart of the classical random walks is the quantum random walks, which have been the subject of an intense research activity [8–14]. The dynamics of quantum random walks significantly departs from that of their classical counterparts. The discreteness of space often assumed when studying quantum random walks immediately suggests a connection between these processes and the spread of a wave-packet from a highly localized initial state in the tight-binding model. According to this idea the roles of "coin" and "walker" are naturally associated with the spin and translational degrees of freedom in the (discrete) space of tight-binding systems.

Quantum random walks exhibit surprising connections with other, apparently unrelated, physical phenomena. For instance, as was recently pointed out in [15–17], a free Dirac particle that is initially highly localized evolves in time by spreading at speeds close to the speed of light. This general phenomenon, and the resulting position probability density along any axis through the point of initial localization, can be interpreted in terms of a quantum random walk. The case of a highly localized initial state has been discussed in detail [15–17].

In the present work we apply several information-theoretical measures to characterize the evolution of quantum wave-packets in the tight-binding model. In particular we consider the Shannon, Wehrl and Leipnik entropies. Shannon's measure is one of the most widely used "spreading measures" to characterize information loss. However, the Wehrl entropy [18] and the Leipnik entropy [19] can also be used to quantify the loss of information associated with the "spreading" of an evolving probability density. Our main interest in the present effort is to make a careful characterization of the spread of highly localized initial quantum states in the tight-binding model. Our results suggest that the Leipnik entropy constitutes a good measure of delocalization, which is here regarded as an information-loss process. It is to be expected that any anomalous behavior exhibited by the system will become manifest in the evolution of this measure. In this work, besides studying the probability distribution characterizing the evolving wave-packet, we also investigate the behavior of the concomitant probability current.

The paper is organized as follows. In Section 1 we briefly review the main properties of the tight-binding model, providing the eigenvectors and eigenvalues of its Hamiltonian as well as the explicit form of the time dependent wave-packet. In Section 2 we compare the exact evolution with an approximate one described by a simple ansatz for the evolving wave-packet. This approximate solution gives some basic, intuitively clear insights concerning the evolution of the probability distribution. In Section 3, various possible characterizations of the spreading of the evolving wave-packet are explored. Finally, in Section 4, we summarize our work making some concluding remarks.

1. Tight-binding Hamiltonian and evolution from a highly localized particle

We consider a particle constrained to a one-dimensional lattice, in the tight-binding model. The Hamiltonian for this problem can be written as follows:

$$H = \sum_{l=1}^{N} E_l |l\rangle\langle l| - \sum_{l=1}^{N} K_l \left(|l+1\rangle\langle l| + |l\rangle\langle l+1|\right), \tag{1}$$

where $N \to \infty$ and, it corresponds to the total lattice points. The basis of states is denoted by the set $\{|l\rangle\}$, where the index $l = 1, \ldots, N$ represents a particular site occupied by the particle. The matrix representation of the Eq. (1) was easily obtained and defines a tridiagonal matrix. Some good examples are discussed in several standard books [20,21]. In a regular chain, $K_l = K$ and $E_l = E_0$, for all l. In such a case, from Eq. (1), the Hamiltonian H accepts the exact solutions like planar waves, which we set as $\{|k\rangle\}$ and it represents a basis of the eigenvectors for the Hamiltonian (1). Then, the projection $\langle k|l\rangle = \exp(\mathrm{i}kal)$.

In addition, the spectrum is

$$E(k) = E_0 - 2K\cos(ka) \tag{2}$$

where $k = -\pi/a, \ldots, \pi/a$, and a is the lattice parameter. Now, if the vector $|\psi\rangle = \sum_{l'} C_{l'}|l'\rangle$ is a general solution of the Eq. (1) for a particle in a tight-binding lattice, the coefficients $C_{l'}$ are arbitrarily defined from an initial distribution in $t = 0$. We can take the explicit time-dependent solution as $\psi_l(t) = \langle l|U(t)|\psi\rangle$, where $U(t) = \exp(-\mathrm{i}Ht/\hbar)$ is the evolution operator. In this manner, we are able to construct the explicit general solution for the problem of a particle in a tight-binding lattice. By applying quantum general properties of operators and basis, we get

$$\psi_l(t) = \frac{a}{2\pi}\sum_{l'} C_{l'} \int_{-\pi/a}^{\pi/a} \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}\left(ka(l-l') + \frac{1}{\hbar}E(k)t\right)}. \tag{3}$$

This general function is a superposition of planar waves, which are solutions of the Hamiltonian of the Eq. (1), whose coefficients evolve in time from the initial distribution. Then, $C_{l'}(k)$ is the initial distribution, *i.e.* $t = 0$. The Eq. (3) is the exact solution of the Hamiltonian (1). If we take into account the explicit form of the spectrum, from the Eq. (2), in the tight-binding model, the wave function has finally got

$$\psi_l(t) = \exp\left(-\mathrm{i}\frac{E_0}{\hbar}t\right)\sum_{l'} C_{l'} i^{(l-l')} J_{l-l'}(2Kt/\hbar), \tag{4}$$

where $J_{l-l'}$ is the Bessel function of the order $l - l'$. A solution similar to (4) has been previously discussed in the literature in connection to continuous-time quantum walks on a line [22,23].

2. Exact solution versus approximate solution

2.1. Exact solution

Starting from the initial distribution, given by a limiting situation that can be identified as a highly localized particle, a suitable choice for $C_{l'}$ is the following: $C_{l'} = \delta_{l,l'}$, where $\delta_{l,l'}$ is the Kronecker delta. Therefore, the wave function can be written as follows

$$\psi_l(t) = i^{(l-l_0)} \exp\left(-\mathrm{i}\left(\frac{E_0}{\hbar}t\right)\right) J_{l-l_0}(2Kt/\hbar), \tag{5}$$

where J_{l-l_0} is the Bessel function of the order $l - l_0$. Therefore, the density of probability is represented in an easy way, by

$$P(l-l_0) = |\psi_l(t)|^2 = [J_{l-l_0}(2Kt/\hbar)]^2. \tag{6}$$

The distribution $P(l - l_0)$ is normalized and evolves with two important properties as quantum random walk. From Eq. (6), according to the general properties of functions it is suggested that:

1. There are several peaks in the distribution. The external peaks are greater than previous ones.
2. The general property of the Bessel function [24], $J_{-n}(x) = (-1)^n J_n(x)$, assures the symmetry of the spread around index $n = 0$, which means $l = l_0$.

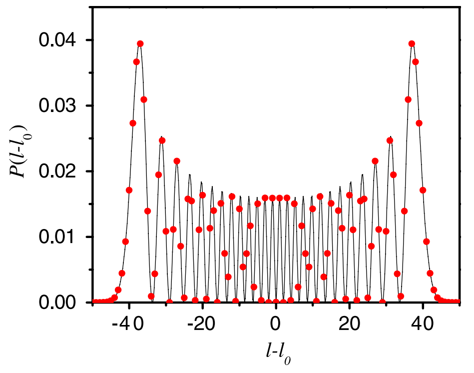

Fig. 1. The exact evolution of the density of the probability is depicted for a particle which is initially localized in l_0. Discrete results (circles) and a theoretical interpolation through Bessel function (solid line) are shown to visualize the trend of the spread of the wave-packet. The numerical values for parameters are $K = 0.1$ (coupling parameter), $t = 200$ (time). The evolution is similar to quantum random walk.

In Fig. 1, the probability distribution $P(l - l_0)$ is depicted as a function of the difference of the position $l - l_0$. On one hand, circles correspond to discrete results that are obtained from numerical calculation, which is thoroughly discussed previously [2]. On the other hand, solid line is obtained from the theoretical interpolation through Bessel function. The coupling parameter $K = 0.1$ and time $t = 200$ and the Planck constant $\hbar$ is set 1.

In addition, there are many ways to characterize the spread of a distribution. However, we are going to use here the standard definition of the square deviation, $\Delta l = \sqrt{\langle l^2\rangle - l_0^2}$. The function Δl is given by,

$$\Delta l = \sqrt{2}\frac{K}{\hbar}t. \tag{7}$$

2.2. Approximate solution

Despite the previous results, where the problem has accepted exact and analytical solutions, we tries to make an effort to write an approximate *expression* of the probability distribution to obtain extra information about the properties of the spread. Restarting from the definition of the following variable,

$$\varphi_l(k) = \frac{E(k)}{\hbar} + ka\frac{l - l_0}{t}, \tag{8}$$

which allows expressing Eq. (3) in the following way $\psi_l(t) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} \mathrm{d}k e^{-\mathrm{i}\varphi_l(k)t}$. Thus, from an extremal in k of the function $\varphi_l(k)$ it is possible to assert that the present approximation claims validity in the following range for l;

$$l_0 - 2\frac{K}{\hbar}t \leq l \leq l_0 + 2\frac{K}{\hbar}t. \tag{9}$$

Now, two additional important approximate results are emphasized from Eq. (9) about the boundaries of the spreading:

1. they are located in $l_0 \pm 2Kt/\hbar$; and,
2. they move in both directions with a speed given by $\pm 2K/\hbar$.

As previously asserted, we can confirm the symmetry of the behavior around l_0. In an expansion in series to the second order of Eq. (8) where the term of the first order is forgotten, the following

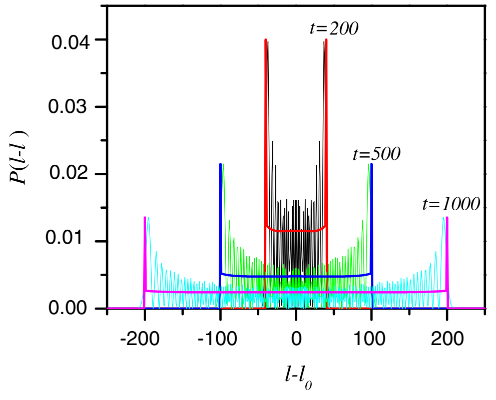

Fig. 2. We compare the evolution of the exact and approximate solutions of the probability density for a particle which is initially localized in the chain center. The approximate boundary of the spread is close to the last peak of the exact solution. We show different distributions for $t = 200, 500, 1000$.

expression for $\psi_l(t)$ is given by:

$$\psi_l(t) = A\frac{a}{2\pi}\mathrm{e}^{-\mathrm{i}\varphi_l(k_{0,l})t}\int_{-\pi/a}^{\pi/a}\mathrm{d}k\mathrm{e}^{-\mathrm{i}(k-k_{0,l})^2\frac{Ka^2t}{\hbar}\cos(k_{0,l}a)}, \tag{10}$$

where A is the normalization constant of the approximate function $\psi_l(t)$ and

$$k_{0,l} = -\frac{1}{a}\arcsin\left(\frac{(l-l_0)}{t}\frac{\hbar}{2K}\right). \tag{11}$$

Taking into account the Fresnel integrals definition [24]

$$\mathcal{S}(\zeta) = \frac{2}{\sqrt{2\pi}}\int_0^{\zeta}\mathrm{d}\rho\sin\rho^2 \quad \text{and} \tag{12}$$

$$\mathcal{C}(\zeta) = \frac{2}{\sqrt{2\pi}}\int_0^{\zeta}\mathrm{d}\rho\cos\rho^2, \tag{13}$$

and if we substitute into Eq. (10), we obtain

$$\psi_l(t) = A\frac{\sqrt{\pi/2}}{\lambda_l}\mathrm{e}^{-\mathrm{i}\varphi(k_{0,l})t/\hbar}(\mathcal{C}(\lambda_l) + \mathrm{i}\mathcal{S}(\lambda_l)), \tag{14}$$

where

$$\lambda_l^2 = \frac{Ka^2t}{\hbar}\cos(k_{0,l}a), \tag{15}$$

and A obeys to the condition

$$|A|^{-2} = \frac{\pi}{2}\sum_{l=l_0-2Kt/\hbar}^{l_0+2Kt/\hbar}\frac{1}{\lambda_l^2}(\mathcal{C}(\lambda_l)^2 + \mathcal{S}(\lambda_l)^2). \tag{16}$$

In Fig. 2, the approximate solution from the Eq. (14) is compared with the exact solution from the Eq. (6), for several values of the time, which are, $t = 200, 500, 1000$. The one-dimensional lattice has N sites, which is the initial state was localized in $l_0 = N/2$ and the lattice parameter is $a = 1$. As before, the coupling parameter is $K = 0.1$. Again, the wave-packet spreads as discrete quantum walks is remarked.

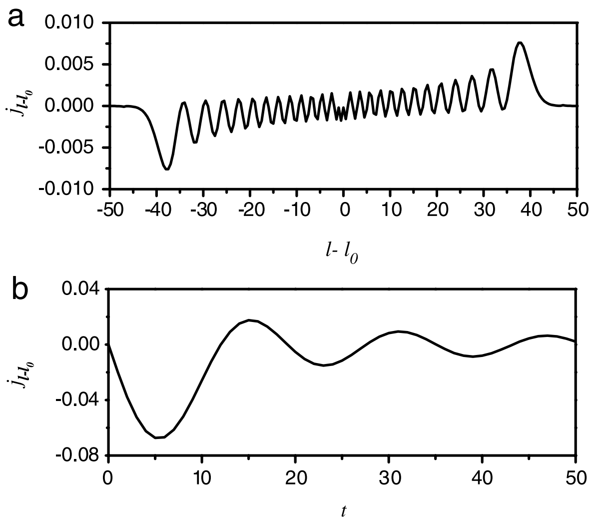

Fig. 3. The probability current at (a) time fixed (*i.e.* $t = 200$) and at (b) position fixed (*i.e.* $l = l_0$) is depicted. Other parameters are $a = 1$, $K = 0.1$ and $\hbar = 1$.

3. Characterization of the spread of the wave-packet

3.1. Probability current

The probability current, $j_l = 2(aK/\hbar)\mathtt{Im}\left(\psi_l(t)\psi^*_{l-1}(t)\right)$ [3], is an important quantity in solid state physics when we are interested in electronic properties of lattices. In this particular case, the probability current is given by

$$j_l = 2\frac{aK}{\hbar}J_{l-l_0}(2Kt/\hbar)J_{l-l_0-1}(2Kt/\hbar). \tag{17}$$

We take two cases, which we show in Fig. 3. We consider parameters like $K = 0.1$ and $a = 1$ and depict the probability current j_l at fixed value of the time, this is $t = 200$ and at fixed value of the position, $l = l_0$ in Fig. 3(a). Moreover, it is noticed that the function j_l takes negative (positive) values for the movement to the left (right) side. An oscillating behavior can be only related to the periodicity of the lattice. A similar observation emerges from different phenomena as interactions [4] and re-examined in a subsequent effort [5]. In the current problem, no interactions are considered. In Fig. 3(b), the evolution of the probability current in the point located in $l = l_0$ is depicted. This is an interesting case because it describes how the central point of the distribution evolves from $t = 0$ to oscillating and damping values close to zero, at $t > 0$.

3.2. Leipnik entropy

The Leipnik entropy [19] constitutes an information measure specially suitable for the characterization of the delocalization process. Rewriting the Eq. (3) in the following way

$$\psi_l(t) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} \mathrm{d}k \exp(-\mathrm{i}kal)\varphi(k;t), \tag{18}$$

where

$$\varphi(k;t) = \exp\left(-\frac{\mathrm{i}}{\hbar}E(k)t\right)\sum_{l'} C_{l'}\exp(\mathrm{i}kal'), \tag{19}$$

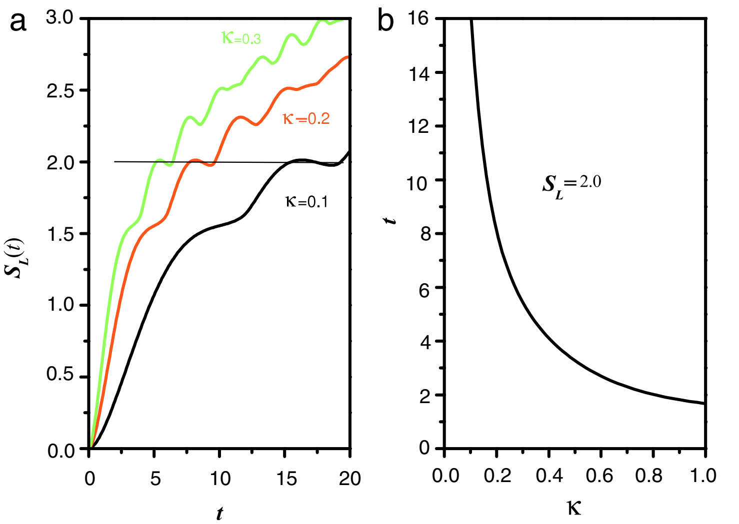

Fig. 4. The evolution in time of the Leipnik entropy is depicted in (a) for three different values of K. The anomalous behavior is evident. A decrease in the entropy is observed when it reaches the value 2. The value of the time t, where $S_L = 2$ as a function of the coupling (K), is shown in (b). This value of the time decreases as K increases.

we obtain an exact expression for $\varphi(k; t)$, which is the Fourier transform that represents the distribution function in wave-vector space. The exact solution of Eq. (18) was already mentioned in Eq. (5) when the same initial condition $C_l = \delta_{l,l_0}$ in Eq. (19) is taking into account.

The functions given by $|\psi_l(t)|^2$ and $|\varphi(k, t)|^2$ stand for the quantum probability densities for the position and wave-vector coordinates, respectively. Hence, Leipnik proposed to consider the product function $\rho_L(l, k; t) = |\psi_l(t)|^2|\varphi(k, t)|^2$, where $\rho_L(l, k; t)$ can be regarded as a probability density in phase space. This probability density is used to define the entropic functional [19],

$$S_L(t) = \frac{1}{N!} \sum_l \int dk \rho_L(l, k; t) \log \rho_L(l, k; t), \tag{20}$$

which is called the Leipnik entropy.

The evaluation of the previous definition of entropy for a special case is one goal of the present contribution. In the current study, the spread of a wave-packet, in a tight-binding lattice, is seen starting from an initial state with known localization and its evolution characterizes the delocalization (loss of localization), through a kind of an uncertainty relation and the Leipnik entropy as semi-classical measures of delocalization. It is seen that the Leipnik entropy increases, starting from zero at $t = 0$. According to the definition of $\rho_L(l, p; t)$ we see that $\rho_L(l, p; 0) = 1$, thus $S_L(0) = 0$, which represents full localization or full information about the position of the particle in $t = 0$. For $t > 0$, $S_L(t) > 0$ and corresponds to the measure of the loss of information about of the localization of the particle.

As seen in Fig. 4, S_L does not increase monotonically in time, surprisingly its tendency decreases in short intervals, anomalies are more evident as K increases in the trend of the entropy. The increase seems to oscillate in time and changing locally its concavity in a point to reach the value 2, in current units, where the curve shows a first local maximum. A typical trend of the Leipnik entropy as a function of the time is depicted in Fig. 4(a), emphasizing a point where the entropy S_L is seriously anomalous, for $K = 0.1$, 0.2 and 0.3. The time t, related to the anomaly, decays with K and it is shown in Fig. 4(b).

It is necessary to emphasize that in this particular case the Leipnik and Shannon entropies numerically coincide because $\varphi(k, t)\,|^2 = 1$. Therefore, Shannon entropy is also a good measure of the localization of one particle evolving in the tight-binding lattice.

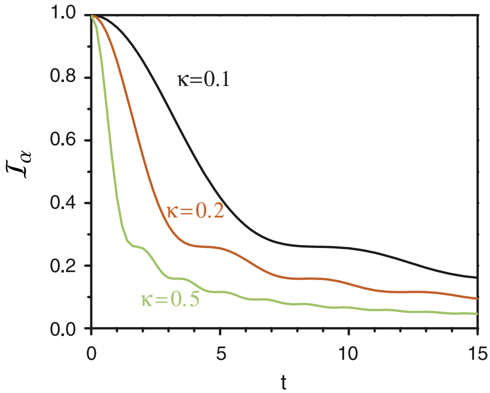

Fig. 5. The inverse participant ratio is depicted as a function of the time. Three values of the coupling parameter are considered and the curves are compared. These are $K = 0.1$, 0.2 and 0.5.

3.3. Inverse participant ratio

We calculate the inverse participant ratio [25,26] as another measure of the localization of the wave function in position space. The inverse participation ratio $\mathcal{I}_\alpha$ is related to the effective number of significant "participants" in a probability distribution $\{p_i\}$. Its inverse $\frac{1}{\mathcal{I}_\alpha}$ gives a rough idea of the number of "events" having an appreciable probability p_i.

This measure of the eigenvector $\psi_l(t)$ is defined as

$$\mathcal{I}_\alpha = \sum_{l=-L}^{L} |\psi_l(t)|^4. \tag{21}$$

The meaning of inverse participant ratio is clarified when considering two limiting cases. In the first case the modulus of the coefficients appearing in the eigenvector are identical; then, $\mathcal{I}_\alpha = 1/(2L+1)$. In the second case there is only one coefficient in the eigenvector different to zero, and the others are 0, in this case by normalization $\mathcal{I}_\alpha = 1$, which is the current case for the highly localized particle at $t = 0$, where the localization is maximum. Therefore, the value of the inverse participant ratio as a function of the time is associated with the localization of particles in a lattice. In Fig. 5, the inverse participant ratio is depicted as a function of the time taking three different values of the coupling parameter, these are $K = 0.1$, 0.2 and 0.5. It is noticed that the delocalization is more gradual when K is large.

3.4. Rényi entropy and statistical complexity measures

The Rényi entropies [27] constitute an important family of information measures that have been found useful in the study of several areas of physics, such as chaotic dynamics [28], statistical physics [29], entanglement theory [30], complex systems [31], among many others. The Rényi entropy of order q, where $q > 0$, is defined as

$$S_q = \frac{1}{1-q} \log \left(\sum_{l=-L}^{L} P_l^q \right). \tag{22}$$

The Rényi entropies are a generalization of Shannon's entropy and reduce to Shannon's measure in the limit case $q = 1$.

If probabilities are defined in the same way as Eq. (6). In Fig. 6, at (a) we present the Rényi entropy, which represents another measure of the delocalization (uncertainty). In addition, at (b) we show the deviation between the Rényi entropy, S_q of q order, from the Shannon entropy, S_1 where $q = 1$.

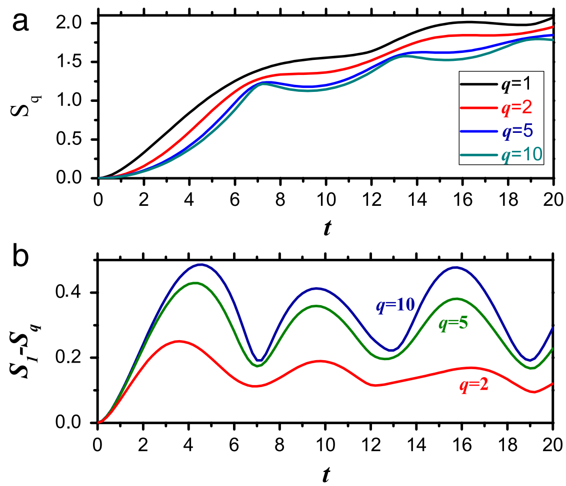

Fig. 6. It is depicted in (a) the Rényi entropy, a measure of the delocalization of the wave-packet. we show in (b) the deviation between the Rényi entropy, S_q, from the Shannon entropy, S_1, where S_1–S_q denotes the increasing of the delocalization as a function of time.

This kind of deviations S_1–S_q denotes the behavior of the increasing delocalization as a function of time. The differences can be regarded as complexity measures. They comply with one of the most basic properties of a statistical measure of complexity [32]: they vanish at "certainty" (when one has one probability p_i equal to one and the rest equal to zero) and also at equiprobability. In fact, the difference $S_1 - S_2$ is closely related to the LMC statistical measure of complexity introduced in 1995 by López-Ruiz et al. [32]. The study of the LMC and related complexity measures [33,34] and their multiple applications have been the focus of intense research activity in recent years (see [31] for a recent review on this subject).

We observe in Fig. 6 that the curves corresponding to the time evolution of S_1–S_q exhibit much more structure than those corresponding to the evolution of the entropies S_q themselves. The entropies S_q have a general tendency to increase (corresponding to the delocalization process) with small superimposed "oscillations". On the other hand, the evolution of the entropic differences S_1–S_q exhibit clearly defined local (in time) maxima and minima, reflecting the changing structure of the spatial probability distribution associated with the evolving wave-packet.

4. Concluding remarks

In this work we have investigated various aspects of the quantum evolution in a tight-binding lattice of a wave-packet corresponding to a highly localized initial state. This problem admits an exact solutions. However, to achieve an intuitive understanding of this process we also considered an approximate ansatz and complemented it with numerical computations.

We have shown that the spread of a wave-packet from a highly localized initial state in a tight-binding lattice in one-dimension is very similar to the evolution of quantum random walk in one dimension. Specifically, for the highly localized initial condition, the distribution of probability spreads symmetrically around the initial location of the particle, having several peaks, where the external peaks are greater than the other ones. The two external peaks are approximately located in $l_0 \pm 2Kt/\hbar$, whose speed of spreading is close to a constant given by $\pm 2K/\hbar$. Every property discussed here is also observed in the evolution of the quantum random walk in one dimension. The deviation of the position of a particle in the tight-binding lattice increases linearly in time, $\Delta l = \sqrt{\langle l^2 \rangle - l_0^2} \propto t$, as the discrete quantum random walk in opposition to the classical walker, which increases in time as $\Delta l \propto \sqrt{t}$.

The probability current was numerically evaluated to get certain internal properties that can be useful to characterize the structure of the system.

The Leipnik entropy was also evaluated to find a measure of the delocalization of the wave-packet. It is emphasized its value in $t = 0$, where delocalization is minimum because the entropy vanishes, $S_L = 0$, which means that the wave-packet is highly localized. As the delocalization takes place the entropy increases, giving finite values $S_L > 0$ for $t > 0$, indicating the amount of delocalization. Anomalies are clearly evident in the behavior of S_L. Indeed, the oscillations observed in Fig. 4(a) indicate that the entropy exhibits a non-monotonic behavior. An important remark is that in the present case the Leipnik entropy numerically coincides with the Shannon's one.

The inverse participant ratio was also used here as a quantitative measure of the loss of localization. This measure also tends to decrease as the delocalization takes place. This behavior becomes more gradual as the coupling parameter K increases.

The Rényi entropy was evaluated to quantify the behavior of the delocalization of the system. A kind of oscillations is seen similar to the one observed in the case of the Leipnik entropy. Nevertheless, we can characterize the increase of the delocalization by comparing the behaviors of different Rényi entropies evaluated for several values of the entropic parameter q. In fact, the differences S_1–S_q, which can be interpreted as statistical complexity measures (related to the LMC measure) turn out to be statistical indicators that are particularly sensitive to the details of the delocalization process. In this sense, our present results suggest that the study of the kind of processes considered here may constitute a new area where the LMC-like complexity measures can be successfully applied.

The extension of our present treatment to scenarios including disorder and interactions in one, two or three dimensions are interesting matters for future research. Any further developments along these lines will be very welcome.

Acknowledgments

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