EUROPHYSICS LETTERS 15 September 1992

Europhys. Lett., 20 (2), pp. 95-100 (1992)

Quantum Evolution in a Dynamical Quasi-Crystal.

D. SHEPELYANSKY(*) and C. SIRE

Laboratoire de Physique Quantique, Université Paul Sabatier
31062 Toulouse Cedex, France

(received 18 March 1992; accepted in final form 24 July 1992)

PACS. 05.45 – Theory and models of chaotic systems.
PACS. 61.50E – Crystal symmetry; models and space groups, and crystalline systems and classes.
PACS. 71.55J – Localization in disordered structures.

Abstract. – We investigate a quantum model of dynamical 2D five-fold quasi-crystal, the classical counterpart of which can be integrable or chaotic. This system can also describe the motion of an electron in a quasi-periodic potential with a magnetic field perpendicular to the plane. In the classically integrable bounded regime, we observe quantum diffusion for big values of $\hbar$. In the chaotic regime, a transition from quantum suppression to diffusion is obtained for fixed small $\hbar$ as the perturbation is increased. The analogy with diffusion properties in 2D quasi-crystals is discussed.

Introduction. – Since the discovery of quasi-crystals some attention has been paid to the investigation of quasi-periodic tight-binding models. The 1D case is the most studied [1] and displays nonusual fractal spectra. The wave functions are neither localized nor extended. This leads to anomalous diffusion properties for the time evolution of a wave packet [2]. In higher dimension, the most investigated models are tight-binding Hamiltonians on the Penrose tilings (2D and 3D) [3] and the octagonal tiling [4, 5]. The main difference with the 1D case is that the electronic spectrum is not necessarily a Cantor set, which has some consequences on the physical properties [4]. For instance, it was shown in ref. [4] that for reasonable Hamiltonian parameters the spectrum displays some level repulsion, instead of level clustering. This could be a mark of quantum chaos in such systems. However, the models studied have no simple classical dynamical analogue which permits to understand this phenomenon.

For crystals in a magnetic field, such dynamical systems are known as, for instance, the Harper [6] and kicked Harper [7] models. In the first case, the classical motion is integrable but the existence of an infinite separatrix net leads to normal quantum diffusion. For the kicked model, the classical motion can be completely chaotic, leading to more interesting diffusion properties, namely anomalous diffusion with an exponent depending on the various parameters [7].

(*) On leave from Budker Institute of Nuclear Physics, Novosibirsk.

In the present letter, we investigate a quantum dynamical model of two-dimensional quasi-crystal with a clear classical counterpart.

Dynamical model. – We first present the classical model since its relation to the Penrose lattice will be clearer. So consider the following Hamiltonian first introduced and investigated in [8]

$$\mathcal{H}(p, x) = \frac{1}{2}p^2 + \frac{1}{2}x^2 + K\cos x\,\delta_T(t), \tag{1}$$

where $\delta_T(t)$ is a periodic Dirac peak of period $T = 2\pi/Q$, with Q being an integer. We shall see that $Q = 4$ corresponds to the kicked Harper model, whereas the case under study in this letter is $Q = 5$. Indeed, between two kicks the motion in the phase space is a rotation of the vector $\boldsymbol{v} = (p, x)$ by an angle T. For integer Q, the free evolution of $\boldsymbol{v}$ goes back to the initial position. Therefore, in the rotating frame the Hamiltonian can be written

$$\begin{cases} \mathcal{H}_{\mathrm{RF}}(p, x) = K \sum\limits_{i=0}^{Q-1} \cos(\boldsymbol{e}_i \cdot \boldsymbol{v})\, \delta_T^{(i)}(t), \\ \boldsymbol{v} = (p, x), \qquad \boldsymbol{e}_i = (\alpha_i = \cos(2\pi i/Q),\ \beta_i = \sin(2\pi i/Q)), \end{cases} \tag{2}$$

where the $\delta_T^{(i)}$ kicks are ordered in time. After Q kicks, the phase space and the dynamics of both Hamiltonians are the same. In the case of small K, δ-functions can be eliminated after averaging and the effective Hamiltonian is

$$\mathcal{H}_{\mathrm{eff}}(p, x) = K \sum_{i=0}^{Q-1} \cos(\boldsymbol{e}_i \cdot \boldsymbol{v}). \tag{3}$$

In fig. 1*a*), we show the constant-energy section $\mathcal{H}_{\mathrm{eff}}(p, x) = K$ for $Q = 5$. The structure strongly recalls a Penrose lattice. Note that, contrary to the Harper case ($Q = 4$) and to any other crystallographic symmetry ($Q = 2, 3, 6$), there is no infinite separatrix (see also [8]).

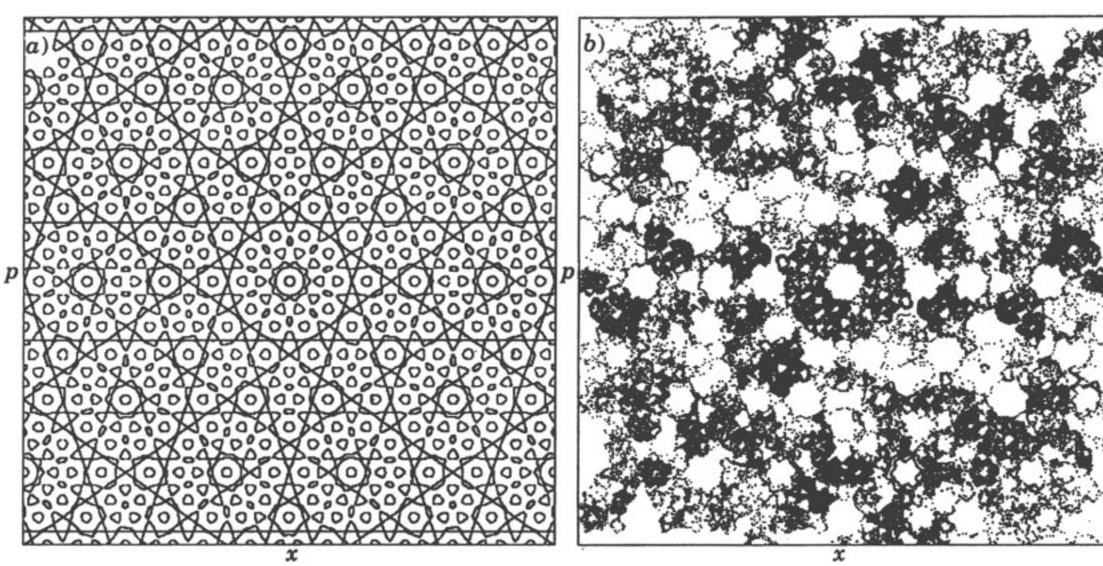

Fig. 1. – *a*) Constant energy surface $\mathcal{H}_{\mathrm{eff}}(p, x) = K$ for $(x, p) \in [-120, 120]^2$. A careful analysis shows the absence of infinite separatrices; *b*) same phase plane region of map (4) for $K = 1.25$ in the chaotic regime.

For Hamiltonian (2), one can write a map relating $\bar{v}$ after a kick to v before it:

$$\bar{p} = p + K\beta_i \sin(\alpha_i p + \beta_i x), \qquad \bar{x} = x - K\alpha_i \sin(\alpha_i p + \beta_i x). \tag{4}$$

From (2) and (4) it is clear that $Q = 4$ corresponds to the kicked Harper model. In our case ($Q = 5$), the motion is bounded and integrable in the limit $K \to 0$. For K of order 1, there is chaotic diffusion in the phase plane and the width of the wave packet in the phase plane $\sigma = \langle p^2 + x^2 \rangle$ behaves like $\sigma \sim Dt$, where t is measured in number of kicks. For $K \geqslant 4$, D is approximately equal to $K^2/2$ which is the diffusion rate in the random phase approximation. Some examples of chaotic trajectories in the phase plane are shown in fig. 1*b*).

One can quantize the model by setting $[\hat{x}, \hat{p}] = i\hbar$. After that, $\hat{p}$ and $\hat{x}$ can be seen as normal 1D momentum and coordinate. Alternatively, (3) represents the motion of the electron in a 2D quasi-periodic potential (with $\hat{X} = \hat{x}$ and $\hat{Y} = \hat{p}$) in a magnetic field (Peierls substitution). Then, $\hbar$ is related to the field flux and $\hat{x}$ and $\hat{p}$ are the two quasi-momenta of the electron. From Hamiltonian (1), one can see that the classical and quantum dynamics of the systems (1), (2) are time reversible.

Now, the quantum map for the wave function after one kick of kind i ($i = 0, ..., 4$) is given by

$$\begin{cases} \bar{\psi} = \exp[-ik\cos(\alpha_i \hat{p} + \beta_i \hat{x})]\psi, \qquad \text{or in } x \text{ representation}, \\ \bar{\psi}(x) = \displaystyle\sum_{m=-\infty}^{+\infty} (-i)^m J_m(k) \exp[i\hbar m^2 \alpha_i \beta_i /2] \exp[im\beta_i x]\, \psi(x + m\hbar\alpha_i), \end{cases} \tag{5}$$

where $k = K/\hbar$ and the classical limit corresponds to $\hbar \to 0$. J_m is the m-th Bessel function.

Numerical results. – The numerical investigation of this model is much more difficult than in the kicked Harper case, since the dynamics leads to spreading in the whole (p, x)-plane and cannot be reduced to a motion on a cylinder. This seems to be the reason why there were practically no attempts to investigate the quantum dynamics of model (1) except in [9], where only the case $Q = 4$ in the representation (1) was considered, and in [10]. In both cases the authors used the harmonic-oscillator representation which does not allow us to treat a large space volume which determines the number of effective quantum states. Here, we used the Hamiltonian in the rotation frame (2), which allows us to work in x representation using the simple map (5) and to reach an effective number of oscillator states of about 10^5. Moreover, by approximating α_i by means of the golden-mean approximants, we were able to work on an integer grid for x which is equivalent to periodic boundary conditions for p (the number of points in the x direction was up to $3 \cdot 10^5$). We took rational approximants with denominator up to 610 for the golden mean which enters in the expression of α_i and β_i. For instance, one has $\alpha_1 = (\tau - 1)/2$, $\alpha_2 = -\tau/2$, and $\beta_1 = \tau \sin(\pi/5)$, $\tau = 1.618\ldots$. This procedure corresponds to the exact numerical treatment of system (2) with rationally twisted e_i's so that the classical phase plane becomes periodic in p with period up to $2\pi \times 610$.

First, we present our results for k small for which the Hamiltonian in approximately the sum of five cosine and the classical motion is essentially bounded. We observed two different situations depending on the value of $\hbar$ which is the only parameter in this regime. For small $\hbar$ we recover the bounded classical behaviour for initial wave packets centred in the stable region as well as near unstable fixed points. More unexpected and interesting was the case of large $\hbar$ for which we observed diffusion in the phase plane (x, p). A typical evolution of the wave packet width σ is shown in fig. 2 for $k = 0.05$ and $\hbar = 10$. We checked that this behaviour really corresponds to the limit of small k by testing several values of k which simply led to rescaling of time (see (3) and (4)). The qualitative interpretation of this result is

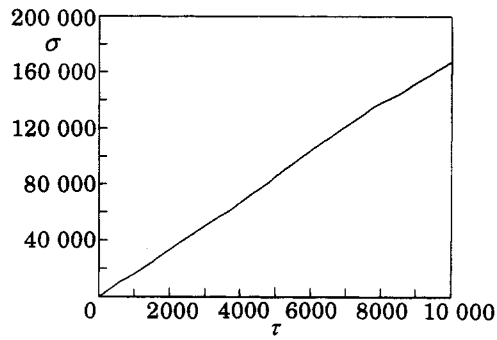

Fig. 2. – Wave packet width in phase space $\sigma = \langle \hat{p}^2 + \hat{x}^2 \rangle$ as a function of the number of time perturbation periods $\tau = 5t$ (the number of kicks is 5 times bigger). For this simulation $k = 0.05$ and $\hbar = 10$. The initial wave packet was a Gaussian centred at $x_0 = 3.1$ and $p_0 = 0$ with width of order 0.5.

the following. For big values of $\hbar$, the Planck cell is comparable to the size of the stability islands for the classical motion. Due to quantum uncertainty, this allows effective transitions between different classically isolated regions. Here, we have an example where quantization leads to diffusion and destroys the classically bounded motion. This is in opposition with the kicked rotator case [11] for which quantization causes the suppression of classical diffusion. Then, increasing k (for example up to $k = 1$ or more for $\hbar = 10$) does not destroy diffusion whatever the nature of the classical regime, integrable or chaotic. Finally, we have verified that in x-space the wave function was roughly Gaussian, confirming a diffusive behaviour.

More complex situations arise when decreasing $\hbar$. Indeed, we have observed quantum suppression even when the classical motion was chaotic. This is illustrated in fig. 3. We cannot conclude about the localization of quasi-energy eigenfunctions, however the quantum suppression is obvious. Some preliminary results giving support to suppression were also obtained in [10]. For bigger values of k and same values of $\hbar$, the diffusive excitation takes

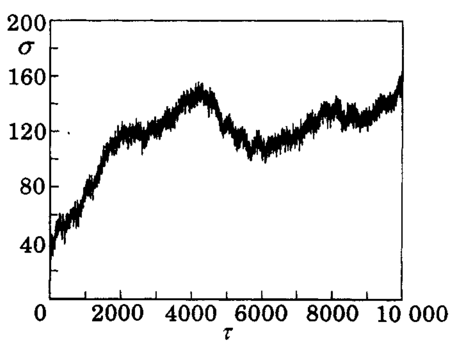

Fig. 3.

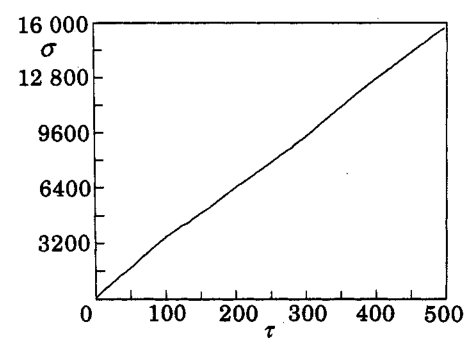

Fig. 4.

Fig. 3. – Same as fig. 2, for $k = 2$ and $\hbar = 1$. The packet was centred at the same position which is in the classically chaotic region. At the end of the evolution ($10^4 \times 5$ kicks) the quantum width is two orders of magnitude less than the classical one.

Fig. 4. – Same as fig. 2, for $k = 5$ and $\hbar = 1$.

place (fig. 4). However, the diffusion rate is less than the classical one which gives support to the quantum nature of this diffusion.

The time reversibility of the system is crucial for Anderson localization in 2D. Due to classical chaos, the phase volume excited after t kicks is $V \sim Dt$ with $D \sim K^2/2$ and the number of quantum states $N \sim V/\hbar$ grows linearly with time. The uncertainty relation between frequency and time [11] leads to the spectrum resolution decreasing like $1/t$. This decay goes in the same way as the average distance between quasi-energies which behaves like $1/N = \hbar/(Dt)$. Since the functional dependence is the same, this case is analogous [12, 13] to a two-dimensional Anderson model in the time reversible case, with a localization length $\ln \xi \sim D/\hbar \sim K^2/2\hbar$ (note that without time reversibility one has Anderson transition from localization to diffusion). However, in our case this estimate does not work, since for large values of $\hbar$ we have observed diffusion (see fig. 2 and 4). This result shows that one cannot consider the present effective potential as random and that the quasi-periodic structure produces important effects. In fact the situation seems to be somehow similar to what is observed for the diffusion in 2D quasi-crystals [4, 14]: for strong quasi-periodic potential (small k and $\hbar$) the spectrum is strongly fractal and diffusion is suppressed, whereas for big coupling between cells (big k and $\hbar$) the diffusion is enhanced. However, in our case we have normal diffusion instead of the anomalous one observed in [14].

Before concluding we would like to mention another approach we also used for the investigation of this system. It is based on the analysis of propagation of pure plane waves in the quantum system (2). In the plane-wave representation, the wave function can be expanded as a superposition of waves of type $\exp[i(n_1\beta_1 + n_2\beta_2)x]$. For an initial wave function of this form, we were interested in the spreading in the (n_1, n_2)-plane. The quantity $p = n_1\beta_1 + n_2\beta_2$ is the momentum and is the relevant physical characteristic. We found that $\langle p^2 \rangle$ was growing diffusively for k bigger than 1 ($\hbar = 1$), whereas for small k we have obtained anomalous diffusion with exponents less than 1. This is also similar to the results of [14]. In the perpendicular nonphysical direction $p_\perp = n_2\beta_1 - n_1\beta_2$ the spreading was going in a ballistic way.

Conclusion. – In this letter we have considered the evolution of a wave packet in a quasi-periodic Hamiltonian system with integrable or chaotic classical dynamics. Quantization can lead to delocalization of classically bounded integrable motion due to big values of Planck cell in comparison to the size of stability islands. On the contrary, for small fixed values of $\hbar$, we go from a regime of quantum suppression to a diffusion spreading as the classical kick amplitude is increased. The obtained results have a certain analogy with similar diffusion properties in 2D quasi-crystals.

Finally, we would like to point out the connection between this model and the question of localization of 2D electrons in a smooth random potential in the presence of a magnetic field. This problem is directly related to the quantum Hall effect. In the limit of strong field, there is no transition between different Landau levels. In that case, it is believed that localization takes place for all values of energy except the centre of the band [15]. The existence of infinite localization length for this energy is due to the occurence of infinite separatrices for the classical system. In our system the limit of strong magnetic field corresponds to $K/\hbar \to 0$, so that there is no transition between oscillator states in (1) associated to Landau levels. Qualitatively, large values of $K/\hbar$ correspond to strong transitions between Landau levels, for which there is no definite prediction. Our result in the case of small $K/\hbar$ (see (3)) shows that there are many energy values with delocalized states, explaining the observed diffusion. This result is different from the random potential picture [15]. The reason for that can be connected to the dynamical nature of the Hamiltonian or to its quasi-crystalline structure.

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We are indebted to J. BELLISSARD, F. BORGONOVI and I. GUARNERI for stimulating discussions and for the communication of the results [10]. We are also grateful to P. LABASTIE for his interest in our work. One of us (DS) would like to thank the LPQT in Toulouse for their kind hospitality.

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