Eur. Phys. J. B **29**, 437–440 (2002)
DOI: 10.1140/epjb/e2002-00276-8

THE EUROPEAN
PHYSICAL JOURNAL B

The CPA solution of the anomalous Lyapunov exponent for disordered binary chains

I. Avgin[a]

Electrical and Electronics Engineering Department, Ege University, Bornova 35100, Izmir, Turkey

Received 22 April 2002

Abstract. The Coherent Potential Approximation (CPA) self-consistent equation is calculated for a binary disordered chain introducing a simple transformation. The transformation reduces the CPA equation to a cubic polynomial whose complex roots are related to the Green function and their relation to the complex Lyapunov exponent is also established. This solution fruitfully captures essential aspects of the well-known anomalous scaling behaviors in a different and advantageous way. It is found that the anomalous behavior is strongly effected by the nature of these roots. A small disorder expansion is carried out for comparison with the previous weak disorder calculations. We found that the CPA reproduced the anomalous behavior of the exact calculations.

PACS. 75.10.Hk Classical spin models – 78.30.Ly Disordered solids – 71.23.-k Electronic structure of disordered solids

1 Introduction

One-dimensional disordered systems have been studied for a long time due to their applicability to a variety of systems and the simulation can be extended to long chains of 10^8 atoms. Recently experiments are available to test some of the results obtained from the one-dimensional disordered systems. The the random microwave transmission in a single-mode wave-guide experiment [1], the transport studies with GaAs-AlGaAs random dimer super lattice systems [2], and the one-dimensional photonic band-gap structures [3] represent a few examples.

Over the years many numerical and analytical tools were developed to study these systems. Recently, Izrailev *et al.* [4] suggested classical Hamiltonian maps for the tight binding chain model. They reproduced analytically the exact calculations for the weak disorder case [16]. They also studied the localization properties of the electronic states of the one-dimensional Kroning-Penny model with the correlated random potential [5]. Heinrichs investigated the relation between the random tight binding chain and the phase and delay time distributions for continuous disordered chains [6]. The variance of the Lyapunov exponent for the random tight binding model with the Cauchy distribution has been investigated by another group lately [7]. Despite all of these efforts there is no analytical solution to this problem for the entire range of the random potentials.

Here using the Coherent Potential Approximation (CPA), an effective medium theory, we are able to obtain a solution for the binary random potential essentially for the whole range of the random potential strengths (however the CPA is only able to reproduce behavior on the mean field level except for the weak random potential strengths.) We have been studying low-energy excitations in disordered magnetic and spin glass chains using numerical and analytical methods [8,9]. The CPA, although a mean field theory, is still the best tool for disordered systems with known ground states describing the overall spectrum qualitatively. Moreover, we have found that the CPA reproduced the low-energy anomalous singularity in the density of states [9]. This is surprising since a mean field theory [10] usually cannot account the singularity and instead averages it out. Here the CPA reproduces in a clear and advantageous way the essential ingredients of the anomalous behavior of the Lyapunov exponent as shown below. A general expression for the Lyapunov exponent as a function of energy and arbitrary potential strength is obtained through the transformation introduced below. This expression will be useful for many interesting quantities such as transmission coefficients and conductivity [4,5].

2 The solution of the CPA equation

The CPA amounts to replacing a random environment with an effective environment, calculated self consistently [10]. The self-consistent equations are a nonlinear and one usually needs to use computer to solve them. An exact solution of the self-consistent equation is possible for certain types of disorder. The behavior of the one-dimensional disordered systems formulated in different contexts [11] (using proper transformations [9]),

[a] e-mail: avgin@bornova.ege.edu.tr

magnetic, electronic and vibrational can be described mathematically by the discrete, one-dimensional Schrödinger equation given by

$$(E - \xi_n V)\psi_n = \psi_{n+1} + \psi_{n-1}, \tag{1}$$

where E is energy, V is the strength of the random potential and ξ_n is equal to ∓ 1 with equal probability. The solution below can also be extended to asymmetric distributions of the signs, which will be presented elsewhere. The CPA self consistent equation for general case [9] is read

$$(1-c)\frac{V - V_c}{1-(V-V_c)\overline{G}} - c\frac{V + V_c}{1+(V+V_c)\overline{G}} = 0, \tag{2}$$

where c is the probability of $\xi_n = -1$. For equal probability it takes the form

$$-V_c(E) + (V^2 - V_c^2)\overline{G}(E, V_c) = 0, \tag{3}$$

where V_c is the potential describing the behavior of the random potential on a mean field level and is generally a complex function of energy. This equation is also valid for two and three dimensions with equal probability. $\overline{G}$ is the configurationally averaged Green function given by

$$\overline{G}(E, V_c) = [(E - V_c - 2)(E - V_c + 2)]^{-1/2}. \tag{4}$$

There exists some efforts to solve this equation for the three-dimensional case for diluted magnetic semiconductors [15] which can be achieved for a particular Green function obtained from the semicircular density of states and produces a disorder averaged Green function directly. Herein is described more convenient approach where we define a transformation that is related to the Green function and which we established in relation to the Lyapunov exponent. This method is also applicable to the three-dimensional case studied by reference [15] and gives the exact solution. Now we can introduce the following transformation [12]

$$E - V_c = 2\mathrm{cosh}\phi, \tag{5}$$

then the Green function and the self-consistent equation take the following forms [12],

$$\overline{G} = (2\mathrm{sinh}\phi)^{-1} \tag{6}$$

and using equation (5) and equation (6)

$$(t^2 - Et + t)(t - E/2) - V^2 t = 0 \tag{7}$$

respectively, where $t \equiv \mathrm{e}^{-\phi}$. This is a cubic polynomial whose roots can easily be found from any standard mathematical handbook [13]. The coherent potential $V_c(E)$ can be obtained from the roots of the equation (7). Once the coherent potential is known, various quantities can be calculated: the shift in energy due to disorder, the damping of the zero mode [12] and the line shape and the dynamic structure factor can be calculated. One can easily show that the density of states is proportional to the root of this cubic equation which is

$$\rho = -\frac{1}{\pi}\Im\frac{t_0}{1 - t_0^2} \tag{8}$$

where t_0 is the root of the cubic polynomial. If the roots are real, then the density of states is simply zero. This will enable the study of the gaps in the density of states as a function of energy and of the strength of the disorder. Generally, a cubic equation has complex roots if it holds the condition [13]

$$q(E,V)^3 + r(E,V)^2 \geq 0 \tag{9}$$

which is the case here, where $q(E,V) = 1/3 - V^2/6 - E^2/12$ and $r(E,V) = 3EV^2/8$. Otherwise, all the roots are real indicating a gap in the density of states. In the absence of disorder, *i.e.*, $V_c = V = 0$, the Green function correctly reduces to the regular form.

The solution, a function of $r(E,V)$ and $q(E,V)$, has a cumbersome, closed form [13]. However, a weak disorder (small V) expansion can be made to compare with exact calculations [16]. It also reveals fruitfully the reason behind the anomalous power law in a different but more insightful perspective. To do this, the complex Lyapunov exponent is required. This can be obtained by integrating the Green function over E [17]. The real and imaginary part of the Lyapunov exponent are related to the integrated density of states and the inverse localization length, respectively.

3 The Lyapunov exponent

In this section the relation between ϕ and the Lyapunov exponent $\gamma(E,V)$ is established. It was shown by reference [17] that the disorder averaged green function is related to the Lyapunov exponent which is given by

$$\frac{\mathrm{d}}{\mathrm{d}E}\gamma(E, V_c) = \overline{G}(E, V_c). \tag{10}$$

Changing variables from E to ϕ and using equations (5, 6) we obtain the following differential equation:

$$\frac{\mathrm{d}\gamma}{\mathrm{d}\phi} = 1 + \frac{1}{2\mathrm{sinh}\phi}\frac{\mathrm{d}V_c}{\mathrm{d}\phi}\cdot \tag{11}$$

One can obtain the coherent potential V_c as a function of ϕ by solving equations (3) namely

$$V_c = -\mathrm{sinh}\phi + \sqrt{\mathrm{sinh}^2\phi + V^2}. \tag{12}$$

The Lyapunov exponent takes this form by substituting equation (12) into equation (11)

$$\frac{\mathrm{d}\gamma}{\mathrm{d}\phi} = 1 - \frac{1}{2}\mathrm{coth}\phi + \frac{\mathrm{cosh}\phi}{2\sqrt{\mathrm{sinh}^2\phi + V^2}}\cdot \tag{13}$$

The Lyapunov exponent is obtained by integrating equation (13) yielding

$$\gamma(E) = \phi + \frac{1}{2}\ln\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{V^2}{\sinh^2\phi}}\right), \quad (14)$$

where the integration constant is chosen so as to produce the regular case when the random potential's strength $V = 0$. The Lyapunov exponent is then simply obtained by inserting ϕ, the solution of equation (7). In case $V = 0$, equation (7) yields a solution (complex root) $t = e^{-i\theta}$ where θ is conveniently defined by

$$E = 2\cos\theta, \quad (15)$$

and the Lyapunov exponent is pure imaginary $\Im\gamma = \Im\phi = \theta = \cos^{-1}\frac{E}{2}$ which is related to the integrated density of states (IDOS). Clearly, the inverse localization proportional to $\Re\gamma(E)$ is zero within the band $E \in [-2, 2]$ indicating no disorder.

Equation (14) has the interesting consequence that one does not need to introduce the CPA self energy with an artificial coefficient. This point is discussed in reference [19], and the coherent potential should be divided by 2 supposing the problems related to averaging.

4 Weak disorder expansion

Analyses are carried out below for small disorder as $V \to 0$ and the complex root of equation (7) is used since the real root implies that the integrated density of states is zero, which may not be true. For positive E not equal to the band edge value 2, using the equation (15), the self-consistent equation (7) becomes

$$(t - e^{i\theta})(t - e^{-i\theta})(t - \cos\theta) = \frac{V^2}{2}t. \quad (16)$$

for small V. One can solve this equation by perturbation methods [20] where t can be expanded

$$t = t_0 + \epsilon t_1 + \epsilon^2 t_2 + \cdots, \quad (17)$$

where $\epsilon = \frac{V^2}{2}$ and for the equation (16) $t_0 = e^{i\theta}$. We are subsequently only concerned first order terms and thus the solution of t takes the form

$$e^{-\phi} = t \simeq e^{i\theta}\left(1 - \frac{V^2}{4\sin^2\theta}\right). \quad (18)$$

Substituting this into the equation (16), the Laypunov exponent can be written as

$$\gamma = -i\theta + \frac{V^2}{8\sin^2\theta}\,. \quad (19)$$

The real part of the above result is reproduced by reference [4] using classical maps. Derrida *et al.* [16] for certain discrete energies obtained $-i\frac{\pi}{2} + \frac{V^2}{8}$ for $E = 0$ at the band center and $-i\frac{\pi}{3} + \frac{V^2}{6}$ for $E = 1$. These results are in good agreement with those obtained from equation (19).

For $E = 2$ at the band edge, equation (16) becomes $(t - 1)^3 = (V^2/2)t$. We can again use the perturbation method but care must be taken since we have multiple roots [20]. In this case the expansion $t = 1 + \epsilon^\alpha t_1 \ldots$ where α will be obtained through balancing the terms [20]. We obtain, $\epsilon^{3\alpha}t_1^3 - \epsilon^{\alpha+1}t_1 - \epsilon = 0$ for t_1. This equation will be balanced for $\alpha = 1/3$ and then, t is given by

$$t \simeq 1 + e^{-i2\pi/3}(V^2/2)^{1/3}. \quad (20)$$

The Lyapunov exponent takes the form

$$\gamma \simeq -i\frac{3\sin\frac{\pi}{3}}{2^{7/3}}V^{2/3} + \frac{3\cos\frac{\pi}{3}}{2^{7/3}}V^{2/3}, \quad (21)$$

where $IDOS = -\frac{1}{\pi}\Im\gamma = 0.164V^{2/3}$ and inverse localization length $\Re\gamma = 0.297V^{2/3}$. The so-called anomalous power-law behavior [16] is successfully reproduced. The coefficients are close to values given in reference [16] which are in turn $IDOS = -\frac{1}{\pi}\Im\gamma = 0.159V^{2/3}$ and $\Re\gamma = 0.289V^{2/3}$ and which was obtained rather by complex detailed analyses.

We remark here that the CPA solution clearly predicts when the anomalous scaling occurs as a function of energy in a more insightful and clear way. Anomalous scaling occurs if the polynomial equation (16) of the CPA self-consistent equation has multiple roots. It can be checked quite easily whether the cubic equation (7) has multiple roots for $V = 0$. This can be probed by setting [13] $q(E,V)^3 + r(E,V)^2 = 0$. This will show that at $E = \pm 2$ anomalous scaling appears. Similar anomalous scaling of the Lyapunov exponent was also observed in chaotic billiards systems [14]. Note that for the negative values of E, the same results also hold except that the imaginary part of the Lyapunov exponent picks up a constant term equal to π.

5 Summary and discussion

We have obtained a solution for the nonlinear, self-consistent equation of the CPA. The solution can be obtained from the roots of third order polynomials that has a cumbersome, closed form. We have shown here that for the weak disorder, the CPA solution correctly reduces to the exact calculation of Derrida *et al.* [16]. The solution can predict the energies at which the power law scaling may occur. This method is also easily extendible to asymmetric distributions of the random signs. There are constant efforts to develop an understanding of the spectrum of the one-dimensional discrete Schrödinger equation and thus many different techniques [18,21–23] have been developed. The CPA results can be compared to equations (40) and (50) of reference [21] where the correct anomalous power-law was obtained with a coefficient larger by a factor of two. Using the method of [18] again a cubic polynomial is obtained but one cannot produce the correct power-law behavior. In the past using the replica method the Lyapunov exponent was calculated [22]. A cubic equation was also obtained which led to the 2/3 power-law behavior but again with a coefficient twice that of the exact one. Paladin *et al.* also studied this anomalous scaling behavior using transfer matrix techniques where they recover the correct power, 2/3, but with the coefficient for the inverse localization length 0.6299 [23] almost twice that of the exact coefficient. The CPA solution reproduces correctly the power-law behaviors and coefficients, giving a better performance than some of the cited works above. It proves to be a useful tool to investigate disordered problems.

I would like to thank Professor D.L. Huber for helpful discussions. This work is partially sponsored by the Scientific and Technical Research Council of Turkey (TUBITAK).

References

1. U. Kuhl, H.J. Stöckmann, Physica E **9**, 384 (2001)
2. F. Kuckar, H. Heinrich, G. Bauer, *Localization and confinement of electrons in semiconductors* (Berlin, Heidelberg, New York, Springer, 1990)
3. M. Bayindir, S. Tanriseven, E. Ozbay, Appl. Phys. A **72**, 117 (2001)
4. F.M. Izrailev, S. Ruffo, L. Tessieri, J. Phys. A **31**, 5263 (1998)
5. F.M. Izrailev, A.A. Krokhin, S.E. Ullo, Phys. Rev. B **63**, 41102 (2001)
6. J. Heinrichs, Phys. Rev. B **65**, 075112 (2002)
7. L.I. Deych, D. Zaslavsky, A.A. Lisyansky, Phys. Rev. Lett. **81**, 5390 (1998)
8. I. Avgin, Phys. Rev. B **59**, 13554 (1999)
9. I. Avgin, J. Phys. Cond. Matt. **8**, 8379 (1996), I. Avgin, D.L. Huber, Phys. Rev. B **48**, 13625 (1993)
10. J.M. Ziman, *Models of disorder* (Cambridge, 1982), p. 341
11. K. Ishii, Prog. Theor. Phys. Suppl. **53**, 77 (1973)
12. I. Avgin, D.L. Huber, *Frontiers in magnetism of reduced dimension systems*, edited by V.G. Bar'yakhtar, P.E. Wigen, N.A. Lesnik (Dordrecht, Kluwer Academic Publisher, 1998), p. 317
13. M. Abramowitz, I.R. Stegun, *Handbook of Mathematical Functions* (New York, Dover, 1972)
14. G. Benettin, Physica D **13**, 211 (1984)
15. M. Takahashi, J. Phys. Cond. Matter **13**, 3433 (2001)
16. B. Derrida, E. Gardner, J. Phys. France **45**, 1283 (1984)
17. D.J. Thouless, J. Phys. C **5**, 77 (1972)
18. A. Bulatov, J.L. Birman, Phys. Rev. B **54**, 16305 (1996)
19. E.N. Economou, C.M. Soukoulis, A.D. Zdetsis, Phys. Rev. B **30**, 1686 (1984)
20. E.J. Hinch, *Perturbation Methods, Cambridge Texts in Applied Mathematics* (Cambridge, 1991)
21. J. Heinrichs, Phys. Rev. B **50**, 5295 (1994)
22. J.P. Bouchaud, A. Georges, D. Hansel, P. Le Doussal, J.M. Maillard, J. Phys. A **19**, L1145 (1986)
23. G. Paladin, G. Vulpani, Phys. Rev. B **35**, 2015 (1987)