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Wave-Packet Dynamics in Chains with Disorder-Type Ornstein–Uhlenbeck and Static Electric Field

*Jose Luis S. Soares, Adhemar Ranciaro Neto, Messias O. Sales, and Francisco A. B. F. de Moura**

Herein, the electronic dynamics in a 1D model with correlated disorder and under the influence of a static electric field is considered. In the framework, the diagonal disorder is obtained from an Ornstein–Uhlenbeck (OU) process. The Schrödinger equation considering an initial Gaussian wave packet with width *l* located at the center of chain will be solved. To understand the competition between the OU-like disorder and the electric field, the time evolution of the electronic mean position is calculated. The results suggest that chains with diagonal disorder generated from OU process with small viscosity coefficient seem to exhibit apparent Bloch oscillations (BO) with dominant frequency roughly $\omega \approx E$. In addition, the stability of these apparent BO along the time is investigated.

1. Introduction

The presence of a static electric field acting on a periodic lattice promotes the dynamic localization of a given wave packet. Furthermore, the localized wave packet exhibits an oscillatory behavior called "Bloch oscillations" (BO).[1,2] The period of these oscillations is inversely proportional to the magnitude of the static electric field. In the recent literature, it is possible to find a wide collection of works in which it is possible to "visualize" BO in several kinds of systems.[3–16] The first real direct observation of BO was done in semiconductor superlattices.[12] Following this discovery, other Bloch-like phenomena were detected in matter waves,[13] acoustic waves,[14] optical systems,[15] and also in plasmonic waveguide arrays.[16] Recently, the problem of many-body quantum dynamics in optical lattices was experimentally investigated.[17] The authors have used an amazing experimental framework to access to essential features of many-body systems (such as particle–particle interaction, electric field effects; by the way, disorder can also be included within this setup). They experimentally demonstrate the dependence of the frequency of BO with the intensity of the particle–particle interaction. In general, Preiss et al.[17] confirmed the theoretical prediction of frequency doubling of BO[18] due to electron–electron Coulomb interaction. In a theoretical overview, some attention was driven to the possible existence of BO in disordered systems[19,20] with intrinsic correlations in the disorder distribution. These results indicate that, at the limit of strong correlations, these systems may exhibit BO even at the complete absence of internal periodicity.

In this work, we provide further progress along those lines. We investigate the electronic dynamics in a chain with correlated disorder under the influence of a static electric field E. In the current model, the diagonal disorder is constructed using an Ornstein–Uhlenbeck (OU) process. This stochastic process describes the dynamics of a Brownian motion under the influence of friction.[21,22] In general, the OU process is a random series in which the power spectrum displays a Lorentzian shape.[21,22] The presence of disorder distributions based on the OU process was investigated in classical transmission lines (TL)[23] and also in classical harmonic chains.[24] Within the framework of TL systems, it was shown that the OU disorder can promote the appearance of a transition from nonconducting to conducting states.[23] However, calculations in 1d classical harmonic chains with the mass distribution constructed from an OU process indicate that only the zero-frequency mode can propagate through the chain.[24] In our work, we will use the OU process to introduce correlations within the on-site electronic potential. We will solve the Schrödinger equation considering an initial Gaussian wave packet with width l located at the center of chain. To understand the competition between the OU-like disorder and the electric field, we monitor the mean electronic position along the time. Our results suggest that chains with diagonal disorder generated from OU process with small viscosity coefficient seem to exhibit apparent BO with frequency roughly $\omega \approx E$. We analyze the survival of this apparent BO by comparing the localization length of eigenstates with the size of region in which the wave packet remains trapped.

J. L. S. Soares, Dr. F. A. B. F. de Moura
Instituto de Fsica
Universidade Federal de Alagoas
57072-970 Maceió-AL, Brazil
E-mail: fidelis@fis.ufal.br

Dr. A. R. Neto
Faculdade de Economia
Administração e Contabilidade
Universidade Federal de Alagoas
57072-970 Maceió-AL, Brazil

Dr. A. R. Neto
Ministry of Economy – Special Secretariat for Finance
Esplanada dos Ministérios, BL P, Braslia, DF 70297-400, Brazil

Dr. M. O. Sales
Instituto Federal do Maranhão (IFMA)
Campus São João dos Patos
rua Padre Santiago, s/n, Centro, São João dos Patos, MA 65665-000, Brazil

The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/pssb.202000096.

DOI: 10.1002/pssb.202000096

2. Model and Formalism

We consider the problem of a one-electron moving on a disordered chain under the influence of a static electric field. The electronic Hamiltonian in our model is given by[19,20]

$$H = \sum_{n=1}^{N}[\epsilon_n + E(n - N/2)]|n\rangle\langle n| + \sum_{n=1}^{N}(|n\rangle\langle n+1| + |n\rangle\langle n-1|) \tag{1}$$

where ϵ_n is the on-site energy, E represents the electric field acting parallel to the chain, and $E(n - N/2)$ is the energy interaction between an electron with charge $e = 1$ and the electric field E (take the lattice spacing as $a = 1$). The term $|n\rangle$ is a Wannier state at the nth site. If electronic wave function at time t was $|\psi(t)\rangle = \sum_n f_n(t)|n\rangle$, then we write the time-dependent Schrödinger equation as ($\hbar = 1$)

$$[\epsilon_n + E(n - N/2)]f_n + f_{n+1} + f_{n-1} = i\frac{df_n}{dt} \tag{2}$$

In our study, the diagonal disorder distribution is obtained from an OU process. This stochastic process is defined from the following stochastic differential equation[21–26]

$$\frac{dz}{dt} = -\gamma z(t) + \sqrt{D}\lambda(t) \tag{3}$$

succinctly, where γ represents the system viscosity, D is the diffusion coefficient, and finally $\lambda(t)$ is known as the stochastic term.[23,25] The quantity $\lambda(t)$ is termed as a white Gaussian noise produced by the Box–Muller method such that $\langle\lambda(t)\rangle = 0$ and $\langle\lambda(t)\lambda(t+\tau)\rangle = \delta(\tau)$. It is possible to show that $\langle z(t)\rangle = z_0 e^{-\gamma t}$ and $\langle z(t)z(t+\tau)\rangle = (D/2\gamma)e^{-\gamma\tau}$.[26] A discrete form of Equation (3) is constructed based on the study by Gillespie.[26] Then, $z(t)$ is reduced to z_m, where m expresses the number of time increments ($t = m\Delta t$). Using this discrete variable, we get another version of Equation (3)

$$z_{m+1} = \mu z_m + \sigma_m \alpha_m \tag{4}$$

where μ is written in the form

$$\mu = e^{-\gamma\Delta t} \tag{5}$$

and that σ is a function of the process-specific parameters OU (γ and D)

$$\sigma_m = \sqrt{\left(\frac{D}{2\gamma}\right)(1 - \mu^2)} \tag{6}$$

We emphasize that α_m is a white Gaussian noise obtained by a Box–Muller algorithm.[23,25] In our calculations, we consider $D = \gamma^2$.[23,25] We start Equation (4) with a random seed z_0 and therefore generate all values $z_1, z_2, \ldots, z_N$. After the set of values of $\{z_m\}$ be generated, we performed a normalization done on this set $\{z_m\}$ in order to construct the on-site energy terms. We initially calculate the normalized sequence of $\{z_m\}$ values, i.e., $\{\tilde{z}_m\}$ defined by $\tilde{z}_m = (z_m - \langle z_m\rangle)/\sqrt{\langle z_m^2\rangle - \langle z_m\rangle^2}$. The on-site energies ϵ_n will be defined as $\epsilon_n = \tilde{z}_m$ with $n = \equiv m$. We emphasize that there are a wide range of techniques that can construct disordered sequences with internal correlations. Some of them use a Fourier-transform formalism (like in ref. [19]). The kind of formalism used in the study by Domínguez-Adame et al.[19] does not contain disorder in the amplitudes of the Fourier decomposition; the source of disorder is, in general, introduced at the phases of the Fourier formalism. The OU stochastic process can generate correlated disorder without the Fourier formalism. Therefore, this is a key difference between the OU disorder and the disorder distribution considered in the study by Domínguez-Adame et al.[19] If we calculate the Fourier transform of the OU series, we will find disorder in both amplitudes and phases of the Fourier decomposition. Moreover, we need to point out again that the correlation function here is roughly an exponential with correlation length of about $1/\gamma$. Therefore, the disorder distribution here exhibits a typical finite correlation length. The disorder distribution obtained via Fourier formalism[19] does not contain a typical finite correlation length due to its power law spectrum.

Our calculations are done by numerical solution of Equation (2). These differential equations were solved using a high-order Taylor expansion of the evolution operator[25,27]

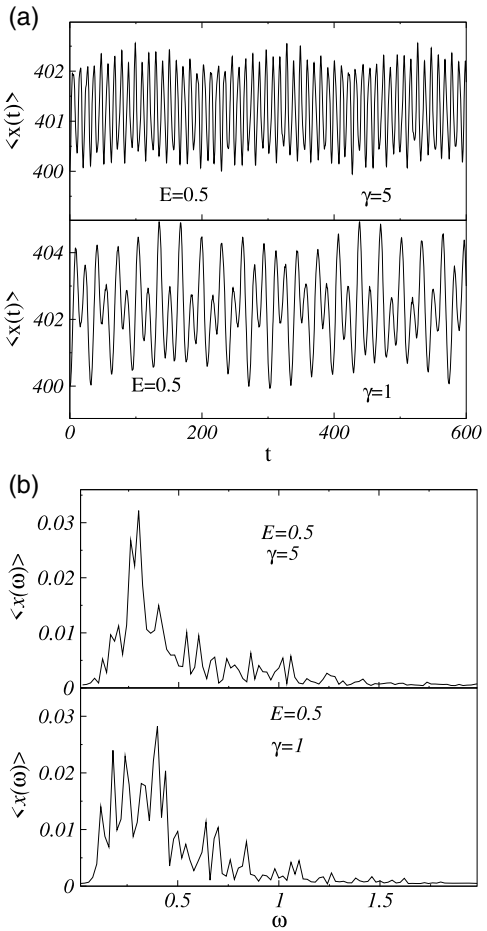

Figure 1. a) Electronic mean position $\langle x(t)\rangle$ versus time t and b) its Fourier transform for $E = 0.5$ and $\gamma = 1$ and 5. The electron remains localized around the initial position and the Fourier spectrum does not exhibit a single-frequency profile.

$$U(\Delta t) = \exp(-iH\Delta t) = 1 + \sum_{l=1}^{R_0} \frac{(-iH\Delta t)^l}{l!} \quad (7)$$

where H represents the Hamiltonian of the system. The electronic state at time Δt is obtained from the initial state as $|\psi(\Delta t)\rangle = U(\Delta t)|\psi(t=0)\rangle$. We can apply the evolution operator successively to find the electronic wave function at time t. This formalism is faster and is more accurate than, for example, fourth-order Runge–Kutta formalism. In our calculations, we use $R_0 = 12$ and $\Delta t = 0.01$. To characterize the electronic dynamics, we calculate the electronic position along the time, i.e.

$$\langle x(t)\rangle = \sum_n n|f_n(t)|^2 \quad (8)$$

The electronic position gives useful information about the general electronic dynamics under the influence of correlated disorder and electric field.

3. Results

We performed calculations in a chain with $N = 800$ sites immersed in a static electric field value E. It is worth mentioning that we are using units such that $e = a = \hbar = 1$ and the terms ϵ_n and $E(n - N/2)$ are in units of the electronic hopping. In our calculations, the electron was initially set in a Gaussian state, i.e., $|\psi(t=0)\rangle = \sum_n f_n(t=0)|n\rangle$ with $f_n(t=0) = Ae^{[-(n-N/2)^2/4]}$ and A being a normalization constant. In **Figure 1**a,b, we plot results for $\gamma = 1$ and 5 and $E = 0.5$. In case Figure 1a, we plot the electronic position versus time and in Figure 1b, we plot its Fourier transform. According to the figure, the electron remains dynamically localized around the initial position. Moreover, the Fourier spectrum exhibits a broadening range of frequencies, thus indicating an incoherent dynamics (in good agreement with the dynamics profile shown in Figure 1a). We stress that for $\gamma \gg 1$, the on-site disorder does not contain correlations; it behaves roughly as a uncorrelated disorder similar to the kind of disorder previously used in the standard Anderson model. Therefore, the electron also remains localized even in the absence of electric field. By decreasing the value of γ, our results change drastically. In **Figure 2**, **3**, and **4**, we show our calculations for $\gamma = 0.001$ and 0.0001 with $E = 0.5$, 0.7, and 0.9. **Figure 2**a, 3a, and 4a show an apparent coherent electronic dynamics around the initial position. We observe that the wave packet remains trapped in a region with size L_0; L_0 is the mean size of region in which the electron keeps its oscillatory dynamics. By observing

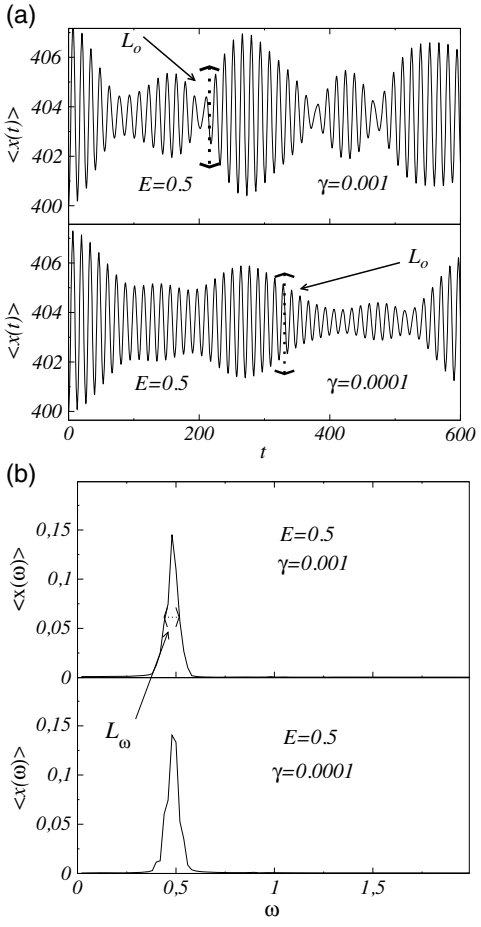

Figure 2. a) Electronic mean position $\langle x(t)\rangle$ versus time t and b) its Fourier transform for $E = 0.5$ and $\gamma = 0.001$ and 0.0001.

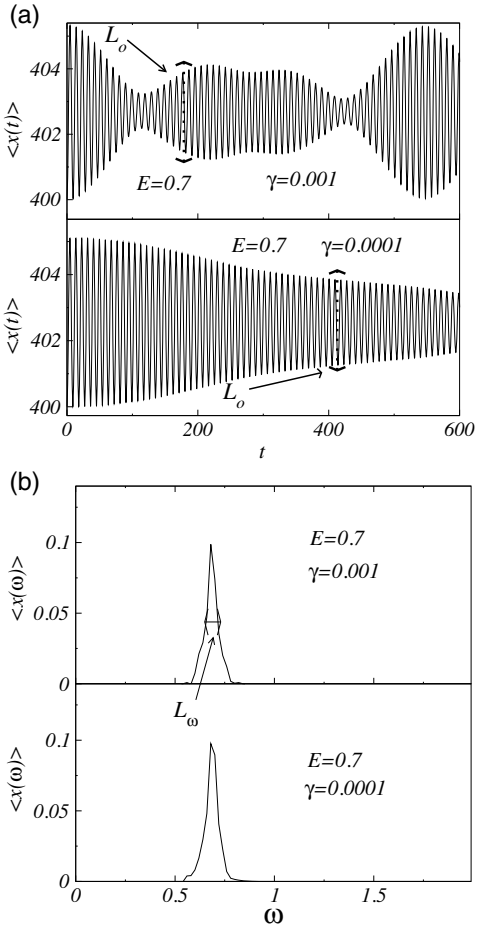

Figure 3. a) Electronic mean position $\langle x(t)\rangle$ versus time t and b) its Fourier transform for $E = 0.7$ and $\gamma = 0.001$ and 0.0001.

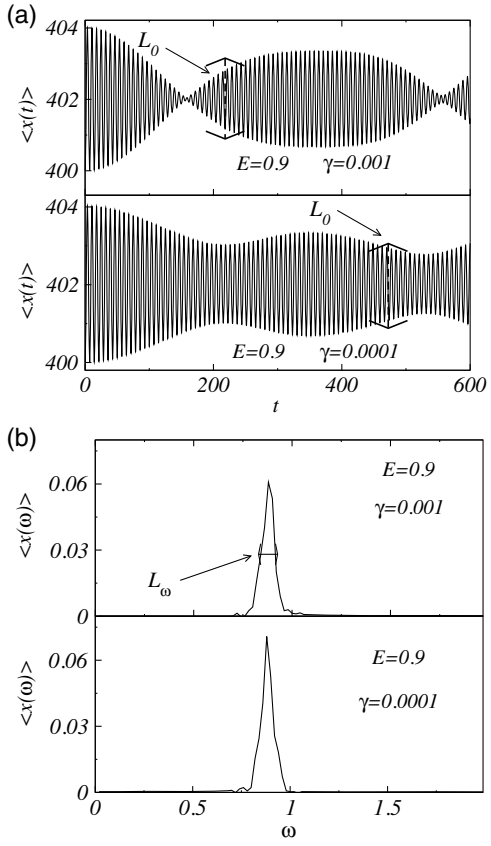

Figure 4. a) Electronic mean position $\langle x(t)\rangle$ versus time t and b) its Fourier transform for $E = 0.9$ and $\gamma = 0.001$ and 0.0001.

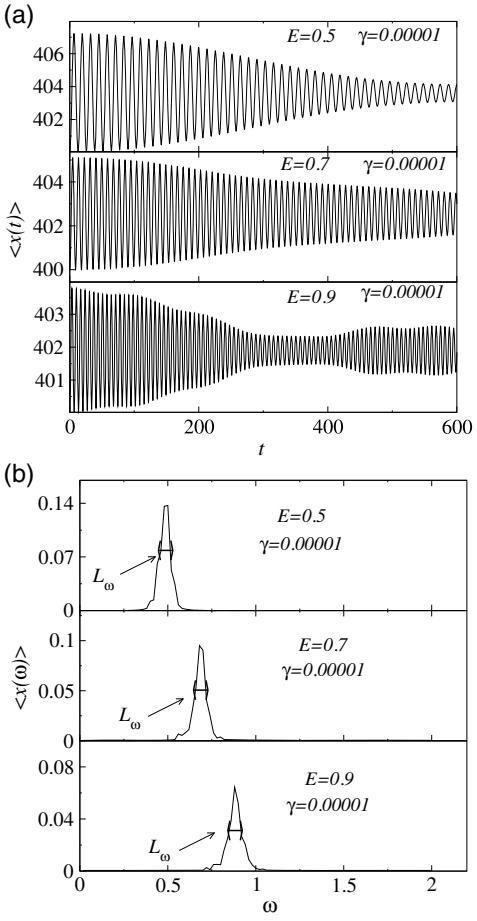

Figure 5. a) Electronic mean position $\langle x(t)\rangle$ versus time t for $\gamma = 0.00001$ and $E = 0.5$, 0.7, 0.9; b) the Fourier transform of part (a).

Figure 2a, 3a, and 4a, we can see the vertical dashed line illustrating the quantity L_0. We emphasize that L_0 is obtained by calculation of the dispersion of the electronic position $\langle x(t)\rangle$ along the time; our calculations indicate that the value of L_0 for these cases is approximately $L_0 = 6$.

The Fourier transform (Figure 2b, 3b, and 4b) showed a single peak around the $\omega \approx E$ and thus in good agreement with the coherent electronic dynamics shown in Figure 2a, 3a, and 4a. The single narrow peak around $\omega \approx E$ suggests that the results found are, indeed, apparent BO[3–11] with frequency roughly equal to the frequency predicted by the semiclassical formalism.[28,29] In **Figure 5**a,b, we show our results for $\gamma = 0.00001$ and $E = 0.5$,0.7, and 0.9. Based on Figure 5a,b, we note that the electron remains trapped around the initial position and exhibits an oscillatory behavior with frequency roughly $\omega = E$. We did a lot of calculations for several values of E and γ, and analyzed the Fourier transform of the electronic position. To detect the existence of a single frequency at the oscillatory electronic dynamics, we found the width L_ω of the Fourier spectrum. If $L_\omega \gg 0$, we are dealing with a Fourier transform with several frequencies within the electronic dynamics; therefore, we have an incoherent oscillatory behavior. However, if $L_\omega = 0$, the Fourier spectrum contains a single frequency and, therefore, the oscillatory behavior should be coherent. In **Figure 6**, we plot the width L_ω of the Fourier spectrum versus the correlation degree γ. We plot our calculations for $E = 0.5$, 0.7, and 0.9 in the plane $(L_\omega, \log(\gamma))$. For $\gamma > 1$, the Fourier spectrum is strongly wide, thus indicating the complete absence of Bloch-like oscillations. For $\gamma < 1$, the width of Fourier spectrum decreases, thus pointing to the existence of a single-frequency dynamics. However, the complete vanishing of the width L_ω is not obtained within the range of values of γ used here. Within our numerical tolerance, the values of L_ω seem to saturate for $\gamma < 0.001$ in a value $L_\omega = 0.04(2)$. We think that, in our numerical precision, this extremely narrow Fourier spectrum indicates the presence of apparent Bloch-like oscillations with a single frequency ($\omega \approx E$). In **Figure 7**, we illustrate the effect of the OU correlated disorder and the static electric field on the electronic dynamics. We plot the square modulus of the electronic wave function ($|f_n|^2$) versus time t and n with $E = 0.5$, $\gamma = 0.0001$, and $\gamma = 1$. We clearly observe the Bloch-like oscillations for $\gamma = 0.0001$. The coherent oscillatory patterns with frequency $\omega = 0.5$ are shown in Figure 7a. Moreover, for $\gamma = 1$ (Figure 7b), there is possible to note the localization dynamics of the electronic wave packet with no coherent profile. Therefore, our results indicate that, for $\gamma < 0.001$, this model exhibits Bloch-like oscillations with frequency $\omega \approx E$.

Before concluding this work, we need to write some words on the stability of these oscillations along the time. The OU-like

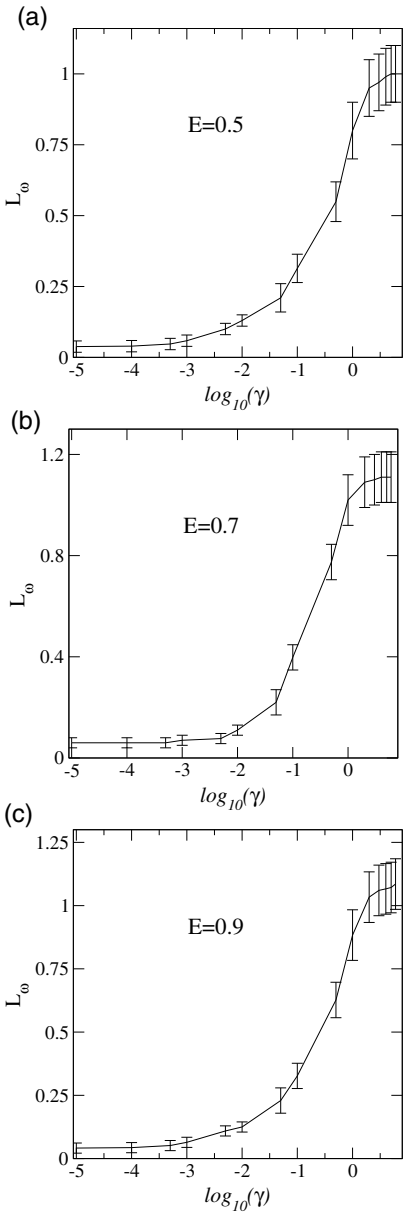

Figure 6. The width L_ω of the Fourier spectrum versus the logarithm of correlation degree $\log(\gamma)$ for a) $E = 0.5$, b) $E = 0.7$, and c) $E = 0.9$. Our calculations suggest that, for $\gamma < 0.001$, L_ω saturates in a small value (about $L_\omega = 0.04(2)$), thus pointing to the presence of apparent Bloch-like oscillations with a single frequency ($\omega = E$).

disorder contains a power spectrum fitting a Lorentzian profile; the autocorrelation functions exhibit an exponential decay. The correlations' length is proportional to $1/\gamma$. Therefore, formally, the disorder displays short-range correlations. However, at the presence of static electric field, the size of regions in which the electron remains trapped is extremely smaller than $1/\gamma$ at the limit of small viscosity. Therefore, the oscillatory behavior may hold for intermediate time span (the time limit in our numerical calculations was about 10^5). Moreover, at the thermodynamic limit, there is no extended states within this model.[24]

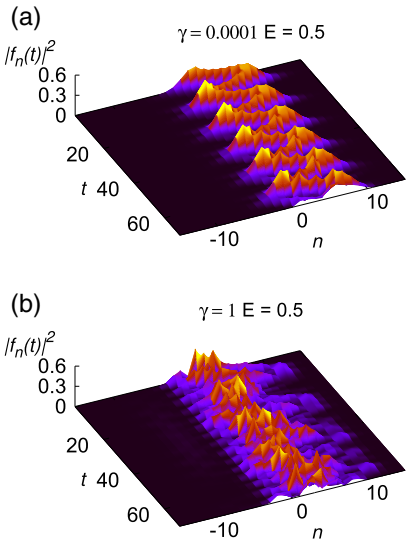

Figure 7. The square modulus of the electronic wave function ($|f_n|^2$) versus time t and n considering $E = 0.5$, a) $\gamma = 0.0001$ and b) $\gamma = 1$.

For γ close to zero, the states around the band center are weakly localized (not fully extended), so the oscillatory behavior might not be sustained indefinitely. To understand the nature of eigenstates better, we solve the problem with no electric field ($E = 0$) calculating the scaled participation number defined as $\xi/N = (1/N)[\sum_n Y_n^4]^{-1}$, where Y_n are the components of the eigenstate $|\psi\rangle$ (i.e., $|\psi\rangle = \sum_n Y_n|n\rangle$).

Computation were done for $N = 800$ up to 6400, $\gamma = 0.0001$, and $E = 0$. In **Figure 8**, we plot the scaled participation number versus the electronic energy E_c. We see that ξ/N decreases as the system size N is increased. It is a clear signature of localized states. However, for eigenstates with energy E_c close to zero, the localization length seems large (it is roughly about $N/3$). Therefore, these states around the band center remain weakly localized and promote the appearance of this oscillatory behavior for intermediate time span. These states around $E_c = 0$ have a localization length larger than the region in which the electron remains trapped and oscillating. Analyzing Figure 2 and 3, we note that the electron oscillates in a region with size

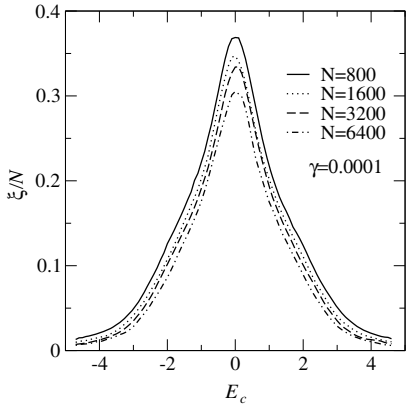

Figure 8. The scaled participation number versus energy E_c for $N = 800$ up to 6400 with $\gamma = 0.0001$ and in the absence of electric field ($E = 0$).

$L_0 < 10$ sites. However, it is shown in Figure 8 that the cases with size $N = 800$ (same size as in Figure 2 and 3) have some eigenstates with localization length ξ over 100 sites. Therefore, the difference between the localization length (over 100 sites) and the size of region in which the electron wave packet remains trapped ($L_0 < 10$ sites) is the key issue behind the apparent oscillatory dynamics found.

4. Conclusion

We studied the electronic dynamics in a 1D model with correlated disorder and under the influence of a static electric field. Here, the diagonal disorder was obtained from an OU process. We solved the Schrödinger equation using a Taylor expansion of the evolution operator. The initial condition was a Gaussian wave packet with width l located at the center of chain. We calculated the mean electronic position along the time. Our results suggest if the diagonal disorder distribution was generated from an OU process with small viscosity coefficient, then the electronic dynamics seem to exhibit apparent BO with frequency roughly equal to the magnitude of the electric field. However, due to the absence of real extended states within this model, it is possible that this oscillatory behavior could not be kept indefinite. For $1/\gamma$ larger than the size of the region in which the electron wave packet remains trapped, this Bloch-like oscillation may survive for intermediate times (the maximum time used here was about 10^5). From the experimental point of view, we think that these results could be observed in appropriately designed random microwave waveguides[30,31] or optical lattices.[17,32]

Acknowledgements

This work was partially supported by CNPq, CAPES, and FINEP (Federal Brazilian Agencies), CNPq-Rede Nanobioestruturas, as well as FAPEAL (Alagoas State Agency).

Conflict of Interest

The authors declare no conflict of interest.

Keywords

correlated disorder, localization, wave-packet dynamics

Received: February 20, 2020
Revised: May 5, 2020
Published online: May 20, 2020

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