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in Equilibrium and Nonequilibrium Systems

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in Equilibrium and Nonequilibrium Systems

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Professor Masuo Suzuki

Faculty of Science, Department of Physics, University of Tokyo,
7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

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Foreword

Speech by Toyosaburo Taniguchi

Dr. Kubo, Chairman, Distinguished Guests, and Friends,

I am very happy, pleased and honored to be here this evening with so many distinguished guests, friends, and scholars from within this country and from different parts of the world. The Taniguchi Foundation wishes to extend a warm and sincere welcome to the many participants of the Ninth International Symposium on the Theory of Condensed Matter, which series was inaugurated eight years ago through the strenuous efforts of Dr. Ryogo Kubo, who is gracing us today with his presence.

We are deeply indebted to Dr. Kubo, Dr. Suzuki, and their associates, who have spent an enormous amount of time and effort to make this particular symposium possible. We are convinced that the foundation should not be considered as what makes our symposium a success. The success is entirely due, I feel, to the continuous efforts of the Organizing Committee and of all those who have lent their support to this program. In this sense, your words of praise about the symposium, if any, should be directed to all of them.

So far, I have met in person a total of 62 participants in this Division from 12 countries: Argentina, Belgium, Canada, Denmark, the Federal Republic of Germany, France, Ireland, Israel, Rumania, Switzerland, the United Kingdom, and the United States of America, with 133 participants from Japan. Those friends I have been privileged to make, I shall always treasure.

Whenever I meet with the participants in our symposia, both young and old, I am deeply impressed by the unselfish and sincere dedication they display in pursuing their vocation. To those younger people who are made welcome by world-famous scholars as their friends, we offer our hopes that even after climbing the ladder of academic fame within, say, the next 10, 20 or 30 years, you will join forces, and help to forge closer bonds of friendship and cooperation in a manner that will make a major contribution not only to academia but also to permanent world peace. And, it is our hope that our symposia be continued as long as the fund permits, for several more years at least.

In conclusion, we sincerely trust that all the participants, both Japanese and foreign, will return home with pleasant memories of the symposium and of our enjoyable time together.

Thank you.

Preface

This volume contains papers presented at the Ninth Taniguchi Symposium on the Theory of Condensed Matter, which was held 14–18 November, 1986, at Susono, Japan. The topic of the symposium was "Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems".

The field of quantum Monte Carlo methods in equilibrium and nonequilibrium systems, namely quantum statistical Monte Carlo methods, has been studied only for about ten years. Quite recently many physicists began to work in this field, partly because larger-scale and higher-speed computers are now available, and partly because many important problems cannot yet be solved analytically. The basic idea of quantum statistical Monte Carlo methods is to transform the relevant d-dimensional quantum system into the corresponding (d+1)-dimensional classical system, using the generalized Trotter formula.

This volume consists of three parts. In the first paper of Part I, quantum statistical Monte Carlo methods are reviewed generally with great emphasis on methodology and some mathematical aspects such as the convergence and correction of the so-called ST transformation. The following four papers treat some general aspects of quantum systems, which are related to the quantum Monte Carlo approach. Part II contains ten papers which treat quantum spin systems using quantum statistical Monte Carlo methods, and two papers which treat quantum spin glasses. The five papers in Part III treat fermion systems, including nuclear systems.

The present Taniguchi Symposium was supported by the Taniguchi Foundation. Mr. Toyosaburo Taniguchi, who is the former president of Toyobo Co., Ltd., has supported various academic activities in the natural and human sciences for many years. His speech delivered at the reception in Kyoto after the symposium appears as the Foreword to this volume to illustrate the philosophy behind this support.

On behalf of all the participants we would like to express our hearty thanks to Mr. Taniguchi and the members of the Taniguchi Foundation.

Tokyo, 1 March 1987 *Masuo Suzuki*

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Part I

General Aspects of Quantum Monte Carlo Methods

General Review of Quantum Statistical Monte Carlo Methods

M. Suzuki

Department of Physics, Faculty of Science, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan

1. INTRODUCTION

The main purpose of the present paper is to explain the methodology of quantum statistical Monte Carlo Simulations to those who are coming into this rather new field of quantum Monte Carlo at finite temperatures.

Until quite recently, physics has been classified into the two categories, namely theoretical physics and experimental physics. Now there exists another category, so-called computational physics mainly based on computer simulations with use of Monte Carlo methods [1-5]. The classical Monte Carlo method was introduced by Metropolis et al. [6]. Numerical simulations of quantum systems at zero temperature were started in rather early days after quantum mechanics was established [5]. There have been proposed many methods such as the Green-function Monte-Carlo method by Kalos [7], variational Monte Carlo methods [5], and diffusion equation Monte Carlo methods [5], in order to study quantum-mechanical properties at zero temperature.

However, quantum Monte Carlo at finite temperatures had been believed to be quite difficult except a special symmetric system of the isotropic Heisenberg model [8], until the present author [9-12] proposed a general approach of "quantum statistical Monte Carlo" in which d-dimensional quantum systems are mapped onto (d+1)-dimensional classical systems using the following Trotter-like formula of exponential operators [9-12]:

$$e^{A_1+A_2+\cdots+A_p} = \lim_{n\to\infty}(e^{A_1/n}e^{A_2/n}\cdots e^{A_p/n})^n . \qquad (1.1)$$

The above general approach was first applied to quantum spin systems by Suzuki, Miyashita and Kuroda [11,13]. Barma and Shastry [14] applied this general idea to find equivalent classical models of one-dimensional fermi lattices. Hirsch et al. [15] performed explicitly Monte Carlo simulations in fermi systems. On the other hand, De Raedt and Lagendijk [16,17] studied extensively quantum spin, fermi and bose systems, and polaron problems, using the above general transformation method (1.1).

Many numerical investigations of the validity and convergence of the above general approach based on (1.1) have been reported by De Raedt-De Raedt [18], Wiesler [19], Cullen-Landau [20]. There have been reported many other interesting applications of the above idea to S = 1/2 spin systems by Satija-Wysin-Bishop [21], Marcu-Müller-Schmatzer [22], Sakaguchi-Kubo-Takada [23], to higher-spin systems by Takano [24] and Marcu-Wiesler [25], and to fermi gas by Takahashi and Imada [26]. Kolb [27] performed Monte Carlo renormalization group calculations in the two-dimensional quantum transverse Ising model by transforming it to the corresponding three-dimensional Ising model, as was suggested by the present author [28]. Betsuyaku [29] performed calculations of the linear quantum spin systems numerically by using the quantum transfer-matrix method [29,30]. Tsuzuki [31] applied this transfer-matrix method to the case of higher-spin chains using the cluster decomposition method [12,30]. Quite recently Nagai et al. [32] applied the above general method to the transverse Ising model.

In Section 2, basic ideas of the quantum statistical Monte Carlo will be explained in detail. Namely we discuss generalized Trotter-like approximations, decomposition formulae of exponential operators and convergence theorems [33], and moment- and cumulant-expansions of sliced exponential operators. The equivalence theorem by the present author [10,12] will be also reviewed in Section 2. In Section 3, the thermofield quantum Monte Carlo method [34-39] will be presented. In Section 4, the thermofield transfer-matrix methods will be discussed. The decomposition of the Trotter-like formula (1.1) is not unique and consequently it has the merit that cluster decompositions are also applicable in (1.1), as will be discussed in Section 6. In Section 7, the quantum Monte Carlo renormalization approach will be discussed. In Section 8, quantum spin glasses will be discussed briefly using some equivalent classical random spin systems. In Section 9, Fisher's finite-size scaling law is discussed in connection with Monte Carlo simulations. A finite-Trotter-number scaling ansatz is proposed in Section 10. This is originally proposed in the present paper. In Section 11, correlation identities by the present author [41] will be presented in a completely general form with possible applications to testing of Monte Carlo calculations. They take the following general form

$$\langle fg \rangle = \langle f \langle g \rangle_{\mathcal{H}_g} \rangle \tag{1.2}$$

for arbitrary classical functions f and g under the conditions that f and g do not contain common variables that $\langle g \rangle$ is the canonical average of g over the partial Hamiltonian $\mathcal{H}_g$ which is connected to the variables contained in g. This is a complete generalization of Callen's identity [42]. These correlation identities are very useful to test the accurary of Monte Carlo calculations, as was discussed by Mouritsen [3]. In Section 12, symmetry properties of Kubo's canonical correlations with respect to Trotter's number n will be studied in detail. In Section 13, quantum dynamics via Monte Carlo will be discussed. In Section 14, summary and future problems will be given.

2. GENERAL THEORY OF QUANTUM MONTE CARLO

2.1 Generalized Trotter-like Approximations

As was briefly mentioned in Section 1, the quantum statistical Monte Carlo method [10-13] is based on Trotter's formula [43] or the generalized Trotter formula (1.1). It is convenient to introduce here the following extremely generalized Trotter-like formula [44,45]

$$e^{-\beta\mathcal{H}} = (e^{-\beta\mathcal{H}/n})^n = \lim_{n\to\infty}(f_m[-\tfrac{1}{n}\beta\mathcal{H}])^n, \tag{2.1}$$

where the approximant $f_m[-(1/n)\beta\mathcal{H}]$ satisfies the following condition

$$e^{-\beta\mathcal{H}/n} = f_m[-\tfrac{1}{n}\beta\mathcal{H}] + O(\tfrac{1}{n^m}) \tag{2.2}$$

for large n, with some positive integer m.

2.2 Decomposition Formulae of Exponential Operators and Convergence Theorems

Now we have the following theorem concerning the above generalized Trotter-like decomposition.

Theorem 1 [12]: With the condition (2.2), we have

$$e^{-\beta\mathcal{H}} = (f_m[-\tfrac{1}{n}\beta\mathcal{H}])^n + O(\tfrac{1}{n^{m-1}}), \tag{2.3}$$

or more explicitly

$$\| e^{-\beta\mathcal{H}} - (f_m[-\tfrac{1}{n}\beta\mathcal{H}])^n \| \le nM^{n-1} \| e^{-\beta\mathcal{H}/n} - f_m[-\tfrac{1}{n}\beta\mathcal{H}] \|, \tag{2.4}$$

where

$$M \equiv \max\{\| \exp(-\tfrac{1}{n}\beta\mathcal{H})\|, \| f_m[-\tfrac{1}{n}\beta\mathcal{H}]\| \}. \tag{2.5}$$

These are very useful in performing quantum Monte Carlo simulations of many-body quantum systems in equilibrium, as shown in previous papers [10-32].

The partition function of the relevant system described by the Hamiltonian is given by

$$Z = \mathrm{Tr}\, e^{-\beta\mathcal{H}} = \mathrm{Tr}(f_m[-\tfrac{1}{n}\beta\mathcal{H}])^n + O(\tfrac{1}{n^{m-1}}). \tag{2.6}$$

A more non-uniformly generalized form of Eq. (2.3) is given by

$$e^{-\beta\mathcal{H}} = e^{-(\beta-\beta_n)\mathcal{H}} e^{-(\beta_n-\beta_{n-1})\mathcal{H}} e \cdots e^{-(\beta_1-\beta_0)\mathcal{H}} e^{-\beta_0\mathcal{H}}$$

$$= f_m[-(\Delta\tau)\mathcal{H}] f_m[-(\Delta\tau_n)\mathcal{H}] \cdots f_m[-(\Delta\tau_0)\mathcal{H}] + O(\overline{\Delta\tau}^{m-1}), \tag{2.7}$$

where

$$\overline{\Delta\tau} = \max\{\Delta\tau,\ \Delta\tau_n,\ ---,\ \Delta\tau_0\} \text{ and } \Delta\tau=\beta-\beta_n,\ \Delta\tau_n=\beta_n-\beta_{n-1},\ ---,\ \Delta\tau_0=\beta_0. \tag{2.8}$$

There are many different ways to express the approximate operator $f_m[-\beta\mathcal{H}/n]$ explicitly, and to evaluate $\mathrm{Tr}(f_m[-\beta\mathcal{H}/n])^n$ numerically, as in [10-32]. Many people have been trying to find new approximate expressions of $f_m[-\beta\mathcal{H}/n]$ and efficient evaluation methods of them in the above general scheme of generalized Trotter-like approximations (2.3).

For example, we have [9,10,12,33]

$$f_2[A_1+A_2+---+A_p] = e^{A_1}e^{A_2}---e^{A_p}\ . \tag{2.9}$$

These Trotter-like approximations have been used frequently [10-33].

It will be instructive to summarize here some useful decomposition formulae.

Theorem 2 [33]: For any set of operators $\{A_j\}$ in a Banach algebra (i.e., normed space),

$$\left\| \exp\left(\sum_{j=1}^{p} A_j\right) - \left(\prod_{j=1}^{p} e^{(1/n)A_j}\right)^n \right\| \le \frac{1}{2n}\left(\sum_{j>k} \left\| [A_j, A_k] \right\|\right) \exp\left(\sum_{j=1}^{p} \left\| A_j \right\|\right) \tag{2.10}$$

with an arbitrary positive integer p.

In particular, for p=2, we obtain Trotter's formula

$$e^{A+B} = \lim_{n\to\infty}(e^{A/n}\, e^{B/n})^n. \tag{2.11}$$

Theorem 3 [33]: For any operators A and B in a Banach algebra,

$$\left\| e^{A+B} - (e^{A/2n}\, e^{B/n}\, e^{A/2n})^n \right\| \le \frac{1}{n^2}\Delta_2(A,B), \tag{2.12}$$

where

$$\Delta_2(A,B) = \frac{1}{12}\left\{ \left\| [[A,B],B] \right\| + \frac{1}{2}\left\| [[A,B],A] \right\| \right\} \times \exp(\|A\| + \|B\|). \tag{2.13}$$

Now we discuss higher order decompositions of the general exponential operator $\exp(A_1+A_2+\cdots+A_p)$. For this purpose, we may find $f_m(\{\frac{1}{n}A_j\})$ which satisfies the condition

$$\exp\left(\frac{1}{n}\sum_{j=1}^{p} A_j\right) = f_m\left(\left\{\frac{1}{n}A_j\right\}\right) + O\left(\frac{1}{n^m}\right), \tag{2.14}$$

according to the generalized Trotter-like formula (2.1) with (2.2). It is convenient to note that the (m+1)th approximant defined by

$$f_{m+1}\left(\frac{A}{n},\frac{B}{n}\right) = e^{A/n}\, e^{B/n}\, e^{C_2/n^2} \cdots e^{n^{-m}C_m} \tag{2.15}$$

satisfies the condition (2.14), if the coefficients $\{C_j\}$ are given by [9]

$$C_2 = \frac{1}{2}[B,A],\ C_3 = \frac{1}{3}[C_2, A+2B], \cdots. \tag{2.16}$$

Thus, we can obtain formally any higher order decompositions of the exponential operator (2.14).

Up to now, we have discussed the convergence of decomposed operators. We are, however, practically interested in the trace of such decomposed operators. Then, we may have more convenient theorems which assure more rapid convergence. The following correction formula is now well known [15,30,33,44-46]:

$$\mathrm{Tr}e^{A+B} = \mathrm{Tr}(e^{A/n}e^{B/n})^n + O(n^{-2}). \tag{2.17}$$

This is generalized as follows [44]:

Theorem 4: If $f_m(\{A_j\})$ satisfies the condition

$$f_m(\{-A_j\})^{-1} = f_m(\{A_j\})^t \tag{2.18}$$

then the approximant

$$Z_m(n) \equiv \mathrm{Tr}[f_m(\{\tfrac{1}{n}A_j\})]^n \tag{2.19}$$

is an even function of n, namely,

$$Z_m(-n) = Z_m(n). \tag{2.20}$$

Theorem 5 (corollary of Theorem 4)[44]: With the conditions (2.14) and (2.19), we have

$$Z_{exact} = Z_{2m}(n) + O(\frac{1}{n^{2m}}). \tag{2.21}$$

In particular, if we put $f_m(\{A_j\})$ as (2.9) for symmetric $\{A_j\}$ (namely, $A^t{}_j = A_j$), then we have the following theorem:
Theorem 6 [44]: If $\{A_j\}$ are symmetric operators (i.e., $A^t{}_j = A_j$), then we have

$$Z_2(n) \equiv \mathrm{Tr}(e^{A_1/n}e^{A_2/n}\cdots e^{A_p/n})^n = Z_2(-n). \tag{2.22}$$

Consequently we have

$$Z_{exact} = Z_2(n) + O(\frac{1}{n^2}). \tag{2.23}$$

This was first obtained by Fye [45] for a general integer p in a different condition.

Theorem 6 suggests [44] the following new extrapolation method:

$$Z_{exact} \simeq Z(n) + \frac{a}{n^2+b}. \tag{2.24}$$

Theorem 7 [43]: If $Q^t = Q$ with the condition (2.18), the average of any quantum operator Q defined by

$$\langle Q\rangle_m(n) \equiv \mathrm{Tr}Q[f_{2m}(\{\tfrac{1}{n}A_j\})]^n/Z_{2m}(n) \tag{2.25}$$

is an even function of n, namely

$$\langle Q\rangle_m(-n) = \langle Q\rangle_m(n). \tag{2.26}$$

In particular, we have