Spectrum and diffusion for a class of tight-binding models on hypercubes

1999 J. Phys. A: Math. Gen. 32 2361

(http://iopscience.iop.org/0305-4470/32/12/009)

J. Phys. A: Math. Gen. **32** (1999) 2361–2367. Printed in the UK PII: S0305-4470(99)99703-2

Spectrum and diffusion for a class of tight-binding models on hypercubes

Julien Vidal†, Rémy Mosseri† and Jean Bellissard‡§

† Groupe de Physique des Solides, Universités Pierre et Marie Curie P6 et Denis Diderot P7, Tour 23, 2 place Jussieu, 75251 Paris Cedex 05, France
‡ Institut Universitaire de France
§ Laboratoire de Physique Quantique, UMR5626 associée au CNRS, IRSAMC, Université Paul Sabatier, 118 route de Narbonne, F-31062 Toulouse Cedex 4, France

Received 27 November 1998

Abstract. We propose a class of exactly solvable anisotropic tight-binding models on an infinite-dimensional hypercube. The energy spectrum is computed analytically and is shown to be fractal and/or absolutely continuous according to the value of the hopping parameters. In both cases, the spectral and diffusion exponents are derived. The main result is that, even if the spectrum is absolutely continuous, the diffusion exponent for the wave packet may be anything between 0 and 1 depending upon the class of models.

The interplay between the energy spectrum and the diffusion process for quantum systems is still an open question. Indeed, recent studies have shown that the spreading of a wave packet is determined by several exponents that depend on the nature of the spectrum (absolutely continuous, singular continuous, pure point, or any mixture) [1, 2]. More recently, it has been shown that the correlation dimension of the eigenstates also plays a crucial role in this process [3]. In particular, for quasiperiodic systems, such as quasicrystals (QCs), it has been shown that an anomalous behaviour of the wave packet spreading occurs when the spectrum is singular continuous [4] (see below).

In such systems, scaling laws occur at many levels. We will concentrate upon two classes of scaling exponents due to their importance for electronic and transport properties. The first one concerns *spectral exponents*, defined as $\int_{E-\delta E}^{E+\delta E} \mathrm{d}\mathcal{N}(E') \sim \delta E^{\alpha(E)}$ as $\delta E \to 0$, where $\mathcal{N}$ is the local density of states (LDOS). An absolutely continuous spectrum in some interval I of energy implies $\alpha(E) = 1$ for $E \in I$ and E in the spectrum. A pure point spectrum in I, namely the LDOS is a sum of Dirac peaks in I, implies $\alpha(E) = 0$ on the part of the spectrum contained in I. Finally, if $0 < \alpha(E) < 1$ for E in some part of the spectrum implies a singular continuous spectrum there. This is actually what happens for one-dimensional (1D) QCs [5, 6] such as the Fibonacci chain. Such a singular continuous spectrum occurs for 1D chains with a potential given by a substitution sequence [7–10]. The problem of two-dimensional (2D) electrons on a square lattice under magnetic field that can be mapped onto a 1D Harper equation [11] also displays a singular continuous spectrum [12] for incommensurate fluxes, and the spectral exponents have been computed numerically [13]. A number of non-rigorous results suggesting singular spectra were obtained for models on higher-dimensional QCs such as the *labyrinth model* [14], the *octagonal tiling* [15], in the small-hopping regime. Finally, we also mention

0305-4470/99/122361+07$19.50

recent studies on Jacobi matrices associated with *iterated function systems* (IFSs) [17, 18] generalizing Julia sets [19, 20] leading to the calculation of the spectral exponents.

The next class concerns *diffusion exponents*, given by $L_E(t) \sim t^{\beta(E)}$ as $t \to \infty$ where $L_E(t)$ characterizes the spreading of a typical wave packet of energy E after time t [21] (see equation (16) for a definition of the exponents). *Ballistic* motion such as the electronic motion in a perfect crystal, corresponds to $\beta = 1$. *Strong localization* is defined by demanding that $\sup_{t>0} L_E(t) < \infty$ implying $\beta(E) = 0$. The *weak-localization* regime appearing in weakly disordered metals generally corresponds to $\beta = \frac{1}{2}$, namely to the case for which the quantum evolution mimicks classical diffusion such as Brownian motion. Such behaviour of the quantum diffusion also occurs in the random-phase approximation (RPA) [21]. If β takes on values different from $0, \frac{1}{2}, 1$ we shall speak of *anomalous diffusion*. In QCs for instance, numerical results show that β may be anything between 0 and 1 and is model dependent [4, 16]. For realistic QCs, such as i-AlCuCo, an *ab initio* calculation leads to $\beta = 0.375$ at the Fermi level [22].

The spectral and diffusion exponents are related through the *Guarneri inequality* [2]

$$\beta(E) \geqslant \frac{\alpha(E)}{d} \tag{1}$$

where d is the dimension of the system. This inequality implies that for an absolutely continuous spectrum, ballistic motion always occurs in one dimension†, whereas for higher dimensions $\beta \geqslant 1/d$. One of the main question addressed recently in this respect is whether β can be computed more directly from α. It seems that this is indeed the case for Jacobi matrices [17, 18], namely 1D chains with nearest-neighbour interactions. One important result of this paper is precisely to show the opposite in the extreme case for which $d = \infty$, namely that there is no relation whatsoever between the α's and the β's. This gives a negative answer to the question raised by Lebowitz (see [23]). This is due to the fact that the spectral exponents characterize only the spectral measure (the LDOS) of the Hamiltonian H, independently of any other type of observable. On the other hand, the diffusion exponents involves the interplay between the Hamiltonian (through the quantum evolution) and the *position operator* $\boldsymbol{X}$, or even better, the *current* (or *velocity*) operator $\boldsymbol{J} = \mathrm{i}[H, \boldsymbol{X}]/\hbar$. The link between the diffusion exponent β and the pair $(H, \boldsymbol{J})$ is still not precisely established, even though it has been related to the *current-current correlation function* [24, 21]. However, Jacobi matrices are very special since the position operator is defined by mean of the orthogonal polynomials associated with the spectral measure (the LDOS), so that β is defined through purely spectral properties.

In this paper, we consider a family of anisotropic tight-binding models in an infinite-dimensional hypercubic structure and show that, depending upon the explicit form of the hopping parameters, it is possible to shift from an absolutely continuous spectrum to a singular continuous spectrum. Moreover, we are able to adjust the fractal dimension of this spectrum, fine-tuning a single parameter that drives the transition. In addition, we show that depending on the hopping term law, one can face an absolutely continuous spectrum and a somewhat anomalous diffusion for which the mean square deplacement $L(t)$ can either scale as $\log t$ or as t^α with $0 < \alpha < 1$. We first introduce some mathematical tools that are useful for a careful analysis of the structure we are dealing with. We then characterize the energy spectrum for different types of tight-binding Hamiltonians and discuss the nature of their spectral measures. Finally, we compute the autocorrelation function and the mean square displacement of a wave packet for the different models.

† However, $\beta(E) = 0$ does not necessarily implies that $L_E(t)/t$ converges to a positive constant as $t \to \infty$. Because $\beta(E)$ is the infimum of the γ's such that $\int_1^\infty \mathrm{d}t\, L(t)/t^{1+\gamma} < \infty$ (see equation (16)). A counter-example can be found in [23].

A d-dimensional hypercube Δ_d is the set of vertices of a cube of size 1 in a d-dimensional space. The infinite-dimensional hypercube Δ is defined by: $\Delta = \bigcup_{d>1} \Delta_d$. It can therefore be seen as the set of sequences $\varepsilon = (\varepsilon_k)_{k=0}^{\infty}$ where $\varepsilon_k \in \{0, 1\}$ and $\varepsilon_k = 0$ for all but a finite number of k's. We endow the set $\{0, 1\}$ with the group structure given by the addition modulo 2, so that Δ becomes a discrete countable group for the coordinatewise addition. It is also convenient to introduce its dual group $\mathcal{B}$ ($\mathcal{B}$ stands for Brillouin), which is the counterpart of the quasimomentum space in a perfect crystal. $\mathcal{B}$ can be described as the set of all sequences $\sigma = (\sigma_k)_{k=0}^{\infty}$ with $\sigma_k = \pm 1$. $\mathcal{B}$ is a compact abelian group with the pointwise multiplication and the product topology. The duality between Δ and $\mathcal{B}$ is given by the characters

$$\forall \sigma \in \mathcal{B} \quad \forall \varepsilon \in \Delta \qquad \chi_\sigma(\varepsilon) = \prod_{k=0}^{\infty} \sigma_k^{\varepsilon_k}. \tag{2}$$

In this formula, the product is finite by construction. Moreover, $\chi_\sigma(\varepsilon + \varepsilon') = \chi_\sigma(\varepsilon)\chi_\sigma(\varepsilon')$ and $\chi_{\sigma+\sigma'}(\varepsilon) = \chi_\sigma(\varepsilon)\chi_{\sigma'}(\varepsilon)$. These characters play the role of the Bloch phase $\exp(\mathrm{i}ka)$ in a crystal, where a is the period of the translation group, and k is a quasimomentum. While on Δ the Haar measure is the counting one, the integral of a continuous function f on $\mathcal{B}$ is defined as

$$\int_{\mathcal{B}} \mathrm{d}\sigma\, f(\sigma) = \lim_{K\to\infty} \frac{1}{2^K} \sum_{\sigma_0=\pm1,\ldots,\sigma_K=\pm1} f(\sigma). \tag{3}$$

The Hilbert space of physical states is $\mathcal{H} = \ell^2(\Delta)$, namely the set of sequences $\psi(\varepsilon)$ indexed by Δ (the wavefunctions), such that

$$\|\psi\|^2 = \sum_{\varepsilon\in\Delta} |\psi(\varepsilon)|^2 < +\infty. \tag{4}$$

A canonical orthonormal basis is provided by the states $|\varepsilon\rangle$ vanishing everywhere but on the 'site' ε. The Fourier transform of the wavefunction $\psi \in \mathcal{H}$ is the function on $\mathcal{B}$ formally defined by

$$\mathcal{F}\psi(\sigma) = \sum_{\varepsilon\in\Delta} \chi_\sigma(\varepsilon)\psi(\varepsilon). \tag{5}$$

This function actually belongs to $L^2(\mathcal{B})$, namely it is square integrable on $\mathcal{B}$ (with respect to the Haar measure) and the Parseval identity holds true namely $\|\psi\|^2 = \|\mathcal{F}\psi\|^2 = \int_{\mathcal{B}} \mathrm{d}\sigma\, |\mathcal{F}\psi(\sigma)|^2$. Therefore we get two unitarily equivalent representations of the Hilbert space of states.

The translation operators $T(a)$, $(a \in \Delta)$ are acting on $\mathcal{H}$ as follows:

$$T(a)\psi(\varepsilon) = \psi(\varepsilon - a). \tag{6}$$

Equivalently, $T(a)|\varepsilon\rangle = |\varepsilon - a\rangle$. Note that $a = -a$ in Δ due to the addition modulo 2, so that $T(a)^2 = 1, \forall a \in \Delta$. In addition $T(a) = T(a)^\dagger$ as can be easily checked, so that there is an infinite set of mutually commuting unitary and self-adjoint operators. The spectrum of such operators is made of two eigenvalues (with infinite multiplicities) namely ± 1. Through a Fourier transform, $T(a)$ becomes the operator of multiplication by $\chi_\sigma(a)$. Particularly, if $a = e_k$, where e_k is the sequence in Δ with all coordinates vanishing except the kth one, $T_k = T(e_k)$ becomes simply the operator of multiplication by σ_k.

We consider the following class of tight-binding Hamiltonians on $\mathcal{H}$:

$$H = \sum_{k=0}^{\infty} t_k T_k. \tag{7}$$

In order that H be self-adjoint we need $t_k \in \mathbb{R}$. By a simple unitary tranformation, one can choose $t_k \geqslant 0$. The coefficient t_k denote the 'transfer' or 'hopping' term in the kth direction.

H is bounded if and only if $\sum t_k < +\infty$. It is self-adjoint (but not necessarily bounded) if $\sum t_k^2 < +\infty$. In what follows, we will assume that this latter condition holds. By Fourier tranform, H becomes the operator of multiplication by $E(\sigma)$ where E is called the *band function* and is given by

$$E(\sigma) = \sum_{k=0}^{\infty} \sigma_k t_k. \tag{8}$$

This function is real and square integrable on $\mathcal{B}$ with $\mathcal{L}^2$ norm:

$$\int_{\mathcal{B}} \mathrm{d}\sigma \, E(\sigma)^2 = \sum_{k=0}^{\infty} t_k^2. \tag{9}$$

The spectrum of H (its spectral measure), is then given by the image of $\mathcal{B}$ in $\mathbb{R}$ (of the measure $\mathrm{d}\sigma$) under the function E. Note that if H is bounded, E is continuous with $\|H\| = \sup_{\sigma\in\mathcal{B}} |E(\sigma)| = \sum_{k=0}^{\infty} t_k$.

The spectral properties can be studied through the autocorrelation function

$$P(s) = |\langle 0|\mathrm{e}^{\mathrm{i}sH}|0\rangle|^2 = \left(\int_{\mathbb{R}} \mathrm{d}\mu(E)\, \mathrm{e}^{\mathrm{i}sE}\right)^2 \tag{10}$$

where $|0\rangle$ denotes an origin site where we initially localize a wave packet and μ the corresponding spectral measure. Note that the translation invariance of H allows us to choose any site of Δ as initial condition. If P is integrable over $\mathbb{R}$, then μ is absolutely continuous (the converse may not be true). Alternatively, one can use the temporal correlation function:

$$C(t) = \frac{1}{t}\int_0^t \mathrm{d}s\, P(s) \tag{11}$$

that is the time-averaged version of P. The spectral measure is purely continuous (singular or absolutely continuous) if and only if $C(t) \to 0$ as $t \to \infty$ (the Wiener criterion).

An elementary computation using (3) leads to

$$P(s) = \prod_{k=0}^{\infty} \cos^2(st_k). \tag{12}$$

This infinite product converges since $\sum t_k^2 < +\infty$.

We define the position operator as follows. For $k \in \mathbb{N}$, X_k denotes the operator of multiplication by ε_k in $\mathcal{H}$. It commutes with T_l for $l \neq k$ whereas $T_k X_k T_k^{-1} = \mathbf{1} - X_k$, and since $T_k^2 = \mathbf{1}$ it follows that:

$$\mathrm{e}^{\mathrm{i}sT_k} = \cos s + \mathrm{i}T_k \sin s. \tag{13}$$

Let us define the mean square displacement by

$$L_E^2(s) = \sum_{k=0}^{\infty} \langle\varphi|\,(X_k(s) - X_k(0))^2\,|\varphi\rangle \tag{14}$$

where $X_k(s) = \exp{(\mathrm{i}sH)} X_k \exp{(-\mathrm{i}sH)}$ denotes the Heisenberg representation of X_k and $|\varphi\rangle$ is an initial state with energy close to E. This expression does not depend upon the explicit choice of φ as it turns out. Using the previous relations, for any E one gets

$$L_E^2(s) = L^2(s) = \sum_{k=0}^{\infty} \sin^2(st_k). \tag{15}$$

The diffusion exponent β is given by $L(s) \sim s^{\beta}$ as $s \to \infty$. It does not depend on E. A rigourous way to define a power-law asymptotic behaviour is given as follows (see [21, 25] for more details): a function f of a real variable s behaves as s^{β} when $s \to \infty$ if

$$\int_c^{\infty} \frac{\mathrm{d}s}{s^{1+b}} f(s) \qquad c > 0 \tag{16}$$

converges for $b > \beta$ and diverges for $b < \beta$. In addition, if the function f can be written as a series:

$$f(s) = \sum_{k=0}^{\infty} F(st_k) \tag{17}$$

where F is a positive bounded real function, such that $F(x) = \mathrm{O}(x^2)$ for $x \sim 0$, and $(t_k)_{k\in\mathbb{N}}$ is a set of positive number such that $\sum_{k=0}^{\infty} t_k^2 < \infty$, then the exponent β is given by

$$\beta = \inf\left\{ b \in \mathbb{R}_+; \sum_{k=0}^{\infty} t_k^b < \infty \right\}. \tag{18}$$

It is clear that this definition is particularly convenient for our purpose since L^2 is exactly of the form (17). The closed forms obtained for the three observables previously discussed (energy, autocorrelation function, mean square displacement), allows us to study the spectrum and the quantum diffusion for various classes of hopping terms.

The first interesting class of models consists of choosing an algebraic scaling of the hopping parameters $t_k \sim k^{-\gamma}$, namely $\lim_{k\to\infty} k^{\gamma} t_k = t$, with $\gamma > \frac{1}{2}$. In this case, the spectrum is bounded if $\gamma > 1$ whereas it is unbounded if $\gamma \leqslant 1$. Moreover, one can prove (see the appendix) that

$$P(s) \leqslant c_1 \mathrm{e}^{-c_2 s^{1/\gamma}} \tag{19}$$

where c_1, c_2 are two positive constants. This shows that the spectral measure is always absolutely continuous and also infinitely differentiable. This also implies that the correlation function decays as $1/t$. In addition, according to expression (18), it is obvious that

$$L^2(s) \sim s^{1/\gamma}. \tag{20}$$

Hence, the diffusion exponent is $\beta = 1/2\gamma$ which can take any value in $]0, 1[$ even though the spectrum is always absolutely continuous.

Another interesting case is $t_k = (q-1)/q^{(k+1)}$ (geometrical scaling) with $q > 1$, for which $\|H\| = 1$.

(i) For $1 < q \leqslant 2$, the spectrum is nothing but the $q-$adic decomposition of real numbers in the interval $[-1, +1]$. It is therefore gapless and absolutely continuous.

(ii) For $q > 2$, the image of E is a Cantor set of zero Lebesgue measure, constructed by removing the central interval of width $2(1 - 2/q)$ in the interval $[-1, +1]$ and repeating the operation on each of the intervals left. The spectrum is a monofractal set with a Hausdorff dimension $D_H = \ln 2/\ln q$ [26]. The spectral measure is the Cantor one and gives the same weight to each subinterval. Note that the classical tryadic Cantor set is obtained for $q = 3$.

For such Cantor spectra, it is shown in [1] that the temporal correlation function decays as $C(t) \sim t^{-D_2}$, where D_2 is the correlation dimension of the spectral measure (i.e. of the local density of states). In this example, one has: $D_2 = 1$ for $1 < q \leqslant 2$, since the spectrum is absolutely continuous, and $D_2 = D_H = \log 2/\log q$ for $q > 2$ since the spectrum is then a monofractal set. It is important to consider C because the behaviour of P is much more complex. In particular, P is sensitive to the nature of q. Indeed, it is shown in [27] that

$$\lim_{s\to\infty} P(s) = 0 \quad \Leftrightarrow \quad q \notin S \setminus \{2\} \tag{21}$$

where S denotes the set of algebraic integer numbers defined by Pisot and Vijayaraghavan [28, 29].

Note that the functional relation

$$\forall q \in \mathbb{R} \qquad P(qs) = \cos^2(s(q-1))P(s) \tag{22}$$

allows us to exactly determine P for $q = 2$ since

$$P(2s) = \cos^2(s)P(s) \quad \Leftrightarrow \quad P(s) = \sin^2(s)/s^2. \tag{23}$$

According to the identity (18) one obtains a diffusion exponent $\beta = 0$ for any $q > 1$, whereas the spectrum can be either absolutely continous or singular continuous. In addition, one can show that $L^2(s) \sim \ln(s)$, with a criterion similar to the one given in (16).

In conclusion, these toy models defined on infinite-dimensional hypercubes allows us to carefully analyze the possible relationships between the spectral measure and the diffusion exponents. The first class of Hamiltonians (algebraic scaling of the hopping terms), shows that it is possible to face an absolutely continuous spectrum and an anomalous diffusion with a β exponent that can take any value between 0 and 1. On the other hand, the second case (geometrical scaling of the hopping parameters), displays a zero β exponent whereas the spectrum can be either absolutely or singular continuous. Finally, we emphasize upon the importance of these exponents in transport properties, especially in quasicrystals, where they should be responsible for the anomalous behaviour of their conductivity.

Appendix. Proof of equation (19)

Let us consider $K > 0$ large enough so that $t/2k^\gamma \leqslant t_k \leqslant 2t/k^\gamma$ for $k \geqslant K$. Then choose $s_0 > 0$ large enough so that $s_0 t/K^\gamma \leqslant \pi/2 \leqslant s_0 t/(K-1)^\gamma$. For $s \geqslant s_0$ let $K_1 \geqslant K$ be such that $st/2K_1^\gamma < \pi/2 \leqslant st/2(K_1-1)^\gamma$. Then

$$\ln P(s) \leqslant \sum_{k=K_1}^{\infty} \ln\cos^2 st/2k^\gamma$$

If one sets $x_k = k\,(2/st)^{1/\gamma}$, the right-hand side is dominated by an integral of the form

$$\ln P(s) \leqslant (ts/2)^{1/\gamma} \int_{(2/\pi)^{1/\gamma}+\mathrm{O}(s^{1/\gamma})}^{\infty} \mathrm{d}x\ \ln\cos^2(1/x^\gamma)$$

for $s > s_0$, leading to equation (19).

References

[1] Ketzmerick R, Petschel G and Geisel T 1992 *Phys. Rev. Lett.* **69** 695
[2] Guarneri I 1993 *Europhys. Lett.* **21** 729
[3] Ketzmerick R *et al* 1997 *Phys. Rev. Lett.* **79** 1959
[4] Zhong J X and Mosseri R 1995 *J. Phys.: Condens. Matter* **7** 8383
[5] Sütö A 1989 *J. Stat. Phys.* **56** 525
[6] Bellissard J, Iochum B, Scoppola E and Testard D 1989 *Commun. Math. Phys.* **125** 527
[7] Bellissard J 1989 *Number Theory and Physics (Les Houches Mars 89, Springer Proc. in Physics, vol 47)* ed J M Luck, P Moussa and M Waldschmidt (Berlin: Springer) p 140
[8] Bellissard J, Bovier A and Ghez J M 1991 *Commun. Math. Phys.* **135** 379
[9] Bovier A and Ghez J M 1995 *J. Phys. A: Math. Gen.* **28** 2213
[10] Hof A, Knill O and Simon B 1995 *Commun. Math. Phys.* **174** 149
[11] Hofstadter D R 1976 *Phys. Rev.* B **14** 2239
[12] Last Y 1994 *Commun. Math. Phys.* **164** 421
[13] Hiramoto H and Kohmoto M 1989 *Phys. Rev.* B **40** 8225

[14] Sire C 1989 *Europhys. Lett.* **10** 483
[15] Benza V G and Sire C 1991 *Phys. Rev.* B **44** 10343
[16] Passaro B, Sire C, and Benza V G 1992 *Phys. Rev.* B **46** 13751
[17] Guarneri I and Schulz-Baldes H 1998 *Preprint* mp_arc 98-382
Guarneri I and Schulz-Baldes H 1998 *Preprint* mp_arc 98-457
[18] Schulz-Baldes H and Barbaroux J M 1998 Anomalous quantum transport in presence of self-similar spectra *Ann. Institut Henri Poincaré* submitted
[19] Bellissard J, Bessis D and Moussa P 1982 *Phys. Rev. Lett.* **49** 701
[20] Barnsley M, Geronimo J and Harrington A N 1985 *Commun. Math. Phys.* **99** 303
[21] Schulz-Baldes H and Bellissard J 1998 *Rev. Math. Phys.* **10** 1
[22] Roche S and Fujiwara T 1998 *Phys. Rev.* B **58** 11338
[23] Simon B 1990 *Commun. Math. Phys.* **134** 209
[24] Khorunzhy A and Pastur L 1993 *Commun. Math. Phys.* **153** 605
Wegner F 1979 *Phys. Rev.* B **19** 783
[25] Zhong J X, Bellissard J and Mosseri R 1995 *J. Phys: Condens. Matter* **7** 3507
[26] Kahane J P and Salem R 1963 *Ensembles parfaits et séries trigonométriques* (Paris: Hermann) p 72
[27] Salem R 1943 Set of uniqueness and sets of multiplicity *Trans. Am. Math. Soc.* **54**
Salem R 1944 *Trans. Am. Math. Soc.* **56**
Salem R 1948 *Trans. Am. Math. Soc.* **63**
[28] Pisot C 1938 La répartition modulo 1 et les nombres algébriques *Annali di Pisa* **7**
[29] Pisot C 1955 Sur une famille remarquable d'entiers algébriques formant un ensemble fermé *Colloque sur la théorie des nombres, Bruxelles*