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A Result Not Dependent on Rationality for Bloch Electrons in a Magnetic Field[2])

By

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There are some facts known about the wave functions of a Bloch electron in a magnetic field. A great deal more is known for a special model. All results are restricted to rational fields and depend heavily on the denominator of the representative fraction. A result is described below which is independent of rationality. It is the statistical weight of identifiable regions in an energy versus field plot. In fact if one goes further and plots instead of the energy the integrated density of state versus field a set of computable polygons results for these regions.

Es existieren einige Kenntnisse über die Wellenfunktionen von Blochelektronen im Magnetfeld. Etwas mehr ist für ein spezielles Modell bekannt. Alle Resultate sind auf rationale Felder beschränkt und hängen sehr stark vom Nenner des eingehenden Bruchs ab. Es wird ein Ergebnis beschrieben, das nicht von der Rationalität des Feldes abhängt: das statistische Gewicht der identifizierbaren Gebiete in einer Darstellung, die die erlaubte Energie als Funktion des Feldes darstellt. Wenn man noch weiter geht und anstatt der Energie die integrierte Zustandsdichte aufträgt, so bekommt man berechenbare Polygone für diese Gebiete.

1. Introduction

For some years now, this writer and collaborators [1 to 6] have been engaged in analyzing the energy spectrum which results when a charged particle is acted upon simultaneously by a periodic potential and a homogeneous magnetic field. We are interested in the high field region where the field contributes more than a minor correction to the Bloch band structure. The papers have been of two kinds: papers dealing with a general periodic potential, and papers discussing a special simple model equation.

This paper belongs to the second class. The model has been discussed very fully be Hofstadter in his thesis [5] and a paper [6] (referred to here as H1 and H2, respectively). The equation is a difference equation; it is, curiously enough, subject to a double interpretation. In the framework of the Peierls-Onsager method [7, 8] it shows, within an assumed Bloch band, the allowed energies as function of the field. In the Regensburg interpretation [1 to 4][4]) it shows, for an assumed periodic potential, the fine structure of a free electron Landau level as a function of the reciprocal field. The first interpretation is easier, but only in the second is the basic function space clearly defined.

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[4]) Section 3 of paper [4] is incorrect because a diagonal matrix element depending on k_z was omitted.

The model has the full complexity of the general problem, but involves only one parameter which will be called Φ. It equals

$$\Phi = \frac{eHa^2}{hc} \quad \text{or} \quad \frac{hc}{eHa^2} \tag{1}$$

depending on the interpretation chosen. a is the spacing of the square mesh periodic potential, and the other letters have their usual meaning. Thus, Φ equals the magnetic flux through a unit cell in natural flux units.

We have now ample numerical results for the model. They are shown in Fig. 1, taken from H1. The figure appears as an infinite strip periodic in the parameter Φ. This is physically surprising because it implies that certain finite magnetic fields are equivalent to either zero or infinite field. This periodicity feature should not be taken too seriously in either interpretation. In the case of the Onsager interpretation it has been shown [9, 10] that the method is correct to all powers of the field only if, in addition, the band structure is allowed to vary parametrically as function of the field. By the time Φ has reached 1 (an impossibly large field by today's laboratory standards) such changes are no doubt very drastic. In the Regensburg interpretation there could be some truth in a periodic repetition of the fine structure with $1/H$ (in addition to a very rapid shrinking of the total width which is normalized away here). But it is not very likely that such a pattern is quantitatively the same as that for strong fields. The method suppresses the inter-level matrix elements which are responsible for the transformation of the free electron Landau levels into the Bloch band Landau levels. This must involve a thorough scrambling of the levels at intermediate fields.

It is therefore more realistic to accept as evidence only the first rectangle in the periodic sequence, the one adjoining $\Phi = 0$. It is shown in detail in Fig. 2. Close inspection of the figure shows that the spectrum is actually worked out only along a discrete set of verticals, that is a small number of values of Φ. This number could no doubt be augmented, but continuity in Φ cannot be achieved in principle because the calculation can only be performed for rational Φ, and the rationality plays an essential role. In fact, if we set

$$\Phi = \frac{p}{q}; \qquad p, q \text{ integer and prime to each other}, \tag{2}$$

then the number of allowed energy bands equals q.

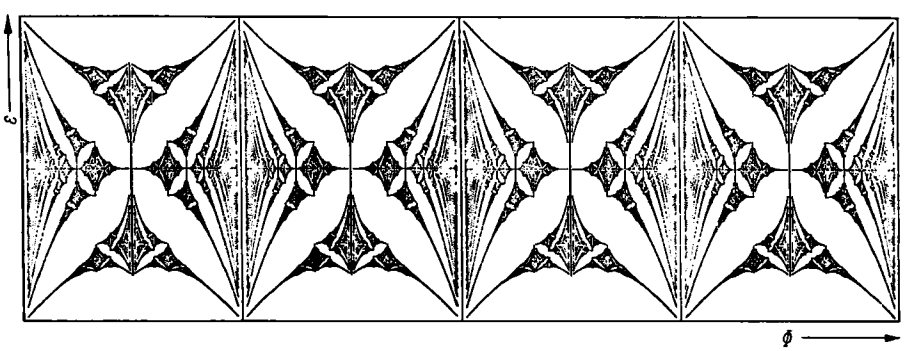

Fig. 1. Allowed energies versus field for the model treated by Hofstadter. The abscissa Φ is subject to a double interpretation which makes it respectively proportional or reciprocal to the magnetic field

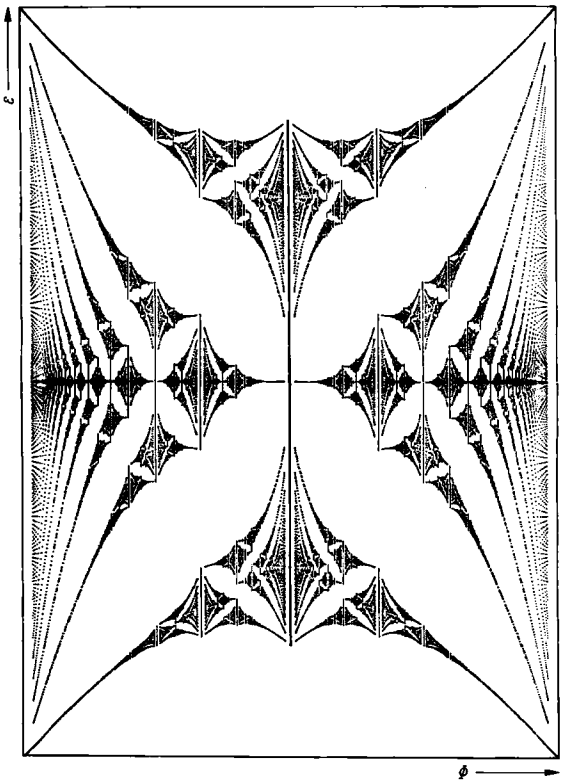

Fig. 2. Enlarged view of the first cell of Fig. 1. The graph is restricted to certain verticals representing "rational" fields. Replicas of the graph seem to be contained within the graph (nesting hypothesis)

Fortunately Hofstadter has pushed his calculations up to $q = 49$ and thus rendered the values of Φ dense enough to permit a perception of structure even in the Φ direction. One can distinguish a lower and an upper arm, ending in the four corners of the rectangle. In the center is a figure almost breaking in two in the middle but firmly anchored on the two long bands at $\Phi = 0$ and $\Phi = 1$; the figure is called C chain in H1 and H2. In the diagonal directions, there are wide gaps of forbidden energies which are only interrupted at $\Phi = \frac{1}{2}$. Further secondary gaps open up for $q > 3$, $q > 4$ etc. One observes that, once formed, these gaps never close for higher q. The distressing aspect of these observations is the preponderant role played by the denominator q. It is the purpose of this paper to bring in new aspects of the model equation in which only Φ, not q, plays a role. This has always been a primary purpose of the Regensburg group.

2. Construction of the Transformed Graph

We shall now achieve a simplified replica of Fig. 2, and perhaps a simplified approach to the entire problem, by injecting a new variable into the problem: the statistical weight in the form of the integrated density of states of certain pieces.

We must here anticipate the result which has opened up the thinking in this direction. It was found by Ray and Obermair and was published elsewhere [11]. The result is that for a given Φ, the integrated density of states for each band has the same value. For the purpose of this paper, we shall take the total integrated density of states as 1. The statistical weight of a band is then $1/q$. This result pertains inspite of a widely different spread of these bands on an energy scale.

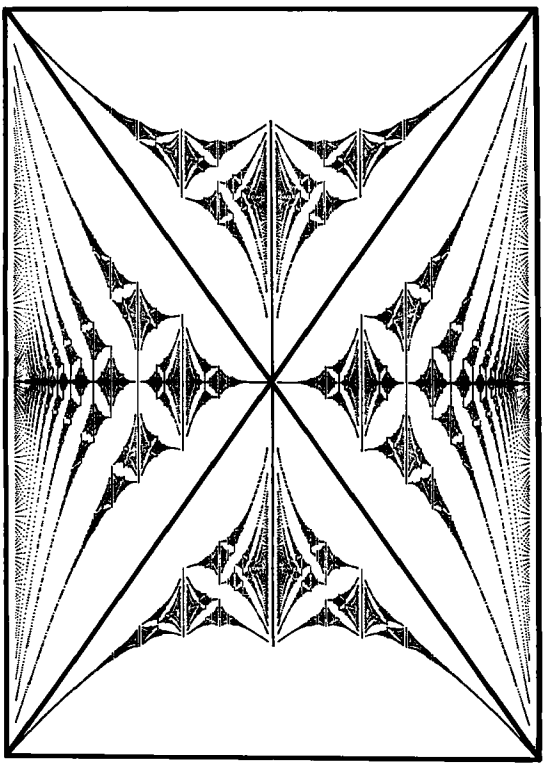

Fig. 3. The diagonals in Fig. 2 divide it into four parts. The statistical weight of each part is a simple linear function of Φ

For further progress we now invoke Hofstadter's nesting hypothesis, still unproven, but highly likely. In H1 and H2 the rectangle of Fig. 2 is called a *cell*. The nesting hypothesis sums up the observation that this cell contains within itself duplicates of itself which form subcells. We are mainly interested here in using the mappings which this observation produces, dividing the figure into subregions. The change in the abscissa scale is quite clear; questions about it are answered in H1 and H2 and will not be taken up here. The change in the ordinate gave the author more difficulties. We shall show in the following that if one discards the energy as a variable and puts in its place the accumulated statistical weight these difficulties disappear, and the change in the ordinate becomes obvious.

Let us start out by considering the outer arms. To get the cells lined up along the arms we must replace Φ by a local mapping variable β defined as follows [5, 6]:

$$\beta = \frac{1}{\Phi} - \left[\frac{1}{\Phi}\right], \quad \text{if} \quad 0 < \Phi \leqq \frac{1}{2} \tag{3a}$$

and

$$\beta = \frac{1}{1-\Phi} - \left[\frac{1}{1-\Phi}\right], \quad \text{if} \quad \frac{1}{2} \leqq \Phi < 1\,. \tag{3b}$$

Here $[x]$ is the integer closest to x and not larger than x. The bracketed quantity is a constant within each subcell, making β vary between 0 and 1. It thus fulfills in the subcell the function which Φ fulfills in the graph as a whole. For a particular Φ of the form (2) in a particular subcell having $[1/\Phi] = N$, (3a) takes the form

$$\beta_N = \frac{q}{p} - N\,.$$

In other words β_N is at that point a rational proper fraction of denominator p. If it is a proper mapping variable this means that at that particular location within the subcell there are p bands. But we have seen previously that each band has statistical weight $1/q$. The total weight of all bands is thus p/q. But p/q equals Φ. The argument can be repeated for any Φ in the left part of one of the arms. The total statistical weight of the energy states is Φ, clearly a continuous function of Φ, independent of its rational decomposition. In fact, the relationship is also defined for irrational Φ; if we expect that properties for irrational Φ can be obtained by proceeding to the limit, if existing, over a series of rational values of Φ, then Φ is the statistical weight along the entire left part of the two arms.

We have thus found a result which is independent of the rationality of the field, the statistical weight of a recognizable piece of substructure in Fig. 2. Similarly the right part of the arms has weight $1 - \Phi$, and the two pieces of the C chain $1 - 2\Phi$ and $2\Phi - 1$, respectively. If we superimpose this cumulated weight W over Fig. 2 we find $W = \Phi$ in the lower left, $W = (1 - 2\Phi) + \Phi = 1 - \Phi$ in the upper left, $W = 1 - \Phi$ in the lower right and $W = (2\Phi - 1) + (1 - \Phi) = \Phi$ in the upper right. In other words the straight lines

$$W = \Phi\,, \tag{4a}$$

$$W = 1 - \Phi \tag{4b}$$

subdivide Fig. 2 into the four subregions separated by the wide gaps. These lines are inserted in Fig. 3 on a background showing Fig. 2. It will now be shown that if the substitution of variables initiated above is continued the graph will be gradually transformed: the gaps of Fig. 2 will disappear and be replaced by straight lines acting as boundary lines of the various regions. A quantitative spirit is thereby substituted for the qualitative description contained in H1.

We prove the following theorem (based on the nesting hypothesis):

If, in Fig. 2, one substitutes for the energy the cumulated weight, letting the energy only determine relative position, then all regions in Fig. 2 bounded by bands or gaps will be bounded by straight line segments.

The statement is trivial for the bands which are vertical straight line segments in either representation. The statement is more difficult to prove for the upper and lower borders. It is best approached by studying weights of identifiable pieces in Fig. 2.

An identifiable piece will be one obtained by repeated nesting, the first stage of which was described above in detail. This means that we select our piece in a series of recursive operations. These operations are described in detail in H1 and H2. They furnish us a set of recursively defined mapping variables $\beta_1, \beta_2, \beta_3, \ldots \beta_n$, each of which varies between 0 and 1. The weight of the piece selected will have the form of a product $W_n = w_1 w_2 w_3 \ldots w_n$. We assert for this product that it is a linear function of Φ. The assertion is clearly true at the stage 1 discussed above. It is also true at the stage 0 where we have just one square graph having weight 1 along each vertical. Let us assume that the statement is true for the stage $m-1$ and the stage m; we shall then prove it to be true for the stage $m+1$. In other words, if W_{m-1} and W_m are linear in Φ then W_{m+1} is linear in Φ.

The proof requires detailed examination of the stage m. The cell m may be located (a) in the left part of one of the arms of the cell $m-1$, or (b) in the right part of one of the arms, or (c) in the left part of the C chain, or (d) in the right part of the C

chain. This gives rise to four possible relations:

$$W_m = \beta_m W_{m-1}\,, \tag{5a}$$

$$W_m = (1 - \beta_m)\, W_{m-1}\,, \tag{5b}$$

$$W_m = (1 - 2\beta_m)\, W_{m-1}\,, \tag{5c}$$

$$W_m = (2\beta_m - 1)\, W_{m-1}\,. \tag{5d}$$

With these four weights there are associated four formulas for β_{m+1}:

$$\beta_{m+1} = \frac{1}{\beta_m} - N_{\mathrm{a}}\,, \tag{6a}$$

$$\beta_{m+1} = \frac{1}{1 - \beta_m} - N_{\mathrm{b}}\,, \tag{6b}$$

$$\beta_{m+1} = \frac{\beta_m}{1 - 2\beta_m} - N_{\mathrm{c}}\,, \tag{6c}$$

$$\beta_{m+1} = \frac{1 - \beta_m}{2\beta_m - 1} - N_{\mathrm{d}}\,. \tag{6d}$$

Now whichever piece we work on in the cell $m+1$ its weight is linear in β_{m+1}, that is

$$W_{m+1} = (A + B\beta_{m+1})\, W_m\,. \tag{7}$$

Combination of (7), (6) and (5) yields four expressions for W_{m+1}:

$$W_{m+1} = (A - BN_{\mathrm{a}})\, W_m + BW_{m-1}\,, \tag{8a}$$

$$W_{m+1} = (A - BN_{\mathrm{b}})\, W_m + BW_{m-1}\,, \tag{8b}$$

$$W_{m+1} = \left(A - B(N_{\mathrm{c}} + \tfrac{1}{2})\right) W_m + \tfrac{1}{2}BW_{m-1}\,, \tag{8c}$$

$$W_{m+1} = \left(A - B(N_{\mathrm{d}} + \tfrac{1}{2})\right) W_m + \tfrac{1}{2}BW_{m-1}\,. \tag{8d}$$

In all four cases W_{m+1} is a linear combination of W_m and W_{m-1}. Therefore, by induction, W_{m+1} is also linear in Φ. The same holds then for the cumulative weights where

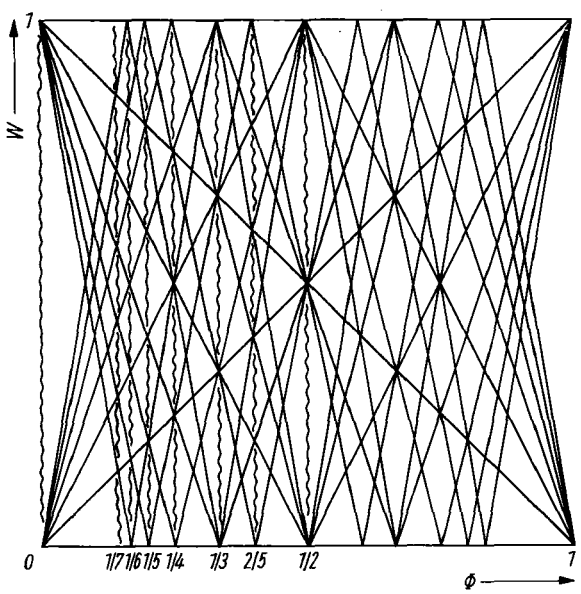

Fig. 4. Continuation of the subdivision of Fig. 2 by the nesting method. A priori dividing lines are shown if statistical weight W is plotted as ordinate instead of energy. For all possible lines W is a linear function of Φ with integer coefficients. Some large bands are shown as wiggly lines in the left portion of the graph

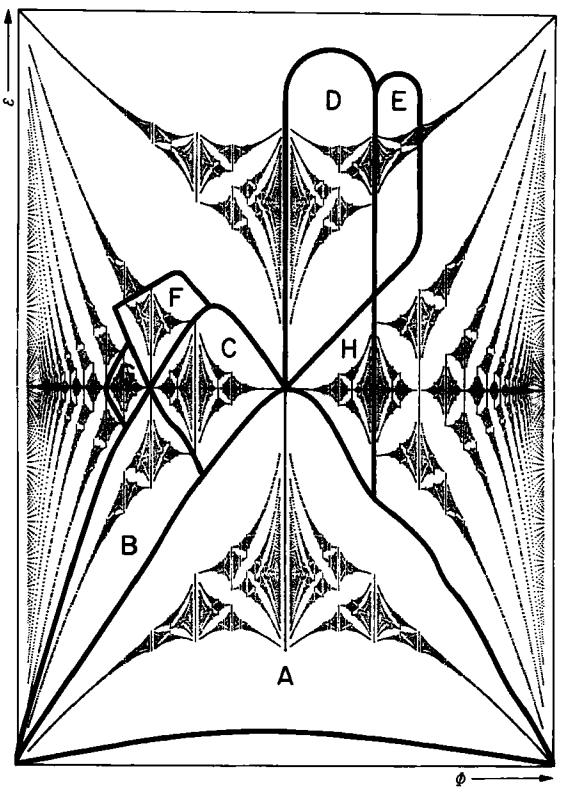

Fig. 5. Repetition of Fig. 2, emphasizing certain regions, labelled A, B, C, D, ...

such linear expressions are added, starting with $W = 0$. The borders of the regions will therefore also be piecewise linear in Φ. This terminates the proof.

The determination of these borders piece by piece is of course a task that can never be finished if the nesting hypothesis holds. It is also unnecessarily cumbersome because we can use instead a priori reasoning to determine what sort of straight lines can serve as regional boundaries.

One type of boundary is represented by the vertical walls of the cells which are the allowed energy bands. The scale along those bands has been changed but they remain vertical straight line segments.

More interesting are the former gaps which are collapsed by our transformation into sloping straight line segments. These sloping straight lines are subject to the important constraint that they must never cross a band. Thus they can cross the verticals $\Phi = 0$ and $\Phi = 1$ only at $W = 0$ and $W = 1$ and the vertical $\Phi = 1/2$ at $W = 0, 1/2, 1$. The diagonals of Fig. 3 clearly obey this constraint. More generally, for $\Phi = p/q$ (p, q prime to each other), the lines must cross at p'/q where p' need not be prime to q. A little consideration of the resulting situation easily shows that the only admissible straight lines are

$$W = M + N\Phi; \qquad M, N \text{ integer}. \tag{9}$$

In Fig. 4 a few of these straight lines are shown, namely the ones having $|N| \leqq 6$. They form bundles emerging from the most prominent band edges, such as the four corners of the square and points like (1/2, 0), (1/2, 1/2), (1/3, 0), (1/3, 1/3), (1/3, 2/3), (1/4, 1/4), etc. Thus, the gaps of Fig. 2 are converted into a network of straight lines.

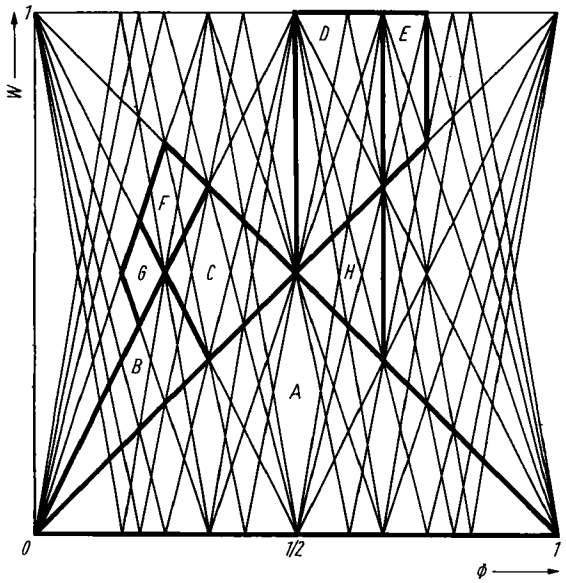

Fig. 6. Repetition of Fig. 4, emphasizing the same regions as in Fig. 5, and using the same labels. A superficial similarity is manifest, but the regions are now polygons

Inversely, the bands of Fig. 2 now show up as gaps, the gaps at $\Phi = 0, 1, 1/2, 1/3, 2/3$ being the most prominent. Thus Fig. 2 and Fig. 4 have a certain duality. The most prominent bands fit into these conspicuous gaps. To make this point clear some of them have been fitted in as wiggly lines into the left half of the figure.

To sum up the nature of the achieved transformation I have placed Fig. 2 and Fig. 4 side by side in Fig. 5 and Fig. 6. Some of the most prominent regions of Fig. 2 have been identified by a heavily outlined boundary in Fig. 5 and designated by letters A, B, C, ... The same regions have been outlined in the same way and designated by the same letter in Fig. 6, on a background showing Fig. 4. It is seen that something of the basic design of Fig. 2 has been preserved in Fig. 6 and some of Hofstadter's qualitative assertions have been quantified. In particular, the "cells" in H1 and H2, already then tentatively termed "trapezoids", are now true trapezoids with easily computed straight lines as boundaries.

Of course a simplification of this sort cannot be accomplished without a certain loss. There is first an esthetic loss: Fig. 6 appears as a "trivialized" form of Fig. 2. There is also a loss of information. Fig. 4 no longer contains the actual value of the energy, but only its location in terms of input parameters and quantum numbers. If one tries to bring back the energy one finds that it has discontinuities at all straight lines shown except the verticals. To find these discontinuities requires the solution of the original eigenvalue problem. What has been achieved here is that the statistical weight of the eigenstates has been extracted out from Fig. 2 and made accessible to independent computation. What comes to one's mind in this connection is that if the rational decomposition of the graph is pushed far enough it might be a good approximation to assign to each piece a constant energy value.

The status of Fig. 4 in the general theory has not yet been investigated. There is a strong possibility that it is valid not just for this model case, but for a general periodic function. If this comes out to be true the same basic graph would apply to all related problems, and only the energy values would be distributed differently.

3. Conclusion

The entire analysis presented here is based on the nesting principle enunciated by Hofstadter [5, 6]. It would be very satisfying to have a proof of it, but none has been forthcoming so far. In the meantime, the next best thing is to use it, and thereby gain a probability feeling concerning its validity. In this context the present work definitely increases the probability for the truth of the hypothesis. Some things have been deduced from it which are manifestly true, and some other things which are not manifestely untrue. In addition, one of the main objections to the hypothesis has been removed by this work. In Fig. 2 the two central bands for even q "kiss" at $\varepsilon = 0$ while in the nested images they do not. No mapping by a topological function can achieve such a result. But now, by the change of variable carried out here all neighboring bands belonging to the same Φ "kiss". Topological mapping is thereby not only rendered possible in principle, but it can actually be performed with the help of simple functions. So this originally strong objection has been converted naturally into an argument in favor of nesting. Of course, infinite nesting has perhaps something to do with the mathematics of this or related difference equations. In physics, it must stop somewhere. However, here again, it is my feeling that one should look for the natural way to resolve this question rather than resort to some forced procedure such as blurring of the energy states to remove this feature artifically.

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