Volume 372, issue 2 15 December 2006 ISSN 0378-4371

Nonlinearity, Nonequilibrium and Complexity: Questions and Perspectives in Statistical Physics

A festschrift dedicated to Alberto Robledo on occasion of his 60th birthday

Guest Editors:

Sumiyoshi Abe
Hans J. Herrmann

Available online at
ScienceDirect
www.sciencedirect.com

http://www.elsevier.com/locate/physa

Available online at www.sciencedirect.com
ScienceDirect
Physica A 372 (2006) 243–248
PHYSICA A
www.elsevier.com/locate/physa

New trends in localization theory

Gerardo G. Naumis*

Instituto de Fisica, Universidad Nacional Autónoma de México, Apdo. Postal 20-364, 01000, México D.F., Mexico

Available online 8 September 2006

Abstract

In this article we discuss some recent trends in the research of electron and phonon localization, specially in the field of quasiperiodic potentials. Then, a new scheme to detect and classify localization is developed by studying the band scaling of a related supercrystal made from replicas of the system. For one dimension, this leads to the use of dynamical systems theory to obtain the localization length and the scaling exponents of the wave functions.

Keywords: Dynamical systems; Localization; Quasicrystals; Quasiperiodic

1. Introduction

Right after the initial development of quantum mechanics, it was not clear how an electron is able to travel inside a crystal. The answer was provided by Bloch [1]. He showed that the eigenfunctions ($\psi_{\mathbf{k}}(\mathbf{r})$) of the Schröedinger equation for an electron in a periodic potential ($V(\mathbf{r})$), where $\mathbf{r}$ is the position vector, are given by the product of a function $u_{\mathbf{k}}(\mathbf{r})$ that has the same periodicity of the lattice [1], and a plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$, and $\mathbf{k}$ is the corresponding wave-vector. Such states are called extended since the probability of finding an electron does not decay with the distance. When Bloch's theorem was combined with the Fermi–Dirac statistics, the result was a very successful model for the electronic properties of solids. However, many materials do not have a periodic potential [2], as happens for example with glasses, disordered alloys, etc. This situation was considered unsatisfactory, and a lot of research has been done since 1950 [2]. An important step was made by Anderson [3]. He showed that for a simple random potential model, it is possible to have exponentially localized solutions of the type [3] $\psi(r) \simeq e^{-|r|/\xi}$, where ξ is a characteristic localization length. The main feature of a localized state is that the probability of observing the electron decays with the distance. There is no equivalent for the Bloch's theorem in disordered solids, instead a collection of models is available to provide clues and answers for different situations [2]. For example, the Anderson model was fundamental to understand the role of dimensionality. The renormalization group has been used as a powerful tool in order to study such effects [4], where the Anderson transition from extended to localized states was recognized by finding the fixed point of a renormalization procedure [4]. The common knowledge about localization in terms of the dimensionality is the following [2]: in one dimension (1D), all states are localized, even for an

*Fax: +52 5 616 15 35.
E-mail address: naumis@fisica.unam.mx.

0378-4371/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.physa.2006.08.012

infinitesimal degree of disorder. In 3D, localized states are separated from extended ones. The energy where this occurs is known as a mobility edge, and is usually at the band edges [2]. In 2D the scaling theory of Abrahams et al. [4] predicts weak localization, and thus metallic conductivity and quantum percolation is not observed for disordered systems. We remark that still there is a discussion about this subject [5]. The electron–electron interaction is a different source of localization [6]. This field is very active at the moment, like for example the research in the Hubbard Hamiltonian for disordered systems [7], due to the importance of the problem for high temperature superconductors. Another field related to many body effects, is the investigation of non-linear Hamiltonians for phonon localization. In this case, even for periodic potentials few things are known [8]. Fermi, Pasta and Ulam were among the firsts to tackle the problem [9]. They tried to understand how non-linearity leads to energy equipartition [9]. Recently, it has been proved that for periodic potentials with non-linear terms, some states are localized [8]. This kind of localization is known as intrinsic [8]. Another active field is the study of quasiperiodic potentials, which are systems that are neither disordered, nor periodic [10]. In this paper, we present the main features of such systems, and then we will show how some ideas taken from dynamical systems are useful for the study of localization.

2. Quasiperiodic potentials

In the last years, there has been a progressive recognition that not all ordered systems are periodic. Mathematicians already knew that; a function $f(x)$ is periodic if there is a T such that $f(x) = f(x+T)$; and as a consequence, $f(x)$ can be developed using a Fourier series. However, there are non-periodic functions which have a Fourier expansion, as for example $f(x) = \cos(x) + \cos(\alpha x)$ when α is an irrational number. Such functions are called quasiperiodic (QP). The first example of a QP potential in physics was given by the Frenkel–Kontorova model, which is a system of coupled oscillators inside an external periodic field [10]. If the ratio between the period of the system and the modulation is not a rational number, the resulting potential is not periodic [10]. A second important example was the Harper equation [11], that describes an electron that travels in a 2D crystal under a uniform magnetic field [12]. It can be reduced to the solution of the following 1D tight-binding equation [12],

$$t\psi_{n-1} + t\psi_{n+1} + V_n\psi_n = E\psi_n, \tag{1}$$

where $V_n = 2\cos(2\pi\sigma n)$ is the on-site potential at site n in the lattice, t the hopping integral between contiguous sites, ψ_n is the wavefunction at site n, and σ is the ratio between lattice and quantum magnetic flux in a unitary cell [12]. If σ is an irrational number, the period of V_n is not commensurate with the lattice. The resulting spectrum is called singular continue and is a fractal set [12]. The corresponding wave functions show a fractal behavior, with a power law envelope decay of the type $\psi(r) \simeq r^{\beta}$. This behavior is known as critical. There are many interesting open questions for this model, like the nature of the quantum phase diagram [13], or the effects of an applied electric field [14].

Quasicrystals (QC), which are solids that were discovered in 1984 [15], also display quasiperiodicity and thus they have a non-periodic long range order. As a consequence, their diffraction patterns present Bragg peaks with forbidden rotational symmetries for a crystal [10]. The most simple model of a QC is the Fibonacci chain [10] (FC), in which two kinds of atoms, A and B, are arranged following a Fibonacci sequence (FS) [10], i.e., if one defines the first generation sequence as $\mathscr{F}_1 = A$ and the second one $\mathscr{F}_2 = BA$, the subsequent generations are given by joining two previous generations $\mathscr{F}_n = \mathscr{F}_{n-1} \oplus \mathscr{F}_{n-2}$. For instance, $\mathscr{F}_3 = ABA$. A tight-binding model like Eq. (1) can be defined to model the FC, where V_n takes two possible values: V_A and V_B following a FS. In fact, using a Fourier expansion, we can show that the Fibonacci potential is a sum of Harper potentials,

$$V(n) = \overline{V} + 2\delta V \sum_{s=1}^{\infty} \widetilde{V}(s)\cos(\pi s\sigma(2n+1)), \tag{2}$$

where now σ is the golden mean $\sigma = (\sqrt{5}+1)/2$, $\overline{V} = (V_A/\sigma) + (V_A/\sigma^2)$, $\delta V = V_A - V_B$, and $\widetilde{V}(s)$ is the s harmonic of the Fourier series, $\widetilde{V}(s) = \sin(\pi s\sigma)/s\sigma$.The corresponding spectrum is singular continuous [16], i.e., almost full of gaps. This result follows from the reciprocal space structure of a QC, which is dense filled with diffraction spots since the number of reciprocal basis vectors is higher than the dimensionality of the

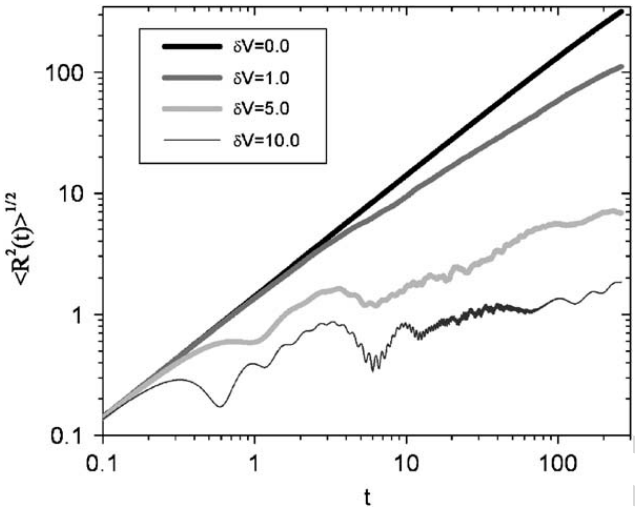

Fig. 1. Dispersion of a wave packet as a function of time for a FC with $N = 10\,000$ sites, obtained by solving Eq. (1) with $t = 1$, $V_A = 0$ and for different values of $\delta V = V_A - V_B$.

system [10], as can be obtained from Eq. (2). To understand the relationship between this fact with the gap opening mechanism, let us approximate the irrational number σ with a sequence of rational approximants $F(l)/F(l-1)$, where $F(l)$ is the l-esim Fibonacci number (defined through the recursive relation $F(l) = F(l-1) + F(l-2)$, with $F(0) = 1$, and $F(1) = 1$). Under this approximation, $V(n)$ has period $T = F(l-1)$ and $F(l-1)$ bands. There is a general relationship between the density of states $\rho_n(E)$, and the structure of the reciprocal space [1],

$$\rho_l(E) = \int_{S_l(E)} \frac{\mathrm{d}S}{4\pi^3} \frac{1}{|\nabla_{\mathbf{k}} E(\mathbf{k})|},$$

where $S_l(E)$ is an isoenergetic surface of the l-band in the reciprocal space and $E(\mathbf{k})$ is the dispersion relation. A singularity occurs whenever the group velocity is zero, $\nabla_{\mathbf{k}} E(\mathbf{k}) = 0$, i.e., when $\mathbf{k}$ has a value that corresponds to a lattice characteristic length, since travelling waves with such a wave length do not propagate, instead they are diffracted. There are as many singularities in the spectrum as bands [1], but since $F(l-1) \to \infty$ as $l \to \infty$, in the limit of irrational σ the spectrum is full of singularities. In one dimension, the singularities are not integrable, and a spectral gap of size $\Delta E_k \simeq 2|\widetilde{V}(k)|$ is open for each Fourier component $\widetilde{V}(k)$ of the potential [1]. In the present case, almost for all values of k it is obtained that $\widetilde{V}(k) \neq 0$ and thus the spectrum is almost full of gaps. The corresponding wave-functions of the FC are also critical [16]. As a consequence, the dispersion of an electron wave-packet is anomalous, as shown in Fig. 1, where the evolution of the quadratic mean displacement, defined as $\langle R^2(t)\rangle \equiv \sum_{n=1}^{N} \|\psi_n(t)\|^2 (n - n_0)^2$, is plotted as a function of the time (t) for a packet that has a delta shape centered at site n_0 at $t = 0$. From Fig.1, for long times we observe a power law behavior of the type: $\sigma(t) = Dt^{\upsilon}$. As expected, the periodic case ($\upsilon = 1$) is recovered for $\delta V = 0$.

The corresponding most simple quasiperiodic structures for 2D and 3D are the well known Penrose tilings [10]. However, the nature of their spectrum and localization properties are still open questions, although it has been shown [17] that the topological disorder and the associated frustration of the wave-function makes the problem very different from the 1D case. For the Penrose, there is numerical evidence that points to the existence of extended, critical and localized states [17]. The critical nature of some wave functions in quasiperiodic potential leads to the question of how to calculate the critical exponents and their relation with the spectrum. As we will see in the next section, some answers are related with an associated dynamical system.

3. Dynamical systems and localization

Although many things are known about QP potentials, even in 1D it has not been possible to find the scaling properties for all the wave-functions. Here we present an approach that uses the band scaling of a related supercrystal, and in 1D this turns out to be closely connected with the stability of a map.

The usual procedure to investigate localization in 1D is as follows: Eq. (1) can be rewritten in terms of a transfer matrix $M(n,E)$ and a vector $\mathbf{\Psi}_n$ with components (ψ_n,ψ_{n-1}), that satisfies,

$$\mathbf{\Psi}_{n+1} \equiv \begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \begin{pmatrix} \dfrac{E-V_n}{t_n} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \equiv M(n,E)\mathbf{\Psi}_n. \tag{3}$$

The wave-function at site n, is given by a successive application of Eq. (3), $\mathbf{\Psi}_n = M(n,E)M(n-1,E)\ldots M(1,E)\Psi_1 \equiv T(n,E)\mathbf{\Psi}_1$, and the spectrum is the set for which the trace norm $|\tau_n(E)| \equiv |\mathrm{tr}\, T(n,E)| \leqslant 2$ [16]. This comes from the following line of thought. The Lyapunov exponent ($\gamma(E)$), that measures the growth of $\mathbf{\Psi}_n$ is [18], $\gamma(E) = \lim_{n\to\infty} \ln \|T(n,E)\|/n = \lim_{n\to\infty} \ln|\lambda_{\max}|/n$, where $\lambda_{\max}$ is the greatest eigenvalue of $T(n,E)$. The two eigenvalues of $T(n)$ are,

$$\lambda_{\pm}(E) = \frac{\tau_n(E) \pm \sqrt{\tau_n^2(E)-4}}{2}. \tag{4}$$

In an energy that belongs to the spectrum, $\lambda_+(E)$ and $\lambda_-(E)$ are complex numbers [19], and thus E must satisfy $|\tau_n(E)| \leqslant 2$. The points where $|\tau_n(E)| = 2$ and $\mathrm{d}\tau(E)/\mathrm{d}E \neq 0$ are the band edges (energies that we denote by E_s). Since from Eq. (4) $\|T(n,E)\|$ is always 1, when $n \to \infty$ the condition $|\tau_n(E)| \leqslant 2$ imply that $\gamma(E) = 0$, no matter what is the localization present in the system. Thus, the question is how to use the trace to detect a localized or a critical state. This issue can be related with the scaling of bands of an associated supercrystal, using as unitary cell a piece of the chain of length n; this cell can be amorphous, quasiperiodic or crystalline. The resultant supercrystal has Bloch solutions and a spectrum within principle n bands. Each bandwidth W_n depends on the overlap and localization of the wave-functions at contiguous cells. Then we can analyze how W_n scales with n to obtain the localization properties. To show how the idea works, let us write the trace of the supercrystal in terms of the roots of $\tau_n(E) - 2 = 0$,

$$\tau_n(E) - 2 = C_n \prod_{i=1} (E - E_i). \tag{5}$$

In fact, the E_i's are band edges, and C_n is a constant. From this we get,

$$\ln\left(\frac{\mathrm{d}\tau_n(E)}{\mathrm{d}E}\right)_{E=E_s} = \sum_{i\neq s} \ln(E_s - E_i). \tag{6}$$

Since the E_i's are the points where $\tau_n(E) = 2$, from Eq. (3) it is easy to show that these values satisfy a cyclic boundary condition for the same finite cell of size n. Taking into account this observation and that each state has a weight $1/n$ in the density of states, the sum in Eq. (6) can be performed by using the density of states ($\rho_n(E)$) of the cyclic problem,

$$\frac{1}{n}\ln\left(\frac{\mathrm{d}\tau_n(E)}{\mathrm{d}E}\right)_{E=E_s} = \int_{-\infty}^{\infty} \rho_n(E')\ln(E_s - E')\,\mathrm{d}E'. \tag{7}$$

Using the Thouless formula [19] for the localization length $\xi(E_s)$, we get an expression that now depends on the trace,

$$\frac{1}{\xi(E_s)} = \lim_{n\to\infty} \frac{1}{n}\ln\left(\frac{\mathrm{d}\tau_n(E)}{\mathrm{d}E}\right)_{E=E_s}. \tag{8}$$

The relation with the stability of the trace map is evident, since now the localization length corresponds to a Lyapunov exponent, used in the sense of dynamical systems [20], i.e., it tells how much two trajectories diverge under the action of $\tau_n(E)$. For a localized state, the band shrinks in an exponential way as the system grows due to a decreasing overlap between neighboring cells.

For quasiperiodic systems, the wave-function decays as $n^{\beta(E)}$ [16]. To obtain $\beta(E)$, instead of dividing by n in Eq. (7), we divide by $\ln n$, since the wave-function overlap is of order $W_n \approx n^{2\beta(E)}$. Then we get the scaling

exponent of the wave-function that is appropriate for quasiperiodic systems,

$$\beta_n(E) \equiv \frac{1}{2\ln n}\ln\left(\frac{\mathrm{d}\tau_n(E)}{\mathrm{d}E}\right) = \frac{n}{2\ln n}\int_{-\infty}^{\infty}\rho_n(E')\ln(E-E')\,\mathrm{d}E'. \tag{9}$$

This expression is very useful for quasiperiodic systems, since there are recurrence relations of the trace of a certain size of the chain as a function of the trace of m smaller chains [21], $\tau_n(E) = f(\tau_{l_1}(E), \tau_{l_2}(E), \ldots, \tau_{l_m}(E))$. These types of relations are called trace maps. Using the approach presented here, the localization properties are determined by the stability of the trace map around the points $\tau_n = \pm 2$, since in a localized state the bands shrink as the cell size grows; this corresponds to a repulsive fixed point of the trace map. For extended states, the band edges do not change with the system size because the overlap is size-independent, and $\tau_n(E_s) = \pm 2$ for any n and fixed E_s. $\tau_n(E_s) = \pm 2$ is a fixed point of the trace map, and must satisfy $\pm 2 = f(\pm 2, \pm 2, \pm 2, \ldots)$. The point $\tau_n(E_s) = \pm 2$ is hyperbolic in nature, since as the system is scaled, the iterations of the map for energies inside the band remain bounded, while for the other energies go to infinity.

As an example of the use of the technique proposed, we will obtain the analytic scaling exponents of the wave-function for the FC. For this system, it has been proved that the spectrum is singular continue, with critical wave-functions [16]. However, the problem of determining the scaling exponents of the wave-function has been approached from numerical calculations and only for a certain state, the exact scaling exponent is known [22]. Here we will apply the technique proposed in the last section to show how it works for the case of the Fibonacci potential. In this case, it has been proved that the trace of a chain with length $F(l)$ is given by a map [21],

$$x_l(E) = x_{l-1}(E)x_{l-2}(E) - x_{l-3}(E), \tag{10}$$

where $x_l = \tau_l(E)/2$. The map has as initial conditions [21], $x_{-1}(E) = 1$, $x_0(E) = (E+\lambda)/2$ and $x_1(E) = (E+\lambda)/2$, where $\lambda = |(V_A - V_B)|/2$. The nature of the states is easily obtained from the approach presented. First one needs to obtain the fixed points of the map. If we denote the fixed point as x^*, from Eq.(10), $x^* = 2(x^*)^2 - x^*$, two solutions are found, $x^* = 0$ and $x^* = 1$. However, 0 is not consistent with the initial conditions, since the map has an invariant [21]

$$x_{l+1}^2(E) + x_l^2(E) + x_{l-1}^2(E) - 2x_{l+1}(E)x_l(E)x_{l-1}(E) = \lambda^2 + 1.$$

From the invariant, it is easy to show that $x^* = 1$ occurs only when $\lambda = 0$ and $V(n) = V_A = V_B$. To investigate the nature of localization, we study the stability of the map around $x^*(E) = 1$. Thus we make a linear stability analysis, using that the map can be seen as a trajectory in 3D [21], where the coordinates of a point $\mathbf{p} = (x_{n+1}, x_n, x_{n-1})$ are iterated to form a 3D map,

$$x_{n+2} = x_{n+1}x_l - x_{l-1}, \quad x_{n+1} = x_l, \quad x_n = x_{l-1}.$$

By making a Taylor expansion around the fixed point, and since the map is a vectorial function, the derivative is a 3×3 matrix. The three eigenvalues of the derivative matrix [20] at the point $\mathbf{p} = (1,1,1)$ are $r_1 = -1, r_2 = \sigma^2, r_3 = 1/\sigma^2$. Thus, $x^* = 1$ is classified as an hyperbolic fixed point. The hyperbolic nature of the flux means that the states are extended for $\lambda = 0$, as expected. Localized states are not observed since there are no repulsive fixed points. The only remaining possibility is to have critical states for $\lambda \neq 0$, as is revealed from the fact that the map contains two cycles: one with period two and the other with period six [22]. A similar linear stability analysis can be made for the cycles, except that the derivative is obtained by multiplying the matrices in each point of the cycle. For the period six cycle, which corresponds to energies at the center of the spectrum, the eigenvalues of the resulting matrix are

$$r_1 = -1, r_{2,3} = [(1 + 4(1+\lambda^2)^2)^{1/2} \pm 2(1+\lambda^2)]^2.$$

From this, one can show that the trace scales as $\tau_{l+6}(E) = (\tau_l(E))^{\alpha}$, where

$$\alpha = \ln\sigma^6/\ln(r_2) = \ln\sigma^3/\ln((1 + 4(1+\lambda^2)^2)^{1/2} + 2(1+\lambda^2)).$$

Using Eq. (9), the stability of the map predicts that the scaling exponent of the wave-function is $\beta = \alpha/2$. This result is similar to that obtained using a direct multiplication of transfer matrices [22] at the special energy

$E = 0$, which is a special energy that follows the six cycle. However, the method presented here can be applied to the other energies as well.

4. Conclusions

In conclusion, this work shows that still there are many unanswered questions in localization theory. Nowadays, correlations, non-linearity and quasiperiodic systems are among the most studied subjects. The tools of dynamical systems are very useful for studying localization, and give a natural classification for the types of localization in terms of fixed points and stability around them.

Acknowledgments

I would like to thank Alberto Robledo for his beautiful science at the edge of chaos, which has been a source of inspiration for young physicists in Mexico. Financial support was provided by DGAPA-UNAM project IN-117806 and 41538 USA NSF-CONACyT joint project.

References

[1] Ch. Kittel, Introduction to Solid State Physics, seventh ed., Wiley, New York, 1996.
[2] R. Zallen, The Physics of Amorphous Solids, Wiley, New York, 1998.
[3] P.W. Anderson, Phys. Rev. 109 (1958) 1492.
[4] E. Abrahams, P.W. Anderson, D.C. Licardello, T.V. Ramakrishnan, Phys. Rev. Lett. 42 (1979) 673.
[5] G.G. Naumis, Ch. Wang, R.A. Barrio, Phys. Rev. B 65 (2002) 134203.
[6] N.F. Mott, Proc. Phys. Soc. (London) A 62 (1949) 416.
[7] K. Byczuk, W. Hofstetter, D. Vollhardt, Phys. Rev. B 69 (2004) 045112.
[8] D.K. Campbell, S. Flach, Y.S. Kivshar, Phys. Today January (2004) 43.
[9] M. Toda, Theory of Non-Linear Lattices, Springer, Berlin, 1988.
[10] C. Janot, Quasicrystals: A Premier, second ed., Oxford Science, Oxford, 1994.
[11] P.G. Harper, Proc. Phys. Soc. London A 68 (1955) 874.
[12] D.R. Hofstadter, Phys. Rev. B 14 (1976) 2239.
[13] D. Osadchy, J.E. Avron, J. Math. Phys. 42 (2001) 5665.
[14] A. Kunold, M. Torres, Phys. Rev. B 61 (2000) 9879.
[15] D. Shechtman, I. Blech, D. Gratias, J.W. Cahn, Phys. Rev. Lett. 53 (1984) 1951.
[16] A. Sütö, in: F. Axel, D. Gratias (Eds.), Beyond Quasicrystals, Les Editions de Physique, France, 1994.
[17] G.G. Naumis, Ch. Wang, R. Barrio, Phys. Rev. B 50 (1994) 9834.
[18] A. Crisanti, G. Paladin, A. Vulpiani, Products of Random Matrices, Springer, Berlin, 1993.
[19] J.M. Ziman, Models of Disorder, Cambridge University Press, Cambridge, 1979.
[20] G. Nicolis, Introduction to Non-linear Science, Cambridge University Press, Cambridge, 1995.
[21] M. Kohmoto, L.P. Kadanoff, Ch. Tao Phys. Rev. Lett. 50 (1983) 540.
[22] M. Kohmoto, B. Sutherland, Ch. Tang, Phys. Rev. B 35 (1987) 1023.