Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

# Metal–insulator transition in a ternary model with long range correlated disorder

**A Esmailpour[1], H Cheraghchi[2], Pedro Carpena[3] and M Reza Rahimi Tabar[4,5,6]**

[1] Department of Physics, Shahid Rajaei University, Lavizan, 16788, Tehran, Iran
[2] School of Physics, Damghan University of Basic Sciences, Damghan, Iran
[3] Departamento de Física Aplicada II, ETSI de Telecomunicación, Universidad de Málaga, Málaga, Spain
[4] Department of Physics, Sharif University of Technology, 11365-9161 Tehran, Iran
[5] Institute of Physics, Carl von Ossietzky University, D-26111 Oldenburg, Germany
[6] CNRS UMR 6529, Observatoire de la Côte d'Azur, BP 4229, 06304 Nice Cedex 4, France
E-mail: esmailpour@iust.ac.ir, cheragh2000@yahoo.com, pcarpena@ctima.uma.es, mohammed.r.rahimi.tabar@uni-oldenburg.de and rahimitabar@iust.ac.ir

Received 6 June 2007
Accepted 31 August 2007
Published 20 September 2007

Online at stacks.iop.org/JSTAT/2007/P09014
doi:10.1088/1742-5468/2007/09/P09014

**Abstract.** We study the metal–insulator transition of the one-dimensional diagonal Anderson ternary model with long range correlated disorder. The starting point of the model corresponds to a ternary alloy (i.e. with three possible on-site energies), and shows a metal–insulator transition when the random distribution of site energies is assumed to have a power spectrum $S(k) \propto 1/k^{(2\alpha-1)}$. In this paper, we define a purity parameter for the ternary alloy which adjusts the occupancy probability of site potentials, and for any given $\alpha$ we calculate the critical purity parameter for which extended states are obtained. In this way, we show that the ternary alloy requires weaker correlations than the binary alloy to present a phase transition from localized to extended states. A phase diagram which separates the extended regime from the localized one for


1742-5468/07/P09014+11$30.00

J. Stat. Mech. (2007) P09014

the ternary alloy is presented, obtained as the critical purity parameter in terms of the corresponding correlation exponent.

**Keywords:** Anderson model (theory), disordered systems (theory)

## Contents



## 1. Introduction

It was believed for about forty years [1] that all electron states in one-dimensional (1D) disordered systems are exponentially localized for any amount of uncorrelated diagonal disorder. Recently, the interest in 1D disordered models with correlated disorder has been growing, as it has become progressively clearer that correlations of the random potential can deeply affect the electronic localization properties. Spatial correlations of disorder can unexpectedly create extended states at some particular energies. In a system with short range correlation of the on-site disordered energies, e.g. in the random dimer model [2], one can have a discrete number of extended states. This demonstration attracted a great deal of attention to investigating the existence of a metal–insulator transition (MIT) in 1D disordered systems. Experimental evidence of the delocalization effect produced by these short range correlations in semiconductor superlattices was recently found [3]. Special attention has been recently paid to the presence of a continuum of extended states and mobility edges in the *long range* correlated disordered model. In [4] de Moura and Lyra considered the discrete Anderson model in which the diagonal energies of the Hamiltonian are generated by considering the potential as the trace of a fractional Brownian motion and imposing a normalization condition that kept fixed the variance of potentials for all system sizes (see also [5]). They showed how long range correlated sequences of site energies could result in a continuum of extended states (although these results caused some controversy [6]). Long range correlations also affect the level statistics of the system, which can also experience a transition from Poissonian to non-Poissonian phase [7]. Recent works study the delocalization effects produced when long range correlations are introduced in the hopping terms of the Hamiltonian [8].

Several stochastic processes in Nature are known to generate long range correlated random sequences which have no characteristic scale, for example, in the nucleotide sequence of DNA molecules [9]. The relevance of the underlying long range correlations



J. Stat. Mech. (2007) P09014

for the electronic transport in DNA was first introduced in [10], and later works confirm this result [11, 12]. To understand the effect of long range correlations of the disorder on a phase transition, Izrailev *et al* [13] perturbatively derived an analytical relationship between localization length and potential pair correlators. They showed how specific long range disorder correlations lead to the appearance of mobility edges in 1D discrete models. An experimental confirmation of these findings was obtained by studying the transmission of microwaves in a single-mode waveguide with a random array of correlated scatterers [14]. In addition, there have been several theoretical and numerical studies of these problems in various systems [15]–[20].

The works on correlated disorder referred to above have been carried out for continuous and binary disordered systems, i.e., systems in which the site energies can take any value or only two different values respectively. In the present paper, we introduce and study the one-dimensional Anderson model with long range correlated disorder chosen as a ternary model. The starting point of the model is a ternary alloy, i.e. a model in which, with some probability, the on-site energies can have only three different values. If the sequence of on-site energies is generated totally at random the system is naturally an insulator. Nevertheless, we create long range correlated ternary models by generating a correlated sequence of on-site energies continuously distributed, which is mapped into three different values with some probability which is adjusted via the purity parameter.

We show below how the purity parameter can change the localization properties of the system, and show also that for a fixed system size and for a certain value of the correlations, there exists a critical value of the purity parameter for which a transition from localized to extended states is observed. By performing finite-size scaling, we obtain the asymptotic value of the purity parameter in the thermodynamic limit for any value of the long range correlations imposed in the system. With these data, we present below a phase diagram separating the localized phase from the extended one given as a function of the relevant magnitudes: the purity parameter and the correlation exponent of the system. This is the fundamental result of this paper.

## 2. Model and method

We consider non-interacting electrons in 1D disordered systems within a nearest-neighbor tight-binding formalism. The Schrödinger equation projected on site $i$ becomes

$$\varepsilon_i\psi_i + t_{i,i+1}\psi_{i+1} + t_{i-1,i}\psi_{i-1} = E\psi_i, \tag{1}$$

where $E$ is the energy of the incoming electron. The norm $|\boldsymbol{\psi}_\mathbf{i}|^2$ is the probability of finding an electron at site $i$, $\varepsilon_i$ is the potential at site $i$ and $t_{i-1,i} = t_{i,i-1}$ is the hopping integral from site $i-1$ to site $i$. In this work, the disorder is applied to the site energies $\{\varepsilon_i\}$ and the hopping terms are taken to be unity ($t_{i-1,i} = 1$), thus fixing the energy scale of the disordered system. The site energies are extracted as the $\{\varepsilon_i\}$ for the ternary alloy with different probabilities. Without losing any generality, the ordered system is considered to have zero on-site energy. A binary disorder is introduced on the site energies. Therefore, three potential energies are possible at any site: $\varepsilon_i = \varepsilon_A, \varepsilon_B$ or zero (see below for the details of the model).



J. Stat. Mech. (2007) P09014

The above equation (1) can be easily expressed by using the conventional transfer matrix method as the following recursive matrix form:

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \begin{pmatrix} E-\varepsilon_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \tag{2}$$

The wavefunctions of the two ends can be related together by calculating a product of matrices as $P_{N,1} = \prod_{i=1}^{N} P_{i,i-1}$. In this equation, $N$ is the sample length and $P_{i,i-1}$ is the transfer matrix which connects the wavefunctions of sites $i$ and $i-1$. According to the component of this matrix, the Lyapunov exponent is defined in the following way:

$$\gamma = \lim_{N \longrightarrow \infty} \frac{1}{N} \langle \ln \parallel P_{N,1} \parallel \rangle. \tag{3}$$

The Lyapunov exponent is a suitable variable for describing localization properties because it is related to the exponential decreasing of the wavefunction. The localization length corresponds to the inverse of the Lyapunov exponent ($\lambda \propto 1/\gamma$).

We want to study the localization properties of a ternary model with long range correlated disorder. Thus, we need first to generate long range correlated sequences of site energies. A sequence of long range correlated potentials $\{\varepsilon_i\}$ is produced by the Fourier filtering method [21]. This method is based on a transformation of the Fourier components $\{u_k\}$ of a random number sequence $\{u_i\}$ which is uncorrelated random numbers with a Gaussian distribution. A sequence of $\{\varepsilon_k\}$ is generated for a given $\alpha$ using the formula $\varepsilon_k = k^{-(2\alpha-1)/2} u_k$. Inverse Fourier transformation of the sequence $\{\varepsilon_k\}$ leads to the sequence of interest $\{\varepsilon_i\}$. The resulting sequence of potential energies are spatially correlated with spectral density

$$S(k) \propto k^{-(2\alpha-1)} \tag{4}$$

and they follow a Gaussian distribution. The exponent $\alpha$ is called the correlation exponent, and quantifies the degree of correlation imposed in the system. With the definition in (4) $\alpha$ corresponds to the exponent provided by detrended fluctuation analysis (DFA), which is one of the most widely used methods for quantifying long range correlations [22]–[24]. Note that the case $\alpha = 0.5$ corresponds to uncorrelated disorder (white noise), while the case $\alpha > 0.5$ indicates positive correlations. Several examples of sequences of site energies for different values of the correlation exponent $\alpha$ are shown in figure 1.

We would like to note that, once the sequences of site energies are generated using the method referred to above, we normalize them so that the mean value $\langle \varepsilon_i \rangle$ is set to zero, and the variance is set to unity. This choice is maintained in all the numerical calculations in this paper.

### 2.1. The ternary model

The sequence of site energies of the ternary alloy is produced by applying a map on the correlated sequences $\{\varepsilon_i\}$ with Gaussian distribution generated with the Fourier filtering method described above. By using a purity parameter ($a$), the Gaussian probability distribution $P(\varepsilon)$ of the correlated sequence is divided into three regions. Any value of the correlated series which is in the interval $-a \leq \varepsilon_n \leq a$ is mapped to zero. Furthermore,



J. Stat. Mech. (2007) P09014

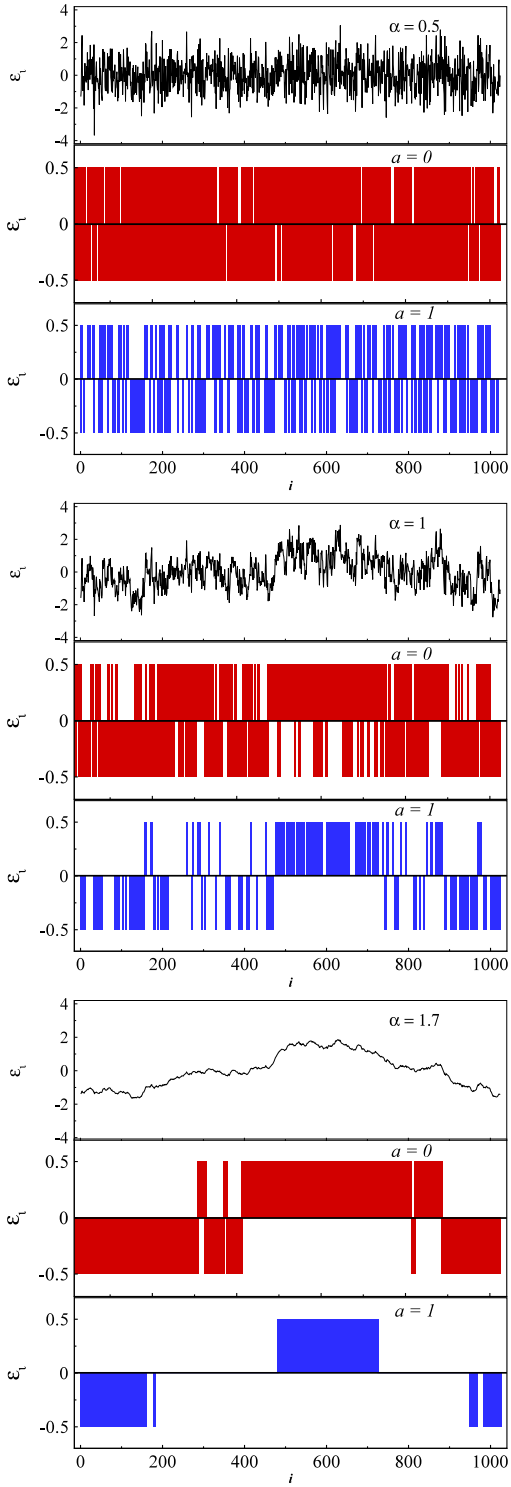


**Figure 1.** Three examples of series of site energies generated with the Fourier filtering method for different values of the correlation exponent $\alpha$ and impurity parameter $a$ for the ternary model.

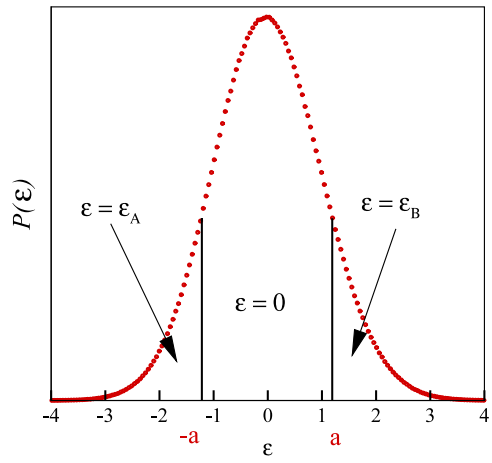


**Figure 2.** Probability distribution of the correlated random sequence with a correlation exponent $\alpha = 1.0$. The purity parameter $a$ determines how many ordered sites are in the system.

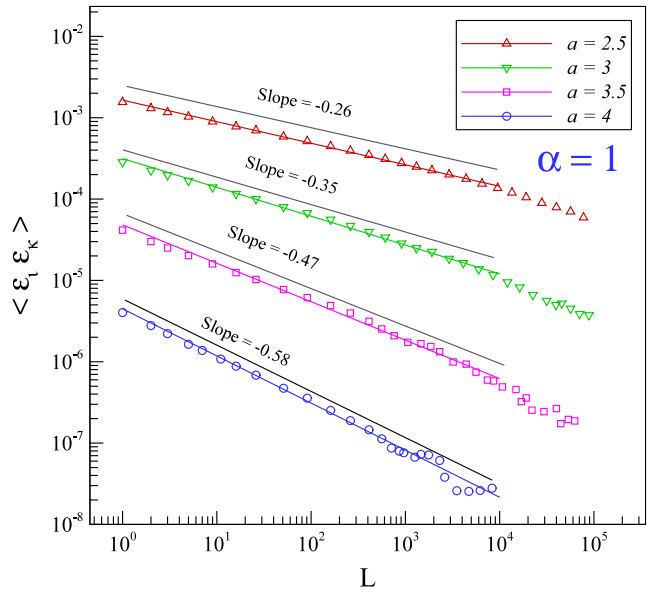


**Figure 3.** Correlation function of on-site energies $\langle \varepsilon_i \varepsilon_k \rangle$ versus $L = |k - i|$ for the ternary model with exponent $\alpha = 1$ and different impurity parameters $a$.

any value greater than $a$ and less than $-a$ is mapped into $\varepsilon_A$ and $\varepsilon_B$, respectively. In summary,

$$\varepsilon_n = \begin{cases} \varepsilon_A, & \varepsilon_n < -a, \\ 0, & -a \leq \varepsilon_n \leq a, \\ \varepsilon_B, & \varepsilon_n > a. \end{cases} \tag{5}$$

Figure 2 shows the Gaussian distribution of the correlated potentials with exponent $\alpha = 1.0$. The purity parameter seen in figure 2 determines the concentration of the ordered sites (see also figure 1). In the limit $a \longrightarrow 0$, the system tends to be completely

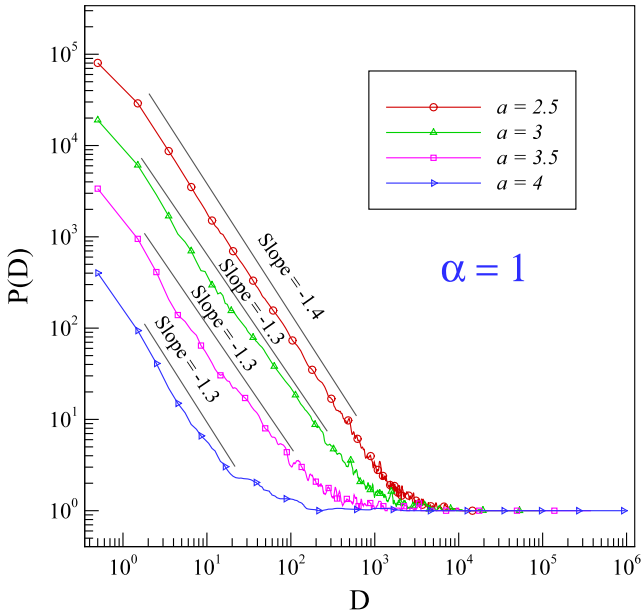


**Figure 4.** Length distribution of sequences of sites with the same energy, which shows that it has scaling behavior with exponent $\simeq -1.3$, for on-site energies with exponent $\alpha = 1$.

disordered. In this case, we have a binary alloy chain with the same concentration for both of the on-site energies. The occupation probabilities of the sites with potentials $\varepsilon_A$ and $\varepsilon_B$ are the same, as $P_A = P_B$. We consider the site energies of $A$ and $B$ to be $\varepsilon_A = -\varepsilon_B = 0.5$.

In figure 3 we have plotted the correlation function of on-site energies $\langle \varepsilon_i \varepsilon_k \rangle$ versus $L = |k - i|$ for the ternary model with exponent $\alpha = 1$ and different impurity parameters $a$. For white noise $\alpha = 0.5$ we find that the on-site energy correlations are zero except for the case $i = k$, which gives the variance of the on-site energies. Figure 4 shows the length distribution of sequences of sites with the same energy, which shows that it has scaling behavior with exponent $\simeq -1.3$, for $\alpha = 1$ and different impurity parameters.

In the following, we show that for the ternary case, for any value of the correlation exponent $\alpha$ one can find some well defined $a$ in the limit of $N \to \infty$ for which the system undergoes a transition from a localized to an extended phase. As we show below, we find that for systems with many ordered sites (i.e., for large $a$), the transition from the extended regime to the localized one requires weaker correlations (smaller $\alpha$) than that for the binary case (equivalent to $a = 0$).

## 3. Numerical results

Now, we study numerically the localization properties of the ternary model described above. In the numerical calculations, the localization properties and the possibility of a phase transition from localized to extended states in the band center are investigated. For all of the calculations, the average of the Lyapunov exponent is obtained in the energy region $-\epsilon \leq E \leq \epsilon$ with finite and small $\epsilon$ (with $\epsilon = 0.1$), from which the average localization length is obtained as the inverse of the Lyapunov exponent.



J. Stat. Mech. (2007) P09014

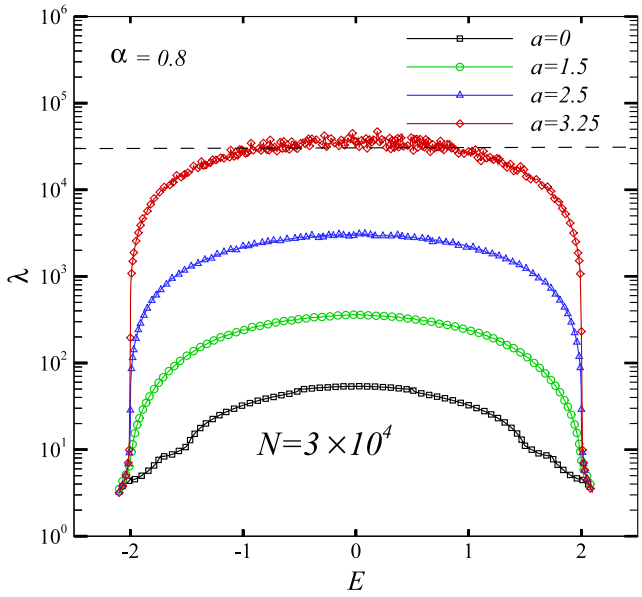


**Figure 5.** Localization length as a function of energy with $\alpha = 0.8$ and for different values of the purity parameter ($a$). The system size is fixed at $N = 3 \times 10^4$, and the variance of the series of site energies is fixed at unity. The averaging is taken over 5000 realizations.

For a fixed system size $N$ there are two parameters which control the localization length of the system: the purity parameter $a$ and the correlation exponent $\alpha$. For a specific correlation exponent $\alpha$, the localization length increases when raising the purity parameter $a$ (see figure 5), because the system becomes more ordered. For a finite system size $N$, the extended regime is produced by the set of values of $a$ for which the localization length $\lambda$ has a value greater than the system size ($\lambda \geq N$). Therefore, the phase transition at finite $N$ will occur at a critical value of the purity parameter ($a_c(N)$) where the localization length is equal to the system size.

Figure 5 shows the localization length $\lambda$ around the band center as a function of energy for the correlation exponent $\alpha = 0.8$ for a system with $N = 3 \times 10^4$ sites. As shown in figure 5, the localization length increases with $a$, and for large $a$ (see the case $a = 3.25$), around the band center, the existence of mobility edges separating localized states from extended ones can be appreciated. This means that there exists a continuum spectrum of extended states around of the band center, at least for finite $N$. To determine the critical value of purity parameter $a$ for fixed $N$, we take averaged localization lengths in the interval $-0.1 \leq E \leq 0.1$, e.g. $\overline{\lambda(E)}$, and compare with size $N$. For $\overline{\lambda(E)} > N$ the system will be in a delocalized state.

For the special case of $a = 0$, it has been shown by [4, 13] that there exists a continuum of extended states located around of the band center just for the range of correlation exponents $\alpha \geq 1.5$. We show below that this result changes in the case of the ternary model, for which the critical value of $\alpha$ at which the transition occurs is also controlled by the purity parameter $a$.

Up to now, we have described the transition from localized to extended states for finite $N$, and we have defined the transition operationally as the point where the localization



J. Stat. Mech. (2007) P09014

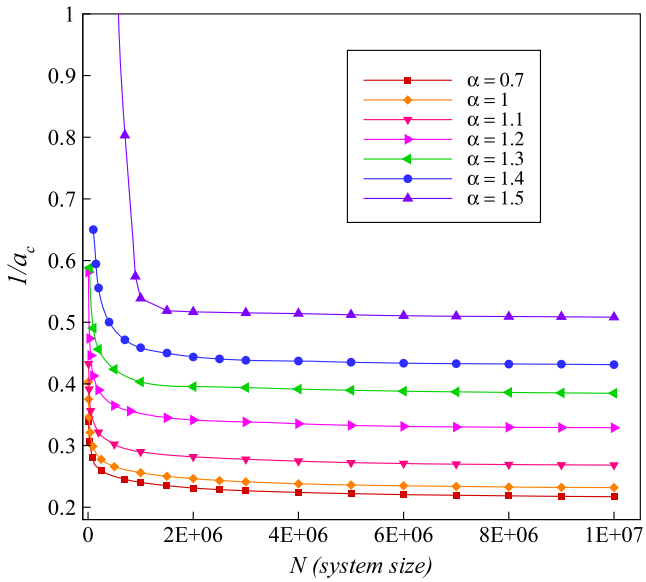


**Figure 6.** Inverse of the critical purity parameter ($a_c$) as a function of the system size $N$ for correlation exponents $\alpha = 0.7, 1.0, 1.1, 1.2, 1.3, 1.4$ and 1.5. The average is obtained using 5000 realizations. The variance of the series of site energies is fixed at unity.

length equals the system size ($\lambda = N$). However, the phase transition condition should be generally defined as $\lambda \propto N^{\beta}$, where $\beta = 1$ and $\beta < 1$ correspond to extended and localized states respectively, since in this way we guarantee that in the thermodynamic limit, the localization length diverges with the system size. Therefore, we have to calculate also our transition point given by $a_c(N)$ in the thermodynamic limit $N \to \infty$ for any value of the correlation exponent $\alpha$, in order to prevent the delocalization effect shown in figure 5 from being simply a finite-size effect.

For a certain correlation exponent $\alpha$, a system with larger size $N$ needs a higher critical purity parameter $a_c$ for the occurrence of the transition. Thus, for any value of $\alpha$ we calculate systematically the behavior of $a_c(N)$ for increasing system size $N$. Figure 6 shows the inverse of the critical purity parameter $a_c(N)$ versus the system size $N$ for different correlation exponents. According to this figure, for a fixed size, the higher the correlation exponent $\alpha$ (the stronger the long range correlations), the lower the purity parameter $a_c$ needed by the system to experience a phase transition.

Using the results shown in figure 6, we see that $a_c$ presents an asymptotic behavior and in the thermodynamic limit $N \to \infty$, it tends to a constant value $a_c(\infty)$ for a specified $\alpha$. To obtain numerically the value of $a_c(\infty)$ by extrapolating the data shown in figure 6 (we have run up to $N = 100\,000\,00$) we have fitted the data for $a_c(N)$ versus the system size $N$ with an expression of the form

$$\frac{1}{a_c} = u + \frac{w}{N^c}. \tag{6}$$

According to this expression, $u^{-1}$ is the value of $a_c$ in the limit $N \to \infty$, i.e. $a_c(\infty) = u^{-1}$. When using expression (6) to fit data of the type shown in figure 6, we obtain at least a



J. Stat. Mech. (2007) P09014

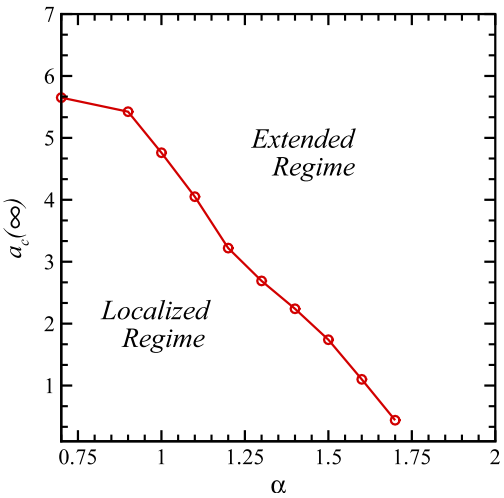


**Figure 7.** Phase diagram separating localized from extended states in the thermodynamic limit given in terms of the purity parameter ($a_c(\infty)$) as a function of the correlation exponent ($\alpha$).

correlation coefficient of 0.999, and therefore the value of $a_c(\infty)$ is obtained consistently. We also find that the exponent $c$ in (6) is almost independent from the correlation exponent $\alpha$ and is $c = 0.28 \pm 0.02$. All the results for the critical purity parameter at infinity ($a_c(\infty)$) and the corresponding correlation exponents are summarized in the phase diagram shown in figure 7. This phase diagram is the main result of this paper, and contains all the information on the localization properties of the long range correlated ternary model. For $\alpha \simeq 1.8$, we find $a_c(\infty) = 0$.

## 4. Conclusion

In summary, we have studied a one-dimensional Anderson model with long range correlated disorder when the disorder is introduced as a ternary model. The ternary model is a binary alloy with partly ordered on-site energies, the proportion of which is controlled by the purity parameter. The localization length of this ternary model increases with the purity parameter and finally a phase transition from localized to extended states can occur. The critical purity parameter for which the transition takes place depends also on the degree of correlation introduced in the system, controlled via the correlation exponent $\alpha$. For a certain correlation exponent $\alpha$, the system with larger size needs a higher purity parameter to show a phase transition. Finally, we have shown that the purity parameter tends asymptotically to a critical value in the thermodynamic limit. As our main result, we present a phase diagram which separates the localized regime from the extended one given in terms of the two relevant magnitudes of the system: the critical purity parameter in the thermodynamic limit and the correlation exponent.

## Acknowledgments

MRRT would like to express his deep gratitude to the Alexander von Humboldt Foundation and Universitat Oldenburg for their financial support and providing an

excellent environment for research. PC acknowledges financial support from the Spanish Government (grant no. BFM2002-00183).

## References

[1] Anderson P W, 1958 *Phys. Rev.* **109** 1492
[2] Dunlap D H, Wu H L and Philips P W, 1990 *Phys. Rev. Lett.* **65** 88
[3] Bellani V, Diez E, Hey R, Toni L, Tarricone L, Parravicini G B, Domýnguez-Adame F and Goméz-Alcala R, 1999 *Phys. Rev. Lett.* **82** 2159
[4] de Moura F A B F and Lyra M, 1998 *Phys. Rev. Lett.* **81** 3735
de Moura F A B F and Lyra M L, 1999 *Physica* A **266** 465
[5] Izrailev F M and Krokhin A A, 1999 *Phys. Rev. Lett.* **82** 4062
Izrailev F M, Krokhin A A and Ulloa S E, 1999 *Phys. Rev.* B **63** 41102
[6] Kantelhardt J W, Russ S, Bunde A, Havlin S and Webman I, 2000 *Phys. Rev. Lett.* **84** 198
de Moura F A B F and Lyra M, 2000 *Phys. Rev. Lett.* **84** 199
[7] Carpena P, Bernaola-Galván P and Ivanov P Ch, 2004 *Phys. Rev. Lett.* **93** 176804
[8] de Moura F A B F, Malyshev A V, Lyra M L, Malyshev V A and Dominguez-Adame F, 2005 *Phys. Rev.* B **71** 174203
Cheraghchi H, Fazeli S M and Esfarjani K, 2005 *Phys. Rev.* B **72** 174207
[9] Peng C K, Buldyrev S V, Goldberger A L, Havlin S, Sciortino F, Simons M and Stanley H E, 1992 *Nature* **356** 168
[10] Carpena P, Galvan P B, Ivanov P Ch and Stanley H E, 2002 *Nature* **418** 955
[11] Roche S, Bicout D, Macia E and Kats E, 2003 *Phys. Rev. Lett.* **91** 228101
[12] Albuquerque E L, Vasconcelos M S, Lyra M L and de Moura F A B F, 2005 *Phys. Rev.* E **71** 021910
[13] Izrailev F M and Krokhin A A, 1999 *Phys. Rev. Lett.* **82** 4062
[14] Kuhl U, Izrailev F M, Krokhin A A and Stöckmann H-J, 2000 *Appl. Phys. Lett.* **77** 633
[15] de Moura F A B F, Coutinho-Filho M D, Raposo E R and Lyra M L, 2002 *Phys. Rev.* B **66** 014418
de Moura F A B F, Coutinho-Filho M D, Raposo E R and Lyra M L, 2003 *Phys. Rev.* B **68** 012202
[16] Dominguez-Adame F, Malyshev V A, de Moura F A B F and Lyra M L, 2003 *Phys. Rev. Lett.* **91** 197402
[17] Shima H, Nomura T and Nakayama T, 2004 *Phys. Rev.* B **70** 075116
[18] Diaz E, Rodriguez A, Dominguez-Adame F and Malyshev V A, 2005 *Europhys. Lett.* **72** 1018
[19] Shahbazi F, Bahraminasab A, Mehdi Vaez Allaei S, Sahimi M and Reza Rahimi Tabar M, 2005 *Phys. Rev. Lett.* **94** 165505
Bahraminasab A, Mehdi Vaez Allae S, Shahbazi F, Sahimi M, Niry M D and Reza Rahimi Tabar M, 2007 *Phys. Rev.* B **75** 064301
[20] Esmailpour A, Esmaeilzadeh M, Faizabadi E, Carpena P and Reza Rahimi Tabar M, 2006 *Phys. Rev.* B **74** 024206
[21] Makse H A, Havlin S, Schwartz M and Stanley H E, 1996 *Phys. Rev.* E **53** 5445
[22] Hu K, Chen Z, Ivanov P-Ch, Carpena P and Stanley H E, 2001 *Phys. Rev.* E **64** 011114
[23] Chen Z *et al*, 2005 *Phys. Rev.* E **71** 011104
[24] Coronado A V and Carpena P, 2005 *J. Biol. Phys.* **31** 121

J. Stat. Mech. (2007) P09014