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Electronic dynamics in chains with Ornstein–Uhlenbeck correlated disorder

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In this paper, we present a detailed study of the electronic dynamics in systems with correlated disorder generated from the Ornstein–Uhlenbeck process (OU). In short, we used numeric methods for solving the time-dependent Schrödinger equation. We apply a Taylor's expansion of the evolution operator in order to solve the differential equation. We calculate some typical tools, such as the participation function $\xi(t)$, the mean square displacement $\sigma(t)$ and the probability of return $R(t)$. In our analysis, we show that for low correlations the system behaves as in the standard Anderson model (i.e. all eigenstates are localized). For strong correlations, our results suggest the existence of a quasi-ballistic dynamics.

Keywords: Correlated disorder; localization; dynamics.

1. Introduction

The dynamics of electrons, phonons, magnons and other elementary excitation in disordered systems have significant implications in the solid state sciences. One of the pioneering and interesting work was done by Anderson, the "Localization theory"; Anderson has developed a model that can explain the general aspects of electronic localization in systems with impurities.[1] Two decades later, in 1979, Abrahams *et al.* proposed the scale theory for the Anderson transition. By using the scale theory, it is possible to understand the dependence of the localization theory with the topological dimension of the system.[2] In the following decades, a range of papers has been published about the localization properties within disordered systems.[3–11] In the recent literature, a lot of works has proved that the presence of correlated disorder can promote the existence of weakly localized states (or some times extended states) in low-dimensional systems $(d <= 2)$.[12–29] Some of these previous works were

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experimentally verified by Bellani *et al.*[30] and Kuhl.[31] They have studied the effect of short- and long-range correlations on the transport properties of low-dimensional disordered systems. Both works concluded that indeed correlations within the disorder distribution promote the amplification of transport properties.

In this paper, we will provide some advances along with these above lines. We will study the electronic dynamics in a 1D model with correlated disorder distribution. We construct the diagonal disorder distribution by using the Ornstein–Uhlenbeck (OU) process. We apply a Taylor's expansion of the evolution operator in order to solve the time-dependent Schrödinger equation and then calculate the time evolution of an initially localized wave packet. The spreading of the electronic wave packet is measured by using standard tools like the participation number and the mean square displacement. Our results suggest that for OU process without correlations this model is similar to the Anderson Model with uncorrelated disorder. Within the limit of strong correlations, our results suggest the existence of a quasi-ballistic dynamics for initial times. After this initial quasi-ballistic dynamics, we observed a crossover for a localized behavior at the limit of long times. The wave packet saturates in a region with increasing size as the degree of correlations within the OU process is increased.

2. Model

In our model, we will consider the electronic Hamiltonian given by[33]:

$$H = \sum_{n=1}^{N} E_n |n\rangle\langle n| + \sum_{n=1}^{N} (|n\rangle\langle n+1| + |n\rangle\langle n-1|), \tag{1}$$

where $|n\rangle$ is the Wannier state at site n and E_n represents the *on-site* energy. By assuming the electronic state as $|\psi(t)\rangle = \sum_n C_n |n\rangle$, we can write the time-dependent Schrödinger equation and ($\hbar = 1$),

$$E_n C_n + C_{n+1} + C_{n-1} = i \frac{dC_n}{dt}. \tag{2}$$

In our model, the *on-site* energies will be described by an OU process. The OU process is defined by using the following stochastic differential equation:

$$\frac{dx}{dt} = -\gamma x(t) + \sqrt{\mathcal{D}}\lambda(t), \tag{3}$$

where γ represents the system viscosity, $\mathcal{D}$ is the diffusion coefficient and $\lambda(t)$ represents a stochastic term.[18,32] In general, $\lambda(t)$ is generated from a white Gaussian noise with $\langle\lambda(t)\rangle = 0$ and $\langle\lambda(t)\lambda(t+\tau)\rangle = \delta(\tau)$ (this sequence can be constructed by using the well-known *box-muller* method). Based on Refs. 33–35, it is possible to take a discrete form of Eq. (3) as

$$x_{n+1} = \mu x_n + \sigma_x \lambda_n. \tag{4}$$

Therefore, within the discrete form, $x(t)$ is reduced to x_n, where n expresses the number of time increments ($t = n\Delta t$). The quantity μ is written as

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

and σ is a function of the parameters γ and $\mathcal{D}$ as

$$\sigma_x^2 = \left(\frac{\mathcal{D}}{2\gamma}\right)(1 - \mu^2). \tag{6}$$

We emphasize again that λ_n represents Gaussian numbers generated using a *box-muller* algorithm. The on-site energies E_n will be obtained from x_n as: $E_n = (x_n - <x_n>)/\sqrt{<x_n^2> - <x_n>^2}$. Therefore, E_n contains all properties of an OU process, however, it contains zero mean value ($<E_n> = 0$) and standard deviation fixed ($\sqrt{<E_n^2> - <E_n>^2} = 1$. In our calculations, we will consider $\mathcal{D} = \gamma^2$ therefore, the degree of correlation of the on-site energies E_n becomes controlled by the parameter γ.[34] The Schrödinger equation will be solved by using a Taylor expansion for the evolution operator i.e. $U(\Delta t) = \exp(-iH\delta t) = 1 + \sum_{l=1}^{L_0} \frac{(-iH\delta t)^l}{l!}$. By considering the initial state as $|\psi(t = 0)\rangle$, the state at time Δt is given by: $|\psi(\delta t)\rangle = U(\delta t)|\psi(t = 0)\rangle$.[18,36–38] In order to analyze the time evolution, we will measure the participation number defined as[18]

$$\xi(t) = \frac{1}{\sum_n |C_n(t)|^4} \tag{7}$$

the participation function provides an estimate of the number of sites that participates within the wave packet. For localized states, the participation number remains finite for long times (i.e $\xi(t) \propto t^0$). On the other hand, for extended states the participation number diverges for long time as $\xi \propto t^1$. In addition, we also calculate the electronic mean position as ($\langle n \rangle(t) = \sum_n n|C_n(t)|^2$); the wave-packet profile ($|C_n(t)|^2 \times n \times t$); the mean square displacement $\sigma(t) = \sqrt{\sum_n (n - n_0)^2 |C_n(t)|^2}$ and the return probability $R(t) = |C_{N/2}(t)|^2$.

3. Results and Discussion

Now, we will show our results regarding the electronic dynamics within our 1D model. We emphasize that we initially locate the wave package ($t = 0$) in the center of the chain. In our calculation, we used the self-expanded chain in order to avoid border effects. In our calculations, we have used $L_0 = 10$ and $\delta t = 0.05$. The accuracy of our numerical integration was checked along the time. Within all calculations, the wave function norm was kept as $|1 - \sum_n |C_n(t)|^2| < 10^{-10}$. In Fig. 1, we plot the time evolution of the participation number for several values of correlation intensity ($\gamma = 0.001, 0.005, 0.05, 0.5, 2.5, 7.5$). All calculations were done for times up to 10^6 time units. Independent of the value of γ we observe that the participation number exhibits a ballistic dynamics for initial times and saturates in a plateau for long times. For larger γ, the intrinsic correlations within the on-site disorder are almost
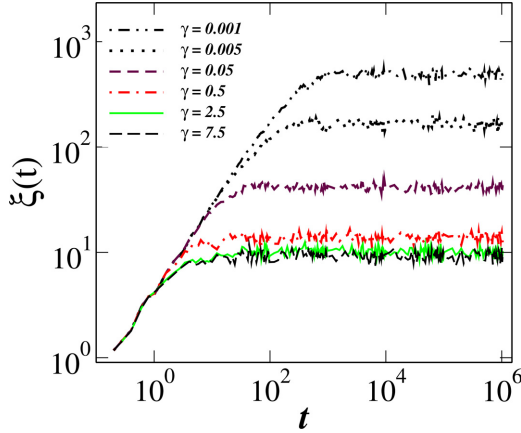
Fig. 1.   (Color online) Time evolution of the participation function $\xi(t)$ for $\gamma = 0.001$ up to 7.5.

absent. Therefore, the participation number is about 10 sites (i.e. the electron remains localized in a small portion of the chain). On the other hand, as we reduce γ, there is a substantial increase in the degree of correlation and therefore, the participation number increases until over one hundred sites. The results found in Figs. 2(a) and 2(b) corroborate the calculations found in Fig. 1. The mean square displacement (Fig. 2(a)) exhibits a behavior similar to that found in Fig. 1. For initial short times σ evolves ballistically and saturates in a plateau at the limit of longer times. For larger γ, the width σ saturates in a small value about 6 or 8 sites; for small γ the mean square displacement increases over 100 sites. We emphasize that ξ and σ are distinct ways of measuring the width of the wave packet, therefore, $\xi(t \to \infty)$ and $\sigma(t \to \infty)$ are expected to have some quantitative differences, however, the qualitative behavior is similar. The results for the return probability (Fig. 2(b)) are
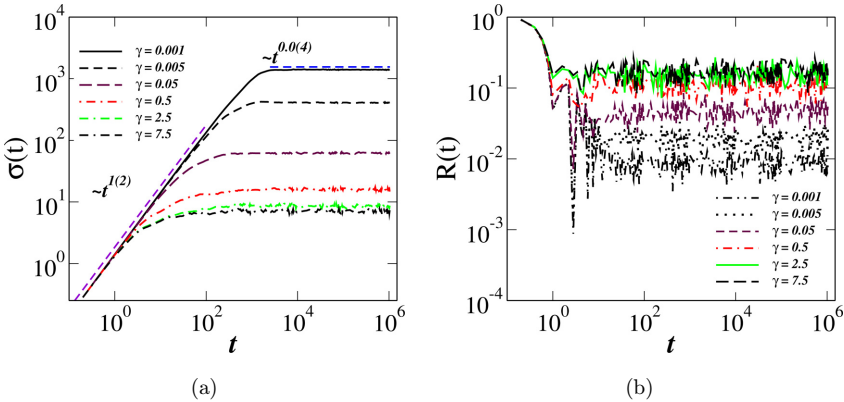

(a)

(b)

Fig. 2.   (Color online) (a) Mean square displacement $\sigma(t)$ and (b) the return probability $R(t)$ for $\gamma = 0.001$ up to 7.5.
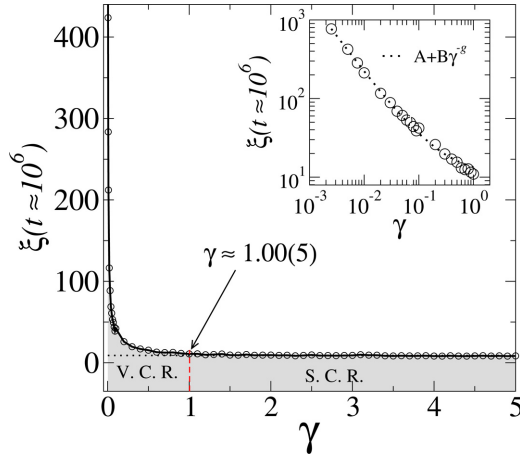
Fig. 3. (Color online) Long time participation function vs. the correlation parameter γ (i.e. $\xi(t \approx 10^6)$ vs. γ); inset: the scaling behavior of $\xi(t \to 10^6)$ for $\gamma < 1$.

also in good agreement with results found in Figs. 1 and 2(a): as the γ tends to zero, the return probability decreases thus indicating the increase in the localization length.

In Fig. 3, we plot $\xi(t \to 10^6)$ vs. γ. Our calculations were done by considering the electron initially localized at center of chain (i.e. $C_n(t = 0) = \delta_{n,N/2}$). We integrated
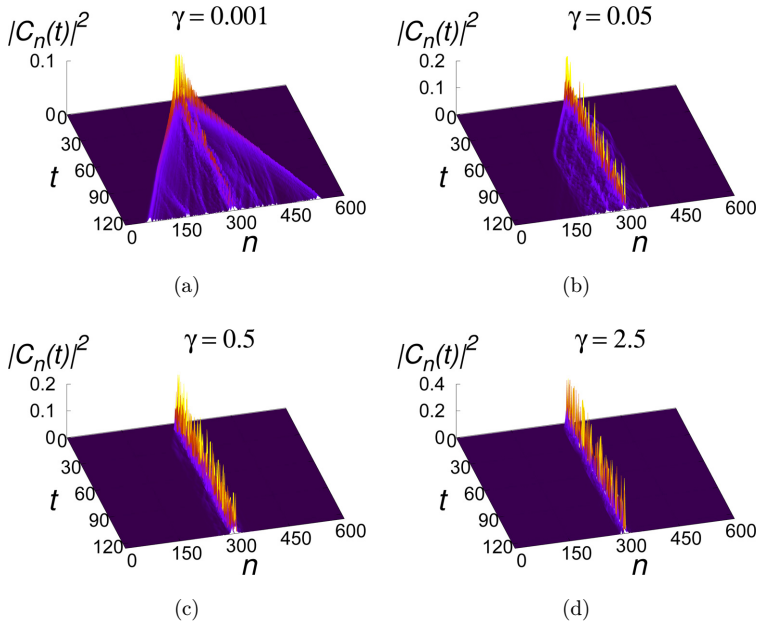

Fig. 4. (Color online) The spatial profile of the wave function using a plot $|C_n(t)|^2$ vs. t and n.

the Schrödinger equation until $t = 10^6$ time units. The calculations of $\xi(t \to 10^6)$ were done by considering the average of $\xi(t)$ using a small range of times close to the end of times (i.e. $\xi(t \to 10^6) = (1/N_t)\sum_{(10^6 - \Delta t) < t \leq 10^6} \xi(t)$ where Δt was about 10000 time units and $N_t = \Delta t/\delta t$). We consider γ as 0.001 up to 5. Our calculations indicate that, for $\gamma > 1.0$ the participation number does not exhibit any substantial modifications (i.e. is roughly independent of γ). These results suggest that for $\gamma > 1.0$ the intrinsic correlations that exist within the OU process are weak such that they become irrelevant within the context of localization behavior of electron eigenstates. In the "inset" of Fig. 3, we analyze the scaling behavior of $\xi(t \to 10^6)$ for $\gamma < 1$. Our best fitting (dotted lines) shows that $\xi(t \to 10^6) = A + B\gamma^{-g}$ with $g = 0.92(1)$. Before concluding, we show in Figs. 4(a)–4(d) the spatial profile of wave packet considering $\gamma = 0.001, 0.05, 0.5, 2.5$. For $\gamma <<< 1$ (see Figs. 4(a) and 4(b)), we can observe that the wave packet exhibits a spreading in good agreement with calculations of ξ, σ and R. For $\gamma = 0.5$ and 2.5, the wave packet remains trapped around the initial site.

4. Summary

We studied the electronic dynamics in a 1D model with correlated disorder distribution. The diagonal disorder distribution was obtained by using the OU process. In order to understand the localization aspects within this model, we numerically integrate the Schrödinger equation using a Taylor's expansion of the evolution operator. The spreading of an initially localized electronic wave packet was measured along the time. Our results suggest that for OU process within the limit of weak correlations, it is similar to the Anderson Model with uncorrelated disorder. By using our calculations, we obtained for which degree of correlations the OU model behaves as a standard Anderson Model. Within the limit of strong correlations, we numerically demonstrated that the electron remains localized. However, we shown that the localization length increases as the degree of correlations is increased.

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