Repeat Space Theory Applied to Carbon Nanotubes and Matrix Art

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In conjunction with the series of papers entitled "Repeat space theory applied to carbon nanotubes and related molecular networks. I, II, III" published in the J. Math. Chem., Springer, two Challenging Problems E and F have been formulated and discussed. The Matrix Art pictures of carbon nanotube energy band curves played a significant role as a heuristic trigger in formulating Problem E, and the pattern analysis of matrices in the repeat space was crucial in providing a conjecture in Problem F. The visual and audible data analysis are playing a significant role in the international, interdisciplinary, and intergenerational Second Generation Fukui Project and in its special new part, the Niagara Project.

Key Words: Repeat Space Theory (RST), Asymptotic Linearity Theorem (ALT), Analytic Curves, Resolution of Singularities, Fourier Expansions of Absolutely Continuous Functions

1. Introduction

The Repeat Space Theory (RST) [1-24] is a central unifying theory in the First and Second Generation Fukui Project [1-4], which was initiated in August 1992 by Kenichi Fukui (1918 - 1998, Nobel Prize 1981). The Matrix Art Program in the Niagara Project, which is a special new part of the Fukui Project started in 2010, and this program has merged to part III of the series of papers entitled "Repeat space theory applied to carbon nanotubes and related molecular networks" published in the J. Math Chem. Springer [7-9]. In conjunction with this series, two challenging problems E and F have been formulated and discussed in the present paper. The Matrix Art pictures of carbon nanotube energy band curves played a significant role as a heuristic trigger in formulating Problem E, and the pattern analysis of matrices in the repeat space was crucial in providing Problem F, which together with other challenging problems from refs. [4,9] are enriching the interdisciplinary and inter-generational investigations in the field between mathematics and chemistry. We remark that the visual and audible data analyses are playing a significant role in the international, interdisciplinary, and inter-generational Second Generation Fukui Project and in its special new part, the Niagara Project.

2. Preliminaries and Challenging Problem E

Before formulating the problem, we need some preparations. Throughout, let $\mathbb{Z}^+$, $\mathbb{Z}_0^+$, $\mathbb{Z}$, $\mathbb{R}$, and $\mathbb{C}$ denote respectively the set of all positive integers, nonnegative integers, integers, real numbers, and complex numbers. (In the present paper, we retain the notation given in the "Nanotube Series, parts I ~ III" published in the Journal of Mathematical Chemistry [7-9]. The reader is referred to refs. [25-27] and references therein for the science and technology of carbon nanotubes.)

Let Arg: $\mathbb{C} \to]-\pi, \pi]$ denote the function defined by

$$\operatorname{Arg}(z) = \begin{cases} 0 & \text{if} \quad z = 0 \\ \theta & \text{if} \quad z \in \mathbb{C} - \{0\}, \end{cases} \tag{2.1}$$

where $\theta \in]-\pi, \pi]$ and

$$z = |z| \exp(i\theta). \tag{2.2}$$

(Note that for each $z \in \mathbb{C} - \{0\}$, there is a unique $\theta \in]-\pi, \pi]$ such that (2.2) holds.)

For each $n \in \mathbb{Z}^+$, let Sg_n: $\{1,\ldots, 2n\} \to \{-1, 1\}$ denote the function defined by

$$\mathrm{Sg}_n(j) = \begin{cases} 1 & \text{if } j \in \{1, \ldots, n\}, \\ -1 & \text{if } j \in \{n+1, \ldots, 2n\}. \end{cases} \tag{2.3}$$

In part III of the "Nanotube series" [9], we proved the

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following theorem using the technique of what is called the spectral symmetry (cf. [28,20] and references therein for the notion of the spectral symmetry and theorems related to it):

Theorem B. *Let $n \in \mathbb{Z}^+$, let $t \in \mathbb{Z}$, let $c, d \in \mathbb{C}$, and let $\theta \in \mathbb{R}$. Let $\rho := \rho(d, \theta) = 1 + d^* \exp(-i\theta)$. Then, for $1 \le j \le 2n$, the eigenvalue $\lambda_j^{n,t,c,d}(\theta)$ of the $2n \times 2n$ Hermitian matrix $F^{n,t,c,d}(\theta)$ is given by*

$$\lambda_j^{n,t,c,d}(\theta) = \mathrm{Sg}_n(j)\sqrt{|c|^2+|\rho|^2+2\,\mathrm{Re}\left(c\rho\exp\left(i\left(\frac{t\theta+2\pi j}{n}\right)\right)\right)}$$

$$= \mathrm{Sg}_n(j)\sqrt{|c|^2+|\rho|^2+2|c||\rho|\cos\left(\mathrm{Arg}(c)+\mathrm{Arg}(\rho)+\frac{t\theta+2\pi j}{n}\right)}. \tag{2.4}$$

Let us now recall the notion of an envelope of a family of curves (cf. e.g. [29]). An envelope of a one-parameter family of curves given implicitly by

$$U(x, y, \alpha) = 0, \tag{2.5}$$

where α is the parameter, is a curve that is tangent to every member of the family at some point. (Here, the differentiability of U and other smoothness conditions of U are usually assumed.) Define the two variable function with the parameter α by

$$V^{(\alpha)}(x, y) := U(x, y, \alpha). \tag{2.6}$$

Recall that the singular locus of the function $V^{(\alpha)}(x, y)$ is the collection of all the points (x, y) where the gradient vector of $V^{(\alpha)}$ vanishes:

$$(\mathrm{grad}V^{(\alpha)})\,(x, y) = (V_x^{(\alpha)}(x,y), V_y^{(\alpha)}(x,y)) = (0, 0). \tag{2.7}$$

In what follows, let U_α stand for the partial derivative of U with respect to α. It is well known that for a family of curves represented implicitly, the envelope is given by the following simultaneous equations with the unknowns x, y with the parameter α:

$$\begin{cases} U(x, y, \alpha) = 0, \\ U_\alpha(x, y, \alpha) = 0, \end{cases} \tag{2.8}$$

with the additional condition that

$$(\mathrm{grad}V^{(\alpha)})\,(x, y) \neq (0, 0). \tag{2.9}$$

Thus, at first, one has to solve the above simultaneous equations (by using e.g. the implicit function theorems) to obtain the parametric solution:

$$(x, y) = (x(\alpha), y(\alpha)) \tag{2.10}$$

that satisfies (2.8). Second, one has to check for each α if the solution is not a singularity of $V^{(\alpha)}$.

For example, if a family of curves is given implicitly by

$$U(x, y, \alpha) = (x-\alpha)^2 + y^2 - 1 = 0, \tag{2.11}$$

then, we have

$$U_\alpha(x, y, \alpha) = -2x + 2\alpha = 0, \tag{2.12}$$

so that $\alpha = x$. By solving the simultaneous equations (2.11) and (2.12), one has

$$(x, y) = (x(\alpha), y(\alpha)) = (\alpha, 1), (\alpha, -1). \tag{2.13}$$

Since

$$(\mathrm{grad}V^{(\alpha)})\,(x, y) = (2x - 2\alpha, 2y), \tag{2.14}$$

the singularity of $V^{(\alpha)}$ is $(\alpha, 0)$. So, neither of the parametric solutions $(\alpha, 1)$ and $(\alpha, -1)$ coincides with the singularity of $V^{(\alpha)}$. Thus, each parametric line $(\alpha, 1)$ and $(\alpha, -1)$ is an envelope of the given families of curves.

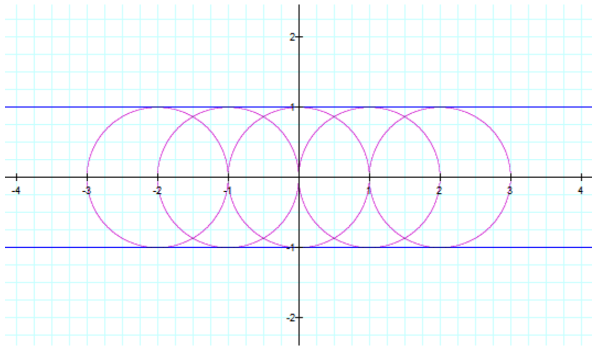

Fig. 1. Envelopes of (2.11)

On the other hand, if a family of curves is given implicitly by

$$U(x, y, \alpha) = (y-\alpha)^2 - x^2(x+1) = 0, \tag{2.15}$$

then, we have

$$U_\alpha(x, y, \alpha) = -2y + 2\alpha = 0, \tag{2.16}$$

so that $\alpha = y$.

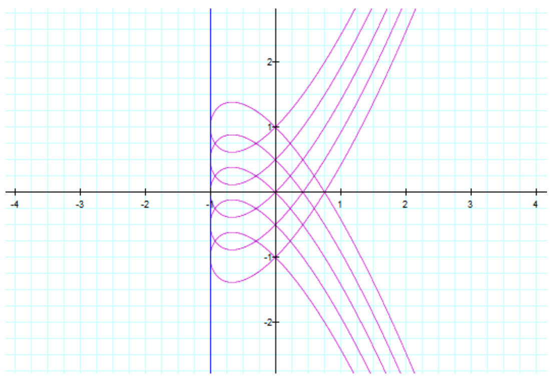

Fig. 2. Envelope of (2.15)

By solving the simultaneous equations (2.15) and (2.16), one obtains

$$(x, y) = (x(\alpha), y(\alpha)) = (-1, \alpha), (0, \alpha). \tag{2.17}$$

Since

$$(\mathrm{grad}V^{(\alpha)})(x, y) = (-3x^2 - 2x, 2(y-\alpha)), \tag{2.18}$$

the singularities of $V^{(\alpha)}$ are $(-\frac{2}{3}, \alpha)$ and $(0, \alpha)$. The parametric solution $(-1, \alpha)$ coincides with none of the singularities of $V^{(\alpha)}$, whereas the parametric solution $(0, \alpha,)$ coincides with one of the singularities of $V^{(\alpha)}$. Thus, only the parametric line $(-1, \alpha)$ is an envelope of the given families of curves, and the parametric line $(0, \alpha)$ is the locus of one of the singularities of $V^{(\alpha)}$.

Now in Theorem B, fix $n \in \mathbb{Z}^+$, $t \in \mathbb{Z}$, $c \in \mathbb{C}$, and $d \in \mathbb{C}$, and set

$$\theta = x, \tag{2.19}$$

$$\rho = \rho(x) = 1 + d^* \exp(-ix), \tag{2.20}$$

$$\alpha = \frac{2\pi j}{n}. \tag{2.21}$$

Let

$U(x, y, \alpha) :=$

$$y^2 - \left(|c|^2 + |\rho|^2 + 2|c||\rho|\cos\left(\mathrm{Arg}(c) + \mathrm{Arg}(\rho) + \frac{tx}{n} + \alpha\right)\right)$$

$$= 0. \tag{2.22}$$

First, notice the fact that the eigenvalues $\lambda_j^{n,t,c,d}(\theta)$ given in Theorem B are the solution of the quadratic equations (2.22) with α given by (2.21).

Second, notice that the following easily verifiable inequality holds:

$$\big||c| - |\rho|\big| \le |y| \le |c| + |\rho|. \tag{2.23}$$

Third, we remark that via the Matrix Art pictures of CNTs and associated computer experiments, one observes that the following four curves are parts of four highly smooth (real-analytic) curves.

$$y = |c| + |\rho(x)| = f_1(x), \tag{2.24}$$

$$y = \big||c| - |\rho(x)|\big| = f_2(x), \tag{2.25}$$

$$y = -\big||c| - |\rho(x)|\big| = f_3(x), \tag{2.26}$$

$$y = -\left(|c| + |\rho(x)|\right) = f_4(x). \tag{2.27}$$

Moreover, for each $\alpha \in \mathbb{R}$, there seem to exist two highly smooth (real-analytic) functions $\tilde{g}^{\alpha}$ and $\tilde{h}^{\alpha}$ on $\mathbb{R}$ which form the solution of (2.22).

We are now ready to formulate our Challenging Problems E (Envelope).

Challenging Problems E. Prove or disprove the following conjectures, and investigate the envelopes of the family of curves implicitly defined by $U(x, y, \alpha) = 0$, where $U(x, y, \alpha)$ is given by (2.22).

Conjecture 1. There exist four real analytic functions $\tilde{f}_1$, $\tilde{f}_2$, $\tilde{f}_3$, and $\tilde{f}_4$ defined on $\mathbb{R}$ such that the identity

$$(y - f_1(x))(y - f_2(x))(y - f_3(x))(y - f_4(x))$$

$$= (y - \tilde{f}_1(x))(y - \tilde{f}_2(x))(y - \tilde{f}_3(x))(y - \tilde{f}_4(x)) \tag{2.28}$$

holds for all $x \in \mathbb{R}$, where $f_1(x)$, $f_2(x)$, $f_3(x)$, and $f_4(x)$ are given by (2.24) ~ (2.27).

Conjecture 2. For each $\alpha \in \mathbb{R}$, there exist two real analytic functions $\tilde{g}^{\alpha}$ and $\tilde{h}^{\alpha}$ such that the following identity

$$y^2 - \left(|c|^2 + |\rho|^2 + 2|c||\rho|\cos\left(\mathrm{Arg}(c) + \mathrm{Arg}(\rho) + \frac{tx}{n} + \alpha\right)\right)$$

$$= (y - \tilde{g}^{\alpha}(x))(y - \tilde{h}^{\alpha}(x)) \tag{2.29}$$

holds for all $x \in \mathbb{R}$, where the left-hand side is $U(x, y, \alpha)$ given by (2.22).

We give preliminary considerations on the above problem, we invite the reader to tackle the problem further.

By taking the partial derivative of (2.22) with respect to α, we have

$U_{\alpha}(x, y, \alpha)$

$$= 2|c||\rho|\sin\left(\mathrm{Arg}(c) + \mathrm{Arg}(\rho) + \frac{tx}{n} + \alpha\right)$$

$$= 0. \tag{2.30}$$

By (2.22) and (2.30), we have

$$\left(y^2 - |c|^2 - |\rho(x)|^2\right)^2 - 4|c|^2|\rho(x)|^2 = 0. \tag{2.31}$$

This is a monic quartic equation with real coefficients analytically dependent on x. Note that the left-hand side of (2.31) can be factored as follows:

$$(y - f_1(x))(y - f_2(x))(y - f_3(x))(y - f_4(x)) = 0. \tag{2.32}$$

3. Challenging Problems F

In ref. [14], entitled ‘Proof of the Fukui conjecture via resolution of singularities and related methods. V’, the theory of analytic (highly smooth) curves and resolution of singularities has been applied to prove the Fukui conjecture originating in chemistry. We remark that the investigations of highly smooth functions and of highly irregular functions are complementary in the repeat space theory (RST).

In contrast to Challenging Problem E formulated in Section 2, the following Challenging Problem F is related to absolutely continuous functions (generally highly irregular) and to their Fourier expansions.

Challenging Problem F is closely related to the Asymptotic Linearity Theorems (ALTs) in the repeat space theory (RST). The reader is referred to [19-24] for the ALTs and for the definitions of the original alpha space $X_\alpha(q)$ and of other symbols given in the following conjecture.

Conjecture 3. (OALT-$X_\alpha(q)$ $AC(I)$ version). *Let $q \in \mathbb{Z}^+$, let $s \in \mathbb{Z}$, let $\{A_N\} \in X_\alpha(q)$, and let I be a closed interval compatible with $\{A_N\}$. Then, for any $\varphi \in AC(I)$, there exists an $\alpha_s(\varphi) \in \mathbb{R}$ such that*

$$\mathrm{Tr}[(P_N^s \otimes I_q)(\varphi(A_N))] = \alpha_s(\varphi)N + o(1) \tag{3.1}$$

as $N \to \infty$. Moreover the real number $\alpha_s(\varphi)$ is represented by the integral given by

$$\alpha_s(\varphi) = \frac{1}{2\pi}\int_0^{2\pi} \exp(is\theta)\mathrm{Tr}\varphi(F(\theta))d\theta\ . \tag{3.2}$$

Challenging Problem F. Prove or disprove Conjecture 3.

Let $P(I)$ denote the subspace of $AC(I)$ of all the polynomial functions with real coefficients. The Conjecture 3 with $AC(I)$ replaced with $P(I)$ is called Off-diagonal ALT, OALT-$X_\alpha(q)$, $P(I)$ version. The reader is invited to prove or disprove this simpler version first.

We note that in investigating the above and related conjectures, MATLAB and audio frequency analysis software called “Spectrogram” have been used to analyze the Matrix pattern of various “functions” of repeat sequences $\varphi(A_N)$. Using a MATLAB function, one can convert numerical data to audible sound data and one can use the latter heuristically to discover patterns in various “functions” of repeat sequences $\varphi(A_N)$. The new development along these lines of investigation is now under way. The frequency analysis of various sound data is now part of the Second Generation Fukui Project and in the Niagara Project. The reader is referred to the link [30], in which bio-electrical signals from muscle cells are analyzed via frequency analyzer.

4. Matrix Art and Computer Experiments for Challenging Problem E and Related Problems

In this section, we provide Matrix Art pictures (see the envelopes in *Figs*. 3, 4, and 5) that triggered discovering the envelopes discussed in Section 2. These pictures also serve to solve Challenging Problem A# formulated in the recent paper [9], entitled ‘Repeat space theory applied to carbon nanotubes and related molecular networks. III’. The reader is also referred to the Matrix Art pictures and notes given in [31].

Matrix Art pictures, or Math Digital Art pictures, have been so far created by mainly using MATLAB in Matrix Art Challenge Seminar in Tsuyama National College of Technology (TNCT). Cf. refs. [4-6,9,14] for the Matrix Art pictures created in TNCT and for the heuristic role played by the pictures. We have recently been extending the range of contributors of Matrix Art from the members of TNCT to include members of the Fukui Project Association. We are also extending the means by which we create such digital art pictures, beginning to use MATHEMATICA especially assessing its new capability of creating interactive files called CDFs, which can be opened and interactively used by anyone who can download a free CDF Player through the internet.

After finding the envelopes in several Matrix Art pictures, simple computer experiments have been made using Graphing Calculator. The following *Figs*. 6, 7 are snapshots of the screens of Graphing Calculator files which can be opened and interactively used by anyone who can download a free Graphing Calculator Viewer through the internet.

In connection to the fractal Matrix Art [4-6,9], the reader is invited to refer to Prof. H. Hironaka’s public speech entitled ‘Mathematics and the Sciences’ [32] for an instructive account of the notion of self-similarity, fractal geometry, and of mathematical sciences.

The reader is also referred to Prof. R. Hoffmann’s public speech entitled ‘One Culture’ [33], which expounds the cross-disciplinary interaction between science and art. We remark that two refs. [32,33] formed an important source of inspiration for the Fukui Project, which is devoted to cultivating a new interdisciplinary region in science, often utilizing dialectic interplay between a complementary pair of opposite notions and ideas. These two refs. [32,33] are also playing the role of a guideline for the Matrix Art Program of the Niagara Project (cf. [4,6,14,] for details), which is a special new part of the on-going international, interdisciplinary, and inter-generational Second Generation Fukui Project.

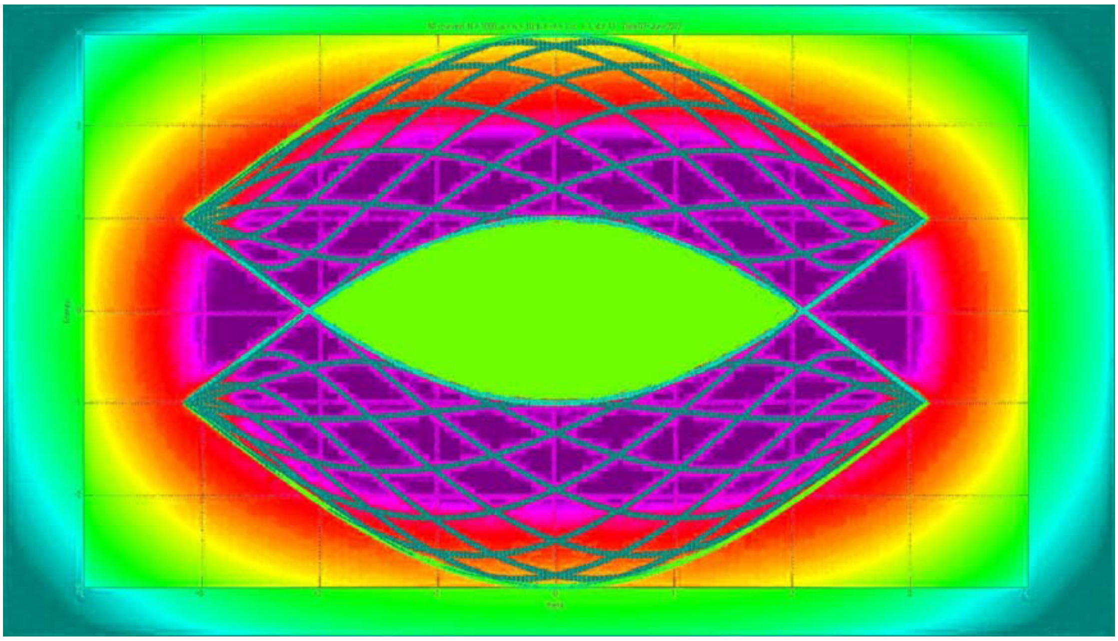

Fig. 3. Matrix Art picture 1 of CNT energy band curves

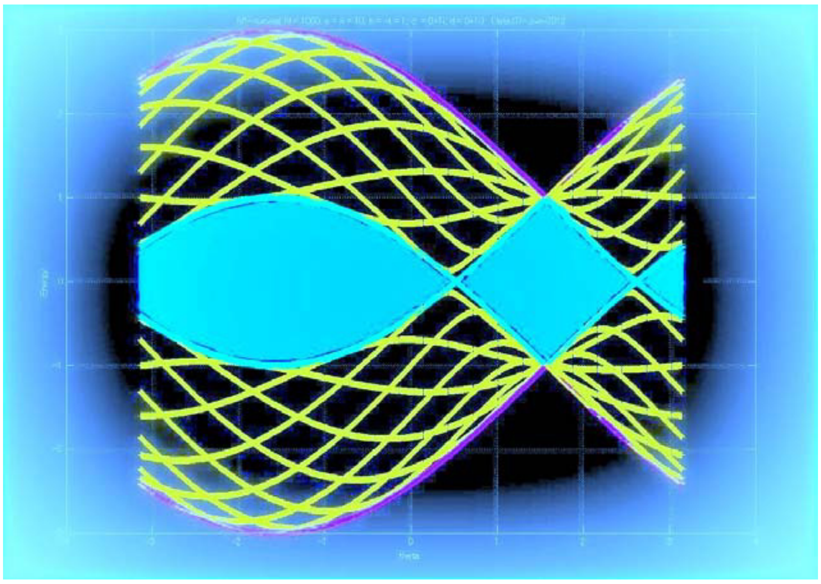

Fig. 4. Matrix Art picture 2 of CNT energy band curves

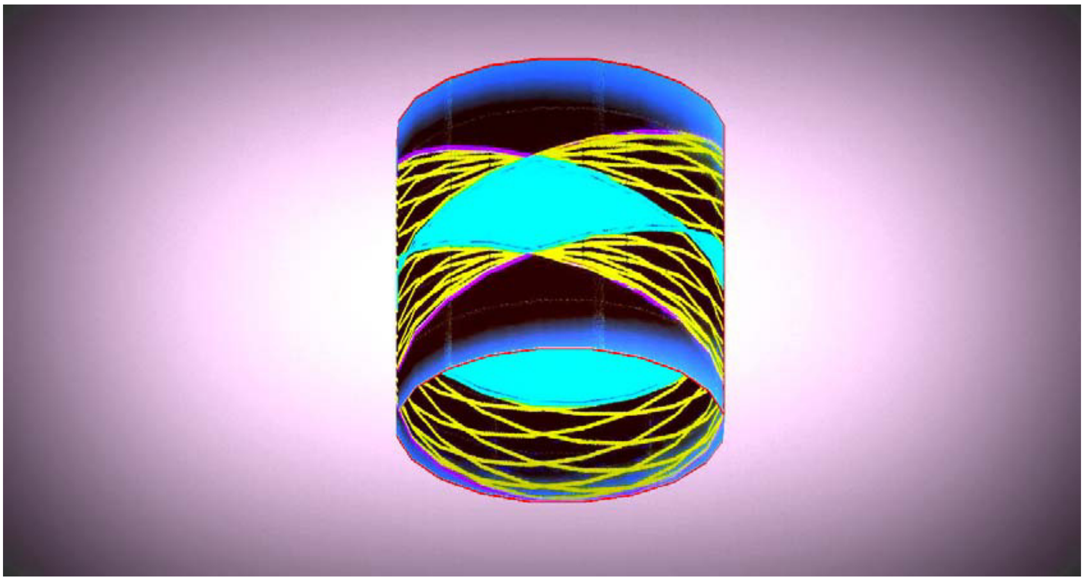

Fig. 5. Matrix Art picture 3 of CNT energy band curves on a cylinder

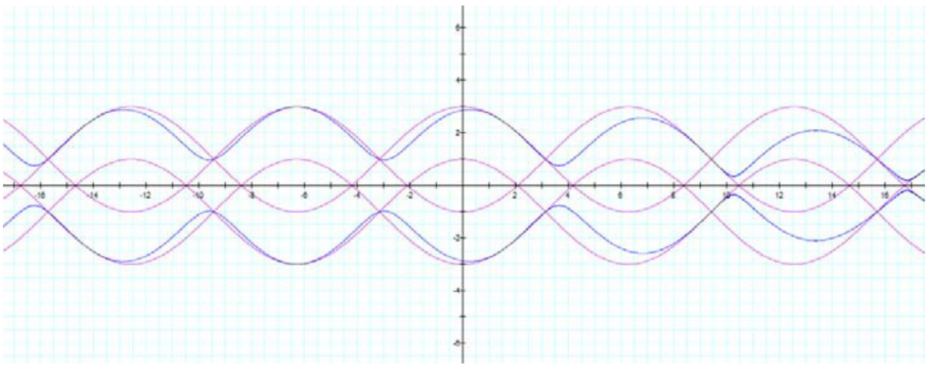

Fig. 6. Envelopes 1

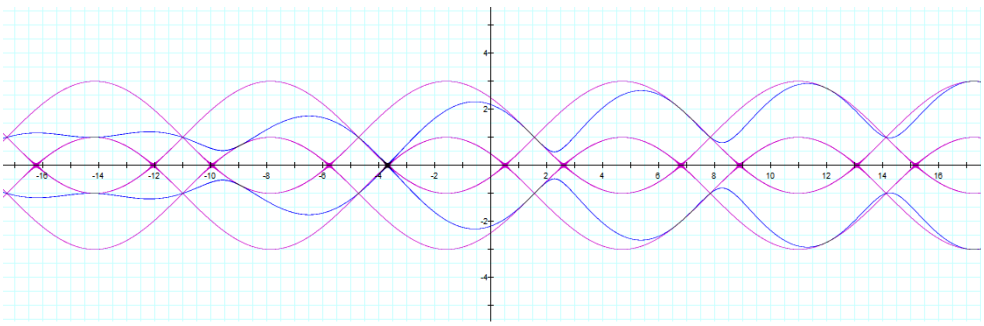

Fig. 7. Envelopes 2

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