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ABSORPTION SPECTRA AND LEVEL SPACING STATISTICS IN A TERNARY ALLOY WITH AN ORNSTEIN–UHLENBECK DISORDER DISTRIBUTION

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In this paper, we study the dynamics of a one-electron in a one-dimensional (1d) alloy with a correlated Ornstein–Uhlenbeck (OU) disorder distribution. The model considered here corresponds to an alloy with three types of atoms where the position of each atom is obtained using a stochastic rule based on the OU process. We analyze in detail the effect of this correlated disorder in the optical absorption spectrum and the level spacing statistics near the band center. Our results reveal a new collection of optical absorption peaks. We explain in details the appearance of each peak. Our calculations about the level spacing's distribution reveals a Poisson distribution thus contradicting previous statements about the existence of extended states in ternary electronic models with correlated disorder distribution.

Keywords: One-electron; correlated disorder; wave-packet.

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1. Introduction

The dynamics of a one-electron in disordered lattices is a key issue which has attracted the scientific interest during several decades.[1–24] According to the Anderson scaling theory there are no extended eigenstates in low-dimensional systems for any degree of uncorrelated disorder. Since the end of 1980s, it has been shown that low-dimensional disordered systems can support extended states or a

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localization–delocalization transition in the presence of short-or long-range correlations in the disorder distribution.[25–48] Furthermore, the theoretical prediction that it is possible to *see* the localization in a random multilayered filter[49,50] opened a wide field to investigate the effects of correlated disorder in optical systems. The theoretical formalisms of random dielectric multilayers can be mapped on the one-electron Hamiltonian in a disordered media with close connections with the random dimers and off-diagonal disorder versions of the Anderson model.[51] The effect of correlated disorder within general transport problems, not only for models with one-electron, became a very interesting field of study. For example, it was studied the effects of correlated disorder on the magnon eigenstates in random ferromagnetic[52,53] and collective vibrational motion of one-dimensional (1d) disordered harmonic chains.[54–58] In both cases, it was demonstrated that the correlated disorder lead to a new set of nonscattered modes. In general, previous works about correlated disorder were done considering systems in which the site energies are uniformly distributed in a finite range $[-W, W]$. Some authors[44,45,59–61] have considered models where the on-site energy can assume two or three different values i.e., the binary and ternary models, respectively. In particular, the Anderson model with long-range correlated disorder chosen as a ternary sequence was studied in Ref. 45. If the sequence of the on-site energies is generated totally random, the system is an insulator. Nevertheless, by creating a ternary diagonal disorder with long-range correlations, it was observed a localized–delocalized phase transition.[45] The effect of long-range correlations in the sequence of capacitances of classical transmission lines (TL) has been studied by Lazo and Diez.[59,60] To generate the ternary correlated distribution of capacitances it was used the Fourier filtering method[59] and also the Ornstein–Uhlenbeck (OU) process.[60] In both cases, it was observed a transition from nonconducting to conducting state of the TL induced by strong correlations. More recently, a 1d classical ternary harmonic chain with the mass distribution constructed from an OU process was studied.[61] The localization aspects of all vibrational eigenstates were obtained by using the transfer matrix formalism. The authors concluded that only the zero frequency mode can propagate through the chain, thus contradicting previous works.[45,59,60]

Moreover, the effect of correlated disorder on the optical spectroscopy properties[62–68] is a key problem in the context of condensed matter physics. Usually, it is well-known that the optical spectroscopy fails in detecting localization–delocalization transitions. However, in Ref. 64 it was numerically reported an anomalous behavior of the absorption spectrum in a 1d lattice with long-range correlated diagonal disorder. The double-peak absorption spectrum found is the unique spectroscopic tool to monitor the Anderson transition. Furthermore, in Ref. 65 a double-peak absorption spectrum was numerically observed in 1d lattice with long-range off-diagonal correlated disorder. In Ref. 66, a detailed study about optical properties in 1d models with heavy-tailed Levy disorder distribution was done. The authors found a broadening of optical line and a nonuniversal scaling of the distribution of exciton localization lengths. The scaling of the optical absorption bandwidth and the

nonuniversality of the localization length within models with Levy disorder distribution were re-visited in Refs. 67 and 68. We would like to stress that from the best of our knowledge, the study of optical spectroscopy properties in low-dimensional systems with ternary correlated disorder is completely absent in the literature.

We emphasize that the existence or nonexistence of a phase transition in ternary models with correlated disorder represents a interesting and controversial issue[45,59–61] with considerable interest from the experimental and theoretical point of view. The possibility to generate real systems with a ternary correlated disorder can be a possible tools to compare theory and experiment procedures and also allows designing new materials with adjustable properties. However, a more detailed statistical analysis of the eigenmodes and a description of the optical properties in electronic ternary models is still absent. In this paper, we will provide some advances along these lines. We will study the optical absorption and the levels spacing distribution in 1d models with a ternary correlated disorder distribution. Here, we will study a 1d model with a ternary diagonal disorder distribution following the OU process. We construct the ternary diagonal disorder distribution by initially generating the OU process and mapping it into a sequence of three different values. The probability of each value is controlled by a fixed parameter b. In that way, we will generate a ternary diagonal potential with long-range correlations. We perform exact numerical diagonalization to compute the level spacing distribution and the optical absorption spectrum. Our results shown that the level spacing distribution near the band center shows a well defined Poisson distribution. This result indicate that all eigenstates are localized thus contradicting previous works that pointed out the existence of extended states in models with ternary diagonal correlated disorder.[45] Within the context of optical absorption spectrum our results show a set of unexpected peaks within absorption spectrum. We explain in detail the origin of each peak.

2. Model and Formalism

We consider a tight-binding one-electron Hamiltonian with hopping J and on-site disorder distribution ϵ_n,[69]

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

where $|n\rangle$ is a Wannier state localized at site n with the on-site energy ϵ_n. The intersite coupling J is restricted to nearest-neighbors and assumed to be uniform over the entire lattice ($J = 1$). The source of disorder is the stochastic fluctuations of the on-site terms, which we are going to consider to follow the OU process.[60,61] The OU process is defined by the stochastic differential equation:

$$\frac{dx}{dt} = -\gamma x(t) + \sqrt{C}\beta(t), \tag{2}$$

where γ is the viscosity coefficient, C is the diffusion coefficient and $\beta(t)$ is the stochastic term.[60,61] $\beta(t)$ is a Gaussian white noise generated by the Box–Muller process with the following properties: $\langle\beta(t)\rangle = 0$ and $\langle\beta(t)\beta(t\tau)\rangle = \delta(\tau)$. This stochastic process contains correlations between each step defined as $\langle x(t)x(t\tau)\rangle = \frac{C}{2\gamma}e^{-\gamma\tau}$.[60,61] In order to generate the diagonal disorder from the OU process we will consider the numerical formalism obtained in Ref. 70 based on the discrete version of Eq. (2). In the discrete form, $x(t)$ is written as x_n where n denotes the time step number ($t = n\Delta t$). Therefore, the discrete form of Eq. (2) is given by[70]

$$x_{n+1} = (e^{-\gamma\Delta t})x_n + \left[\sqrt{\frac{C}{2\gamma}(1 - e^{-2\gamma\Delta t})}\right]\beta_n. \tag{3}$$

Using the Box–Muller algorithm, we calculate β_n in the following way

$$\beta_n = \left(\sqrt{2\ln\frac{1}{r_n}}\right)\cos 2\pi a_n, \tag{4}$$

where r_n and a_n are uniform random numbers defined in the interval $[0, 1]$. We have normalized x_n in order to impose zero average and keep the variance equal to unity. Following Refs. 60 and 61, we will consider $C = \gamma^2$ and, therefore, the degree of correlation of the OU process becomes controlled by a single parameter γ. For $\gamma \to \infty$ the OU sequence evolves into the Gaussian white noise. For $\gamma \to 0$ the degree of correlation of the disordered sequence will increase. Using the normalized sequence x_n generated by OU process, we will construct a ternary on-site energy distribution as follows

$$\epsilon_n = \begin{cases} -\zeta & \text{if } x_n < -b, \\ 0 & \text{if } -b \le x_n \le b, \\ \zeta & \text{if } x_n > b, \end{cases} \tag{5}$$

where $b > 0$ controls the probability of each possible value of the on-site energy. The width of the disorder distribution depends on the value of ζ, a tunable parameter.[60,61]

2.1. *Magnitudes of interest*

In order to investigate the absorption spectrum and the level spacing distribution for this model we perform an exact diagonalization procedure on finite chains. The absorption spectrum is defined as,[64,65]

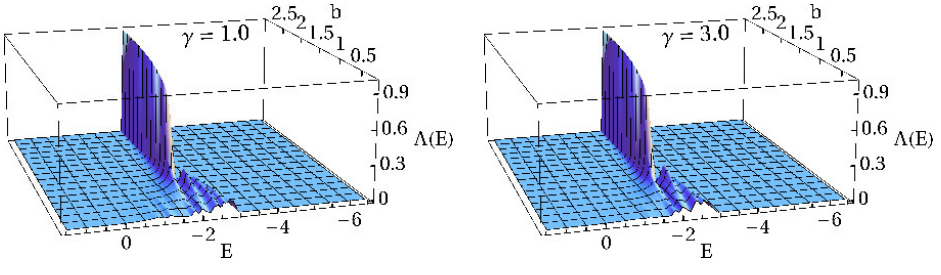
$$A(E) = \frac{1}{N}\sum_{\beta}\delta(E - E_\beta)F_\beta, \tag{6}$$

where F_β is the oscillator strength associated with the eigenvalue β, namely $F_\beta = [\sum_n \psi_n(E_\beta)]^2$. When the off-diagonal term is negative and the diagonal is a disordered uncorrelated distribution, the eigenstates with higher oscillator strength are those at the bottom of the band. Moreover, we will analyze the level spacing

statistics near the band center. In one-electron systems, localized states are uncorrelated in energy and distributed following a Poisson law $P(s) = e^{-s}$, where s is the level spacing measured in units of the mean spacing. In contrast, delocalized eigenfunctions repel each other and their level spacing distribution assumes the Wigner form $P(s) \propto se^{-Cs^2}$.[71,72] At the Anderson transition a new universal critical statistics intermediate between Wigner and Poisson has been suggested as a consequence of the multifractality of critical wave functions.[73] To obtain the level spacing distribution, we used an energy window near the band center $(-0.5, 0.5)$. A spectral unfolding procedure was employed to keep the average level spacing equal to unity in each segment of the energy window.[73]

3. Results and Discussions

To solve numerically Eq. (6) we used $N = 10\,000$ sites, $\zeta = 1$ and 100 realizations of disorder for each value of γ and b. Figures 1 and 2 show the output of these calculations. We observe that for $b \gg 0$ and all γ values considered here, the absorption spectrum displays a single peak slightly above the lower band edge $E = -2$ of the periodic lattice. Our results suggest that only the lowest states of the band contribute to the absorption spectrum. Therefore, we have obtained a similar trend observed to those that was obtained in 1d systems with weak diagonal disorder. For all γ considered in Figs. 1(a) and 1(b) and $b \to 0$ we observed that the absorption spectrum displays a wide peak slightly under the lower band edge $E = -2$. Therefore, for $b \to 0$ we recovered the absorption spectrum similar to those obtained in a 1d lattice with an uncorrelated diagonal disorder. In Figs. 2(a) and 2(b) we show our calculations for $\gamma \to 0$ (i.e. the strongly correlated limit). We can see that for small values of b, our results show that $A(E)$ displays an unexpected set of narrow peaks. We also observed



(a) (b)

Fig. 1. (Color online) Numerical calculations of Eq. (6) by using $N = 10\,000$ sites, $\zeta = 1$, 100 realizations of disorder, $\gamma = 1$ and 3. We observe that for $b \gg 0$ in both (a), (b), the absorption spectrum displays a single peak slightly above the lower band edge $E = -2$. At this limit, the value $\epsilon_n = 0$ is most frequent than other values and therefore, we recovered a 1d model with weak diagonal disorder. This framework corroborates this single narrow peak found. For $b \to 0$ the OU process becomes an uncorrelated series therefore, we will obtain also a uncorrelated binary diagonal potential. Therefore, it explains the single wide peak in the absorption spectrum at this limit.

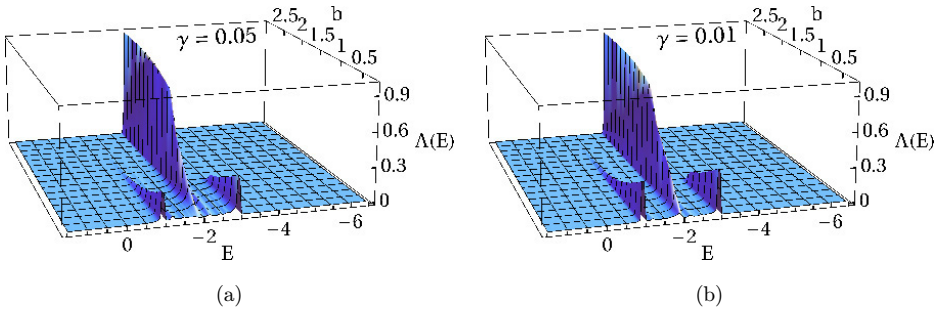


Fig. 2. (Color online) Numerical investigation of the absorption spectrum at limit of strong correlations ($\gamma \to 0$). Calculations of Eq. (6) were done by using $N = 10\,000$ sites, $\zeta = 1$ and 100 realizations of disorder. We can see that for small b we obtained a nonintuitive absorption spectrum profile. We can see that our results for $b \approx 0.5$ indicate the existence of a well defined triplet. For $b \to 0$ our calculations reveals a well defined doublet.

that at this limit of strong correlations ($\gamma \to 0$) depending on the b value, we can get to a well defined triplet (about $b \approx 0.5$). We emphasize that in disordered models traditionally is obtained a single peak around the lower state.[64,65]

To understand this new set of peaks of the absorption spectrum we will need to study in details the local properties of the diagonal disorder and apply a heuristic procedure.[64] Let us start by remembering that the parameter b governs the probability distribution of each value $-\zeta, 0, \zeta$ of the diagonal distribution. For all values of γ and $b > 1$, the value $\epsilon_n = 0$ is most frequent than the other values and therefore, we recovered an 1d model with weak diagonal disorder. The single narrow peak found in Figs. 1(a) and 1(b) for large b is in good agreements with the $A(E)$ for a 1d model with weak diagonal disorder.[64] For $b \to 0$ we obtained a binary disorder distribution i.e. two values $(-\zeta, \zeta)$ randomly distributed. For $\gamma \gg 0$ and $b \to 0$ the OU process becomes uncorrelated and the binary sequence of values $(-\zeta, \zeta)$ obtained using the mapping defined in Eq. (5) becomes also an uncorrelated sequence. Therefore, it explains the single wide peak in the absorption spectrum found in Figs. 1(a) and 1(b) for $\gamma \gg 0$ and $b \to 0$. For $\gamma \to 0$ and $b \to 0$ (see Figs. 2(a) and 2(b)) we can also follow a similar analysis to understand the double peak structure found. For $\gamma \to 0$ the OU process becomes correlated. Previous works[60,70] have demonstrated that the OU process is characterized by a power law spectrum $S(k) \propto k^{-2}$ for $\gamma \to 0$. We know[30,74,75] that a stochastic sequence with power law spectrum $S(k) \propto k^{-2}$ has its increments in the edge between the persistent and anti-persistent behavior. Formally, a random sequence becomes persistent if its spectrum behaves as $S(k) \propto k^{-\nu}$ with $\nu > 2$. The value $\nu = 2$ is the crossing point between the persistent and anti-persistent behaviors. Therefore, at this limit the random sequence displays a initial smoothing and starts to follow a harmonic-like behavior. In this way, when $\gamma \to 0$ and $b \to 0$ the diagonal terms ϵ_n exhibit an almost regular structure of finite segments with values $-\zeta$ and ζ. Therefore, by using the heuristic arguments considered in Ref. 64 we can decouple this 1d model in a collection of two inter-penetrating

chains, one of them with on-site energy $-\zeta$ and another one with diagonal term ζ. Once we have used $\zeta = 1$ there are two sub-band, the first one is within the interval $[-3, 1]$ and a second one within the interval $[-1, 3]$. Following Ref. 64, the absorption spectrum of such a system is expected to have two peaks caused by the transitions from the ground state to the bottom state of each sub-band. We stress that these values i.e. -3 and -1 are in good agreement with the numerical calculations presented in Figs. 2(a) and 2(b) for $b \to 0$. Moreover, the triplet observed in the absorption spectrum for $b \approx 0.5$ (see Figs. 2(a) and 2(b)) can also be understand by using a similar methodology. For $b \approx 0.5$, the probability of each value in the diagonal distribution is approximately the same therefore, we can decouple the system in three inter-penetrating chains, each of them with on-site energies $-\zeta$, 0 and ζ.

For the value $\zeta = 1$ used in our calculations we will have three sub-bands, respectively $[-3, 1]$, $[-2, 2]$ and $[-1, 3]$. Following again Ref. 64, the absorption spectrum is expected to have three peaks related to the bottom state of each sub band i.e. $-3, -2, -1$. This prediction is again in good agreements with our numerical results (see Figs. 2(a) and 2(b)). Before concluding this part, it is interesting to study the dependence of the optical properties with the ζ parameter. We can repeat the heuristic arguments for $b \to 0$ and any ζ to obtain that the positions of the peaks should be respectively $-2J - \zeta$ and $-2J + \zeta$. In order to a numerically verification of our arguments we will solve Eq. (6) for $N = 10\,000$ sites, 100 realizations of disorder and $\zeta = 2$ and 3. In Fig. 3, we plot the results of these calculations. We can observe that our heuristic methodology are in good agreements with our numerical results. As the ζ value is increased, the distance between each peak increases following our heuristic prediction.

In Figs. 4 and 5 we plot our results for the level spacing statistics near of the band center. Calculations were done for $\zeta = 1$ and Figs. 4(a) and 4(b) with $\gamma = 1, 3$ and Figs. 5(a) and 5(b) with $\gamma = 0.05, 0.01$. We stress that we have used in our

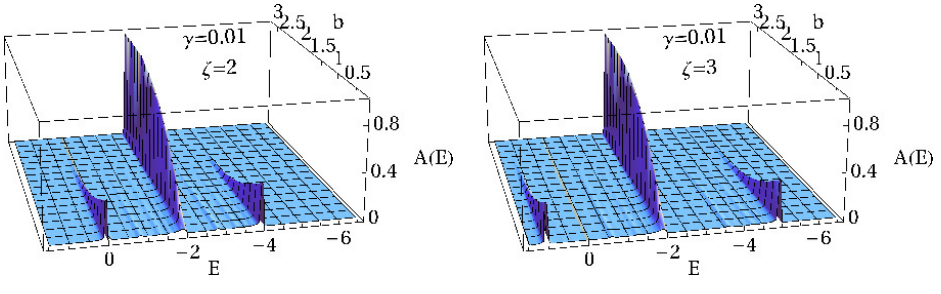


Fig. 3. (Color online) Numerical calculations of the absorption spectrum for $N = 10\,000$ sites, 100 realizations of disorder, $\zeta = 2$ and 3. Our numerical calculations confirm that the optical absorption peak structure is strongly dependent of the possible transitions from the ground state to the bottom state of each sub-band. For $b \to 0$ the positions of the two peaks is in good agreement with the bottom of each sub-band i.e. $[-2J - \zeta]$ and $[-2J + \zeta]$.

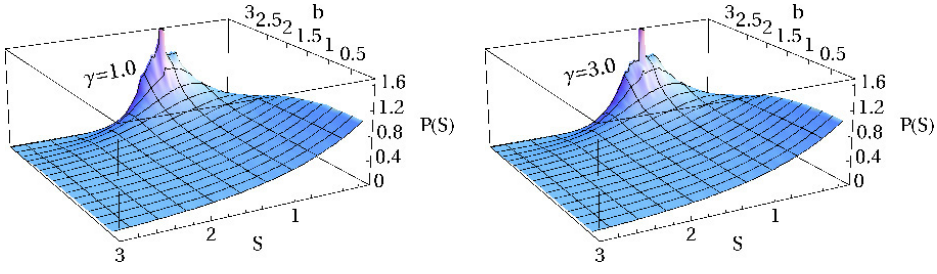


Fig. 4. (Color online) Numerical calculations of the level spacing statistics near of the band center for $\zeta = 1$ and $\gamma = 1, 3$. Our numerical calculation for $b \gg 0$ reveals a single peak around the average level spacing unity ($s = 1$). This level spacing statistics is similar to that found in chains without disorder. For the limit $b \to 0$ all calculations of the $P(s)$ indicate a standard Poisson distribution $P(s) = e^{-s}$ thus corroborating the localized nature of eigenstates.

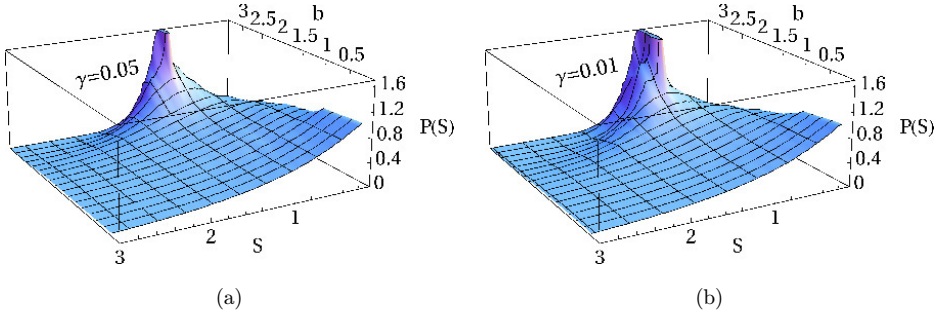


Fig. 5. (Color online) Level spacing statistics near of the band center for $\zeta = 1$ and $\gamma = 0.05, 0.01$. For large b we obtained a peak around $s = 1$, a clear signature of a pure chain. For $b \to 0$, even at the limit of strong correlations, our results reveals a Poisson Law behavior thus corroborating the localized nature of all eigenstates.

calculations an energy region around the band center $(-0.5, 0.5)$ and also a spectral unfolding procedure to keep the average level spacing equal to unity.[71–73,76] We observe that for all values of γ considered here, our numerical calculations for $b \gg 0$ reveals a level spacing statistics similar to those found in chains without disorder,[73] i.e. a single peak around the average level spacing unity ($s = 1$). We stress that in Ref. 61, it was pointed out the existence of a disorder–order transition in ternary OU sequences for $b > 4$. Therefore, our calculations of the level spacing statistics corroborates the existence of this disorder–order transition for large b.[61] For the limit $b \to 0$ all calculations of $P(s)$ indicate a standard Poisson distribution $P(s) = e^{-s}$ even for strong correlations $\gamma \to 0$ (see Figs. 4 and 5). Therefore, the Poisson distribution obtained in our calculations for $b \to 0$ unveil the absence of extended electronic eigenstates in ternary alloys with OU correlated disorder distribution. We emphasize that our results contradict previous works that pointed out the existence

of an Anderson phase transition in 1d electronic models with ternary correlated disorder.[52]

4. Summary and Conclusions

In summary, we have studied a 1d ternary electronic chain with the on-site distribution constructed from an OU process. The ternary diagonal disorder distribution was generated from a mapping of the correlated OU process into a sequence of three different values. The probability of each value is controlled by a fixed parameter b. In that way, we have generated a ternary diagonal potential with long-range correlations. By using exact diagonalization, we computed the optical absorption spectrum and the level spacing distribution for this ternary model. Within the absorption spectrum context, our results indicating a new collection of peaks within the band of energy. We have shown that the kind of correlations considered here can induce the appearance of several well defined peaks, including peaks far from the bottom of the band. We have explained in detail the origin of each peaks by considering the possible transitions from the ground state to the bottom state of each allowed sub-band. Moreover, we demonstrated that it is possible to control the position of each absorption spectrum peak by changing the on-site disorder intensity. We stress that this multipeak structure of the absorption spectrum was never observed before in 1d disordered models. To finishing, our results about the level spacing distribution reveals a Poisson distribution for small values of b. We stress that this result are in good agreement with previous statements about the absence of extended states in ternary models with OU correlated disorder distribution.[61] Therefore, our calculations contradict previous works[45,59,60] that pointed out the existence of an Anderson metal-insulator phase transition in models with ternary correlated disorder distribution. We stress that the choice of the OU process as the source of disorder does not restricts our main results to this class of long-range correlated disorder. In general lines, the OU process consists of an easy way to generate a disorder distribution with long-range correlations. Basically, any random process with power law spectral density could be used as the source of disorder to construct the ternary atomic distribution with long-range correlations. Therefore, based on our present calculations, we are confident that our results are valid for another ternary disorder distributions with long-range correlations. We stress that it is possible[37,38] by using molecular beam epitaxy, the construction of a correlated disordered array of three types of barriers following the correlations rules considered here. In fact, we think that an experimental setup like this should be very useful to reproduce our results about the optical absorption in the presence of a correlated ternary disorder distribution. However, within optical absorption framework, we stress that we have theoretically calculated the absorption by Frenkel excitons while that at semiconductor super-lattices we can found only Wannier–Mott excitons due to the large dielectric constant generally considered. We expect that the present work will stimulate further theoretical and experimental investigations along this line.

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