Diffusion in infinite and semi-infinite lattices with long-range coupling

Alejandro J Martínez\textsuperscript{1,2} and Mario I Molina\textsuperscript{1,2}

\textsuperscript{1} Departamento de Física, Facultad de Ciencias, Universidad de Chile, Santiago, Chile
\textsuperscript{2} Center for Optics and Photonics (CEFOP), University of Concepción, Casilla 4016, Concepción, Chile

E-mail: mmolina@uchile.cl

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Abstract

We prove that for a one-dimensional, infinite periodic lattice, with long-range coupling among sites, the diffusion of an initial delta-like pulse in the bulk is ballistic at all times, with a ‘speed’ that depends on the ‘smoothness’ of the dispersion relation. We obtain a closed-form expression for the mean square displacement (MSD), and show some relevant examples including finite-range coupling, exponentially decreasing coupling and power-law decreasing coupling. For the case of an initial excitation at the edge of the lattice, we find an approximate expression for the MSD that predicts ballistic behavior at long times in agreement with numerical results.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The physics of discrete systems has been a topic of interest for many years, because it can give rise to completely different phenomenology in comparison with that present in homogeneous continuous systems. In particular, discrete periodic systems are found in many different contexts including condensed matter physics, optics, Bose–Einstein condensates and magnetic metamaterials among others. One of the classical problems in this context is that of the diffusion of an initially localized excitation propagating on a $D$-dimensional discrete lattice in the (possible) presence of one or several possible effects: the presence of impurities, extended defects, nonlinearities and the presence of boundaries, to name a few. Due to its intrinsic importance as well as its technological applications, this topic has received ample coverage in the literature [1].

Under the appropriate approximation, many discrete periodic systems can be described by some variant of the discrete Schrödinger (DS) equation [2]. In that way, many of these
systems display the phenomenology common to periodic systems such as the presence of a band structure, discrete diffraction, Bloch oscillations, dynamic localization, Zener tunneling, to name a few.

Usually, the DS equation is used in the weak-coupling limit, where the interaction among constituent units includes nearest-neighbors only. This is a good approximation in cases where the coupling among sites decays very quickly with distance, like the exponentially decreasing coupling found in optical waveguide arrays. However, there are cases where it is advisable to go beyond this approximation. An example of that is a split-ring resonator array, where the interaction among the basic units is dipolar in nature, and therefore, the coupling decreases as the inverse cubic power of the mutual distance [3].

In particular, when regarding the effect of coupling beyond nearest-neighbors, the number of possible routes of energy exchange increases. The dynamical evolution of excited pulses in finite one- and two-dimensional lattices with anisotropic couplings and including up to second nearest neighbor couplings has been explored in [4] by means of Green’s function formalism. Experimental observation of the influence of second-order coupling in linear and nonlinear optical zig-zag waveguide arrays has been recently carried out [5]. In a different context, a recent work [6] shows that long-range coupling in a low-dimensional system can induce a phase transition from delocalized to localized modes. Another interesting scenario that can be modeled as a discrete system with long-range couplings is that of complex networks [7], where the distances between nodes are not necessarily physical ones.

In this work, we carry out an analytical and numerical study on the diffusion of an initially localized pulse propagating in a one-dimensional discrete periodic lattice, in the presence of arbitrary long-range couplings. We focus on two cases of interest: a delta-like pulse in the bulk and a delta-like pulse at the edge of the lattice. The analytical work centers on the evaluation of the mean square displacement (MSD) of the excitation, which is obtained in exact form for the bulk excitation, and in an approximate form for the edge excitation.

2. Model

Let us consider the (dimensionless) DS equation, describing the evolution of an excitation along a one-dimensional periodic lattice:

\[ i \frac{du_n}{dz} + \sum_{m \neq n} V_{n,m} u_m = 0, \]  

(1)

where \( u_n \) is the complex amplitude of the excitation at the \( n \)th site and \( z \) is the evolution coordinate (‘time’ in the tight-binding model for electrons or ‘longitudinal distance’ for coupled waveguide arrays in optics). The matrix element \( V_{n,m} \) denotes the coupling between the \( n \)th and \( m \)th sites. This matrix is periodic in space and obeys \( V_{n,m} = V_{m,n} = V_{|n-m|} \). Model (1) is the starting point of many studies dealing with the diffusion of excitations in discrete periodic systems, found in several different physical contexts [1]. Equation (1) conserves the Hamiltonian \( H = \sum_{n \neq m} V_{n,m} [u_n u_m^* + u_m u_n^*] \) and the norm \( P = \sum_{-\infty}^{\infty} |u_n(z)|^2 \), which can then be set without loss of generality, as unity, \( P = 1 \). The dispersion relation of the linear waves is obtained by inserting a solution of the form \( u_n = A e^{i(kz + \lambda)} \) in equation (1), obtaining

\[ \lambda = \sum_{m \neq n} V_{n,m} e^{ik(m-n)} = 2 \sum_{m=1}^{\infty} V_m \cos(mk). \]  

(2)

The convergence of this series for all \( k \) values constrains \( V_n \) to decrease faster than \( 1/n \). From equation (2), we immediately obtain some basic properties of \( \lambda(k) \): \( \lambda(k) = \lambda(-k) \), \( \lambda(k) = \lambda(k + 2\pi q), \) \( q \in \mathbb{Z} \), and \( \partial_k \lambda(k) |_{k=0} = \partial_k \lambda(k) |_{k=\pm \pi} = 0 \).
The dynamical evolution of an initially localized pulse in a lattice, \( u_n(0) = A_0 \delta_{n,n_0} \), can be monitored through the MSD of the excitation:

\[
\langle n^2 \rangle = \sum_n (n - n_0)^2 |u_n(z)|^2 / \sum_n |u_n(z)|^2.
\] (3)

### 3. Diffusion in the bulk and at the boundary

#### 3.1. Diffusion in the bulk

In this case \(-\infty < n < \infty\) and \( u_n(0) = A_0 \delta_{n,n_0} \). Without loss of generality we take \( n_0 = 0 \). This corresponds physically to the case when the initial excitation is far away from the boundaries of the lattice. By combining Fourier–Laplace transforms to equation (1), followed by the corresponding transformation back to space \( n \) and \( z \) coordinates, one obtains a formal expression for \( u_n(z) \):

\[
u_n(z) = \frac{A_0}{2\pi} \int_{-\pi}^{\pi} e^{i(k n - \lambda(k)z)} dk,
\] (4)

where \( \lambda(k) \) is the dispersion relation. Next, we insert equation (4) into equation (3), and after using the general properties of \( \lambda(k) \), one obtains after some algebra

\[
\langle n^2 \rangle = \left[ \frac{1}{2\pi} \int_{-\pi}^{\pi} \left( \frac{d\lambda(k)}{dk} \right)^2 dk \right] z^2.
\] (5)

Equation (5) implies that the propagation of the excitation is \textit{ballistic at all times}, with a ‘speed’ that depends upon the ‘smoothness’ of the dispersion relation. This result is also valid in any dimension \( d \), where by using the same approach, it can be easily proven that

\[
\langle n^2 \rangle = \left[ \frac{1}{v} \int_{\text{FBZ}} (\nabla_k \lambda(k))^2 d^d k \right] z^2,
\] (6)

where the integral is taken over the first Brillouin zone (FBZ), with volume \( v \). An equivalent expression to equation (6) in ‘real space’ is obtained by substituting (2) in (6)

\[
\langle n^2 \rangle = \left[ \sum_m m^2 |V_{0,m}|^2 \right] z^2.
\] (7)

where \( m \) is the relative position if a lattice node from an arbitrary site \( n \) taken here as 0 without loss of generality because of periodicity and \( V_{0,m} \) is the coupling between sites 0 and \( m \), where \( V_{n,m} \) is periodic in space and obeys \( V_{n,m} = V_{-n,-m} \).

Let us compute now in detail the MSD for several cases of interest.

(a) \textit{Second-order coupling}. In this case, \( V_1 = V, V_2 = \beta V \) and \( V_{i>2} = 0 \), and the dispersion relation is \( \lambda = 2V (\cos(k) + \beta \cos(2k)) \). This implies, according to equation (5)

\[
\langle n^2 \rangle = 2(1 + 4\beta^2)(Vz)^2.
\] (8)

Thus, the inclusion of a second-order coupling (only) always increases the speed of the transversal diffusion.

(b) \textit{Exponentially decreasing coupling}. In this case, \( V_{n,m} = V e^{-\alpha(|n-m|-1)} \), where \( V \) is the coupling between nearest neighbors sites and \( \alpha \) is the long-range parameter.
Figure 1. Exponentially decreasing coupling: discrete diffraction pattern at $V_z = 20$ for spread in the bulk of a delta-like initial condition, for different values of the long-range interaction parameter $\alpha$. High (low) values of $\alpha$ correspond to short (long) interaction range.

Figure 2. Speed of ballistic propagation of initially localized bulk excitation as a function of long-range interaction parameter. The solid (dashed) curve corresponds to exponential (power-law) coupling case. For the power-law coupling case, $g(\alpha) = 2 \zeta (2(\alpha - 1))$.

The linear dispersion relation is
\[
\lambda = V \left( \frac{e^{\alpha} \cos(k) - 1}{\cosh(\alpha) - \cos(k)} \right). \tag{9}
\]

Figure 1 shows some snapshots of the spatial transversal profiles at a given longitudinal propagation distance $z$, for different values of the dispersion parameter. We note that, at small $\alpha$ values, some optical power seems to 'linger' at the initial position [4, 8], in a sort of quasi-self-trapping, while the 'untrapped' portion propagates away from the initial site faster than in the nearest-neighbor case. These observations can be put on a more rigorous basis by computing the MSD directly from equation (5), using equation (9). We obtain $\langle n^2 \rangle = g(\alpha)(Vz)^2$, where
\[
g(\alpha) = \frac{1}{2} \coth(\alpha)(\coth(\alpha) + 1)^2. \tag{10}
\]

This implies a ballistic speed $g(\alpha) \geq 2$, for all finite $\alpha$. However, it only becomes notable larger than 2 for $\alpha \lesssim 2$ (figure 2).

(c) Power-law coupling. Another popular case of long-range interaction is the power-law coupling $V_{n,m} = V/|n - m|^\alpha$. This case was studied numerically in [9], where, among other results, a critical $\alpha$ value was found, above which the propagation was always...
ballistic. This critical value was estimated to lie in the interval $1.5 \leq \alpha_c \leq 2$. Below we prove that $\alpha_c = 3/2$.

In this case, the dispersion relation is given in terms of a polylogarithm function

$$
\lambda(k, \alpha) = V \left( \text{Li}_\alpha(\text{e}^{ik}) + \text{Li}_\alpha(\text{e}^{-ik}) \right) = 2V \sum_{m=1}^{\infty} \cos(mk)/m^\alpha.
$$

For $\alpha = 1$, we can explicitly write

$$
\lambda(k, 1) = -V \log|2 - 2 \cos(k)|,
$$

with the logarithm diverges for $k = 0$. On the other hand, for $\alpha > 1$, the polylogarithm remains bounded at $|k| \leq \pi$. However, the condition on $\alpha$ is more restrictive if we want $\langle n^2 \rangle$ to remain finite. From equation (7), we obtain

$$
\langle n^2 \rangle = 2\zeta(2(\alpha - 1))(Vz)^2,
$$

where $\zeta$ is the Riemann zeta function. Thus, we need $\alpha > 3/2$. Figure 2 shows the ‘speed’ of diffusion as a function of $\alpha$ and compares it with the ‘speed’ obtained for lattices with exponentially decreasing coupling. The discrete diffraction pattern observed in case (b) (figure 1) is also observed in this case.

In all three cases examined, the speed of diffusion is greater than in the case with nearest-neighbors coupling only. For the exponential and power-law cases, we note that as the range of the interaction is increased, the pulse experiences a sort of quasi-localization at the initial site. At the same time, the speed $g(\alpha)$ increases above 2 and tends to diverge at $\alpha = 0$ for the exponentially decreasing case and at $\alpha = 3/2$ for the power-law case (figure 2). We can understand this quasi-localization phenomenon by analyzing the dispersion relations more closely. In cases (b) and (c), as the range increases, the dispersion gets flatter and flatter in the vicinity of $k = \pm \pi$, signaling the emergence of linear modes with very small group velocities. As $\alpha$ is decreased further, this vicinity grows and most of the linear modes acquire negligible velocity, with the exception of a small vicinity of $k = 0$, where the concavity is very high, giving rise to long wavelength modes with high velocity. Since our initial delta-like condition is a superposition of all these linear waves, the pseudo-localization phenomena can be understood as due to those modes with zero velocity, while those few and fast long wavelength modes give rise to the wings that escape at high speed.

In the formal limit $\alpha = 0$ and for a finite number of sites $N$, all sites are connected to one another, and the high degree of degeneracy forces the localization of the wavefunction through the execution of incomplete oscillations between the initial excited site and all the other ones. In this case, the effective dynamics can be mapped to the dynamics of an asymmetric dimer [10]. This system has been solved in closed form and shows partial linear localization at the initial site for finite $N$, which becomes complete in the limit $N \rightarrow \infty$ [8].

### 3.2. Diffusion at the boundary

In this case $u_0(0) = A_0 \delta_{n,1}$, i.e. the initial excitation is at the edge of the lattice. This system can be viewed as an infinite lattice with boundary conditions: $u_n(z) = 0$ for $n \leq 0$, for all $z$. The lack of translational symmetry prevents us from writing a general expression for $u(z)$, similar to equation (5). However, the case of nearest-neighbors coupling can only be solved in a closed form using the method of images [11]. In that case, the boundary conditions are obeyed if we placed an opposite delta-like source at $n = -1$. Then, the propagation for $n > 0$ is then the superposition of the evolution of both sources:

$$
u_n^s(z) = u_n(z) - u_{n+2}(z) = \frac{A_0}{2\pi} \int_{-\pi}^{\pi} \left( 1 - e^{-2ik} \right) e^{i(kn - \lambda(k)z)} \, dk,
$$

(13)
where the superscript $s$ denotes a semi-infinite array. However, when long-range couplings are considered, it is no longer possible to satisfy the boundary conditions by the image method. The reason has to do with the fact that, even though we have $u_{-1}(z) = 0$ for all $z$, the fields of each semi-infinite arrays are still coupled by the range of the interaction.

In spite of this difficulty, and after carrying out a number of numerical simulations for the dynamical evolution of the initially localized edge excitation, we have found that equation (13) provides a good approximation to the asymptotic behavior ($z \to \infty$) for the general case, by just substituting the corresponding dispersion relation for a given long-range coupling into equation (13) (see figure 3). After a bit of algebra, one obtains

$$\langle n^2 \rangle_s \approx \left[ \frac{1}{\pi} \int_{-\pi}^{\pi} \sin^2(k) \left( \frac{dk}{d\lambda(k)} \right)^2 \frac{dk}{d\lambda} \right] z^2,$$

valid for $z \gg 1$.

As expected, the asymptotic behavior is ballistic in all cases, after some transient time, related to the repulsive effect of the boundary. Equation (14) can also be expressed in real space by substituting equation (2) into equation (14), obtaining

$$\langle n^2 \rangle_s \approx \left[ 3V_1^2 + 2 \sum_{m=2}^{\infty} m^2 V_m^2 - 2 \sum_{m=1}^{\infty} m(m + 2)V_mV_{m+2} \right] z^2.$$

These results are confirmed by direct computations of cases (a), (b) and (c), using ‘exact’ equation (1), with an edge excitation as an initial condition, and comparing it with the asymptotic equations (14) and (15). Figure 4 shows this comparison of the MSD for the exponentially decreasing coupling case. In this case, the asymptotic behavior is

$$\langle n^2 \rangle_s \approx 3 \coth(\alpha)(Vz)^2.$$

In figure 5, we show a comparison between this approximation and the numerical results.

We see that for $\alpha \gg 1$ there is a good correspondence between the numerical and analytical approach, while for $\alpha \ll 1$, the exact solution for the bulk, equation (10), constitutes a better fit than the surface approximation, equation (16). This is understandable because in
Figure 4. Numerically exact MSD in logarithmic scale for several values of the long-range parameter $\alpha$, for the exponentially decreasing coupling case. The solid line denotes the approximate solution obtained using the method of images, equation (13), while the gray line shows the slope associated with $z^2$ (to guide the eyes only).

Figure 5. Square of speed of ballistic propagation of initially localized edge excitation as a function of dispersion parameter $\alpha$ for the exponentially decreasing coupling. Triangles correspond to numerical values, continuous line to approximation (16) and dashed line to the exact bulk solution, equation (10).

the long-range coupling regimen, the boundary loses its meaning as such and the edge site behaves effectively like a bulk site.

4. Conclusions

We have examined the propagation of a localized excitation initially placed in the bulk and at the boundary of a one-dimensional periodic lattice, in the presence of general long-range coupling. For the bulk case, we find a novel, closed-form expression showing that the propagation is ballistic at all times, with a ‘speed’ that depends on the ‘smoothness’ of the underlying dispersion relation. In general, this speed increases as the range of the coupling increases. This was clearly evidenced in the examples of second-order coupling, exponentially decreasing coupling and power-law decreasing coupling. For the edge excitation, the behavior is asymptotically similar, after a transient time. The long-range nature of the coupling made
use of the image method not possible, but we proved numerically that it can be applied at long evolution times, thus finding a closed-form asymptotic expression predicting ballistic propagation at long times for any long-range coupling with a speed that, as in the bulk case, depends on the smoothness of the dispersion relation.

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