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Methodology of Analytic and Computational Studies on Quantum Systems

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The concept of "separation of procedures" and the ST-transformation are briefly reviewed together with the equivalence theorem that a d-dimensional quantum system with *finite-range interactions* is equivalent to the corresponding $(d+1)$-dimentional classical system with *finite-range interactions*. This theorem yields the introduction of the quantum transfer-matrix method. Thermo quantum dynamics is formulated using the quantum transfer-matrix method. This new formulation has the great merit that the thermal average $\langle Q \rangle$ for any observable Q in the thermodynamic limit is expressed as an expectation value over a temperature-dependent state vector in the single (conjugate) Hilbert space in the contrast to the usage of the double Hilbert space in thermo field dynamics.

KEY WORDS: Finite-range interactions; ST-transformation; quantum transfer-matrix method.

1. INTRODUCTION

It has been a fascinating subject for long years to study analytically or even numerically quantum many-body systems *at finite temperatures*. Many investigations have been reported on this subject, and many methods to attack this subject have been devised. Among them, the transformation of a quantum system to the corresponding classical system, so-called Suzuki–Trotter transformation(1–3) (ST-transformation) is quite general in the sense that it can be applied to any system in any dimensions. This transformation scheme yields the equivalence theorem(3) that a d-dimensional quantum system with *finite-range interactions* is equivalent to the corresponding $(d+1)$-dimensional classical system with *finite-range interactions*. This theorem gives a general route to the formulation of the

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quantum transfer-matrix method.(1, 4–7) The above ST-transformation is also the essential ingredient of the quantum Monte Carlo method.(3, 8–10) The quantum transfer-matrix method has also been used effectively for *numerical calculations*(11–18) of quantum systems at finite temperatures.

In the present paper, the basic idea of the *separation of procedures*(19) is reviewed in Section 2 to clarify both the background concept in the ST-transformation and the above equivalence theorem. In Section 3, a new formulation of *thermo quantum dynamics* is proposed on the basis of the quantum transfer-matrix method. This has the great merit that any thermal average is expressed in terms of the expectation value on a vector in the *single* Hilbert space in the thermodynamic limit. This is a big contrast to thermo field dynamics,(20–22) in which the introduction of the double Hilbert space is inevitable.

Our new formulation is conceptually related to the C* algebra formulation(23) of thermal equilibrium, because both theories treat quantum systems with infinite degrees of freedom. However, our theory uses this aspect positively. Namely our formulation holds only in the thermodynamic limit.

2. SEPARATION OF PROCEDURES, ST-TRANSFORMATION AND EQUIVALENCE THEOREM

Almost all interesting phenomena occur due to computing or synergetic effects of two or more kinds of interaction. The concept of separation of procedures plays an important role for investigating theoretically many challenging problems of physics concerning cooperative phenomena such as phase transitions.(24–27)

Mathematically, a formal solution of the relevant problem is often expressed in terms of an exponential operator of the form $\exp[x(A+B)]$ for the noncommutable operators A and B. A simple example of the separation of procedures is given by the following exponential product formula(1, 2)

$$e^{x(A+B)} = \lim_{n\to\infty} (e^{\frac{x}{n}A} e^{\frac{x}{n}B})^n. \tag{2.1}$$

The $n=1$ approximant in (2.1), $e^{xA}e^{xB}$ corresponds to the complete separation of the two procedures described by A and B, respectively. In the case of many noncommutable operators $A_1, A_2, \ldots, A_q$, we have

$$e^{x(A_1+A_2+\cdots+A_q)} = \lim_{n\to\infty} (e^{\frac{x}{n}A_1} e^{\frac{x}{n}A_2} \cdots e^{\frac{x}{n}A_q})^n. \tag{2.2}$$

Even the $n = 1$ approximant for q of the order of the particle number $N(\sim 10^{23})$ is complicated enough to calculate the corresponding physical quantities such as the partition function $Z(\beta) = \mathrm{Tr}\exp[-\beta\mathscr{H}]$. Such an approximant was studied first by the present author(1) in studying the critical phenomena of the three-dimensional Heisenberg model. It was called "pair-product approximant (or model)," because the original density matrix $\exp[\beta J \sum_{<i,j>} S_i \cdot S_j]$ is approximated by the product of each exponential operator (namely partial Boltzmann factor) corresponding to the pair interaction, $\exp(\beta J S_i \cdot S_j)$. This very crude approximation still retains the symmetry (O(3) symmetry) of the original Hamiltonian. Therefore, the critical behavior of this system is expected to be described by the "pair-product model." This expectation was partially confirmed by the present author(1) using the high-temperature expansion and the Padé approximants.

In this way, the above exponential product formula (2.2) (the so-called Suzuki–Trotter formula or transformation) has the great merit that the approximant (2.2) for any n retains the symmetry of the original exponential operator such as the unitarity (for pure imaginary x and hermitian operators $\{A_j\}$) and the symplectic property for nonlinear dynamics.

Recently, the present author(28–40) found higher-order exponential product formulas of the form

$$e^{x(A+B)} = e^{t_1 A} e^{t_2 B} e^{t_3 A} e^{t_4 B} \cdots + e^{t_M A} + O(x^{m+1}) \tag{2.3}$$

for an arbitrary positive integer m with the corresponding appropriate positive integer M. The simplest method to construct them is to make use of the following recursive scheme(28, 29)

$$S_{2m}(x) = S_{2m-2}(p_1 x)\, S_{2m-2}(p_2 x) \cdots S_{2m-2}(p_r x) \tag{2.4}$$

with

$$S_2(x) = e^{\frac{x}{2}A} e^{xB} e^{\frac{x}{2}A} \qquad \text{and} \qquad p_j = p_{r-j+1}. \tag{2.5}$$

Here, the requirement that $S_{2m}(x)$ should be of the order $2m$ gives the conditions

$$\sum_{j=1}^{r} p_j = 1 \qquad \text{and} \qquad \sum_{j=1}^{r} p_j^{2m-1} = 0. \tag{2.6}$$

In particular, for the case $r = 5$, we have(28, 29)

$$S^*_{2m}(x) = (S^*_{2m-2}(p_m x))^2\, S^*_{2m-2}((1-4p_m)\, x)(S^*_{2m-2}(p_m x))^2 \tag{2.7}$$

with $S^*_2(x) = S_2(x)$ and $p_m = (4 - 4^{1/(2m-1)})^{-1}$.

These are called “standard higher-order product formulas,” in the sense that the decomposition parameters p_m and $|1-4p_m|$ are both less than unity and consequently that these are stable and desired approximations.

Using these exponential product formulas, a d-dimensional quantum system with *finite-range interactions* can be transformed into the corresponding $(d+1)$-dimensional classical system with *finite-range interactions*. This is our “equivalence theorem.”

3. THERMO QUANTUM DYNAMICS BASED ON THE QUANTUM TRANSFER-MATRIX METHOD

First we explain the quantum transfer-matrix method(5–7) to solve *analytically* quantum systems at finite temperatures.

It is well known that the transfer-matrix method was introduced by Kramers and Wannier,(43) Kubo,(44) and others(4, 45) and that it has been used very effectively in solving several Ising models and other classical systems in one and two dimensions.(47)

Now, according to the equivalence theorem,(3) a d-dimensional quantum system is transformed to the corresponding $(d+1)$-dimensional classical system. For example, a one-dimensional quantum system is transformed into the corresponding two-dimensional system. One direction of the transformed system, which is vertical to the original (real-space) dimension, is called quantum (or Trotter) dimension (namely virtual-space dimension). Then, two kinds of quantum transfer-matrices are defined in this new system. Namely a “real-space” transfer-matrix $\mathscr{T}_{\mathrm{R}}$ is defined in the real space(5) and a “virtual-space” transfer-matrix $\mathscr{T}_m$ is also defined in the virtual space(5) for the Trotter number m.

Thus, the partition function of this transformed system with the periodic boundary condition is given by

$$Z(\beta) = \operatorname{Tr} e^{-\beta\mathscr{H}} = \lim_{m\to\infty} Z_m(\beta); \qquad Z_m(\beta) = \operatorname{Tr} \mathscr{T}_m^N. \tag{3.1}$$

Here, $\mathscr{H}$ denotes the Hamiltonian of the original system and N is the system size. Owing to the exchangeability theorem,(5, 6) we can exchange the above two limits in (3.1). Then, we have(5, 6)

$$\lim_{N\to\infty} \frac{1}{N} \log Z(\beta) = \lim_{m\to\infty} \lim_{N\to\infty} \frac{1}{N} \log Z_m(\beta) \tag{3.2}$$

Let the maximum eigenvalue and the next maximum eigenvalue $\lambda_{\max}^{(m)}$ and $\lambda_2^{(m)}$, respectively. The remaining eigenvalues are denoted by $\lambda_3^{(m)}$, $\lambda_4^{(m)}$,.... Thus, the partition function $Z_m(\beta)$ is expressed as

$$Z_m(\beta) = [\lambda_{\max}^{(m)}]^N \left[1 + \sum_{i=2} \left(\frac{\lambda_i^{(m)}}{\lambda_{\max}^{(m)}} \right)^N \right]. \tag{3.3}$$

Consequently, we obtain

$$\lim_{N \to \infty} \frac{1}{N} \log Z_m(\beta) = \log \lambda_{\max}^{(m)}. \tag{3.4}$$

Therefore, Eq. (3.2) yields the formula$^{(6)}$

$$\lim_{N \to \infty} \frac{1}{N} \log Z(\beta) = \lim_{m \to \infty} \log \lambda_{\max}^{(m)}. \tag{3.5}$$

This formula is quite remarkable in that the free energy of the relevant quantum system is given by the single (namely maximum) eigenvalue of the quantum transfer-matrix, as was exemplified first in the XY spin chain.$^{(6, 7)}$ This is a big contrast to the fact that $Z(\beta)$ is given by all the eigenvalues $\{E_j\}$ of the Hamiltonian $\mathscr{H}$ as

$$Z(\beta) = \sum_j \mathrm{e}^{-\beta E_j}; \qquad \beta = \frac{1}{k_B T}. \tag{3.6}$$

Even the correlation length ξ of the relevant spin system is given by$^{(7)}$

$$\xi^{-1} = \lim_{m \to \infty} \log(\lambda_{\max}^{(m)} / \lambda_2^{(m)}), \tag{3.7}$$

using the first two largest eigenvalues $\lambda_{\max}^{(m)}$ and $\lambda_2^{(m)}$ of the quantum transfer-matrix $\mathscr{T}_m$.

In this way, there has appeared a new possibility$^{(48-59)}$ to find compact exact solutions of one-dimensional quantum systems at finite temperatures such as the Heisenberg chain. It should be remarked here that we can also formulate the quantum transfer-matrix *inversely*, namely starting from a known classical system and that we define the transfer matrix $\tilde{\mathscr{T}}$ of this classical system whose interactions contain an extra parameter m corresponding to the Trotter number and should be determined so that the partition function of the relevant system may be equal to the trace of $\tilde{\mathscr{T}}^m$. This formulation is possible when the equivalent classical system is known in advance, as in the Heisenberg chain$^{(50, 53)}$ (which is equivalent to the six-vertex model). In this sense, the above formulation based on the ST-transformtion is a quite generic tool. Thus, both the formulations are mathematically equivalent. In any formulation, the exchangeability of the two limits $m \to \infty$ and $N \to \infty$ is essential to obtain the nonlinear integral equation$^{(50, 53)}$ on $\lambda_{\max}^{(\infty)}$.

Now, we formulate "thermo quantum dynamics" using the eigenvector $\{|\Psi_m(\beta)\rangle\}$ of the above quantum transfer-matrix $\mathscr{T}_m$ with the maximum eigenvalue $\lambda_{\max}^{(m)}$:

$$\mathscr{T}_m \, |\Psi_m(\beta)\rangle = \lambda_{\max}^{(m)} \, |\Psi_m(\beta)\rangle \tag{3.8}$$

for the Trotter number m with the normalization

$$\langle \Psi_m(\beta) \, | \, \Psi_m(\beta)\rangle = 1 \tag{3.9}$$

The thermal states $\{|\Psi_m(\beta)\rangle\}$ play an essential role in thermo quantum dynamics, as will be shown later.

It is impossible in general situations including a finite system to express the thermal average

$$\langle Q \rangle = \operatorname{Tr} Q \exp(-\beta \mathscr{H}) / \operatorname{Tr} \exp(-\beta \mathscr{H}) \tag{3.10}$$

in terms of an expectation value over a thermal state in a single Hilbert space. Thus, a double Hilbert space was introduced$^{(20, 21)}$ in thermo "field" dynamics, in order to express the thermal average (3.10) or the trace in terms of the expectation value of Q over the thermal vacuum $|O(\beta)\rangle$ as

$$\langle Q \rangle = \langle O(\beta)| \, Q \, |O(\beta)\rangle \tag{3.11}$$

in the double Hilbert space. The above formulation is very tricky, but it can be used even for any finite systems.

In our new formulation, the thermal average $\langle Q \rangle$ of a "local" operator Q in the thermodynamic limit ($N \to \infty$) is expressed as

$$\langle Q \rangle = \lim_{m \to \infty} \langle \Psi_m(\beta)| \, Q \, |\Psi_m(\beta)\rangle \tag{3.12}$$

using the thermal state vectors $\{|\Psi_m(\beta)\rangle\}$ in a single Hilbert space, as will be proven below.

The word "local" means that the thermal average $\langle Q \rangle_m$ for the Trotter number m is expressed as

$$\langle Q \rangle_m = \operatorname{Tr} Q \, \mathscr{T}_m^N / \operatorname{Tr} \mathscr{T}_m^N. \tag{3.13}$$

If Q is not "local" in the above sense (for example, $Q = S_0 S_R$ for the spin operator S_R at the position R), we can easily extend the above formulation (3.12) with (3.13) as follows:

$$\langle Q \rangle_m = \mathrm{Tr}\, Q(\mathcal{T}_m)\, \mathcal{T}_m^N / \mathrm{Tr}\, \mathcal{T}_m^N. \tag{3.14}$$

with some appropriate operator $Q(\mathcal{T}_m)$ modified by the transfer-matrix $\mathcal{T}_m$. For example, if $Q = S_0 S_R$, then

$$Q(\mathcal{T}_m) = S_0 \mathcal{T}_m^R S_R \mathcal{T}_m^{-R}. \tag{3.15}$$

Thus, we arrive at the following expression

$$\langle Q \rangle = \lim_{m \to \infty} \langle \Psi_m(\beta) |\, Q(\mathcal{T}_m)\, | \Psi_m(\beta) \rangle \tag{3.16}$$

for any operator Q.

First we assume that the set of the normalized eigenvectors $\{|\Psi_i\rangle\}$ of $\mathcal{T}_m$ constitutes a complete orthogonal one, where $|\Psi_1\rangle \equiv |\Psi(\beta)\rangle$. Then, the trace $\mathrm{Tr}\, Q\, \mathcal{T}_m^N$ is expressed as

$$\begin{aligned}\mathrm{Tr}\, Q\mathcal{T}_m^N &= \sum_i \langle \Psi_i |\, Q\, \mathcal{T}_m^N\, | \Psi_i \rangle \\ &= \sum_i [\lambda_i^{(m)}]^N \langle \Psi_i |\, Q\, | \Psi_i \rangle \\ &= [\lambda_{\max}^{(m)}]^N \Big[\langle \Psi_1 |\, Q\, | \Psi_1 \rangle + \sum_{i=2} (\lambda_i^{(m)} / \lambda_{\max}^{(m)}) \langle \Psi_i |\, Q\, | \Psi_i \rangle\Big].\end{aligned} \tag{3.17}$$

Therefore, we arrive finally at

$$\begin{aligned}\langle Q \rangle &= \lim_{m \to \infty} (\mathrm{Tr}\, Q\mathcal{T}_m^N / \mathrm{Tr}\, \mathcal{T}_m^N) \\ &= \lim_{m \to \infty} \langle \Psi_1 |\, Q\, | \Psi_1 \rangle = \lim_{m \to \infty} \langle \Psi_m(\beta) |\, Q\, | \Psi_m(\beta) \rangle.\end{aligned} \tag{3.18}$$

This is an extremely interesting result, both conceptually and practically.

Here, it should be remarked that the limit of $\{\mathcal{T}_m\}$ for $m \to \infty$ may not exist and consequently that the limit of $\{|\Psi_m(\beta)\rangle\}$ for $m \to \infty$ may not exist either in some cases. This singular property of the quantum transfer-matrix $\mathcal{T}_m$ is seen explicitly by studying some examples, say, the transverse Ising chain described by the Hamiltonian(3, 61 –65)

$$\mathcal{H} = -J \sum \sigma_j^z \sigma_{j+1}^z - \Gamma \sum \sigma_j^x. \tag{3.19}$$

Clearly, the singular matrix elements

$$\langle \sigma_j | \exp\left(\frac{\gamma}{m}\sigma_j^x\right) | \sigma'_j \rangle = A_m \exp(K_m \sigma_j \sigma'_j) \tag{3.20}$$

with $\gamma = \beta \Gamma$ and

$$A_m = \left\{\frac{1}{2}\sinh\left(\frac{2\gamma}{m}\right)\right\}^{1/2} \quad \text{and} \quad K_m = \frac{1}{2}\log\left\{\coth\left(\frac{\gamma}{m}\right)\right\} \tag{3.21}$$

appear in the quantum transfer-matrix $\mathscr{T}_m$ for the transverse Ising chain. Namely, $A_m \to 0$ and $K_m \to \infty$ for $m \to \infty$.

However, the limit of the maximum eigenvalues $\{\lambda_{\max}^{(m)}\}$ should exist in the limit $m \to \infty$, as a physical requirement. The mathematical structure of this situation will be explained as follows.

If we diagonalize $\mathscr{T}_m$ in terms of the matrix U_m as

$$U_m \mathscr{T}_m U_m^{-1} = \mathscr{T}_m^{(d)}, \tag{3.22}$$

then we have

$$\mathscr{T}_m^{(d)} |\Psi_m^*(\beta)\rangle = \lambda_{\max}^{(m)} |\Psi_m^*(\beta)\rangle \tag{3.23}$$

with $|\Psi_m^*(\beta)\rangle = U_m |\Psi_m(\beta)\rangle$. In this diagonal representation, the limits of $\mathscr{T}_m^{(d)}$ and $|\Psi_m^*\rangle$ should exist for $m \to \infty$. Namely, it is expected that the singularity of $|\Psi_m(\beta)\rangle$ may be canceled by that of U_m. This mathematical aspect will be discussed elsewhere.

The present formulation of thermo quantum dynamics is also valid even in higher dimensions, in which the thermodynamic limit $N \to \infty$ is taken only in one real dimension among d dimensions. The sizes of the remaining $(d-1)$ dimensions may be either finite or infinite.

4. AN ALTERNATIVE FORMULATION OF THERMO QUANTUM DYNAMICS

In the present section, we introduce another quantum transfer-matrix. First, we explain the main idea in one dimension. Let the Hamiltonian of the relevant system $\mathscr{H}_N$ for the system size N.

We consider the limit

$$\mathscr{T}(\beta) = \lim_{N \to \infty} \mathrm{e}^{\beta \mathscr{H}_N} \mathrm{e}^{-\beta \mathscr{H}_{N+1}}. \tag{4.1}$$

If this limit exists, the partition function of the relevant system may be expressed in terms of the above limit (4.1) as

$$Z_N(\beta) = \mathrm{Tr}[\mathscr{T}(\beta)]^N \tag{4.2}$$

for large N. This will be reasoned in the following:

$$\begin{aligned}\lim_{N\to\infty} N^{-1}\log Z_N(\beta) &\equiv \lim_{N\to\infty} N^{-1}\log \mathrm{Tr}\, \mathrm{e}^{-\beta\mathscr{H}_N}\\ &= \lim_{N\to\infty}\lim_{L\to\infty} N^{-1}\log \mathrm{Tr}\, \mathrm{e}^{\beta\mathscr{H}_L}\mathrm{e}^{-\beta\mathscr{H}_{L+N}}\\ &= \lim_{N\to\infty}\lim_{L\to\infty} N^{-1}\log \mathrm{Tr}(\mathrm{e}^{\beta\mathscr{H}_L}\mathrm{e}^{-\beta\mathscr{H}_{L+1}})(\mathrm{e}^{\beta\mathscr{H}_{L+1}}\mathrm{e}^{-\beta\mathscr{H}_{L+2}})\\ &\quad\cdots(\mathrm{e}^{\beta\mathscr{H}_{L+N-1}}\mathrm{e}^{-\beta\mathscr{H}_{L+N}})\\ &= \lim_{N\to\infty} N^{-1}\log \mathrm{Tr}[\mathscr{T}(\beta)]^N.\end{aligned} \tag{4.3}$$

The thermal average $\langle Q\rangle$ of any local observable Q is then given

$$\langle Q\rangle = \langle\Psi(\beta)|\, Q\, |\Psi(\beta)\rangle \tag{4.4}$$

where $|\Psi(\beta)\rangle$ is the eigenvector of $\mathscr{T}(\beta)$ with the maximum eigenvector $\lambda_{\max}$, namely

$$\mathscr{T}(\beta)\,|\Psi(\beta)\rangle = \lambda_{\max}\,|\Psi(\beta)\rangle. \tag{4.5}$$

Physically, $\lambda_{\max}$ should be equal to $\lambda^*_{\max}$ in the preceding section, and $|\Psi(\beta)\rangle$ should be related through the following transformation

$$|\Psi(\beta)\rangle = \mathscr{V}\,|\Psi^*(\beta)\rangle. \tag{4.6}$$

Here, $\mathscr{V}$ is defined by

$$\mathscr{V}^{-1}\mathscr{T}(\beta)\,\mathscr{V} = \mathscr{T}^{(d)}_{\infty}, \tag{4.7}$$

where

$$\mathscr{T}^{(d)}_{\infty} = \lim_{m\to\infty} \mathscr{T}^{(d)}_{m}. \tag{4.8}$$

Mathematical arguments on the convergence of this quantum transfer-matrix and some applications of this formulation will be reported in future.

5. SUMMARY AND DISCUSSION

In the present paper, we have reviewed some basic aspects of the concept of separation of procedures and exponential product formulas which yield the equivalence theorem. This is basic to the general formulation of the quantum transfer-matrix method, which results in the present new formulation of thermo quantum dynamics.

When the present paper was rewritten, the author was informed by Araki(66) that a formula similar to (4.1) was proposed by him and its convergence was proved.

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