Note on the repeat space theory *

– its development and communications with Prof. Kenichi Fukui –

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Dedicated to the memory of Professor Kenichi Fukui (1918–1998)

This note provides a chronological sketch of the development from the early 1990s of
the Repeat Space Theory (RST), which had originated in the study of the zero-point energy
additivity problems of hydrocarbons in 1985. Interacting with the theories of dynamical sys-
tems, operator algebra, and so forth, the RST has developed into a comprehensive theoretical
framework of axiomatic nature, which unites and solves, in particular, what we call globally-
pertaining-type problems, or, for short, g-type problems; these constitute physico-chemical
problems for whose solutions global mathematical contextualization is essential. In conjunc-
tion with the author's communications with Prof. Kenichi Fukui, the genesis of the notion of
g-type problems has also been presented in this note. Through the vision the RST provides,
it is foreseeable that investigations of the peripheral research domains of g-type problems in
chemistry will play a significant role for future investigations, especially for those related to
macromolecules, physico-chemical network systems, and biochemical network systems, in
the vast uncharted interdisciplinary regions between chemistry and modern mathematics.

KEY WORDS: repeat space theory (RST), additivity problems, Asymptotic Linearity Theo-
rem (ALT), zero-point energy

1.   Development of the repeat space theory in the 1990s

In the 1990s, the repeat space theory (RST), which had originated in the formu-
lation of the repeat space $X_r(q)$ in [1] for the zero-point energy additivity problems of
hydrocarbons, developed into a comprehensive theory through which one can analyze
and view a chain of physico-chemical additivity and network problems under a unifying
perspective.

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*An earlier version of this note was distributed to former members of the Institute for Fundamental
Chemistry and to members of the newly inaugurated Fukui Kenichi Memorial Research Center, Kyoto,
Japan.

Joint research between the Institute for Fundamental Chemistry (IFC), Japan, and the Mathematical Chemistry Research Unit (MCRU), University of Saskatchewan, Canada, whose project was referred to as the Fundamental Mathematical Chemistry Joint Project, began in August 1992 through the initiative of the late Prof. Kenichi Fukui in co-operation with the author (on leave from the IFC, August 1990–March 2002) and representatives of the MCRU, Prof. Paul G. Mezey and Prof. Keith F. Taylor.

In the early 1990s, while surveying the development of the RST in conjunction with the above joint project, the author became aware of a noteworthy parallel between his earlier asymptotic analysis of quantum mechanical network systems using the earlier RST and part of his analysis of Fukui's chemical kinetic cyclic network systems whose special version had been given in [2].

From a physico-chemical point of view, these two types of network systems have no common characteristics. In fact, the former are molecular systems governed by a quantum mechanical law, the latter are kinetic dynamical systems consisting of n chemical species whose concentrations at time t are governed by simultaneous differential equations (kinetic equations). Strikingly, however, it turned out that the fundamental methodology of the RST, called the approach via the aspect of general topology, with some additional tools from the theory of Banach algebra, led to a general solution of Fukui's problems of chemical kinetic cyclic networks. Conversely, the theory of Banach algebra used for our chemical kinetic investigations proved to be helpful in the RST, especially in sharpening fundamental existence theorems in the RST.

The RST had initially been developed for the zero-point energy additivity problems of hydrocarbons, which shall be briefly reviewed in section 2. However, around the time when the author introduced tools and techniques of the theories of operator algebra and functional analysis to the RST, it began to transform into a theory of axiomatic nature whose scope of applications comprises not only physico-chemical network systems but also other network systems appearing, for example, in the branch of the theory of Toeplitz matrices and operators (cf. [3] and references therein). This transformation of the RST also brought forth our subsequent new vision on the future of the interdisciplinary research field between chemistry and modern mathematics.

2. Brief review of the Functional Asymptotic Linearity Theorem, a fundamental theorem in the RST

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.

Global contextualization is an essential strategy in tackling the zero-point energy additivity problems of hydrocarbons. In dealing with these problems, which stem from the empirical soil of structural organic chemistry, it is a significant procedure to em-

bed the square root function in the formula (for the zero-point energy $\mathscr{E}_{\text{zero}}$ of a linear oscillator)

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

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 functional version of the Asymptotic Linearity Theorem (ALT), or the Functional ALT, 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:

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

even if the square root function in equality (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 $\mathscr{E}_{\text{zero}}$ were given by

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

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:

$$E_N' = a'N + b' + o(1), \tag{4}$$

where a' and b' are real constants dependent on ξ (cf. section 4).

3. Globally-pertaining-type problems in the interdisciplinary research field between chemistry and modern mathematics

About the middle of the 1990s, after several communications between Prof. Fukui and the author, we reached the following recognition on the implication of the author's newest functional version of the ALT (cf. section 4):

1. From the new ALT and its associated theorems in the RST, one straightforwardly infers and recognizes that the additivity relations and other associated asymptotic relations which empirical chemists initially investigated in the analysis of thermodynamic and spectroscopic data on organic compounds are physical or physico-chemical manifestation of global structural mathematical phenomena. (From an earlier version of the ALT, this recognition had been obtained only through lengthy steps of mathematical inferences.)

2. One also recognizes that a molecular language is not sufficient in order to structurally elucidate the mechanism of this kind of manifestation. For this purpose, it is essential to *globally contextualize a molecular problem into a broader setting and view the physico-chemical problem we face from a more*

general standpoint from which it appears only as a single member of a class of related problems (cf. [4, p. 10]).

To explain the nature of the RST and its relationship with physico-chemical problems to which it is applied, it is instructive to recall the relationship between the theory of field extensions and the following well-known geometric problem from ancient Greece: "Is it possible to construct a cube with a volume equal to twice the volume of a given cube by using ruler and compass only?" This is the so-called Delian Problem; it originated in ancient Greece presumably with the task of constructing a cubical altar at Delos having twice the volume of the original cubical altar. This problem was (negatively) solved only in modern times within the general context of the theory of constructible numbers and field extensions. The Delian Problem is a typical example of a problem for whose solution "a global contextualization" is essential. Although the original problem is formulated in the language of Euclidean geometry, if one remains in the original context of the world of compass and ruler, a solution cannot be reached. However, if one begins to see beyond the original setting, directs one's attention to a broader perspective, and views this geometric problem from a more general standpoint from which it appears only as a single member of a class of related problems, then a right path to the solution of the problem will be found. Moreover, after reaching the solution via a general viewpoint and method, it often happens that solutions of chains of problems related to the original problem are discovered resulting in a theory with a new vista and a broad range of applications.

In the spring of 1995, the author discussed with Prof. Fukui about *a type of problem in chemistry for whose solution a global mathematical contextualization is essential*. For convenience sake, let us call this type of problem a ***globally-pertaining-type problem*** or a ***g-type problem***, for short. Fukui's problems of chemical kinetic cyclic networks and the problems of the zero-point energy additivity of his former teacher, Prof. Haruo Shingu (both sets of problems had been solved by the author) belonged to the category of g-type problems.

In our joint project and other researches, the author frequently came across problems of physico-chemical systems with fundamental equations which are analytically unsolvable. Many such problems deferring conventional approaches, which depended on analytic solutions of fundamental equations, turned out to be g-type problems that could be solved by global mathematical contextualizations. In the course of investigating g-type problems and their associated indigenous physico-chemical problems, one notices a complementary relationship between molecular languages and abstract structural languages of modern mathematics. The domains surrounding g-type problems in chemistry have rarely been investigated despite the fact that in those domains the two disciplines of chemistry and mathematics meet in profoundest manner.

In the author's report on the joint project prepared for Prof. Fukui in 1995, the author emphasized the importance and potentiality of investigations in the *peripheral research domains of g-type problems in chemistry* not only for our immediate joint work but for investigations of future generations, especially for investigations related to macromolecules, physico-chemical network systems, and biochemical network systems,

in the vast uncharted interdisciplinary regions between chemistry and modern mathematics. Prof. Fukui enthusiastically responded to this vision, which imparted a strong influence to the course of the joint project: the theoretical framework of the RST, which illuminates a variety of fundamental physico-chemical problems in a new global context, and solves g-type problems and their associated indigenous physico-chemical problems in a unifying manner, became central to our joint research towards the end of the 1990s (cf. [5] and references therein).

4. Concluding remarks

The reader is referred to article [6] in which a proof of the functional version of the Asymptotic Linearity Theorem mentioned in sections 2 and 3 is made public for the first time.

Acknowledgements

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