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On the convergence of the Trotter formula

R Thieberger

Physics Department, Ben Gurion University of the Negev, Beer Sheva and NRC Negev, PO Box 9001, Beer Sheva, Israel

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Abstract. The convergence of the Trotter formula for the one-dimensional harmonic oscillator is studied. Padé approximants improve the convergence.

1. Introduction

In recent years there has been much interest in solving statistical mechanics problems by a Monte Carlo procedure (Barker 1979, De Raedt *et al* 1982). The approach is based on the path integral formulation due to Feynman (1972). Intimately connected with this approach is the Trotter product formula (Schulman 1981), which we will restate here for the sake of completeness.

The density matrix is defined by

$$\rho = \exp(-\beta H) \tag{1}$$

and the Trotter formula states (Suzuki 1976)

$$\rho = \lim_{N\to\infty} \rho_N \tag{2}$$

where

$$\rho_N = \left[\exp\left(-\frac{\beta H_0}{N}\right)\exp\left(-\frac{\beta H_1}{N}\right)\dots\exp\left(-\frac{\beta H_p}{N}\right)\right]^N \tag{3}$$

$$H = H_0 + H_1 + \dots + H_p.$$

The different H_l do not have to commute with each other. This formula holds if each of the operators H_l is bounded. Let us recall that a linear operator on a finite-dimensional Hilbert space is bounded.

Except for some rigorous inequalities (Lieb and Thirring 1976), little is known about the nature of this formula. The convergence must be studied for each particular case (De Raedt *et al* 1982). In this paper we investigate the convergence of equation (2) in a particularly simple case, the one-dimensional harmonic oscillator. This case is instructive, because we can obtain the explicit expressions of the partition function Z and the expressions for Z_N, where

$$Z_N = \mathrm{Tr}\,\rho_N \tag{4}$$

where, obviously,

$$\lim_{N\to\infty} Z_N = Z.$$

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Let us recall the essential formulae from the literature; we will write the expressions in one dimension. The Hamiltonian is

$$H = \frac{h^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) = T + V. \tag{5}$$

Using equation (3), the density matrix is expressed in the coordinate representation as follows (Schulman 1981):

$$\rho_N(x_0, x_N) = \int \mathrm{d}x_1 \ldots \mathrm{d}x_{N-1} \prod_{j=0}^{N-1} \langle x_{j+1}|\mathrm{e}^{-\beta T/N}\,\mathrm{e}^{-\beta V/N}|x_j\rangle \tag{6}$$

from which

$$\rho_N(x_0, x_N) = \int \mathrm{d}x_1 \ldots \mathrm{d}x_{N-1}\left(\frac{mN}{2\pi\beta\hbar^2}\right)^{N/2} \times \prod_{j=0}^{N-1} \exp\left(-\frac{m(x_{j+1}-x_j)^2 N}{2\beta\hbar^2} - \frac{\beta V(x_j)}{N}\right). \tag{7}$$

The partition function based on equation (7) is then

$$Z_N = \int \mathrm{d}x_0 \ldots \mathrm{d}x_N\, \delta(x_0 - x_N)\left(\frac{mN}{2\pi\beta\hbar^2}\right)^{N/2} \times \prod_{j=0}^{N-1} \exp\left(-\frac{m(x_{j+1}-x_j)^2 N}{2\beta\hbar^2} - \frac{\beta V(x_j)}{N}\right). \tag{8}$$

2. The Z_N for the harmonic oscillator

In this case

$$V(x) = \tfrac{1}{2}m\omega^2 x^2. \tag{9}$$

We can then rewrite Z_N in a form suitable for explicit evaluation:

$$Z_N = \int \frac{\mathrm{d}t_0 \ldots \mathrm{d}t_{N-1}}{\pi^{N/2}} \exp\left[\exp\left(-A_N \sum_{i=0}^{N-1} t_i^2 + 2\sum_{i=0}^{N-1} t_i t_{i+1}\right)\right] \qquad (t_N \equiv t_0) \tag{10}$$

where $A_N = 2 + B^2/N^2$ and $B = \beta\hbar\omega$.

Since all integrals in equation (10) are Gaussians of the form

$$\int_{-\infty}^{\infty} \exp(-p^2x^2 \pm qx)\,\mathrm{d}x = \frac{\sqrt{\pi}}{p}\exp\left(\frac{q^2}{4p^2}\right) \tag{11}$$

we can perform the integration for different values of N. We write our results in the form

$$Z_N = [f_N(A_N)]^{-1/2}. \tag{12}$$

Table 1 gives the expressions for $N \leqslant 7$.

It is instructive to see how these expressions converge for small B; this can be seen in table 2. To understand the rate of convergence we compare it to the convergence of the exact solution, developed in powers of B^2 (Feynman 1972)

$$Z = \frac{1}{2\sinh(\frac{1}{2}B)} = \frac{1}{B + \frac{1}{3}(B/2)^3 + \frac{1}{60}(B/2)^5 + \ldots}. \tag{13}$$

Table 1. The expressions for $f_N(A_N)$.

N	$f_N(A_N)$
1	A_1-2
2	A_2^2-4
3	$A_3^3-3A_3-2$
4	$A_4^4-4A_4^2$
5	$A_5^5-5A_5^3+5A_5-2$
6	$A_6^6-6A_6^4+9A_6^2-4$
7	$A_7^7-7A_7^5+14A_7^3-7A_7-2$

Table 2. $Z_N=B^{-1}[1+\alpha_N B^2+\mathrm{O}(B^4)]^{-1}$.

N	1	2	3	4	5	6	7	∞
α_N	0	$\frac{1}{32}$	$\frac{1}{27}$	$\frac{5}{128}$	$\frac{1}{25}$	$\frac{35}{864}$	$\frac{2}{49}$	$\frac{1}{24}$

In table 3 we compare the results for N Trotter terms (equation (12)) to N terms in the series development (equation (13)) for two values of B, a relatively small value ($B=2$) and a much larger value ($B=20$). As can be seen, in both cases the Trotter formula convergence does not seem to be very fast.

We therefore wish to improve the convergence of the Trotter formula. From the study of Padé approximants one notices that this method improves the convergence of series even in unexpected cases (Killingbeck 1983). Let us recall its definition. The rational fraction P/Q where

$$P=\sum_0^M p_n x^n \qquad Q=\sum_0^N q_n x^n \qquad q_0=1$$

can be formally expanded as a power series in x. If this expansion fits the series expansion of some function $f(x)$ up to the x^{M+N} term, then it is called the $[M/N]$ Padé approximant to $f(x)$.

We tried to apply the method, using a Wynn algorithm (Wynn 1956, Killingbeck 1983) to the Trotter formula results. The best approximation was obtained for

Table 3. The comparison of the partial sums of Z for $B=2$ and 20.

	$B=2$			$B=20$		
N	Z_N	$[\sinh(\frac{1}{2}B)_N^{-1}]$	Padé approx.	Z_N	$[\sinh(\frac{1}{2}B)_N^{-1}]$	Padé approx.
1	0.500 00	0.500 00	—	0.050 00	0.050 00	—
2	0.447 21	0.428 57	—	0.009 81	0.002 83	—
3	0.435 48	0.425 53	0.432 13	0.003 16	0.000 50	0.001 85
4	0.431 17	0.425 46	0.428 67	0.001 38	0.000 17	0.000 72
5	0.429 14	0.425 46	0.427 00	0.000 73	0.000 09	0.000 30
6	0.428 03	0.425 46	0.426 37	0.000 45	0.000 06	0.000 18
7	0.427 35	0.425 46	0.425 99	0.000 31	0.000 05	0.000 12
∞	0.425 46	0.425 46	0.425 46	0.000 05	0.000 05	0.000 05

$[(N/2)/(N/2)]$ for N even and $[((N+1)/2)/((N-1)/2)]$ for N odd. The results are given in table 3.

To examine if this improvement is limited to our special case, we tried to apply it to a different problem: the energy per site of a ring of four spins obtained for the Heisenberg antiferromagnet (De Raedt *et al* 1982, table 4). For the case $\beta = 1$ we obtain for [3/3] the value of -1.954 compared to the exact value -1.944 and the calculated (i.e. [6/0]) value of -1.984.

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