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ENERGY BANDS SPLITTING IN THE KOHMOTO MODEL

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Abstract. Peierls gap is analized in case of a two-dimensional lattice under the influence of a magnetic field, in a tight-binding approximation. By using a non-analytic class of potentials, such as the Kohmoto potential in the Harper model, splitting effect occurs in the energy bands. In the metalinsulator transition point, the charge carriers become separated due to their energy, releasing and expanding the Peierls gap. As a result, the energy bands around the Fermi level become localized in case of the electrons and delocalized coresponding to the holes, since their energy become lowered. These facts are supported by numerical investigations.

Key words: Harper model, quasi-periodic potentials, recursive energy bands.

1. INTRODUCTION

Studies regarding two-dimensional electron systems under the simultaneous influences of a periodic potential and of an external homogeneous magnetic field have received much interest in the last four decades [1–5]. This kind of systems are important in solid state studies, because the nowadays nanoscale technologies are based on the band engineering concept [6, 7] and on the thermodynamic formalism [8]. In order to build heterostructures with a precise distribution of the energy bands, we have to understand the way in which they appear.

The energy bands structure of the carriers in magnetic fields was predicted in 1964 by Azbel, while in 1969 Langbein [9] analyzing the Landau levels, discovered "the butterfly pattern", in fact a new and profound connection between the admissible energy states and the form and size of the latticed pierced by the magnetic field. This phenomenon was analyzed numerically by Hofstadter [10] in 1976. He obtained the self-similar structure of the energy bands, with a shape of a butterfly.

It has been found that electrons moving under the simultaneous influence of a periodic potential and of a magnetic field display a series of mini-bands, separated by corresponding mini-gaps. The energy spectrum due to its unique shape, represent even today a remarkable achievement of the theoretical investigation in physics.

The interpretation given by Hofstadter to the numerical results, highlighted the fact that for a given value of the anisothropy parameter, the system is at a crossroad between the conductive and insulator states. This self-dual point between localized and extended states, have been described by André and Aubry [11] too. In this critical point appears a gap described by Peierls in 1955 [12] known today as the Peierls gap [13, 14]. This represents ever since a cornerstone to any studies connected to transitions between conductive and insulator states [15].

The aim of this paper is to investigate numerically the energy bands distribution of a system in which the Peierls gap create a separation between the charge carriers, leading from conductive to insulator states. For this purpose we intend to analyze the Harper model with the Kohmoto quasi-periodic potential. Similar studies have been done by Hiramoto and Kohmoto [16] by resorting to a generalized Harper model.

The paper is organized as follows: After the Introduction, in Section II we present as a short review of potentials of a two-dimensional lattice. In the following one shows the Harper equation with the Kohmoto quasi-periodic potential. The numerical results are discussed in Section III. In the last Section we present the Conclusions of our research.

2. MODEL DESCRIPTION AND NUMERICAL RESULTS

In order to analyze the Harper equation with the Kohmoto quasi-periodic potential, we have to reiterate the concept of potentials. That's important because we are interested to identify the way in which carriers cross the environment from a point to the other, depending on their conductive properties.

Let us start from a one-dimensional system in a tight-binding approximation, submitted to an external and homogeneous magnetic field [17, 18]. It can be viewed as a conductive media of a free electron gas. By generalizing the above chain into a two-dimensional square lattice, we can describe any particular direction using the Miller indices [*u v w*] [19]. In this way, three kind of periodic potentials arise.

The first kind concerns the periodic potentials [20] which corresponds to the directions [0 1 0] parallel to the *x*-axis, [1 0 0] parallel to the *y*-axis and [1 1 0] for the first and second bisectrices. These directions work in conjurrection with the *NN* (nearest neighbor) and the *NNN* (next nearest neighbor) hoppings. The periodic potentials are described in terms of the Bloch functions. They have a rational

number as slope, but not localized states. The second kind concerns the super-periodic potentials [21], which occur to large u of the corresponding Miller indices [u 1 0]. These potentials have a large integer as slope and lead to localized states.

The third one, the quasi-periodic potentials [22, 23] have a regular but never exactly repeating pattern with an irrational number as slope. In this later case, the translation invariance is lost. One deal instead with local rotational symmetries. It is a kind of long range order potentials, with similarities between tiny bits appearing in different places but slightly modified, from one to the other. The quasi-periodic potentials can be found for instance, between [u_1 1 0] and [u_2 1 0] directions.

At the beginning these kind of potentials where only strange entities without any applicability. Howewer, between 1962 and 1984 they became the major description tool of a sort of quasi-crystals [24]. One of the most intriguing properties of these solid state compounds are connected with their behavior at low temperatures. It is known that any conductive medium responds positively to the influence of low temperatures [25] by increasing its conductivity and giving birth to the superconductor state. The quasi-periodic crystals behave vice-versa, by transforming from a conductor state into an insulator one. Such a crystal is provided by synthetic organic materials like *TTF – TCNQ* (Tetra Thia Fulvalene - Tetra CyaNoQuinodimethane) [26], which have been discovered between 1962 and 1973.

Besides the organic compounds, there are other kind of crystals which exhibit a forbidden five-fold symmetry, such as the Al-Pd-Mn icosahedral quasicrystals [27], discovered in 1984. This alloy, formed with 3 metals, each of them with good conductivity, is in fact almost an insulator.

An experimental attempt to understand the way in which electrons flow through a quasi-periodic crystal have been done by Torres et al. [28] in 2003, resorting to a pulse propagation with a shallow fluid covering a quasiperiodically drilled bottom. In order to implement the quasi-periodicity, we have to resort to the Harper equation [29], given by

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

where ψ_n is the wave functions at site n. Here V_n is a periodic function with the role of potential

$$V_n = 2\Delta \cos 2\pi\left(n\beta + \frac{k_2 a}{2\pi} \right), \tag{2}$$

Δ being the anisothropy parameter and E the allowed energies.

In other words we deal with a two-dimensional system under the influence of an external and perpendicular magnetic field. The quotient $\beta = P/Q = \phi/\phi_0$ is the commensurability parameter expressing the number of flux quanta per unit cell, P and Q are two mutual prime integers and $k_2 a$ stands for the Brillouin phase.

Rational values of the commensurability parameter, result in a finite number of energy bands. When it become an irrational number, the energy bands becomes infinite, the spectrum depending completely on the potential strength played by the anisothropy parameter.

So, for $\Delta > 1$ we have localized solutions, for $\Delta < 1$ we have extended wave functions of a contiguous spectrum and for $\Delta = 1$ we have a singular continuous spectrum.

The Harper equation which originates from the minimal substitution on the energy dispersion law, can be rewritten in terms of transfer matrices [30] as

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}, \tag{3}$$

where the transfer matrix [31] is given by

$$T_n = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}, \tag{4}$$

while the potential is periodic $V_n(x) = V_n(x + 1)$.

3. NUMERICAL STUDIES

In order to investigate the energy bands when the system passes from a conductive state to an insulator one, we chose a particular class of non-analytic potentials, namely the Kohmoto potential [32], proposed independently by Ostlund [33], because it preserves discontinuities and takes only two values

$$V_n \equiv \alpha = \begin{cases} V_A = 1 & \text{for} \quad -\gamma < x \le -\gamma^3 \\ V_B = -1 & \text{for} \quad -\gamma^3 < x \le \gamma^2 \end{cases}, \tag{5}$$

where $\lambda = \left(\sqrt{5} - 1\right)/2$ represents the golden mean ratio. The Kohmoto model was introduced at the beginning as a simple toy model [34, 35], with the purpose to explain the metal-insulator transition. By considering only two kind of possible values of V_n, the Fibonacci sequence can readily established. Accordingly, the potential becomes [36]

$$V_n = V_B + V_A \left(\lfloor (n+1)\beta \rfloor - \lfloor n\beta \rfloor \right), \tag{6}$$

where $\lfloor n\beta \rfloor$ represents the greatest integer lower than $n\beta$. Following the Naumis and Rodrigues work and using the identity $n\beta = \lfloor n\beta \rfloor + \{n\beta\}$ the potential can be rewritten as

$$V_n = V_A\beta + V_B(1-\beta) + (V_A - V_B)\left(\{n\beta\} - \{(n+1)\beta\}\right), \tag{7}$$

where $\{n\beta\}$ denotes the decimal part.

In our numerical calculation the quantity $(V_A - V_B)$ in (7) known as the strength of the quasi-periodicity is taken as $(V_A - V_B) = -1$. The next step is to introduce this potential into the Harper equation, such as

$$T_n = \begin{pmatrix} E - \alpha\beta - \alpha(1-\beta) + \left(\{n\beta\} - \{(n+1)\beta\}\right) & -1 \\ 1 & 0 \end{pmatrix} \tag{8}$$

because the last one has many convenient symmetries, which can facilitate the numerical analysis. In this way the metal-insulator transition can be studied on the two-dimensional lattice, as a splitting effect of the energy bands, corresponding to the electrons and holes concerning energy bands. The numerical results are presented in Fig.1 for several values of n as follows:

a) The energy bands are continuous. The conductive medium exhibits mixed states of both electrons and holes if $n = 1$.

b) One deals with splittings in the energy spectrum, supporting the cosine shape of the dispersion law of the energy if $n = 1.1$.

c) The energy gap tends to increase releasing the Peierls gap if $n = 1.2$.

d) More and more splittings occur in the inner bands distribution releasing incrementally the Peierls gap. The system is still a conductive medium if $n = 1.5$.

e) One deals with the Aubry duality point, which corresponds to the transition state from conduction to the insulator one. The Fermi level is located at the middle of the Peierls gap if $n = 2$.

f) Beyond the critical point the energy gaps tend to increase. By now the system become more and more an insulator for $n = 3$.

g) The lower energy bands tend to decrease in an accentuated chaotic manner, while the top bands tend to gather together around the zero value if $n = 4$.

h) The separations between the energy bands become more pronounced, while the lower energy bands become a cloudy like configuration of points and short range lines if $n = 7$.

i) Separations between energy bands are clear. Since an environment can't be a conductive medium with only one carriers, determine the insulator states. In this case state, the Peierls gap become to large between the energy of the negative carriers and the positive ones, to allow a combination. The conductive environment remain only with one kind of cherge carriers, which leads to the suppression of current flow if $n = 100$.

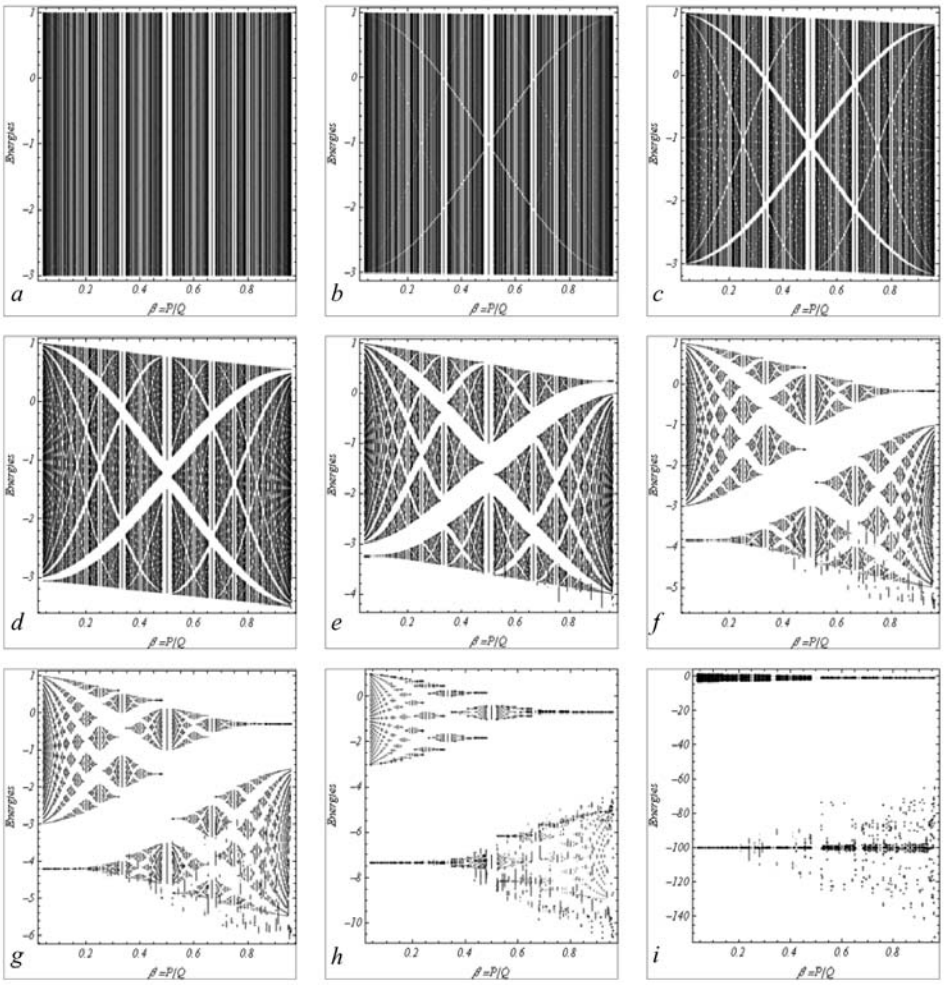

Fig. 1 – The energy spectrum *versus* β showing the band splittings for several n-values.

By virtue of this transition the system exhibits less symmetric states, but with a lower-energy configuration. The energy bands splits, due to the periodic potential, which induce a small gap by releasing and expanding the Peierls distortion. The band splittings take place in such a way that the Fermi energy is always placed in the middle of the gap. The higher energy bands corresponding to the electrons get gathered araund the zero energy, while the negative ones corresponding to the holes lower their energy. This interpretation of the energy band splittings is an atempt to investigate numerically the way in which systems undergo transitions from conductive to insulator states.

4. CONCLUSIONS

In this paper we analyzed numerically the way in which the energy bands get splitting, when the system goes from conductive to the insulator state, i.e. to a less symmetric but lower-energy configuration, passing through the transition point. The energy bands become divided by increasing small gaps in such a way that the Fermi energy will be placed always in the middle of the gap. As result of n continuous variation, the system passes from a symmetric state to symmetry broken ones. The higher energy bands become locked, while the lower energy bands tend to become unlocked.

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REFERENCES

1. M. Y. Azbel, Zh. Eksp. Teor. Fiz., **46**, 939 (1964).
2. G. H. Wannier, Phys. Rev., **117** 432 (1960); Rev. Mod. Phys., **34**, 645 (1962).
3. M. Wilkinson, Proc. Roy. Soc. London, A**403**, 153 (1986).
4. P.G. Harper, Proc. Roy. Phys. Soc. London, A **68**, 874 (1955).
5. Y. Last and M Wilkinson, J. Phys. A: Math. Gen, **25**, 6123 (1992).
6. John H. Davies, *The physics of low-dimensional semiconductors*, Cambridge University Press, 1998.
7. N. W. Ashcroft, N.D. Mermin, Solid State Physics, Saunders College, Phyladelphia, 1976.
8. S. Datta, A. Sharma and R. Ramaswamy, Phys. Rev., E **68**, 036104 (2003).
9. D. Langbein, Phys. Rev., **180**, 633 (1969).
10. D.R. Hofstadter, Phys. Rev., B **14**, 2239 (1976).
11. G. André and S. Aubry, Ann Isr. Phys. Soc., **3**, 133 (1980).
12. R. Peierls, *Quantum theory of solids*, Oxford University Press, Oxford, 1955.
13. Y. Ono and T. Hamano, J. Phys. Soc. Jpn., **69**, 1769 (2000).
14. M. Kohmoto and Y. Hatsugai, Phys. Rev., B **41**, 9527 (1990).
15. M. Kohmoto, Phys. Rev. Lett., **51**, *13*, 1198 (1983).
16. H. Hiramoto and M. Kohmoto, Phys Rev B Condens Matter, **40**, *12*, 8225 (1989).
17. J. F. Weisz, Phys. Rev., B **44**, 6515 (1991).
18. E. Papp and. C. Micu, *Low-Dimensional Nanoscale Systems on Discrete Spaces*, World Scientific, Singapore, 2007.
19. R. J. D. Tilley, *Crystals and crystal structures*, John Wiley, New York, 2006.
20. E. Courtade, O. Houde, Jean-François Clément, P. Verkerk and D. Hennequin, Phys. Rev., A **74**, 031403 (2006).
21. I. Pletikosić, M. Kralj, P. Pervan, R. Brako, J. Coraux, A. T. N'Diaye, C. Busse and T. Michely, Phys. Rev. Lett., **102**, 056808 (2009).
22. F. Borgonovi and D. L. Shepelyansky, Physica D: Nonlinear Phenomena **109**, *1–2*, 24 (1997).
23. J. Bellissard, B. Iochum and D. Testard, Commun. Math. Phys., **141**, 353 (1991).
24. J. M. Luck and D. Petritis, J. of Statist. Phys., **42**, *3–4*, 289 (1986).
25. Hyun-Tak Kim, Kwang-Yong Kang, Bong-Jun Kim, Y. C. Kim, W. Schmidbauer and J. W. Hodby, Physica C: Superconductivity, **341**, 729 (2000).
26. P. W. Anderson, P. A. Lee and M. Saitoh, Solid State Communications, **13**, 595,(1973).
27. D. Shechtman, I. Blech, D. Gratias, J.W. Cahn, Phys. Rev. Lett., **53**, 1951 (1984).

28. M. Torres, J.P. Adrados, J.L. Aragón, P. Cobo and S. Tehuacanero, Phys. Rev. Lett., **90** 114501 (2003).
29. P. G. Harper, Proc. Phys. Soc. London, Sect A **68** 879 (1955).
30. M. Kohmoto, B. Sutherland and C. Tang, Phys. Rev., B **35** 1020 (1987).
31. S. S. Negi and R. Ramaswamy, arXiv:nlin/0104054v1 [nlin.CD] (2001).
32 L.P. Kadano, M. Kohmoto and C. Tang, Phys. Rev. Lett., **50** 1870 (1983).
33. S. Ostlund, R. Pandit, D. Rand, H.J. Schellhuber and E.D. Siggia, Phys. Rev. Lett., **50**, 1873 (1983).
34. Y. Hatsugai and M. Kohmoto, J. Phys. Jpn., **61**, 256 (1992).
35. A. Satou and M. Yamanaka, Phys. Rev., B **63**-21 212403 (2001).
36. G. G. Naumis and F. J. López-Rodriguez, Physica B 1755 (2008).