JOURNAL OF MATHEMATICS

THE UNIVERSITY OF TOKUSHIMA

VOLUME 38 2004

PUBLISHED BY THE
UNIVERSITY OF TOKUSHIMA
TOKUSHIMA, JAPAN

This journal is devoted to the publication of original research papers of our university staff and their joint researchers. One volume is published in each school year.

The journal is the new series of "Journal of Mathematics, Tokushima University" and "Journal of Gakugei, Tokushima University". "Journal of Gakugei, Tokushima University" was published from 1951 to 1966. "Journal of Mathematics, Tokushima University" was published from 1967 to 2000. The new series started in 2001. The volume number of the journal succeeds to that of the former series.

The contents of all papers of the journals from 1967 can be seen at the web site:

http://www-math.ias.tokushima-u.ac.jp/

Any communication with the journal should be addressed to:

The Editorial Committee of Journal of Mathematics The University of Tokushima 1-1, Minamijosanjima-cho Tokushima-shi, 770-8502 JAPAN

JOURNAL OF MATHEMATICS

THE UNIVERSITY OF TOKUSHIMA

VOLUME 38 2004

PUBLISHED BY THE
UNIVERSITY OF TOKUSHIMA
TOKUSHIMA, JAPAN

CONTENTS

SHIHARA, T.: Local Switching of Some Signed Graphs	• 1
TO, Y.: New Notions of Convergence of Directed Families of Points and Convergence of Filters	9
TO, Y. and Md Sharif UDDIN: New Quantum Theory and New Meaning of Specific Heat of a Solid	•17
TO, Y. and Md Sharif UDDIN: New Quantum Theory and New Meaning of Specific Heat of an Ideal Gas	29

Local Switching of Some Signed Graphs

By

Toru Ishihara

Faculty of Integrated Arts and Sciences, The University of Tokushima, Minamijosanjima, Tokushima 770-8502, JAPAN e-mail adress: ishihara@ias.tokushima-u.ac.jp (Received September 30, 2004)

Abstract

Some singed graphs are transformed to trees by a sequence of local switchings. We give some examples of such signed graphs to investigate when signed graphs are transformed to trees by local switching.

2000 Mathematics Subject Classification. 05C22

Introduction

Local switching of signed graphs is introduced by P. J. Cameron, J.J. Seidel and S. V. Tsaranov in [3]. Some singed Fushimi trees are tansformed to trees by a sequence of local switchings [4]. Signed cycles with odd parity are transformed to trees by a sequence of local switchings, but signed cycles with even parity can not be transformed to trees by no means [5]. What kinds of graphs are transformed to trees by a sequence of local switchings? It is important and intresting to give examples of signed graphs which are transformed to trees by a sequence of local switchings. In this note, we give rather simple examples of such signed graphs.

We state briefly basic facts about signed graphs. A graph G=(V,E) consists of an n-set V (the vertices) and a set E of unordered pairs from V (the edges). A signed graph (G,f) is a graph G with a signing $f:E \to \{1,-1\}$ of the edges. We set $E^+=f^{-1}(+1)$ and $E^-=f^{-1}(-1)$. For any subset $U\subseteq V$ of vertices, let f_U denote the signing obtained from f by reversing the sign of each edge which has one vertex in U. This defines on the set of signings an equivalence relation, called switching. The equivalence classes $\{f_U: U\subseteq V\}$ are the signed swithing classes of the graph G=(V,E).

Let $i \in V$ be a vertex of G, and V(i) be the neighbours of i. The local graph of (G, f) at i has V(i) as its vertex set, and as edges all edges $\{j, k\}$ of G for which f(i, j)f(j, k)f(k, i) = -1. A rim of (G, f) at i is any union of connected

2 Toru Ishihara

components of local graph at i. Let J be any rim at i, and let $K = V(i) \setminus J$. Local switching of (G, f) with respect to (i, J) is the following operation:(i) delete all edges of G between J and K; (ii) for any $j \in J$, $k \in K$ not previously joined, introduce an edge $\{j, k\}$ with sign chosen so that f(i, j)f(j, k)f(k, i) = -1; (iii) change the signs of all edges from i to J; (iv) leave all other edges and signs unaltered. Let Ω_n be the set of switching classes of signed graphs of order n. Local switching, applied to any vertex and any rim at the vertex, gives a relation on Ω which is symmetric but not transitive. The equivalence classes of its tansitive closure are called the clusters of order n.

1. Singed graphs which are transformed into trees by local switching

A connected graph G = (V, E) is called Fushimi tree if each block of G is a complete graph. A complete graph is a Fusimi tree of one block. Let a be a cut vertex of a Fushimi tree G. If G is divided exactly m connected components when the cut vertex a is deleted, in the present paper, we say that the Fushimi degree(simply F-degree) of the cut vertex a is m. A connected subgraph of a Fushimi tree G is called a sub-Fushimi tree if it consists of some blocks of G. A block of Fushimi tree is said to be pendant if it has only one cut vertex. It is evident that any Fushimi tree has at least two pendant blocks.

A signed Fushimi tree is called a Fushimi tree with positive sign (or simply a positive Fushimi tree) if we can switch all signs of edges into +1. A tree is always considered as a Fushimi tree with positive sign. A tree with only two leaves is said to be a line tree or simply a line in the present paper.

A k-cycle $C^k = (V, E)$, where $V = \{a_1, a_2, \dots, a_k\}$, $E = \{a_1a_2, a_2a_3, \dots, a_{k-1}a_k, a_ka_1\}$, will be denoted simply $C^k = a_1a_2 \cdots a_ka_1$. For signed cycles, there are two switching classes, which are distinguished by the parity or the balance, where the parity of a signed cycle is the parity of the number of its edges which carry a positive sign and the balance is the product of the signs on its edges [3]. In the forthcoming paper[5], we will show the following two theorems.

Theorem 1. Let G be a positive Fushimai tree whose any cut vertex has F-degree 2. We can transform G into a line tree by a sequence of local switchings.

Theorem 2. Let C^k be a k-cycle. Then, it is transformed to a tree by a sequence of local switchings if and only if its parity is odd.

We will show

Theorem 3.Let G = (V, E) be a signed graph with $V = \{a_1, a_2, \cdots, a_n, b_2, b_3, \cdots, b_{m-1}\}$ and $E = \{a_1a_2, a_2a_3, \cdots, a_{n-1}a_n, a_na_1, a_1b_2, b_2b_3, \cdots, b_{m-1}a_n\}$ Consider two cycles $A^n = a_1a_2 \cdots a_na_1$ and $B^m = a_1b_2 \cdots b_{m-1}a_na_1$. Then, the graph is transformed to a tree by a sequence of local switchings if and only if both parities of A^n and B^m are odd.

Proof. Assume that the parity of A^n is odd. By a sequence of local swithings, $(a_2, J = \{a_3\})$, $(a_3, J = \{a_4\})$, \cdots , $(a_{n-2}, J = \{a_{n-1}\})$, $(a_3, J = \{a_2\})$, $(a_4, J = \{a_3\})$, \cdots , $(a_{n-2}, J = \{a_{n-3}\})$, $(a_{n-1}, J = \{a_1\})$, we get a singned graph with edge set $E = \{a_2a_3, \cdots, a_{n-2}a_{n-1}, a_1b_2, b_2b_3, \cdots, b_{m-1}a_n, a_na_{n-1}, a_{n-1}a_1\}$. The parity of the cycle $a_1b_2b_3\cdots b_{m-1}a_na_{n-1}a_1$ is odd if and only if the parity of B^m is odd. In this case, this cycle is transformed to a tree by a sequence of local swithings. If the parity of A^n is even, by a sequence of local swithings, $(a_2, J = \{a_3\})$, $(a_3, J = \{a_4\})$, \cdots , $(a_{n-2}, J = \{a_{n-1}\})$, $(a_3, J = \{a_2\})$, $(a_4, J = \{a_3\}, \cdots)$, $(a_{n-2}, J = \{a_{n-1}\})$, we get a singned graph with edge set $E = \{a_1a_2, a_2a_3, \cdots, a_{n-2}a_{n-1}, a_{n-1}a_n, a_{n-2}a_1, a_{n-1}a_1, a_1b_2, b_2b_3, \cdots, b_{m-1}a_n\}$. As the sign of the edge $a_{n-1}a_n$ is -1, the cycle $a_1a_{n-1}a_na_1$ can not be transformed to a line.

2. Examples of signed graphs which are transformed into trees

```
For j = 3, 4, ..., 8, set signed graphs T_j = (V, E) as follows. V = \{a_1, a_2, ..., a_{j+2}\}, E^+ = \{a_i a_{i+1}, a_i a_{i+2} (i = 1, 2, ..., j), a_{j+1} a_{j+2}\}, E^- = \emptyset.
```

Then, we have

Proposition 4. The signed graphs T_3 , T_4 , T_5 , T_6 , T_7 are transformed to trees by a sequence of local switchings, but T_8 can not be transformed to a tree by a sequence of local switchings.

Proof. By a sequence of local switchings, $(a_3, J = \{a_2\})$, $(a_5, J = \{a_3\})$, from T_3 , we get a tree with edge set $E = \{a_1a_3, a_3a_5, a_4a_5, a_2a_5\}$.

By a sequence of local switchings, $(a_3, J = \{a_2\})$, $(a_5, J = \{a_3, a_6\})$, $(a_6, J = \{a_2\})$, from T_4 , we get a tree with edge set $E = \{a_1a_3, a_3a_5, a_4a_5, a_5a_6, a_2a_6\}$.

By a sequence of local switchings, $(a_3, J = \{a_2\})$, $(a_5, J = \{a_3, a_6, a_7\})$, $(a_7, J = \{a_5\})$, $(a_6, J = \{a_2\})$, from T_5 , we get a tree with edge set $E = \{a_1a_3, a_3a_5, a_5a_7, a_4a_7, a_7a_6, a_2a_6\}$.

By a sequence of local switchings, $(a_3, J = \{a_2\})$, $(a_5, J = \{a_3, a_6, a_7\})$, $(a_7, J = \{a_5\})$, $(a_8, J = \{a_7\})$, $(a_6, J = \{a_2\})$, $(a_2, J = \{a_8\})$, from T_6 , we get a tree with edge set $E = \{a_1a_3, a_3a_5, a_5a_8, a_8a_2, a_2a_6, a_2a_7, a_7a_4\}$.

By a sequence of local switchings, $(a_3, J = \{a_2\})$, $(a_5, J = \{a_3, a_6, a_7\})$, $(a_7, J = \{a_5, a_8, a_9\})$, $(a_9, J = \{a_7\})$, $(a_2, J = \{a_9\})$, $(a_4, J = \{a_8\})$, $(a_8, J = \{a_9\})$, from T_7 , we get a tree with edge set $E = \{a_1a_3, a_3a_5, a_5a_7, a_7a_9, a_9a_8, a_8a_4, a_8a_2, a_2a_6\}$.

By a sequence of local switchings, $(a_3, J = \{a_2\})$, $(a_5, J = \{a_3, a_6, a_7\})$, $(a_7, J = \{a_5, a_8\})$, $(a_2, J = \{a_7\})$, from T_8 , we get a signed graph with edge set $E^+ = \{a_1a_3, a_3a_5, a_5a_7, a_7a_9, a_9a_{10}, a_8a_{10}, a_8a_2, a_2a_7, a_2a_6\}$, $E^- = \{a_4a_7\}$. But this graph can not be transformed to a tree at all.

It is rather difficult to decide that a given signed graph can not be transformed to a tree by a sequence of local switchings. We describe some facts concerning with this point.

Remark. A signed cycle with even parity can not be transformed to a tree by a sequence of local switchings. Hence, we do not make a 3-cycle with even parity by local switching. Set $G_1 = (V, E)$ be a signed graph with vertex set $V = \{a_1, a_2, b_1, b_2, c\}$ and edge sets $E^+ = \{a_1b_1, a_1b_2, a_2b_1, a_2b_2, a_1c\}$, $E^- = \{a_2c\}$. By local switching at b_1 or b_2 , we get a 3-cycle with even parity, we can not apply it. By local switching at a_1 or a_2 , if b_1 is in J and b_2 is in K or if the reverse holds, we get a 3-cycle with even parity. Similarly, set $G_2 = (V, E)$ be a signed graph with vertex set $V = \{a_1, a_2, b_1, \cdots b_n, c\}$ and edge sets $E^+ = \{a_1b_1, \cdots, a_1b_n, a_2b_1, \cdots, a_2b_n, a_1c\}$, $E^- = \{a_2c\}$. We can no do local switching at any b_i , $(1 \le i \le n)$. If we apply local switching at a_1 or a_2 , all $b_i's$ must be in J or in K.

Let $Q_3=(V,E)$ be a signed graph with $V=\{a_1,a_2,\cdots,a_7,a_8\}, E^+=\{a_1a_2,a_1a_3,\ a_3a_4,a_3a_5,a_5a_6,a_5a_7,a_7a_8\}$ and $E^-=\{a_2a_4,a_4a_6,a_6a_8\}$. and $Q_4=(V,E)$ be a signed graph with $V=\{a_1,a_2,\cdots,a_9,a_{10}\}, E^+=\{a_1a_2,a_1a_3,a_3a_4,a_3a_5,a_5a_6,a_5a_7,a_7a_8,a_7a_9,a_{9}a_{10}\}$ and $E^-=\{a_2a_4,a_4a_6,a_6a_8,a_8a_{10}\}$.

Now we have

Proposition 5. The graph Q_3 is transformed to the graph T_6 , and hence to a tree, by a sequence of local switchings. The graph Q_4 is transformed to the graph T_8 by a sequence of local switchings. Hence this graph can not be transformed to a tree by a sequence of local switchings.

Proof. By a sequence of local switchings, $(a_1, J = \{a_2\})$, $(a_7, J = \{a_8\})$, $(a_6, J = \{a_5\})$, $(a_8, J = \{a_7\})$, we get T_6 from Q_3 . Similarly, by a sequence of local switchings, $(a_1, J = \{a_2\})$, $(a_{10}, J = \{a_9\})$, $(a_7, J = \{a_8\})$, $(a_6, J = \{a_5\})$, $(a_9, J = \{a_{10}\})$, $(a_8, J = \{a_7\})$, $(a_{10}, J = \{a_9\})$, we get T_8 from Q_4 .

Define QH_2 , QH_3 and QH_4 as follows;

 $QH_2 = (V, E), V = \{a_1, a_2, a_3, a_4, b_1, b_2\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_1b_1, a_3b_2\}, E^- = \{a_4a_1\};$

 $QH_3 = (V, E), V = \{a_1, a_2, a_3, a_4, b_1, b_2, b_3\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_1b_1, a_2b_2, a_3b_3\}, E^- = \{a_4a_1\};$

 $QH_4 = (V, E), V = \{a_1, a_2, a_3, a_4, b_1, b_2, b_3, b_4\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_1b_1, a_2b_2, a_3b_3, a_4b_4\}, E^- = \{a_4a_1\};$

We can prove

Proposition 6. The signed graphs QH_2, QH_3, QH_4 are transformed to trees by a sequence of local switchings.

Proof. By a sequence of local switchings, $(a_4, J = \{a_1\})$, $(a_3, J = \{a_1, b_2\})$, $(b_2, J = \{a_3\})$, from QH_2 , we get a tree with edge set $E = \{b_1a_1, a_1a_3, a_3b_2, b_2a_2, b_2a_4\}$. By a sequence of local switchings, $(a_4, J = \{a_1\})$, $(a_3, J = \{a_1, b_3\})$, $(b_3, J = \{a_3\})$, from QH_3 , we get a tree with edge set $E = \{b_1a_1, a_1a_3, a_3b_3, b_3a_2, b_3a_4, a_2b_2\}$. By a sequence of local switchings, $(a_2, J = \{a_3\})$, $(a_3, J = \{a_3\})$

 $\{a_2, a_4\}$, $(b_3, J = \{a_3\})$, $(b_2, J = \{a_4\})$, $(a_4, J = \{a_3, b_4\})$, $(b_4, J = \{a_4\})$, from QH_4 , we get a tree with edge set $E = \{b_1a_1, a_1a_3, a_3a_4, a_4b_4, b_4a_3, b_4b_2, b_3a_2\}$.

Set signed graphs $PH_1, PH_2, PH_3(1), PH_3(2), PH_4, PH_5$ as follows;

 $PH_1 = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_1, a_1b_1\}, E^- = \emptyset;$

 $PH_2 = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1, b_2\}, E = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_1, a_1b_1, a_2b_2\}, E^- = \emptyset;$

 $PH_3(1) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1, b_2, b_3\}, E = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_1, a_1b_1, a_2b_2, a_3b_3\}, E^- = \emptyset$;

 $PH_3(2) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1, b_2, b_3\}, E = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_1, a_1b_1, a_2b_2, a_4b_3\}, E^- = \emptyset;$

 $PH_4 = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1, b_2, b_3, b_4\}, E = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_1, a_1b_1, a_2b_2, a_3b_3, a_4b_4\}, E^- = \emptyset;$

 $PH_5 = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1, b_2, b_3, b_4, b_5\}, E = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_1, a_1b_1, a_2b_2, a_3b_3, a_4b_4, a_5b_5\}, E^- = \emptyset$;

Now we obtain

Proposition 7. The graphs PH_1 , PH_2 , $PH_3(1)$, $PH_3(2)$, PH_4 are transformed to trees, by a sequence of local switchings. The graph PH_5 can not be transformed to a tree by a sequence of local switchings.

Proof. By a sequence of local switchings, $(a_2, J = \{a_3\}), (a_3, J = \{a_4\}),$ $(a_4, J = \{a_5\}), (a_2, J = \{a_1, a_5\}), (a_3, J = \{a_4\}), \text{ from } PH_1, \text{ we get a tree with }$ edge set $E = \{b_1a_1, a_1a_2, a_2a_3, a_2a_5, a_3a_4\}$. By a sequence of local switchings, $(a_3, J = \{a_4\}), (a_4, J = \{a_3, a_5\}), (a_5, J = \{a_2\}), \text{ from } PH_2, \text{ we get a tree}$ with edge set $E = \{b_1a_1, a_1a_5, a_5a_4, a_2a_5, a_3a_4, a_2b_2\}$. By a sequence of local switchings, $(a_4, J = \{a_5\}), (a_5, J = \{a_3\}), (a_3, J = \{a_1, b_3\}), (b_3, J = \{a_3\}),$ from $PH_3(1)$, we get a tree with edge set $E = \{b_1a_1, a_1a_3, a_3b_3, b_3a_2, b_3a_5, a_4b_4, a_5b_4, a_5b_6, a_5b_7, a_5$ a_2b_2, a_5a_4 . By a sequence of local switchings, $(a_3, J = \{a_4\}), (a_4, J = \{a_4\})$ $\{a_2,b_3\}$), $(b_3,J=\{a_4\})$, $(a_5,J=\{a_2\})$, $(b_3,J=\{a_2,a_3\})$, $(a_3,J=\{b_3\})$, from $PH_3(2)$, we get a tree with edge set $E = \{b_1a_1, a_1a_5, a_5a_3, a_3b_3, a_3a_4, a_5a_5, a_5$ b_3a_2, a_2b_2 . By a sequence of local switchings, $(a_5, J = \{a_1\}), (a_4, J = \{a_3, a_5\}),$ $(b_4, J = \{a_4\}), (a_3, J = \{a_1, b_3\}), (b_3, J = \{a_3\}), (a_1, J = \{b_4\}), (a_3, J = \{b_4\}),$ from PH_4 , we get a tree with edge set $E = \{b_1a_1, a_1a_4, a_1a_3, a_3b_3, a_3b_4,$ b_3a_2, a_2b_2, b_4a_5 . By a sequence of local switchings, $(a_3, J = \{a_4\}), (a_5, J = \{a_5\}), (a_$ $\{a_4\}$), $(a_4, J = \{a_1, a_3, b_5\})$, $(b_4, J = \{a_4\})$, from PH_5 , we get a signed graph with edges sets $E^+ = \{b_2a_2, a_2a_4, a_2b_5, b_5b_3, b_5b_4, b_3a_4, b_3a_1, a_1b_1, a_1a_4, a_1b_4, a_1b_4, a_2b_5, b_3a_4, b_3a_4, b_3a_5, a_1b_4, a_1b_4, a_2b_5, b_3a_5, b_3a_5, b_3a_5, b_3a_6, b_3a_$ a_4a_5, a_5a_3, a_3b_4 , $E^- = \{a_4b_4\}$. We can not apply to this graph local switching at vertices a_1 , or a_2 , or b_3 , or b_5 and can not transform it to a tree.

Define H_1 , $H_2(1)$, $H_2(2)$, $H_2(3)$, $H_3(1)$, $H_3(2)$, $H_3(3)$ and $H_4(1)$, $H_4(2)$, $H_4(3)$, as follows;

 $H_1 = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1\}, E^- = \{a_6a_1\};$

 $H_2(1) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_2b_2\}, E^- = \{a_6a_1\};$

6 Toru Ishihara

```
H_2(2) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_5b_2\}, E^- = \{a_6a_1\};
```

 $H_2(3) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_4b_2\}, E^- = \{a_6a_1\};$

 $H_3(1) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_2b_2, a_3b_3\}, E^- = \{a_6a_1\};$

 $H_3(2) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_2b_2, a_4b_3\}, E^- = \{a_6a_1\};$

 $H_3(3) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_3b_2, a_5b_3\}, E^- = \{a_6a_1\};$

 $H_4(1) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_1b_1, a_2b_2, a_3b_3, a_4b_4\}, E^- = \{a_6a_1\};$

 $H_4(2) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_2b_2, a_4b_3, a_5b_4\}, E^- = \{a_6a_1\};$

 $H_4(3) = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1, b_2, b_3, b_4\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_1b_1, a_3b_2, a_4b_3, a_5b_4\}, E^- = \{a_6a_1\};$

Now we obtain

Proposition 8. The graphs H_1 , $H_2(1)$, $H_2(2)$, $H_2(3)$, $H_3(1)$, $H_3(2)$, $H_4(1)$ are transformed to trees, by a sequence of local switchings. The graphs $H_3(3)$, $H_4(2)$, $H_4(3)$ can not be transformed to trees by a sequence of local switchings.

Proof. By a sequence of local switchings, $(a_2, J = \{a_3\})$, $(a_3, J = \{a_4\})$, $(a_4, J = \{a_5\}), (a_3, J = \{a_2\}), (a_4, J = \{a_3\}), (a_5, J = \{a_1\}), \text{ from } H_1, \text{ we get }$ a tree with edge set $E = \{b_1a_1, a_1a_5, a_5a_6, a_5a_4, a_4a_3, a_3a_2\}$. By a sequence of local switchings, $(a_3, J = \{a_4\}), (a_4, J = \{a_5\}), (a_5, J = \{a_6\}), (a_4, J = \{a_3\}),$ $(a_5, J = \{a_4\}), (a_6, J = \{a_2\}), \text{ from } H_2(1), \text{ we get a tree with edge set}$ $E = \{b_1a_1, a_1a_6, a_6a_5, a_6a_2, a_5a_4, a_2b_2, a_4a_3\}$. By a sequence of local switchings, $(a_2, J = \{a_3\}), (a_3, J = \{a_4\}), (a_4, J = \{a_5\}), (a_3, J = \{a_2\}), (a_4, J = \{a_3\}),$ $(a_5, J = \{a_1, b_2\}), (b_2, J = \{a_5\}), \text{ from } H_2(2), \text{ we get a tree with edge set}$ $E = \{b_1a_1, a_1a_5, a_5b_2, b_2a_6, b_2a_4, a_4a_3, a_3a_2\}$. By a sequence of local switchings, $(a_2, J = \{a_3\})$, $(a_3, J = \{a_1\})$, $(a_6, J = \{a_5\})$, $(a_5, J = \{a_1\})$, from $H_2(3)$, we get a signed graph with edge sets $E^{+} = \{a_{1}a_{3}, a_{3}a_{4}, a_{4}a_{5}, a_{1}b_{1}, a_{3}a_{2}, a_{4}b_{2}, a_{5}a_{5}, a_{5}a$ a_5a_6 , $E^- = \{a_1a_5\}$ which is isomorphic to the singed graph QH_4 . Hence, $H_2(3)$ is transformed to a tree, by a sequence of local switchings. By a sequence of local switchings, $(a_6, J = \{a_5\}), (a_5, J = \{a_4\}), (a_4, J = \{a_3\}),$ $(a_5, J = \{a_6\}), (a_4, J = \{a_5\}), (a_3, J = \{a_1, b_3\}), (b_3, J = \{a_3\}), \text{ from } H_3(1),$ we get a tree with edge set $E = \{b_1a_1, a_1a_3, a_3b_3, b_3a_2, a_2b_2, b_3a_4, a_4a_5, a_5a_6\}.$ By a sequence of local switchings, $(a_6, J = \{a_5\})$, $(a_5, J = \{a_4\})$, $(a_5, J = \{a_5\})$ $\{a_6\}$), $(a_4, J = \{a_1, b_3\})$, $(b_3, J = \{a_4\})$, $(a_3, J = \{a_1\})$, $(a_1, J = \{b_1, b_3\})$, $a_5a_6, b_1a_4, b_1a_3, a_3a_2, a_2b_2$. By a sequence of local switchings, $(a_6, J = \{a_5\})$, $(a_5, J = \{a_4\}), (a_5, J = \{a_6\}), (a_4, J = \{a_1, b_4\}), (b_4, J = \{a_4\}), (a_4, J = \{a_4\}), (a_5, J = \{a_4\}), (a_5, J = \{a_6\}), (a_6, J = \{a_6\}), (a_6,$ $\{b_4\}$), $(a_1, J = \{a_2, b_4\})$, $(b_1, J = \{a_1\})$, $(a_4, J = \{a_1\})$, $(a_2, J = \{a_1, b_2\})$, $(b_2, J = \{a_2\})$, from $H_4(1)$, we get a tree with edge set $E = \{b_3a_3, a_3a_1, a_1a_2, a_1a_2, a_2a_1, a_2a_2, a_3a_1, a_3a_2, a_3a_1, a_3a_2, a_3a_1, a_3a_2, a_3a_2, a_3a_2, a_3a_2, a_3a_2, a_3a_3, a_3a_2, a_3a_2, a_3a_2, a_3a_2, a_3a_3, a_3a_2, a_3a_2,$ $a_2b_2, b_2a_4, b_2b_1, b_1b_4, b_4a_5, a_5a_6$.

The graphs $H_3(3)$, $H_4(2)$, $H_4(3)$ can not be transformed to trees by any sequences of local switchings at all.

Define C_{44} , C_{45} , C_{55} and H_{56} as follows;

 $C_{44} = (V, E), V = \{a_1, a_2, a_3, a_4, b_1\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_1, a_1b_1\}, E^- = \{a_3b_1\};$

 $C_{45} = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, b_1\}, E^+ = \{a_1a_2, a_3a_4, a_4a_5, a_5a_1, a_1b_1, a_3b_1\}, E^- = \{a_2a_3\};$

 $C_{55} = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, b_1\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_4a_5, a_5a_6, a_6a_1, a_1b_1, a_4b_1\}, E^- = \emptyset;$

 $C_{56} = (V, E), V = \{a_1, a_2, a_3, a_4, a_5, a_6, a_7, b_1\}, E^+ = \{a_1a_2, a_2a_3, a_3a_4, a_5a_6, a_6a_7, a_1b_1, a_4b_1\}, E^- = \{a_4a_5\};$

Then, we get

Proposition 9. The graphs C_{44} , C_{45} , C_{55} are transformed to trees, by a sequence of local switchings. The graph C_{56} can not be transformed to a tree by a sequence of local switchings.

Proof. By a sequence of local switchings, $(a_1, J = \{b_1\})$, $(b_1, J = \{a_1, a_3\})$, from C_{44} , we get a tree with edge set $E = \{b_1a_1, b_1a_2, b_1a_3, b_1a_4\}$. By a sequence of local switchings, $(a_1, J = \{b_1\})$, $(b_1, J = \{a_2, a_5\})$, $(a_5, J = \{a_3\})$, from C_{45} , we get a tree with edge set $E = \{b_1a_1, b_1a_2, b_1a_5, a_5a_3, a_5a_4\}$. By a sequence of local switchings, $(a_3, J = \{a_4\})$, $(a_5, J = \{a_6\})$, $(a_1, J = \{b_1\})$, $(b_1, J = \{a_2, a_6\})$, $(a_3, J = \{a_4\})$, $(a_5, J = \{a_6\})$, $(a_6, J = \{a_4\})$, $(a_2, J = \{a_4\})$, $(a_4, J = \{b_1\})$, from C_{55} , we get a tree with edge set $E = \{b_1a_1, b_1a_4, a_4a_2, a_4a_6, a_2a_3, a_6a_5\}$. The graph C_{56} can not be transformed to a tree by any sequences of local switchings at all.

References

- P. J. Cameron, J. M. Goethals, J. J. Seidel and E. E. Shult Line graphs, root systems, and Elliptic geometry, J. Algebra, 43(1976), 305-327.
- [2] D. M. Cvetkovic, M. Doob, I. Gutman and A. Torgasev, Recent results in the theory of graph spectra, Annals of Discrete Mathematics, 36(1991), North-Holand, Amsterdam.
- [3] P. J. Cameron, J. J. Seidel and S. V. Tsaranov, Signed Graphs, Root lattices, and Coxeter groups, J. Algebra, 164(1994), 173-209.
- [4] T. Ishihara, Signed graphs associated with the lattice A_n , J. Math. Univ. Tokushima, 36(2002), 1-6.
- [5] T. Ishihara, Local switiching of signed Fushimi tree (in preparation).

New Notions of Convergence of Directed Families of Points and Convergence of Filters

By

Yoshifumi Ito

Faculty of Integrated Arts and Sciences
The University of Tokushima
1-1, Minamijosanjima-cho
Tokushima-shi 770-8502, Japan
e-mail: y-ito@ias.tokushima-u.ac.jp
(Received November 4, 2003)

Abstract

In this article, we introduce new notions of convergence of directed families of points and convergence of filters in a general topological space where we do not necessarily assume any seperation axiom. Then we mention some new properties of them for a Hausdorff topological space.

2000 Mathematics Subject Classification. Primary 54A20.

Introduction

In a Hausdorff topological space which satisfies the first countability axiom, we can also define the topology by way of defining the limit of sequence of countable points. In a general topological space which does not necessarily satisfy the first countability axiom, we cannot define the topology by using sequences of countable points as above. In order to improve this, Moore-Smith indroduced the notion of limit of directed families of points which are not necessarily countable [1],[6],[7],[8]. On the other hand, H. Cartan and N. Bourbaki introduced the notion of limit of filters [2],[3],[4],[7]. Both define the equivalent topology.

Nevertheless, in the topological space where we do not assume any separation axiom, the meanings of both notions of limit in the sense of Moore-Smith and of limit of filters in the sense of Cartan-Bourbaki, are ambiguous. We cannot define their convergence to a certain point clearly. It occurs that they converge to more than one points simultaneously.

Therefore, in this article, we try to improve the notions of limit of directed families of points and of limit of filters so that these notions have reasonable

10

meaning in the topological space where we do not necessarily assume any separation axiom.

Even only for a Hausdorff topological space, we have some new results of convergence.

1. Convergence of sequences of points

Let X be a topological space. For a set S in X, \overline{S} denotes the closure of S. Here we give the definition of new notion of convergence of sequences of points.

Definition 1.1. Let X be a topological space. For a sequence $\{a_n\}$ in X and a nonempty set A of accumulation points of $\{a_n\}$, we say that the sequence $\{a_n\}$ converges to A if A satisfies the following conditions:

- (1) For any neighborhood U of A, there exists some natural number n_0 such that, for every $n \ge n_0$, $a_n \in U$ holds.
- (2) A is the maximum one which satisfies the condition (1).

We say that A is the limit set of $\{a_n\}$ or simply the limit and we denote it as $\lim_{n\to\infty} a_n = A$ or $a_n \to A(n\to\infty)$. We say that every point in A is a limit point of $\{a_n\}$. Then we have the following.

Corollary 1.2. We use the notation in Definition 1.1. Then the set A is calculated by the relation

$$\bigcap_{n=1}^{\infty} \overline{\bigcup_{m \ge n} \{a_m\}} = A.$$

Thus the limit set can be calculated by the set operation. If $A = \{a\}$, the limit point of $\{a_n\}$ is the same as considered until now. In this case, we say that $\{a_n\}$ converges to a in the narrow sense or mearly $\{a_n\}$ converges to a. But if A is composed of more than one points, then the notion of the limit of $\{a_n\}$ is of a new case. In this case, we say that $\{a_n\}$ converges to A in the wide sense. In any way, if the limit set A is composed of one or more than one points, we say that $\{a_n\}$ converges to A. After all the limit set A is the set of all accumulation points of $\{a_n\}$. But, conversely, the set of all accumulation points of $\{a_n\}$ is not necessarily the limit set of $\{a_n\}$. For example, we have the following.

Example 1 (Asaoka). If we put $a_n = 0$ for odd n and $a_n = n$ for even n, then the set of all accumulation points of $\{a_n\}$ is $\{0\}$. Then $\{a_n\}$ does not converges to $\{0\}$.

Here we have another example.

Example 2 (Ito). Let $\{a_n\}$ be the sequence obtained by lining all rational numbers up. Then $a_n \to \mathbf{R}$.

In this case, the limit set is not compact.

Then we have the following.

Proposition 1.3. A sequence of real numbers converges to a nonempty bounded closed set if and only if the sequence is bounded.

As for the convergence of sequence of real numbers in the narrow sense, we have the following.

Theorem 1.4 (Cauchy's Criterion of Convergence). A sequence $\{a_n\}$ of real numbers converges to a certain real number in the narrow sense if and only if, for any positive number ε , there exists some natural number N such that, for every m, n > N, the inequality $|a_m - a_n| < \varepsilon$ holds.

Let X be a topological space. We say that a sequence $\{a_n\}$ of points in X is precompact if the closure of the set of points $\{a_n; n \geq 1\}$ is a compact set in X.

Then we have the following.

Theorem 1.5. Let X be a Hausdorff topological space. Then a sequence $\{a_n\}$ of points in X converges to a certain nonempty compact set A if and only if $\{a_n\}$ is a precompact sequence. Then the limit set A is given by the relation

$$\bigcap_{n=1}^{\infty} \overline{\bigcup_{m \ge n} \{a_m\}} = A.$$

In the above theorem 1.5, the limit set A is not empty because the family of sets in $X \{a_m; m \geq n\}, (n = 1, 2, \cdots)$ has the finite intersection property.

Then we have the following.

Corollary 1.6. Let X be a compact Hausdorff topological space. Then every sequence $\{a_n\}$ of points in X converges to a certain nonempty compact set.

Proposition 1.7. In a Hausdorff topological space X, a sequence $\{a_n\}$ of points in X converges to a point a if, for any neighborhood U of a, there exists some natural number n_0 such that we have $a_n \in U$ for all n such as $n \ge n_0$.

Theorem 1.8. For the convergence of sequences in a topological space X, we have the following properties. We use the above notation.

- (S1) If $a_n = a$ for all n, we have $a_n \to \{a\}$.
- (S2) If $a_n \to A$ for the set A of all accumulation points of $\{a_n\}$, then, for any convergent subsequence $\{a_{k_m}\}$ of $\{a_n\}$, we have

$$\bigcup_{\{k_m\}}^{\infty} \bigcap_{n=1}^{\infty} \overline{\bigcup_{m \geq n} \{a_{k_m}\}} = A.$$

Here $\bigcup_{\{k_m\}}$ means the union for all subsequences $\{k_m\}$ of the sequence of all natural numbers such that $\{a_{k_m}\}$ converges.

(S3) Let $\{a_n\}$ be a sequence in X and A the set of all accumulation points of $\{a_n\}$. If, for any subsequence $\{a_{k_m}\}$ of $\{a_n\}$, we have $a_{k_m} \to A$, we have $a_n \to A$.

For a topological space X which is not Hausdorff, we have the following.

Example 3 (Asaoka). Let X be a set $\{0,1\}$ of 0 and 1. Assume that all open sets in X are \emptyset , $\{1\}$ and $X = \{0,1\}$. Then X becomes a topological space which is not Hausdorff. In X, all closed sets are \emptyset , $\{0\}$ and X. Then if we consider a sequence $\{a_n\}$ such as $a_n = 1$ for all $n \ge 1$, the set of all accumulation points of $\{a_n\}$ is X and $\{a_n\}$ converges to X. In this case, we have,

$$\bigcap_{n=1}^{\infty} \overline{\bigcup_{m \ge n} \{a_m\}} = \{0,1\} = X$$

If we consider a sequence $\{a_n\}$ such as $a_n=0$ for all $n\geq 1$, the set of all accumulation points of $\{a_n\}$ is $\{0\}$ and $\{a_n\}$ converges to $\{0\}$. In this case, we have

$$\bigcap_{m=1}^{\infty} \overline{\bigcup_{m \geq n} \{a_m\}} = \overline{\{0\}} = \{0\}.$$

But the limit set is not the intersection of all neighborhoods of the limit set.

Let X and Y be two topological spaces. In general, we assume that f is a mapping from a certain subset D of X to Y. Let A be a certain set of accumulation points of D. For a certain set B of accumulation points of the set $\{f(x); x \in D\}$, we say that $\lim_{x \to A} f(x) = B$ or $f(x) \to B$ as $x \to A$ if, for any neighborhood V of B, there exists some neighborhood U of A such that we have $f((U \cap D) \setminus A) \subset V$. $\lim_{x \to A} f(x) = B$ is equivalent to say that, for any sequence $\{a_n\}$ in $D \setminus A$ such as $a_n \to A$, B is the union of all limit sets $\lim_{n \to \infty} f(a_n)$. If we have $B = \{b\}$ for a given f and $A = \{a\}$ in X, b is said to be the limit value of f(x) as $x \to a$ or the limit of f(x) as $x \to a$.

In Definition 1.1, we give the definition of new notion of convergence of sequences of points for a general topological space.

2. Covergence of directed families of points

In this section, we consider the new notions of convergence of directed families of points.

Definition 2.1. Let X be a topological space, $\{x_{\alpha}\}_{{\alpha}\in A}$ a directed family of points in X and A a nonempty set of accumulation points of $\{x_{\alpha}\}_{{\alpha}\in A}$. Then we say that $\{x_{\alpha}\}_{{\alpha}\in A}$ converges to A if A satisfies the following conditions:

- (1) For any neighborhood U of A, there exists some $\alpha_0 \in \mathcal{A}$ such that, for every $\alpha \geq \alpha_0$, $x_{\alpha} \in U$ holds.
- (2) A is the maximum one which satisfies the condition (1). Then we denote this as $x_{\alpha} \to A(\alpha \in \mathcal{A})$ or simply $x_{\alpha} \to A$. Then we have the following.

Corollary 2.2. We use the notation of Definition 2.1. Then the set A is calculated by the relation

$$\bigcap_{\alpha_0 \in \mathcal{A}} \overline{\bigcup_{\alpha \ge \alpha_0} \{x_\alpha\}} = A.$$

When A = N, this is nothing but the convergence of a sequence of points $\{x_n\}$ in X. The limit set A is the certain set of accumulation points of $\{x_\alpha\}_{\alpha\in\mathcal{A}}$. But, conversely, any set of accumulation points of $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ is not necessarily the limit set of $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$.

Then we have the following.

Theorem 2.3. Let X be a Hausdorff topological space. Then a directed family of points $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ in X converges to a certain nonempty compact set A if there exists some $\alpha_0 \in \mathcal{A}$ such that the closure of the set of points $\{x_\alpha; \alpha \geq \alpha_0\}$ is a compact set in X.

Corollary 2.4. Let X be a compact Hausdorff topological space. Then every directed family of points $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ in X converges to a certain nonempty compact set.

Proposition 2.5. Assume that X is a Hausdorff topological space. Then a directed family of points $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ in X converges to a point x if, for any neighborhood U of x, there exists some $\alpha_0 \in A$ such that $x_\alpha \in U$ for all $\alpha \geq \alpha_0$.

Theorem 2.6. Let X be a topological space. Let $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ be a directed family of points in X. We use the above notation. Then we have the following:

- (D1) If $x_{\alpha} = x$ for all α , $x_{\alpha} \to \{x\}$ holds.
- (D2) If $x_{\alpha} \to A$ for a nonempty set A of accumulation points of $\{x_{\alpha}\}_{{\alpha} \in \mathcal{A}}$ and $\{y_{\beta}\}\$ is a cofinal directed subfamily of $\{x_{\alpha}\}, y_{\beta} \to A$ holds.
- (D3) If a directed subfamily $\{y_{\beta}\}$ of $\{x_{\alpha}\}$ has always a converginy directed subfamily $\{z_{\gamma}\}$ and $z_{\gamma} \to A$ for a nonempty set A of accumulation points of $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ and A is determined independently of the choice of $\{y_{\beta}\}$, then $x_{\alpha} \to A$ holds.
- (D4) Assume that $x_{\alpha} \to A(\alpha \in A)$ holds for a nonempty set A of accumulation points of $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$ and, for each ${\alpha}\in\mathcal{A}$, $y_{{\alpha}{\beta}}\to x_{\alpha}({\beta}\in\mathcal{B}_{\alpha})$ holds. Then we define a directed set of direct product $C = A \times \prod B_{\alpha}$

and define the projections $p: \mathcal{C} \to \mathcal{A}$ and $p_{\alpha}: \mathcal{C} \to \mathcal{B}_{\alpha}$. If we define $z_{\gamma} = y_{\alpha\beta}$ where $\gamma \in \mathcal{C}, \alpha = p(\gamma), \beta = p_{\alpha}(\gamma)$ hold, then $z_{\gamma} \to A$ holds.

We denote the limit set of x_{α} as $\lim x_{\alpha}$ or $\lim_{\alpha \in \mathcal{A}} x_{\alpha}$. We say that a point in $\lim x_{\alpha}$ is a limit point of x_{α} . $x_{\alpha} \to A$ is equivalent to say that A is the intersection of the closures of sets, each of which is composed of any cofinal directed subfamily of $\{x_{\alpha}\}.$

If a directed subfamily $\{y_{\beta}\}\$ of $\{x_{\alpha}\}\$ is not cofinal with $\{x_{\alpha}\}\$, then some accumulation points of $\{y_{\beta}\}\$ does not belong to the limit set of $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$.

3. Convergence of filters

Definition 3.1. Let X be a topological space and Φ a filter in X and A a nonempty set of accumulation points of every $F \in \Phi$. Then we denote a system of all neighborhoods of A by $\mathfrak{U}(A)$. We say that the filter Φ converges to the set A if A satisfies the following conditions:

(1) $\Phi \supset \mathfrak{U}(A)$ holds.

(2) A is the maximum one which satisfies the condition (1).

Then we denote this $\Phi \to A$ and we say that the set A is the limit set of Φ or simply the limit of Φ . If the filter generated by a filter basis \mathcal{B} converges to A, then we say that the filter basis \mathcal{B} converges to A.

Then we have the following.

Corollary 3.2. We use the notation of Definition 3.1. Then the set A is calculated by the relation

$$\bigcap_{F\in\Phi}\overline{F}=A.$$

Namely, the limit or the limit set can be obtained by the set operation.

Then we have the following.

Theorem 3.3. Let X be a Hausdorff topological space. Then a filter Φ converges to a certain nonempty compact set A if there exists some element F of Φ such that \overline{F} is compact.

Corollary 3.4. Let X be a compact Hausdorff topological space. Then every filter Φ converges to a certain nonempty compact set A.

Proposition 3.5. Assume that X is a Hausdorff topological space. Then a filter Φ converges to a point x if $\Phi \supset \mathfrak{U}(x)$ holds.

Theorem 3.6. Let X be a topological space. We use the above notation. Then we have the following:

- (L1) For a point a in X, a filter $\Phi_a = \{B; a \in B \subset X\}$ converges to $\overline{\{a\}}$.
- (L2) If two filters Φ and Ψ satisfy the conditions $\Phi \to A$ and $\Psi \supset \Phi$, then $\Psi \to A$ holds.
- (L3) If, for a family of filters $\{\Phi_{\lambda}\}$, every $\Phi_{\lambda} \to A$ holds, then $\cap_{\lambda} \Phi_{\lambda} = \Phi$ $\to A$ holds.
- (L4) Assume the following (i) \sim (iii). (i) $X \supset Y$, (ii) For every nonempty closed set B in Y, there exists a filter Φ_B in X such that $\Phi_B \to B$ and (iii) a filter Ψ in X generated by a filter basis $\mathcal B$ in Y converges to A. Then $\bigcup_{B \in \mathcal B} (\bigcap_{\emptyset \neq C = \overline{C} \subset \mathcal B} \Phi_C)$ converges also to A.

4. Relations between various convergences

In this section, we mention relations of various convergences.

We have the following theorems.

Theorem 4.1. Let X be a topological space.

- (1) For a directed family of points $\{x_{\alpha}\}_{{\alpha}\in\mathcal{A}}$, the family of subsets in X $\{\{x_{\alpha}; {\alpha}\in\mathcal{A}, {\alpha}\geq{\alpha}_0\}; {\alpha}_0\in\mathcal{A}\}$ is a filter basis in X.
- (2) For the filter Φ generated by the filter basis defined in (1), $x_{\alpha} \to A$ if and only if $\Phi \to A$.

Then Theorem 3.6 induces Theorem 2.6 and Corollary 3.5 induces Corollary 2.5.

Let X and Y be two topological spaces and $f: X \to Y$ a function (or mapping) and D the domain of f. Let A be a certain set of accumulation points of D. Then $\{f(U \cap D \setminus A); U \in \mathfrak{U}(A)\}$ becomes a filter basis in Y, where $\mathfrak{U}(A)$ means a system of neighborhoods of A. Further assume $U \cap D \setminus A \neq \emptyset$. Let Φ be the filter generated by the above filter basis. Then $f(x) \to B$ as $x \to A$ if and only if $\Phi \to B$.

By the above, the various convergences mentioned until now can be represented by the convergence of filters.

5. Convergence and topology

In a topological space, we could define the notions of convergence of directed families of points and of filters. Conversely, we can introduce a topology using the notion of convergence. We have the following.

Theorem 5.1. Assume that, in a topological space X, all filters are determined to converge or not and that the properties (L1) \sim (L4) are satisfied in X. Then, if we define the convergence of directed families of points in X as above, then the properties (D1) \sim (D4) are satisfied.

Thereby, if we define the union of the limit sets of all directed families $\{x_{\alpha}\}\$ such as $x_{\alpha}\in A$ to be \overline{A} , then the axiom of closures is satisfied for \overline{A} . Thereby we can define a topology of X. With respect to this topology, we have the following properties:

- (i) $B = \overline{B} \subset \overline{A}$ if and only if there exists $\{x_{\alpha}\}(x_{\alpha} \in A)$ such that $x_{\alpha} \to B$.
- (ii) U is a neighborhood of $A = \overline{A}$ if and only if, for any $\{x_{\alpha}\}$ such as x_{α} $\rightarrow A$, there exists to α_0 such that $\{x_{\alpha}; \alpha \geq \alpha_0\} \subset U$ holds.

When we define the convergence of directed families of points by way of the topology, these properties (i) and (ii) as above hold also. Then if we define the new topology by the processes: the topology \rightarrow the convergence of filters \rightarrow the convergence of directed families of points \rightarrow the new topology, the new topology coincides with the first given topology. Further, if we define the new notion of convergence of filters (or directed families of points) starting from the given notion of convergence of filters (or directed families of points), this also coincides with the first given one. By the above, to give the notion of topology and to give the notion of convergence of filters or directed families of points are entirely identical.

When we mention the notions in a topological space using the terminology of convergence, we have the following. The fact that a topological space X is compact is identical with the fact that all perfect directed families of points converge. This is also identical with the fact that all ultrafilters converge. Further this is also identical with the fact that, for every directed family of points, there exists a converging directed subfamilies of points.

Theorem 5.2. Let X and Y be two topological space and $f: X \to Y$ a mapping and D the domain of f. In order that f is continuous at a certain nonempty closed set $A(\subset D)$ of accumulation points of D, it is necessary and sufficient that each one of the following conditions (i) \sim (iii) is satisfied:

- (i) For every directed family of points $\{x_{\alpha}\}$ such as $x_{\alpha} \to A$, we have $f(x_{\alpha}) \to f(A)$.
- (ii) For every filter Φ such as $\Phi \to A$, we have $f(\Phi) = \{f(M); M \in \Phi\} \to f(A)$.
- (iii) In the sense of the limit of values of the function f, if $x \to A$ holds, we have $f(x) \to f(A)$.

The definition of the topology on the basis of the notion of convergence was originated by M. Fréchet[5]. By using the notion of convergence of filters or directed families of points, the correspondence of the convergence and the topology in a topological space becomes perfect. For that purpose, E. H. Moore and H. L. Smith introduced the notion of convergence of directed families of points[8]. Nevertheless, the definition of Moore-Smith is ambiguous in the case other than the case of Hausdorff topological space. Therefore, in this article, we improved these notions as metioned before.

References

- G. Birkhoff, Moore-Smith convergence in general topology, Ann. of Math., 38(1937), 39-56.
- [2] N. Bourbaki, Topologie générale, chap. 1, Actualités Sci. Indust., Hermann, 1940, 4th ed. 1965.
- H. Cartan, Théorie des filtres, C. R. Acad. Sci. Paris, 205(1937), 595-598.
- [4] H. Cartan, Filtres et ultrafiltres, C. R. Acad. Sci. Paris, 205(1937), 777-779.
- [5] M. Fréchet, Sur quelques points du calcul fonctionnel, Rend. Circ. Mat. Palermo, 22(1906), 1-74.
- [6] K. Ito, Iwanami sügaku jiten, 3rd ed, Iwanami Shoten, 1985. (in Japanese).
- [7] Y. Kawada and Y. Mimura, Introduction to modern mathematies, II, Iwanami Shoten, 1965. (in Japanese).
- [8] E. H. Moore and H. L. Smith, A general theory of limits, Amer. J. Math., 44(1922), 102-121.

New Quantum Theory and New Meaning of Specific Heat of a Solid

By

Yoshifumi Ito and Md Sharif Uddin

Department of Mathematical and Natural Sciences, Faculty of Integrated Arts and Sciences, The University of Tokushima, Tokushima 770-8502 Japan

and

Department of Mathematics, Jahangirnagar University, Savar, Dhaka-1342
Bangladesh

e-mail: y-ito@ias.tokushima-u.ac.jp msharifju@yahoo.com (Received December 4, 2003)

Abstract

In this article, we consider the specific heat of a monatomic solid in the view point of the new quantum theory. Thereby we can clarify a new meaning of specific heat. At last, we give a new meaning of the Debye model of specific heat of a solid.

2000 Mathematics Subject Classification. Primary 82B10; Secondary 81Q05

Introduction

In this article, we consider the molar heat of a monatomic solid in the view point of the new quantum theory. We get a reasonable explanation of the molar heat of a monatomic solid. It gives a new explanation of the Debye's model of specific heat of a solid. In the old quantum theory, there are Einstein's theory of specific heat at 1907 and Debye's theory of specific heat at 1912. But they are different from ours with respect to the standing point. The new quantum theory was originated by Y. Ito [2]-[4] at 1998-2000. As for the new quantum theory, we refer the papers [1]-[8] of the references.

1. Axiom of the new quantum theory

Here we remember the axiom of the new quantum theory which is the basis of this article. As for this we refer Ito[2], [3], Ito-Kayama[6], [7] and Ito-Kayama-Kamoshita[8].

Axiom I (quantum system). A quantum system Ω is defined to be a probability space (Ω, \mathbf{B}, P) . Here Ω is a set of microparticles ρ , \mathbf{B} is a σ -algebra of subsets of Ω and P is a completely additive probability measure on \mathbf{B} .

Axiom II (quantum state). The (quantum) state of a quantum system $\Omega = \Omega(B, P) (= (\Omega, B, P))$ is defined to be the state of the quantum probability distribution of the position variables $r(\rho)$ and the momentum variables $p(\rho)$ of microparticles ρ which compose the quantum system. Here, we consider the orthogonal coordinate systems of n-dimensional Euclidean space \mathbb{R}^n and its dual space \mathbb{R}_n . Here we put n = dM, where d denotes the dimension of the physical space and M denotes the number of particles which compose one elementary event ρ .

(II₁) The quantum probability distribution of the position variables $r = r(\rho)$ is determined by an L^2 -density ψ on \mathbb{R}^n such that it satisfies the condition

$$\int_{m{
ho}n} |\psi(m{r})|^2 dm{r} = 1,$$

where $d\mathbf{r}$ denotes the Lebesgue measure on \mathbf{R}^n .

(II₂) The quantum probability distribution of the momentum variable $p = p(\rho)$ is determined by the Fourier transform $\hat{\psi}$ of ψ . Here we put

$$\hat{\psi}(\mathbf{p}) = (2\pi\hbar)^{-n/2} \int \psi(\mathbf{r}) e^{-i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{r},$$

$$\psi(\mathbf{r}) = (2\pi\hbar)^{-n/2} \int \hat{\psi}(\mathbf{p}) e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{p},$$

$$\mathbf{r} = (x_1, x_2, \cdots, x_n), \ \mathbf{p} = (p_1, p_2, \cdots, p_n),$$

$$\mathbf{p} \cdot \mathbf{r} = p_1 x_1 + p_2 x_2 + \cdots + p_n x_n.$$

Here we put $\hbar = \frac{h}{2\pi}$ and h is the Planck constant. (II₃) We put

$$\mu(A) = \int_A |\psi(m{r})|^2 dm{r}$$

for a Lebesgue measurable set A in \mathbb{R}^n . Then we assume that

$$P(\{\rho\in\Omega; \boldsymbol{r}(\rho)\in A\})=\mu(A).$$

Then, $\mu(A)$ denotes the probability of the event " $r(\rho)$ belongs to A". Thereby, we have the probability space $(\mathbf{R}^n, \mathcal{M}_n, \mu)$, where \mathcal{M}_n is the family of all Lebesgue measurable sets in \mathbf{R}^n .

(II4) We put

$$u(B) = \int_B |\hat{\psi}(oldsymbol{p})|^2 doldsymbol{p}$$

for a Lebesgue measurable set B in R_n . Then we assume that

$$P(\{\rho \in \Omega; p(\rho) \in B\}) = \nu(B).$$

Then, $\nu(B)$ denotes the probability of the event " $p(\rho)$ belongs to B". Thereby, we have the probability space $(\mathbf{R}_n, \mathcal{N}_n, \nu)$, where \mathcal{N}_n is the family of all Lebesgue measurable sets in \mathbf{R}_n .

Axiom III (motion of a quantum system). We call the time evolution of the L^2 -density $\psi(\mathbf{r},t)$ of a quantum system the motion of the quantum system. The law of the motion of the quantum system is described by the Schrödinger equation. We call the Schrödinger equation the equation of motion of the quantum system.

A Schrödinger equation is defined by an equation of the form

$$i\hbarrac{\partial\psi}{\partial t}=H\psi.$$

We call the operator H a Hamiltonian, which has a various form corresponding to each quantum system. H is assumed to be a self-adjoint operator on some Hilbert space \mathcal{H} .

2. Physical setting of the system and the problem

We consider a monatomic solid spreaded infinitely. Every atom of the solid is oscillating by the cause of heat. Approximately we may consider every atom as a harmonic oscillator near the equilibrium point. We wish to consider the specific heat of this solid.

We consider the specific heat as molar heat. It is 3N times of the specific heat with respect to one degree of freedom of oscillation, where N is the Avogadro's number.

3. Setting of the mathematical model

We use the notation in chapter 1. Let $\Omega = \Omega(\boldsymbol{B}, P)$ be the probability space which represents the quantum system considered here. An elementary event ρ of Ω is a harmonic oscillator which oscillates harmonically in the 1-dimensional Euclidean space \boldsymbol{R}^1 . Here we consider one degree of freedom of the 3-dimensional harmonic oscillator. Then we denote the position variable of a harmonic oscillator ρ by $x = x(\rho)$, and the momentum variable of ρ by

 $p = p(\rho)$. Here we put n = dM = 1 because the space dimension is d = 1, the number of harmonic oscillators which compose an elementary event ρ is M = 1. The variable x changes in the space R^1 and the variable p changes in its dual space R_1 . Then by the axiom II, the L^2 -density $\psi(x)$ determines the quantum probability distribution law of the position variable x and its Fourier transform $\hat{\psi}(p)$ determines the quantum probability distribution law of the momentum variable p. The total energy of each harmonic oscillator p is determined by the classical mechanics. Its value is

$$\frac{1}{2m}p(\rho)^2 + \frac{m}{2}\omega(\rho)^2x(\rho)^2.$$

Here the first term is the kinetic energy of the harmonic oscillator ρ and the second term is the potential energy of the harmonic oscillator ρ . $\omega(\rho)$ is the angular frequency of the harmonic oscillator ρ and m is the mass of the harmonic oscillator.

This energy variable is considered as a quantum random variable defined on the probability space Ω which represents the quantum system. The evaluation of the expectation value of this energy variable, namely the energy expectation value, is carried out by using the axiom II.

Namely we use the relation

$$egin{aligned} P(\{
ho\in\Omega;x(
ho)\in A\}) &= \int_A |\psi(x)|^2 dx, \ P(\{
ho\in\Omega;p(
ho)\in B\}) &= \int_B |\hat{\psi}(p)|^2 dp \end{aligned}$$

for a subset A in \mathbb{R}^1 and a subset B in \mathbb{R}_1 . Further we assume that the $\omega(\rho)$ is a random variable whose probability distribution law is given by a probability density $D(\omega)$ such as

(1)
$$0 \le D(\omega) \le \infty$$
.
(2) $\int_0^\infty D(\omega)d\omega = 1$.
(3) $\int_0^\infty \omega D(\omega)d\omega < \infty$.

Then we have the energy expectation value \overline{E} :

$$\begin{split} \overline{E} &= E\left[\frac{1}{2m}p(\rho)^2 + \frac{1}{2}m\omega(\rho)^2x(\rho)^2\right] \\ &= \int_0^\infty E\left[\frac{1}{2m}p(\rho)^2 + \frac{1}{2}m\omega(\rho)^2x(\rho)^2; \omega(\rho) = \omega\right]D(\omega)d\omega. \end{split}$$

Then, for an admissible L^2 -density ψ , we have

$$E\left[\frac{1}{2m}p(\rho)^2 + \frac{1}{2}m\omega(\rho)^2x(\rho)^2; \omega(\rho) = \omega\right]$$

$$\begin{split} &= E\left[\frac{1}{2m}p(\rho)^2 + \frac{1}{2}m\omega^2x(\rho)^2\right] \\ &= E\left[\frac{1}{2m}p(\rho)^2\right] + E\left[\frac{1}{2}m\omega^2x(\rho)^2\right] \\ &= \int \frac{1}{2m}p^2|\hat{\psi}(p)|^2dp + \int \frac{1}{2}m\omega^2x^2|\psi(x)|^2dx \\ &= \int \left\{\frac{\hbar^2}{2m}\left|\frac{d\psi(x)}{dx}\right|^2 + \frac{1}{2}m\omega^2x^2|\psi(x)|^2\right\}dx. \end{split}$$

Here we use the Plancherel formula for Fourier transformation. Here we denote this conditional energy expectation value by

$$J[\psi;\omega] = \int \left\{ \frac{\hbar^2}{2m} \left| \frac{d\psi(x)}{dx} \right|^2 + \frac{1}{2} m \omega^2 x^2 |\psi(x)|^2 \right\} dx.$$

We call $J[\psi; \omega]$ the conditional energy functional.

Here we assert the following principle.

Principle I (variational principle). The true physical state of the quantum system is realized as a state such that the energy expectation value of the quantum system takes its stationary value under some conditions.

From this principle, we can choose the true L^2 -density for each quantum system. So that we consider the following problem.

Problem 1. Find out the L^2 -density ψ for which conditional energy expectation value $J[\psi;\omega]$ takes its stationary value under the condition that

$$\int |\psi(x)|^2 dx = 1.$$

4. Mathematical analysis

Solving the problem 1 in chapter 3 under the condition that $\omega(\rho) = \omega$ is fixed by the way similar to Ito-Kayama-Kamoshita [8], we have the Schrödinger equation

$$\left(-rac{\hbar^2}{2m}rac{d^2}{dx^2}+rac{1}{2}m\omega^2x^2
ight)\psi(x)=\mathcal{E}\psi(x)$$

as the Euler equation. Here \mathcal{E} is the Lagrange's unknown constant. Namely, the function ψ which is the solution of the problem is obtained as a solution of the above Schrödinger equation. As solutions of the above eigenvalue problem, we have the eigenfunctions $\psi_n(x)$ corresponding to the eigenvalues \mathcal{E}_n for $n = 0, 1, 2, \cdots$.

Namely we have

$$\mathcal{E}_n = \left(n + \frac{1}{2}\right)\hbar\omega,$$

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!} \sqrt{\frac{1}{\pi} \cdot \frac{m\omega^2}{\hbar}} H_n\left(\sqrt{\frac{m}{\hbar}} \omega x\right) \cdot \exp\left[-\frac{1}{2} \frac{m}{\hbar} \omega^2 x^2\right]},$$

$$(n = 0, 1, 2, \cdots).$$

Here we put

$$H_n(x) = (-1)^n e^{x^2} \cdot \frac{d^n}{dx^n} e^{-x^2}.$$

Then we have

$$J[\psi_n;\omega]=\left(n+rac{1}{2}
ight)\hbar\omega, (n=0,1,2,\cdots).$$

Let $S(R^1)$ be the space of all rapidly decreasing C^{∞} -functions on \mathbb{R}^1 . Then for the system of eigenfunctions $\{\psi_n\}_{n=0}^{\infty}$, we have the following. (see Kuroda [10], Chapter 4).

Theorem 1. The system of eigenfunctions $\{\psi_n\}_{n=0}^{\infty}$ is a complete orthonormal system in $S(R^1)$.

By virtue of theorem 1, for any $\psi \in \mathcal{S}(\mathbb{R}^1)$, there exists only one sequence $\{c_n\}_{n=0}^{\infty}$ of complex numbers such that we can expand $\psi(x)$ as $\psi(x) = \infty$

 $\sum_{n=0}^{\infty} c_n \psi_n(x)$. Here this series converges also in the space $L^2(\mathbf{R}^1)$.

If the true physical state of the total quantum system Ω is determined by some L^2 -density $\psi(x)$ at the initial time point, then we can expand $\psi(x)$ by using $\{\psi_n\}_{n=0}^{\infty}$ as above. Then we have the conditional energy expectation value

$$J[\psi;\omega] = \sum_{n=0}^{\infty} |c_n|^2 J[\psi_n;\omega] = \sum_{n=0}^{\infty} |c_n|^2 \left(n + \frac{1}{2}\right) \hbar \omega.$$

Further, since the function $\psi(x)$ satisfies the normalization condition $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$, we have

$$\sum_{n=0}^{\infty} |c_n|^2 = 1.$$

Then the sequence $\{c_n\}_{n=0}^{\infty}$ is a rapidly decreasing sequence. (see Kuroda [10], p.81). Here, using the experimental facts, we assume

$$|c_n|^2 = (1 - \exp\left[-\frac{\hbar\omega}{k_BT}\right])(\exp\left[-\frac{\hbar\omega}{k_BT}\right])^n, (n = 0, 1, 2, \cdots).$$

Here T is the absolute temperature and k_B is the Boltzmann constant. Therefore we have the conditional energy expectation value

$$J[\psi;\omega] = \sum_{n=0}^{\infty} |c_n|^2 J[\psi_n;\omega]$$

$$\begin{split} &= \left(1 - \exp\left[-\frac{\hbar\omega}{k_BT}\right]\right)\hbar\omega\sum_{n=0}^{\infty}\left(\frac{1}{2} + n\right)\left(\exp\left[-\frac{\hbar\omega}{k_BT}\right]\right)^n \\ &= \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\exp\left[\frac{\hbar\omega}{k_BT}\right] - 1} \end{split}$$

The L^2 -density $\psi(x)$ at the initial time point can be expanded as follows:

$$\psi(x) = \sum_{n=0}^{\infty} c_n \sqrt{\frac{1}{2^n n!} \sqrt{\frac{1}{\pi} \cdot \frac{m\omega^2}{\hbar}}} H_n\left(\sqrt{\frac{m}{\hbar}} \omega x\right) \cdot \exp\left[-\frac{1}{2} \frac{m}{\hbar} \omega^2 x^2\right].$$

Here we follow the method of separation of variables in the reverse. At first we consider the function

$$\psi_n(x,t) = \psi_n(x) \exp \left[-i rac{\mathcal{E}_n}{\hbar} t
ight].$$

Then we differentiate with respect to the time variable t and we have

$$i\hbar\frac{\partial\psi_n(x,t)}{\partial t}=\mathcal{E}_n\psi_n(x)\exp\left[-i\frac{\mathcal{E}_n}{\hbar}t\right].$$

Here we put

$$H = -rac{\hbar^2}{2m}rac{d^2}{dx^2} + rac{m}{2}\omega^2x^2.$$

Then we have

$$H\psi_n(x) = \mathcal{E}_n\psi_n(x), (n = 0, 1, 2, \cdots).$$

Thereby we have

$$i\hbar rac{\partial \psi_n(x,t)}{\partial t} = H\psi_n(x) \cdot \exp\left[-irac{\mathcal{E}_n}{\hbar}t
ight]$$
 $= H\psi_n(x,t).$

Therefore, considering the function

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x,t),$$

we have

$$i\hbar rac{\partial \psi(x,t)}{\partial t} = H\psi(x,t).$$

This is the Schrödinger equation of the time evolution of the total quantum system Ω . This shows that this quantum system satisfies the axiom III in

chapter 1. Therefore we have the energy expectation value of the total quantum system Ω :

$$\begin{split} \overline{E} &= E \left[\frac{1}{2m} p(\rho)^2 + \frac{1}{2} m \omega(\rho)^2 x(\rho)^2 \right] \\ &= \int_0^\infty J[\psi; \omega] D(\omega) d\omega \\ &= \int_0^\infty \left\{ \frac{1}{2} \hbar \omega + \frac{\hbar \omega}{\exp\left[\frac{\hbar \omega}{k_B T}\right] - 1} \right\} D(\omega) d\omega \\ &= \frac{1}{2} \hbar \overline{\omega} + \int_0^\infty \frac{\hbar \omega}{\exp\left[\frac{\hbar \omega}{k_B T}\right] - 1} D(\omega) d\omega. \end{split}$$

Here $\overline{\omega}$ is the mean of angular frequency:

$$\overline{\omega} = \int_0^\infty \omega D(\omega) d\omega.$$

For considering the specific heat of the solid, we should evaluate the derivative $\frac{d\overline{E}}{dT}$.

$$\frac{d\overline{E}}{dT} = \frac{d}{dT} \int_0^\infty \frac{\hbar \omega}{\exp\left[\frac{\hbar \omega}{k_B T}\right] - 1} D(\omega) d\omega.$$

The density $D(\omega)$ of angular frequency should be determined for each solid concretely.

5. Consideration and conclusion

On the true physical system, the quantum system $\Omega = \Omega(B, P)$ of 1-dimensional harmonic oscillators is decomposed into subsystems as follows:

$$\Omega = \bigcup_{i} \Omega(\omega),$$

$$\Omega(\omega) = \{ \rho \in \Omega; \omega(\rho) = \omega \}.$$

Then we have the probability space $\{\Omega(\omega), \mathbf{B}(\omega), P_{\omega}\}$ for every ω . Then, for every angular frequency ω , the subsystem $\Omega(\omega)$ is decomposed into characteristic subsystems as follows:

$$\Omega(\omega) = \sum_{n=0}^{\infty} \Omega_n(\omega), (\text{direct sum}).$$

Then, for every $A \in B(\omega)$, we have

$$P_{\omega}(A) = \sum_{n=0}^{\infty} P_{\omega}(\Omega_n(\omega)) P_{\Omega_n(\omega)}(A).$$

Here $P_{\Omega_n(\omega)}(A)$ denotes the conditional probability. Then, for $n=0,1,2,\cdots$, the probability space $\{\Omega_n(\omega), \mathbf{B}(\omega)\cap\Omega_n(\omega), P_{\Omega_n(\omega)}\}$ is said to be the *n*-th characteristic quantum system.

Here we assume that, for $n = 0, 1, 2, \dots$,

$$P_{\omega}(\Omega_n(\omega)) = |c_n|^2 = \left(1 - \exp\left[-\frac{\hbar\omega}{k_B T}\right]\right) \left(\exp\left[-\frac{\hbar\omega}{k_B T}\right]\right)^n$$

holds.

Then, for $A \subset \mathbb{R}^1$ and $B \subset \mathbb{R}_1$, we have

$$\begin{split} \sum_{n=0}^{\infty} P_{\omega}(\Omega_n(\omega)) &= \sum_{n=0}^{\infty} |c_n|^2 = 1, \\ P_{\Omega_n(\omega)}(\{\rho \in \Omega_n(\omega); x(\rho) \in A\}) &= \int_A |\psi_n(x)|^2 dx, \\ P_{\Omega_n(\omega)}(\{\rho \in \Omega_n(\omega); p(\rho) \in B\}) &= \int_B |\hat{\psi}_n(p)|^2 dp. \end{split}$$

Therefore, for every ω , the conditional energy expectation value of the characteristic quantum system $\Omega_n(\omega)$ is

$$\begin{split} E_{\Omega_n(\omega)} &\left[\frac{1}{2m} p(\rho)^2 + \frac{1}{2} m \omega(\rho)^2 x(\rho)^2; \omega(\rho) = \omega \right] \\ &= \int \left\{ \frac{\hbar^2}{2m} \left| \frac{d\psi_n(x)}{dx} \right|^2 + \frac{1}{2} m \omega^2 x^2 |\psi_n(x)|^2 \right\} dx \\ &= J[\psi_n; \omega] = \left(n + \frac{1}{2} \right) \hbar \omega. \end{split}$$

Then we have

$$E\left[\frac{1}{2m}p(\rho)^{2} + \frac{1}{2}m\omega(\rho)^{2}x(\rho)^{2}; \omega(\rho) = \omega\right]$$

$$= \sum_{n=0}^{\infty} P_{\omega}(\Omega_{n}(\omega))E_{\Omega_{n}(\omega)}\left[\frac{1}{2m}p(\rho)^{2} + \frac{1}{2}m\omega(\rho)^{2}x(\rho)^{2}; \omega(\rho) = \omega\right]$$

$$= \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\exp\left[\frac{\hbar\omega}{k_{B}T}\right] - 1}$$

Therefore we have the energy expectation value \overline{E} of the total quantum system Ω :

$$\begin{split} \overline{E} &= E \left[\frac{1}{2m} p(\rho)^2 + \frac{1}{2} m \omega(\rho)^2 x(\rho)^2 \right] \\ &= \int_0^\infty J[\psi; \omega] D(\omega) d\omega \\ &= \frac{1}{2} \hbar \overline{\omega} + \int_0^\infty \frac{\hbar \omega}{\exp\left[\frac{\hbar \omega}{k_B T}\right] - 1} D(\omega) d\omega. \end{split}$$

Here we put

$$\overline{\omega} = \int_0^\infty \omega D(\omega) d\omega.$$

In the monatomic solid, each atom has 3 degree of freedom as a harmonic oscillation, so that if we consider the molar heat C of the considered monatomic solid, we have

$$C = 3N rac{d\overline{E}}{dT}.$$

Here N is the Avogadro's number.

Here we consider the Debye model of the specific heat of the monatomic solid. So that we put

$$D(\omega) = \begin{cases} \frac{3}{\omega_D^3} \omega^2 &, (\omega < \omega_D), \\ 0 &, (\omega > \omega_D). \end{cases}$$

Here ω_D denotes the Debye frequency.

Then we have the molar heat C as follows:

$$C = 3N \frac{d\overline{E}}{dT}$$

$$= \frac{9N}{\omega_D^3} \frac{d}{dT} \int_0^{\omega_D} \frac{\hbar \omega^3}{\exp\left[\frac{\hbar \omega}{k_B T}\right] - 1} d\omega.$$

$$= \frac{9N}{\omega_D^3} \frac{\hbar^2}{k_B T^2} \int_0^{\omega_D} \frac{\omega^4 \exp\left[\frac{\hbar \omega}{k_B T}\right]}{\left(\exp\left[\frac{\hbar \omega}{k_B T}\right] - 1\right)^2} d\omega$$

$$= \frac{9N}{\omega_D^3} k_B^4 \left(\frac{T}{\hbar}\right)^3 \int_0^{\{\hbar \omega_D\}/\{k_B T\}} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

$$= 9Nk_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx.$$

Here we put

$$\theta_D = \frac{\hbar \omega_D}{k_B}.$$

We call θ_D to be the Debye temperature. This gives the new meaning of the specific heat for the Debye model of a solid.

The Debye model shows the good coincidence between the theoretical result and the experimental result. The Debye model gives a very good model of the true physical phenomena.

References

- Y. Ito, Theory of Hypoprobability Measure, RIMS Kokyuroku 558, pp. 96-113, 1985 (in Japanese).
- [2] Y. Ito, New Axiom of Quantum Mechanics—Hilbert's 6th Problem—, J. Math. Tokushima Univ., Vol.32, pp. 43-51, 1998.
- [3] Y. Ito, New Axiom of Quantum Mechanics—Hilbert's 6th Problem—, Real Analysis Simposium 1998 Takamatsu, pp. 96-103, 1999.
- [4] Y. Ito, Mathematical Principles of Quantum Mechanics, New Theory. Sciencehouse, 2000 (in Japanese).
- [5] Y. Ito, Theory of Quantum Probability, J. Math. Tokushima Univ., Vol.34, pp. 23-50, 2000.
- [6] Y. Ito and K. Kayama, Variational Principle and Schrödinger Equations, Natural Sciences Research, Faculty of Integrated Arts and Sciences, The University of Tokushima, Vol. 15, pp. 1-7, 2002 (in Japanese).
- [7] Y. Ito and K. Kayama, Variatonal Principle and Schrödinger Equations, RIMS Kokyuroku 1278, pp. 86-95, 2002 (in Japanese).
- [8] Y. Ito, K. Kayama and Y. Kamoshita, New Quantum Theory and New Meanings of Planck's Radiation Formula, Natural Science Research, Faculty of Integrated Arts and Sciences, The University of Tokushima, Vol. 16, pp.1-10, 2003 (in Japanese).
- [9] R. Kubo, Statistical Mechanics, Kyoritsu, 1952 (in Japanese).
- [10] S. Kuroda, Mathematical Theory of Quantum Physics, Iwanami, 1994 (in Japnese).
- [11] Y. Nagaoka, Statistical Mechanics, Iwanami, 1994 (in Japanese).

New Quantum Theory and New Meaning of Specific Heat of an Ideal Gas

Ву

Yoshifumi Ito and Md Sharif UDDIN

Department of Mathematical and Natural Sciences, Faculty of Integrated Arts and Sciences, the University of Tokushima, Tokushima 770-8502, Japan

and

Department of Mathematics, Jahangirnagar University, Savar, Dhaka-1342, Bangladesh

> E-mail: y-ito@ias.tokushima-u.ac.jp msharifju@yahoo.com (Received March 5, 2004)

Abstract

In this article, we consider the specific heat of an ideal gas composed of monatomic molecules in the view point of the new quantum theory. Thereby we can clarify a new meaning of specific heat of an ideal gas.

2000 Mathematics Subject Classification. Primary 82B10; Secondary 82B40, 81Q05

Introduction

In this article, we consider the molar heat and the specific heat of constant volume of an ideal gas composed of monatomic molecules in the view point of the new quantum theory. We get a reasonable explanation of them. It gives a new true explanation of the results known until now. We use here the framework of the new quantum theory mentioned in chapter 1 of Ito and Uddin [9]. The new quantum theory was originated by Y. Ito [2]-[4] at 1998-2000. As for the new quantum theory, we refer the papers [1]-[9] of the references.

1. Physical setting of the system and the problem

We consider an ideal gas composed of monatomic molecules spreaded infinitely. There are N molecules in the region of volume V. The ideal gas is so

rarefied that there is no mutual interaction among molecules. They only move freely and no forces act on them. Every molecule moves under the Newtonian equation of motion:

$$m\frac{d^2x}{dt^2} = 0$$

Here m denotes the mass of one molecule.

We wish to consider the specific heat C_V of constant volume and the molar heat C_M of this ideal gas.

Then we have the relation $C_V = nC_M$ where $N = nN_A$ and N_A denotes the Avogadro number.

2. Setting of the mathematical model

We use the notation in chapter 1 of Ito and Uddin [9]. We consider axiom I and axiom III in chapter 1 of Ito and Uddin [9]. Let $\Omega = \Omega(\boldsymbol{B}, P)$ be the probability space which represents the quantum system considered here. An elementary event ρ of Ω is a monatomic molecule which moves freely in the 3-dimensional Euclidean space \boldsymbol{R}^3 . Here we consider one degree of freedom of the 3-dimensional free motion. Then we denote the position variable of a monatomic molecule ρ by $x = x(\rho)$, and the momentum variable of ρ by $p = p(\rho)$. Here we put n = dM = 1 because the space dimension is d = 1, the number of monatomic molecules which compose an elementary event ρ is M = 1. The variable x changes in the space \boldsymbol{R}^1 and the variable p changes in its dual space \boldsymbol{R}_1 .

Here we need the new axiom for the generalized quantum state.

Axiom II' (generalized quantum state).

We consider the generalized quantum state of the quantum system $\Omega = \Omega(\boldsymbol{B}, P)$ as the state of the generalized quantum probability distribution of the position variable $x = x(\rho)$ and the momentum variable $p = p(\rho)$ of monatomic molecules ρ composing the quantum system. Here we consider the orthogonal coordinate system of 1-dimensional Euclidean space \boldsymbol{R}^1 and its dual space \boldsymbol{R}_1 .

The generalized quantum state is determined as follows:

- (II'₁) The generalized quantum distribution state of the position variable $x = x(\rho)$ is determined by L^2_{loc} -function ψ .
- (Π_2') The generalized quantum distribution state of the momentum variable $p = p(\rho)$ is determined by $\hat{\psi}$. Here $\hat{\psi}$ is the function determined as local Fourier transforms of ψ .

Namely

$$\hat{\psi}_S(p) = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \psi_S(x) e^{-ipx/\hbar} dx,$$
 $\psi_S(x) = (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \hat{\psi}_S(p) e^{ipx/\hbar} dp$

where S is an arbitrary compact set in \mathbb{R}^1 and, when we denote the characteristic function of S as

$$\chi_S(x) = \begin{cases} 1, & (x \in S), \\ 0, & (x \notin S), \end{cases}$$

we define ψ_S to be the function $\psi_S(x) = \psi(x)\chi_S(x)$. Namely ψ_S is the cut off function of ψ on S. We put $\hbar = \frac{h}{2\pi}$, here h being the Planck constant. In the above we use the classical Fourier transformation.

 (II'_3) For a Lebesgue measurable set A in \mathbb{R}^1 , we assume

$$P(\{
ho\in\Omega;x(
ho)\in A\cap S\})=rac{\displaystyle\int_{A\cap S}|\psi_S(x)|^2dx}{\displaystyle\int_S|\psi_S(x)|^2dx}=\mu_S(A)$$

This gives the probability that the position variable $x(\rho)$ of a monatomic molecule ρ moving in the region S belongs to $A \cap S$. Thereby we have the relative probability space $(S, \mathcal{M}_1 \cap S, \mu_S)$ corresponding to ψ_S . Here \mathcal{M}_1 is the family of Lebesgue measurable sets in \mathbb{R}^1 .

(II'₄) For a Lebesgue measurable set B in R_1 , we assume

$$P(\{
ho\in\Omega;x(
ho)\in S,p(
ho)\in B\})=rac{\displaystyle\int_{B}|\hat{\psi}_{S}(p)|^{2}dp}{\displaystyle\int_{-\infty}^{\infty}|\hat{\psi}_{S}(p)|^{2}dp}=
u_{S}(B)$$

This gives the probability that the momentum variable $p(\rho)$ of the monatomic molecule ρ moving in the region S belongs to B. Thereby, we have the relative probability space $(\mathbf{R}_1, \mathcal{N}_1, \nu_S)$ corresponding to $\hat{\psi}_S$. Here \mathcal{N}_1 is the family of Lebesgue measurable sets in \mathbf{R}_1 .

Then by the axiom II', the L^2_{loc} -density $\psi(x)$ determines the generalized quantum distribution law of the position variable x and its local Fourier transform $\hat{\psi}_S(p)$ determines the generalized quantum probability distribution law of the momentum variable p. The total energy of each monatomic molecule ρ is determined by the classical mechanics. Its value is $\frac{1}{2m}p(\rho)^2$. Here m is the mass of the monatomic molecule.

This energy variable is considered as a generalized quantum random variable defined on the probability space Ω which represents the quantum system. The evaluation of the local expectation value of this energy variable, namely the local energy expectation value, is carried out by using the axiom II'.

Namely we use the relation

$$P(\{\rho\in\Omega;x(\rho)\in A\cap S\})=\frac{\displaystyle\int_{A\cap S}|\psi_S(x)|^2dx}{\displaystyle\int_{S}|\psi_S(x)|^2dx},$$

$$P(\{
ho\in\Omega;x(
ho)\in S,p(
ho)\in B\})=rac{\displaystyle\int_{B}|\hat{\psi}_{S}(p)|^{2}dp}{\displaystyle\int_{-\infty}^{\infty}|\hat{\psi}_{S}(p)|^{2}dp},$$

for every compact set S in \mathbb{R}^1 and a subset A in \mathbb{R}^1 and a subset B in \mathbb{R}_1 . Then we have the local energy expectation value \overline{E}_S :

$$\overline{E}_S = E_S \left[\frac{1}{2m} p(\rho)^2 \right] = \frac{\int_{-\infty}^{\infty} \frac{1}{2m} p^2 |\hat{\psi}_S(p)|^2 dp}{\int_{-\infty}^{\infty} |\hat{\psi}_S(p)|^2 dp} = \frac{\int_S \frac{\hbar^2}{2m} \left| \frac{d\psi_S(x)}{dx} \right|^2 dx}{\int_S |\psi_S(x)|^2 dx}.$$

Here we use the Plancherel formula for Fourier transformation. Here we denote this local energy expectation value by

$$J_S[\psi_S] = rac{\displaystyle\int_S rac{\hbar^2}{2m} \left| rac{d\psi_S(x)}{dx}
ight|^2 dx}{\displaystyle\int_S |\psi_S(x)|^2 dx}.$$

We call $J_S[\psi_S]$ the local energy functional.

Here we assert the following principle.

Principle II (local variational principle).

In the case of continuous spectrum of the Hamiltonian operator of a quantum system, the stationary state are realized as the state where the energy expectation of the quantum system considered locally takes the stationary value under some conditions.

From this principle, we can choose the true L^2_{loc} -density for this quantum system. So that we consider the following problem I and problem II:

Problem I.

Let $\{r_n\}$ be a certain increasing sequence of positive numbers: $r_1 \leq r_2 \leq$ $\cdots \leq r_n \leq \cdots$

Let $\{K_n\}$ be an exhausting increasing sequence of non-empty compact sets of \mathbf{R}^1 . Namely it satisfy the following conditions (i) and (ii): (i) $\emptyset \neq K_1 \subset K_2 \subset \cdots \subset K_n \subset \cdots \mathbf{R}^1$,

(i)
$$\emptyset \neq K_1 \subset K_2 \subset \cdots \subset K_n \subset \cdots \mathbb{R}^1$$

(ii)
$$\bigcup_{j=1} K_j = \mathbf{R}^1$$
.

For an arbitrary positive number $\mathcal{E} > 0$, determine the locally square integrable function $\psi^{(\mathcal{E})}(x)$ such that the following conditions (1) \sim (5) are satisfied:

- (1) $\psi^{(\mathcal{E})}|_{K_n} = \psi_n$. (2) $\psi_{n+1}|_{K_n} = \psi_n$.

(3)
$$\int_{\mathcal{K}} |\psi_n(x)|^2 dx = r_n > 0, \ (n = 1, 2, \cdots).$$

(3)
$$\int_{K_n} |\psi_n(x)|^2 dx = r_n > 0, \ (n = 1, 2, \cdots).$$
(4)
$$\int_{-\infty}^{\infty} \psi^{(\mathcal{E}')}(x)^* \psi^{(\mathcal{E})}(x) dx = \delta(\mathcal{E}' - \mathcal{E}), \ (\mathcal{E}, \mathcal{E}' > 0).$$

Here $\delta(\mathcal{E})$ denote the delta function.

(5) The functional

$$J_n[\psi_n] = rac{\displaystyle\int_{K_n} \left(rac{\hbar^2}{2m} \left|rac{d\psi_n(x)}{dx}
ight|^2
ight) dx}{\displaystyle\int_{K_n} |\psi_n(x)|^2 dx}$$

takes its stationary value under the conditions (2) and (3).

Problem II.

Find out the L_{loc}^2 -density for which the local energy expectation value $J_n[\psi_n]$ takes its stationary value under the condition that $\int_{\mathcal{L}} |\psi_n(x)|^2 dx$ is equal to a given constant r_n .

3. Mathematical analysis

Solving the problems I and II in chapter 2, we have the Schrödinger equations

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} = \mathcal{E}\psi_n(x), \ x \in K_n(n=1,2,\cdots)$$

as the Euler equations. Here $\mathcal E$ is the Lagrange's unknown constant. By the conditions (1), (2) and (3) of problem I in chapter 2, we have the L^2_{loc} -function $\psi^{(\mathcal{E})}(x)$ such that it satisfies, for some constant $\mathcal{E} > 0$,

$$\psi^{(\mathcal{E})}(x) = \psi_n(x), \ x \in K_n(n = 1, 2, \cdots).$$

Then $\psi^{(\mathcal{E})}(x)$ satisfies the Schrödinger equation

$$-rac{\hbar^2}{2m}rac{d^2\psi^{(\mathcal{E})}(x)}{dx^2}=\mathcal{E}\psi^{(\mathcal{E})}(x),\,\,x\in oldsymbol{R}^1.$$

As solutions of the above generalized eigenvalue problem, we have the generalized eigenfunction $\psi^{(\mathcal{E})}(x)$ corresponding to the eigenvalue $\mathcal{E} > 0$. Namely we have, for every $\mathcal{E} > 0$,

$$\psi_{\pm}^{(\mathcal{E})}(x) = c(\mathcal{E}) \exp\left(\pm \frac{i}{\hbar} x \sqrt{2m\mathcal{E}}\right).$$

For every $\mathcal{E} > 0$, there exist two independent generalized eigenfunctions. Therefore every spectrum \mathcal{E} is degenerated. If we normalize the generalized eigenfunctions in the scale of \mathcal{E} , we have

$$\psi_{\pm}^{(\mathcal{E})}(x) = \left(\frac{m}{2\hbar^2 \mathcal{E}}\right)^{\frac{1}{4}} \exp\left(\pm \frac{i}{\hbar} x \sqrt{2m\mathcal{E}}\right).$$

Then we have the relations, for $\mathcal{E} > 0$ and $\mathcal{E}' > 0$,

$$\int_{-\infty}^{\infty} \psi_{+}^{(\mathcal{E}')}(x)^{*} \psi_{+}^{(\mathcal{E})}(x) dx = \delta(\mathcal{E}' - \mathcal{E}),$$

$$\int_{-\infty}^{\infty} \psi_{-}^{(\mathcal{E}')}(x)^* \psi_{-}^{(\mathcal{E})}(x) dx = \delta(\mathcal{E}' - \mathcal{E})$$

and

$$\int_{-\infty}^{\infty} \psi_{-}^{(\mathcal{E}')}(x)^* \psi_{-}^{(\mathcal{E})}(x) dx = 0.$$

Here c^* denotes the complex conjugate of a complex number c. If we put $k^2 = \frac{2m\mathcal{E}}{\hbar^2}$, for $\mathcal{E} \geq 0$, we have, for $-\infty < k < \infty$,

$$\psi^{(k)}(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}$$

which is normalized in the scale of k:

$$\int_{-\infty}^{\infty} \psi^{(k')}(x)^* \psi^{(k)}(x) dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx = \delta(k'-k), \ -\infty < k, k' < \infty.$$

Then we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi^{(k)}(x)}{dx^2}=\mathcal{E}\psi^{(k)}(x),\,\,x\in\boldsymbol{R}^1.$$

If we put $\psi^{(k)}|_{K_n} = \psi_n$, $(n = 1, 2, \cdots)$, we have

$$J_n[\psi_n] = rac{rac{\mathcal{E}}{2\pi} \int_{K_n} 1 dx}{rac{1}{2\pi} \int_{K_n} 1 dx} = \mathcal{E}, \,\, (n=1,2,\cdots).$$

Thus $\psi^{(k)}(x)$ satisfies all the conditions of problem I. Thus we have the solution of problem I. If we put $p=\hbar k$ and we write

$$\psi^{(p)}(x) = \frac{1}{\sqrt{\hbar}}\psi^{(k)}(x)$$

for $p = \hbar k$. Then we have

$$\psi^{(p)}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}, \ \left(\mathcal{E} = \frac{p^2}{2m}\right)$$

which is normalized in the scale of p:

$$\int_{-\infty}^\infty \psi^{(p')}(x)^*\psi^{(p)}(x)dx = rac{1}{2\pi\hbar}\int_{-\infty}^\infty e^{i(p-p')x/\hbar}dx = \delta(p'-p), \,\, p,p'\in R_1.$$

Then we have

$$-rac{\hbar^2}{2m}rac{d^2\psi^{(p)}(x)}{dx^2} = \mathcal{E}\psi^{(p)}(x), \,\, x \in I\!\!R^1.$$

If we put $\psi^{(p)}|_{K_n} = \psi_n$, $(n = 1, 2, \dots)$, we have

$$J_n[\psi_n] = rac{rac{\mathcal{E}}{2\pi\hbar}\int_{K_n}1dx}{rac{1}{2\pi\hbar}\int_{K_n}1dx} = \mathcal{E}, \,\,(n=1,2,\cdots).$$

This $\psi^{(p)}(x)$ satisfies all the conditions of problem I. Thus we have the solution of problem I. In the above, the L^2_{loc} -densities $\psi^{(\mathcal{E})}(x)$, $\psi^{(k)}(x)$ and $\psi^{(p)}(x)$ are the different representations of the solutions of problem I which differ only in the scale of the normalization.

By virtue of the theory of Fourier transformation, for any $\psi \in L^2(\mathbf{R}^1)$, there exists $c \in L^2(\mathbf{R}_1)$ such that we have

$$\psi(x) = rac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{ipx/\hbar} dp$$

and

$$c(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx.$$

If the true physical state of the total quantum system Ω is determined by some L^2 -density $\psi(x)$ at the initial time point, then we have the generalized eigenfunction expansion of $\psi(x)$ by $\psi^{(p)}(x)$ as follows:

$$\psi(x) = \int_{-\infty}^{\infty} c(p)\psi^{(p)}(x)dp,$$

$$c(p) = \int_{-\infty}^{\infty} \psi^{(p)}(x)^* \psi(x) dx.$$

Then we have the energy expectation value

$$\overline{E}=J[\psi]=\int_{-\infty}^{\infty}rac{p^2}{2m}|\hat{\psi}(p)|^2dp=\int_{-\infty}^{\infty}rac{p^2}{2m}|c(p)|^2dp.$$

Further, since the function $\psi(x)$ satisfies the normalization condition

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1,$$

we have

$$\int_{-\infty}^{\infty} |c(p)|^2 dp = 1.$$

Since we have $\frac{p^2}{2m} = \mathcal{E}$, we have

$$\begin{split} \overline{E} &= J[\psi] = \int_{-\infty}^{0} \frac{p^2}{2m} |c(p)|^2 dp + \int_{0}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp. \\ &= \frac{1}{2} \int_{0}^{\infty} \mathcal{E} \sqrt{\frac{2m}{\mathcal{E}}} |c(-\sqrt{2m\mathcal{E}})|^2 d\mathcal{E} + \frac{1}{2} \int_{0}^{\infty} \mathcal{E} \sqrt{\frac{2m}{\mathcal{E}}} |c(\sqrt{2m\mathcal{E}})|^2 d\mathcal{E}. \\ &= \frac{1}{2} \int_{0}^{\infty} \mathcal{E} \sqrt{\frac{2m}{\mathcal{E}}} (|c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2) d\mathcal{E}. \end{split}$$

If we put

$$I(\mathcal{E}) = \frac{1}{2} \sqrt{\frac{2m}{\mathcal{E}}} (|c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2), \,\, \mathcal{E} > 0,$$

we have

$$\int_0^\infty I(\mathcal{E})d\mathcal{E} = \int_{-\infty}^\infty |c(p)|^2 dp = 1.$$

So that we have

$$\overline{E} = J[\psi] = \int_0^\infty \mathcal{E} I(\mathcal{E}) d\mathcal{E}.$$

If we assume

$$I(\mathcal{E}) = \frac{2}{k_B T} \exp\left(-\frac{2\mathcal{E}}{k_B T}\right),$$

where T denotes the absolute temperature and k_B denotes the Boltzman constant, we have

$$\overline{E} = rac{1}{2}k_BT.$$

Because the degree of freedom of the 3-dimensional free motion is equal to 3, the energy expectation value of the total quantum system Ω in the 3-dimensional case is equal to

$$\overline{E}=rac{3}{2}k_{B}T.$$

Further the L^2 -density $\psi(x)$ of the total quantum system Ω at the state of thermal equilibrium at the temperature T can be represented as follows:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{ipx/\hbar} dp$$

and

$$c(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx.$$

Here we follow the reverse order of the method of separation of variables. At first we consider the function

$$\psi^{(p)}(x,t) = \psi^{(p)}(x) \exp\left(-i\frac{\mathcal{E}}{\hbar}t\right).$$

Differentiating this function with respect to the time variable t, we have

$$i\hbar\frac{\partial\psi^{(p)}(x,t)}{\partial t}=\mathcal{E}\psi^{(p)}(x)\exp\left(-i\frac{\mathcal{E}}{\hbar}t\right).$$

Here we denote the Hamiltonian operator of the Schrödinger equation of stationary state as follows:

$$H = -rac{\hbar^2}{2m}rac{\partial^2}{\partial x^2}.$$

Then we have

$$H\psi^{(p)}(x) = \mathcal{E}\psi^{(p)}(x), \ \mathcal{E} = \frac{p^2}{2m}.$$

Hence we have

$$i\hbar rac{\partial \psi^{(p)}(x,t)}{\partial t} = \{H\psi^{(p)}(x)\} \exp\left(-irac{\mathcal{E}}{\hbar}t
ight) = H\psi^{(p)}(x,t).$$

Therefore, if we put

$$\psi(x,t) = \int_{-\infty}^{\infty} c(p)\psi^{(p)}(x,t)dp,$$

we have

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = H\psi(x,t).$$
 (3.1)

This is the Schrödinger equation of time evolution of the total quantum system Ω . Here, using the condition of completeness, we have

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = \int_{-\infty}^{\infty} |c(p)|^2 dp = 1.$$

By virtue of the conservation law of probability, we can see that the Schrödinger equation of time evolution is nothing else but the equation (3.1) in order that the L^2 -density satisfies this normalization condition.

4. Consideration and conclusion

We can consider that the quantum system (Ω, \mathbf{B}, P) of the 1-dimensional ideal gas composed of monatomic molecules has the following structure at the stationary state. Namely Ω is decomposed into the direct sum

$$\Omega = \bigcup_{-\infty
$$\Omega_p = \{ \rho \in \Omega; p(\rho) = p \}, \ (-\infty
$$P(\Omega_p) = |c(p)|^2, \ (-\infty
(4.1)$$$$$$

Then, we have, for any $A \in B$,

$$P(A) = \int_{-\infty}^{\infty} P(A|p)|c(p)|^2 dp, \tag{4.2}$$

where P(A|p) denotes the conditional probability. Then for $p: -\infty , we call the probability space <math>(\Omega_p, B \cap \Omega_p, P(\cdot|p))$ as the generalized characteristic quantum system. Considering the equations (4.1) and (4.2) and the results of calculation until now, we put the following assumptions. Now for $p: -\infty , we assume that <math>c(p)$ satisfies the following conditions:

$$egin{aligned} I(\mathcal{E}) &= rac{1}{2} \left(\sqrt{rac{2m}{\mathcal{E}}} (|c(-\sqrt{2m\mathcal{E}})|^2) + |c(\sqrt{2m\mathcal{E}})|^2
ight), \ &\int_0^\infty I(\mathcal{E}) d\mathcal{E} = 1, \,\, p^2 = 2m\mathcal{E}. \end{aligned}$$

If we use the notation of the axiom II', we have

$$\begin{split} P(\Omega_p|p) &= 1, \\ P(\{\rho \in \Omega_p; x(\rho) \in A \cap S\}|p) &= \frac{\displaystyle\int_{A \cap S} |\psi_S^{(p)}(x)|^2 dx}{\displaystyle\int_{S} |\psi_S^{(p)}(x)|^2 dx}, \\ P(\{\rho \in \Omega_p; x(\rho) \in S, p(\rho) \in B\}|p) &= \frac{\displaystyle\int_{B} |\hat{\psi}_S^{(p)}(p)|^2 dp}{\displaystyle\int_{-\infty}^{\infty} |\hat{\psi}_S^{(p)}(p)|^2 dp}. \end{split}$$

Therefore, the conditional energy expectation value \overline{E}_p of the generalized characteristic quantum system Ω_p is equal to

$$\overline{E}_p = \lim_{n \to \infty} J_{K_n}[\psi_{K_n}^{(p)}] = \mathcal{E} = \frac{p^2}{2m}.$$

By the relation of the total quantum system and the generalized characteristic quantum systems, we have

$$\begin{split} \overline{E} &= E\left[\frac{1}{2m}p(\rho)^2\right] = \int_{-\infty}^{\infty} \overline{E}_p |c(p)|^2 dp \\ &= \int_{-\infty}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp = \int_{0}^{\infty} \mathcal{E}I(\mathcal{E}) d\mathcal{E}, \ (p^2 = 2m\mathcal{E}). \end{split}$$

If we assume that $I(\mathcal{E})$ is equal to

$$I(\mathcal{E}) = rac{2}{k_B T} \exp\left(-rac{2\mathcal{E}}{k_B T}
ight),$$

we have

$$\overline{E}=rac{1}{2}k_{B}T.$$

Because the degree of freedom of the 3-dimensional free motion is equal to 3, the energy expectation value of the total quantum system Ω in the 3-dimensional case is equal to

$$\overline{E}=rac{3}{2}k_{B}T.$$

 \overline{E} denotes the energy expectation value for one molecule. Now we consider the ideal gas such as there are N molecules in the region of volume V. So that we have the specific heat C_V of constant volume and the molar heat C_M of this ideal gas as follows:

$$C_V = N \frac{d\overline{E}}{dT}$$
 and $C_M = N_A \frac{d\overline{E}}{dT}$

Namely,

$$C_V = rac{3}{2}Nk_B$$

and

$$C_M = \frac{3}{2} N_A k_B.$$

Here N_A denotes the Avogadro number. If we put $N=nN_A$, we have the relation

$$C_V = nC_M$$
.

These results were considered as the specific heats of the ideal gas composed of monatomic molecules. These facts are confirmed in the view point of the new quantum theory. But our results can be derived reasonably in the view point of the new quantum theory. The new and old results are different at the standing points.

References

- Y. Ito, Theory of Hypoprobability Measure, RIMS Kokyuroku 558, pp. 96-113, 1985 (in Japanese).
- [2] Y. Ito, New Axiom of Quantum Mechanics—Hilbert's 6th Problem, J. Math. Tokushima Univ., Vol. 32, pp. 43-51, 1998.
- [3] Y. Ito, New Axiom of Quantum Mechanics—Hilbert's 6th Problem, Real Analysis Simposium 1998 Takamatsu, pp. 96-103, 1999.
- [4] Y. Ito, Mathematical Principles of Quantum Mechanics, New Theory. Sciencehouse, 2000 (in Japanese).
- [5] Y. Ito, Theory of Quantum Probability, J. Math. Tokushima Univ., Vol.34, pp. 23-50, 2000.
- [6] Y. Ito and K. Kayama, Variational Principle and Schrödinger Equations, Natural Sciences Research, Faculty of Integrated Arts and Sciences, The University of Tokushima, Vol. 15, pp. 1-7, 2002 (in Japanese).
- [7] Y. Ito and K. Kayama, Variatonal Principle and Schrödinger Equations, RIMS Kokyuroku 1278, pp. 86-95, 2002 (in Japanese).
- [8] Y. Ito, K. Kayama and Y. Kamoshita, New Quantum Theory and New Meanings of Planck's Radiation Formula, Natural Science Research, Faculty of Integrated Arts and Sciences, The University of Tokushima, Vol. 16, pp.1-10, 2003 (in Japanese).
- [9] Y. Ito and Md Sharif Uddin, New Quantum Theory and New Meaning of Specific Heat of a Solid, Preprint, 2003.

平成16年12月15日 印 刷 平成16年12月20日 発 行

発 行 者 徳島大学 総合科学部 数理科学教室 工 学 部 数 学 教 室

編集委員 伊東由文

印刷所 德島市東沖洲2丁目1-13 徳島県教育印刷株式会社