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Open problem

Magic Mountain and Devil's Staircase swapping problems *

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Two open questions concerning additivity problems in theoretical chemistry have been posed in this article. Each question involves swapping of the square root function (in the formula for the zero-point energy of a linear oscillator) with a highly irregular function. Global contextualization of molecular problems and function swapping are indispensable strategies in tackling additivity problems in theoretical chemistry.

KEY WORDS: additivity problems, zero-point energy, functional spaces, repeat space theory

1. Introduction

Special magnitudes of universal constants and specific forms of functions manifest themselves in the expressions of natural laws. Nevertheless, it is sometimes legitimate and meaningful to embed fixed constants or functions into a broader context and make them change. For example, one can regard the Planck constant as a variable and let it tend to zero so that classical mechanics can be considered as a limit of quantum mechanics[1].

Global contextualization is an essential strategy in tackling additivity problems in theoretical chemistry. In the "repeat space theory" (RST) (cf. [1–5]), which was initially developed for the additivity problems of the zero-point energies of molecules

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[1] George Gamow reversed this process and magnified the Planck constant in his instructive and amusing book *Mr. Tompkins in Wonderland*. In Gamow's book, Mr. Tompkins, the little clerk of a big city bank, experiences a manifestation of Heisenberg's uncertainty principle in a billiard room filled with men in shirt sleeves playing billiards: "As soon as the ball was placed in the enclosure, the whole inside of the triangle became filled up with the glittering of ivory. 'You see!' said the professor, 'I defined the position of the ball to the extent of the dimension of the triangle, i.e. several inches. This results in considerable uncertainty in the velocity, and the ball is moving rapidly inside the boundary.' 'Can't you stop it?' asked Mr. Tompkins. 'No – it is physically impossible. Any body in an enclosed space possesses a certain motion – we call it zero-point motion.' " (G. Gamow, *Mr. Tompkins in Wonderland*, from the chapter *Quantum Billiards*.)

having repeating identical moieties (cf. references in [2]), it is a significant procedure to embed the square root function in the formula (for the zero-point energy $\mathcal{E}_{\text{zero}}$ of a linear oscillator)

$$\mathcal{E}_{\text{zero}} = \frac{\hbar}{2}\sqrt{\frac{k}{m}} \tag{1}$$

into a functional space endowed with a suitable topology, allowing the function to change in the space. One of the fundamental theorems in the RST, referred to as the Asymptotic Linearity Theorem (ALT) [1,2,4,5], implies that the zero-point energy E_N of a hydrocarbon having N repeating identical moieties between two prescribed end moieties will retain its asymptotic linear form:

$$E_N = aN + b + \mathrm{o}(1) \tag{2}$$

even if the square root function in equation (1) is replaced by an arbitrarily given absolutely continuous function. For example, suppose that ξ is any positive real number and that the formula for $\mathcal{E}_{\text{zero}}$ were given by

$$\mathcal{E}_{\text{zero}} = \frac{\hbar}{2}\left(\frac{k}{m}\right)^{\xi}. \tag{3}$$

Then the zero-point energy E'_N of a hydrocarbon having N repeating identical moieties between two prescribed end moieties would have an asymptotic linear form: $E'_N = a'N + b' + \mathrm{o}(1)$, where a' and b' are real constants dependent on ξ.

A negative solution of either of the open problems given in section 3 automatically proves the following conjecture, and the solution of either problem will play a key role in the future development of the repeat space theory (RST). (Cf. [2,3] for the genesis of the RST and a variety of applications of the RST.)

Asymptotic Linearity Theorem Extension Conjecture. (ALTEC, $C(I)$ version.) The Asymptotic Linearity Theorem (ALT) cannot be extended from $AC(I)$ to $C(I)$, where $AC(I)$ denotes the functional space of all real-valued absolutely continuous functions defined on closed interval I, and $C(I)$ denotes the functional space of all real-valued continuous functions defined on closed interval I.

Before formulating our problem, we need some preparation. Let $Ch_N(m, k)$ denote the linear chain with free ends consisting of N particles each of mass m and separation 1 that can vibrate harmonically under a restoring force due to the first-neighbor interaction k. Let

$$E_N(\varphi) = \sum_{i=1}^{N} \frac{\hbar}{2}\,\varphi\left(4\frac{k}{m}\sin^2\frac{(i-1)\pi}{2N}\right), \tag{4}$$

where φ denotes a real-valued continuous function defined on the closed interval $[0, 4(k/m)]$. Setting $(\hbar/2) = k = 1$ and $m = 4$ in equation (4), let

$$F_N(\varphi) = \sum_{i=1}^{N} \varphi\left(\sin^2 \frac{(i-1)\pi}{2N}\right), \tag{5}$$

where φ denotes a real-valued continuous function defined on the closed interval [0, 1].

If ξ is an arbitrarily given positive real number and if $\mathcal{R}_\xi$ denotes the function defined by $\mathcal{R}_\xi(x) = x^\xi$, then $E_N(\mathcal{R}_{1/2})$ expresses the zero-point energy of $Ch_N(m, k)$, and $E_N(\mathcal{R}_{1/2})$ can be explicitly expressed in terms of the cotangent function (cf. [1]):

$$E_N(\mathcal{R}_{1/2}) = \frac{\hbar}{2}\sqrt{\frac{k}{m}}\left(\cot\left(\frac{\pi}{4N}\right) - 1\right). \tag{6}$$

Inspection of the graph of this as a function of N for fixed m and k, reveals a strong primary correlation between N and $E_N(\mathcal{R}_{1/2})$. In fact, $E_N(\mathcal{R}_{1/2})$ has an asymptotic line:

$$E_N(\mathcal{R}_{1/2}) = \frac{\hbar}{2}\sqrt{\frac{k}{m}}\left(\frac{4}{\pi}N - 1\right) + \mathrm{o}(1), \tag{7}$$

where $\mathrm{o}(1)$ denotes a function of N such that $\mathrm{o}(1) \to 0$ as $N \to \infty$. Note that in general a real sequence E_N has an asymptotic line, i.e. $E_N = aN + b + \mathrm{o}(1)$, $N \to \infty$ if and only if the limits $a = \lim_{N\to\infty} E_N/N$, $b = \lim_{N\to\infty}(E_N - aN)$, $a, b \in \mathbb{R}$ exist. For $E_N(\mathcal{R}_{1/2})$, since $\cot\theta = 1/\theta - \theta/3 +$ (higher order terms), for $\theta \in (0, \pi)$, we have $a = (\hbar/2)\sqrt{k/m}(4/\pi)$, $b = -(\hbar/2)\sqrt{k/m}$.

For an arbitrarily given positive real number ξ, the graph of $E_N(\mathcal{R}_\xi)$ as a function of N for fixed m and k, reveals a strong asymptotic linear correlation between N and $E_N(\mathcal{R}_\xi)$. Notice that by the definitions of $E_N(\mathcal{R}_\xi)$ and $F_N(\mathcal{R}_\xi)$ we have

$$E_N(\mathcal{R}_\xi) = \frac{\hbar}{2}\left(\frac{4k}{m}\right)^\xi F_N(\mathcal{R}_\xi). \tag{8}$$

The graphs of $F_N(\mathcal{R}_\xi)$ for $N = 2, 3, \ldots, 200$ and $\xi = 0.1, 0.3, \ldots, 2.9$ presented in figure 1 indicate strong asymptotic linear correlations between N and $F_N(\mathcal{R}_\xi)$.

2. Magic Mountain and Devil's Staircase

Let $\phi : [0, 1] \to [0, 1]$ be the function defined by

$$\phi(x) = \begin{cases} 2x & \text{if } 0 \leqslant x < 1/2, \\ 2(1-x) & \text{if } 1/2 \leqslant x \leqslant 1, \end{cases} \tag{9}$$

let $\mathcal{M}_n : [0, 1] \to \mathbb{R}$ be the function defined by

$$\mathcal{M}_n(x) = \frac{\phi(x)}{2} + \frac{\phi(\phi(x))}{2^2} + \frac{\phi(\phi(\phi(x)))}{2^3} + \cdots + \frac{\phi(\phi(\phi(\phi(\ldots(x)))) \ldots)}{2^n}, \tag{10}$$

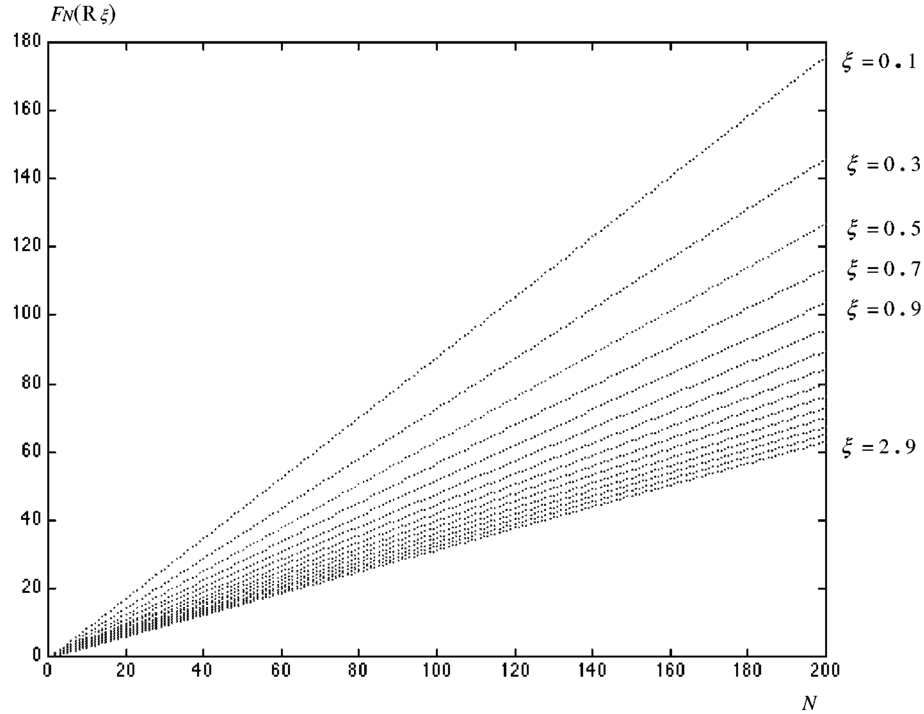

Figure 1. Graphs of $F_N(\mathcal{R}_\xi)$ as functions of N.

and let $\mathcal{M} : [0, 1] \to \mathbb{R}$ be the function defined by

$$\mathcal{M}(x) = \lim_{n\to\infty} \mathcal{M}_n(x). \tag{11}$$

It is easy to check that $\mathcal{M}_n$ is a Cauchy sequence in the Banach space $C([0, 1])$ equipped with the sup norm. Thus $\mathcal{M}$ is a well-defined continuous function on [0, 1]. Getting inspiration from Weierstrass' well-known construction of a continuous and nowhere differentiable function, T. Takagi constructed $\mathcal{M}$ and proved that $\mathcal{M}$ is continuous and nowhere differentiable on its domain [7], and hence $\mathcal{M}$ is often called the Takagi function (cf. [6,8] and references therein). Throughout this article, we shall refer to the function $\mathcal{M}$ as Magic Mountain.

The graph of Magic Mountain is shown in figure 2. The larger square surrounding the graph corresponds to the area $[0, 1] \times [0, 1]$. The part of the graph contained in the smaller square is similar to the entire graph. The graph of Magic Mountain possesses within itself infinitely many reduced-size self-replicas.

Let $\mathcal{D} : [0, 1] \to \mathbb{R}$ denote the well-known Cantor function (often called Devil's Staircase), which is continuous but not absolutely continuous on its domain. Let $0 < \eta \leqslant 1$ and let $\mathcal{D}_\eta : [0, 1] \to \mathbb{R}$ be the function defined by $\mathcal{D}_\eta(x) = \mathcal{D}(\eta x)$. Throughout this article, function $\mathcal{D}_\eta$ shall be referred to as Devil's Staircase of type η.

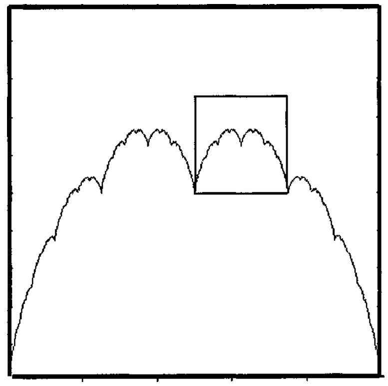

Figure 2. Magic Mountain.

3. Open problems

Now recall the definition of $F_N(\varphi)$ given by equation (5). We know that $(\hbar/2)F_N(\mathcal{R}_{1/2})$ expresses the zero-point energy of the linear chain $Ch_N(4,1)$ and that $F_N(\mathcal{R}_{1/2})$ has an asymptotic line. What if one swaps $\mathcal{R}_{1/2}$ with Magic Mountain or Devil's Staircase of an arbitrarily given and fixed type η, $0 < \eta \leqslant 1$? Here, then, are our two open problems:

(I) Magic Mountain swapping problem.
Does the sequence $F_N(\mathcal{M})$ have an asymptotic line?

(II) Devil's Staircase swapping problem.
Does the sequence $F_N(\mathcal{D}_\eta)$ have an asymptotic line?

Remark. If n is an arbitrarily given and fixed positive integer, then $\mathcal{M}_n$ is absolutely continuous on the closed interval $[0,1]$, and the Asymptotic Linearity Theorem (ALT) implies that the sequence $F_N(\mathcal{M}_n)$ has an asymptotic line.

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