

Applications of the generalized Trotter formula

Hans De Raedt and Bart De Raedt

Physics Department, University of Antwerp, Universiteitsplein 1, B-2610 Wilrijk, Belgium

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We study the properties of Suzuki's systematic approximations to the exponential operator $\exp(-\beta H)$ by calculating the thermodynamic functions of three simple quantum models. We demonstrate that the path-integral representation of the partition function obtained from these approximations can be simplified and made more accurate by constructing Hermitian versions of Suzuki's expressions.

I. INTRODUCTION

The Trotter formula¹

$$e^{-\beta(A+B)} = \lim_{m \rightarrow \infty} (e^{-\beta A/m} e^{-\beta B/m})^m, \quad (1.1)$$

is a convenient starting point for deriving path-integral representations of the partition function

$$Z \equiv \text{Tr} e^{-\beta H}, \quad (1.2)$$

of a quantum (lattice) model defined by the Hamiltonian $H=A+B$. In those cases where it is difficult to write down the classical Lagrangian, the Trotter formula can still be used to construct several equivalent but distinct path-integral representations of the partition function. In particular Suzuki² showed that the partition function of a d -dimensional Heisenberg spin- $\frac{1}{2}$ model is equivalent to the partition function of a $(d+1)$ -dimensional Ising model with complicated four-spin interactions. Formally this Ising model partition function is one of the path-integral representations of the Heisenberg model. Using a slightly modified version of Suzuki's approach, Barma and Shastri derived path-integral representations for fermion lattice models³ and also showed that the eight-vertex model is one of the path-integral representations of the spin- $\frac{1}{2}$ chain.⁴ In addition it has been demonstrated recently⁵⁻⁸ that by using these path-integral representations it is possible to calculate the thermodynamic properties of spin and fermion lattice models. The complexity of the path-integral representation mostly but not always⁹ requires a Monte Carlo simulation technique to calculate estimators of the energy, specific heat, and correlation functions. The basic idea of this computational technique is to calculate the properties of the approximate model defined by

$$Z_m \equiv \text{Tr}(e^{-\beta A/m} e^{-\beta B/m})^m, \quad (1.3)$$

and to study the convergence of the results as a function of m . The number of products m plays the role of the number of (imaginary) time slices that appears in the path integral.^{10,11} In practical applications two different fundamental problems arise. The first one is the numerical problem of subtracting two large numbers¹² (if β/m is small) and reflects the quantum nature of the problem. It is due to the fact that in order to simulate the quantum

model one has to choose a particular representation for the wave functions. The second problem concerns the rate of convergence of the approximant (1.3) as a function of the number of time slices m . This is equally important for practical applications because the computation time of the simulation is at least a linear function of m . Moreover up to now only the simplest form of the Trotter formula has been used in numerical calculations. Therefore, it is worthwhile to examine the possibility of using more complicated forms of the Trotter formula in order to improve the accuracy of the small- m approximants and the rate of convergence.

The aim of the present paper is to study the properties of the generalized Trotter formula derived by Suzuki.¹³ To demonstrate that it is possible to go beyond the simplest form (1.1) we have chosen two simple exactly solvable quantum models for which numerical results can be obtained without the use of a Monte Carlo method. In this way we do not encounter one of the fundamental problems discussed previously. We show that with a modest amount of extra analytic work, considerable improvement can be achieved by modifying Suzuki's generalized approximants.

The basic step in the construction of approximants to the exponential operator $\exp[-\tau(A+B)]$ is to find a product of exponential operators which is correct up to a certain power of $\tau \equiv \beta/m$. Straightforward algebra yields the results

$$\begin{aligned} e^{-\tau(A+B)} &= f_1(A, B) + O(\tau^2) = f_2(A, B) + O(\tau^3) \\ &= f_3(A, B) + O(\tau^4), \end{aligned} \quad (1.4)$$

$$f_1(A, B) \equiv e^{-\tau A} e^{-\tau B}, \quad (1.4)$$

$$f_2(A, B) \equiv e^{-\tau A} e^{-\tau B} e^{\tau^2 C_2}, \quad (1.5)$$

$$f_3(A, B) \equiv e^{-\tau A} e^{-\tau B} e^{\tau^2 C_2} e^{-\tau^3 C_3}, \quad (1.6)$$

where

$$C_2 \equiv [B, A]/2, \quad (1.7)$$

and

$$C_3 \equiv [[B, A], A + 2B]/6. \quad (1.8)$$

We use the expressions (1.4)–(1.6) to define the systematic approximants to the partition function

$$Z_m^{(\alpha)} \equiv \text{Tr}\{[f_\alpha(A,B)]^m\}, \quad \alpha = 1, 2, 3. \quad (1.9)$$

Suzuki¹³ shows that $Z_m^{(\alpha+1)}$ converges faster to Z than $Z_m^{(\alpha)}$. However, the approximants (1.4)–(1.7) are not very well suited to calculate the properties of physical systems because they lead to non-Hermitian approximations to the Hermitian operator $\exp(-\tau H)$. We avoid this problem by introducing the Hermitian approximants

$$e^{-\tau(A+B)} = g_2(A,B) + O(\tau^3) = g_4(A,B) + O(\tau^5),$$

$$g_2(A,B) \equiv e^{-\tau A/2} e^{-\tau B} e^{-\tau A/2}, \quad (1.10)$$

$$g_4(A,B) \equiv e^{-\tau A/2} e^{-\tau B/2} e^{-\tau^3 C_3/4} e^{-\tau B/2} e^{-\tau A/2}. \quad (1.11)$$

Comparing g_2 with f_1 and g_4 with f_3 we see that requiring the product of exponential operators to be Hermitian automatically leads to more accurate approximations. Obviously, the partition function obtained by using g_2 is identical to $Z_m^{(1)}$ because of the cyclic permutation property of the trace. This leads to the conclusion that although f_1 is correct up to order τ , $Z_m^{(1)}$ is correct up to order τ^2 . The operator C_2 is anti-Hermitian ($C_2 = -C_2^\dagger$) and therefore the Hermitian equivalent of f_2 is identical to g_2 . For the same reason C_2 does not appear in g_4 . It can be shown that with or without factors containing C_2 , g_4 is always correct up to fourth order in τ . The use of Hermitian approximants is important for practical applications. The main advantage is most easily seen by comparing f_3 and g_4 . Although the expression for g_4 is simpler than that of f_3 , it is more accurate. We use g_4 to define a fourth approximant to the partition function

$$Z_m^{(4)} \equiv \text{Tr}\{[g_4(A,B)]^m\}. \quad (1.12)$$

Although it is possible to derive higher-order approximations in a systematic manner, the four different approximate partition functions introduced above are sufficient to illustrate the salient features of the approach.

II. SPIN- $\frac{1}{2}$ MODEL

We consider a simple spin- $\frac{1}{2}$ model with Hamiltonian

$$H = A + B, \quad (2.1a)$$

$$A = -h\sigma^z, \quad (2.1b)$$

$$B = -a\sigma^x, \quad (2.1c)$$

where σ^α ($\alpha = x, y, z$) are the usual Pauli matrices. This Hamiltonian is easily diagonalized and the thermodynamic quantities may be calculated rigorously from the partition function $Z = 2 \cosh[\beta(h^2 + a^2)^{1/2}]$. From Eqs. (1.7) and (1.8) we find

$$C_2 = -iah\sigma^y, \quad (2.2)$$

$$C_3 = \frac{2}{3}ah(2a\sigma^z - h\sigma^x). \quad (2.3)$$

We may represent the exponential factors appearing in the expressions for f_α and g_α as 2×2 matrices, because the usual spin states “up” and “down” form a complete set. The approximants of the partition function $Z_m^{(\alpha)}$, $\alpha = 1, \dots, 4$ are evaluated by diagonalizing the matrices f_α and g_α . Here we should mention that for the calculation of g_4 we factorized

$$e^{-\tau^3 C_3/4} = e^{\tau^3 ah^2 \sigma^x/12} e^{-\tau^3 a^2 h \sigma^z/3} e^{\tau^3 ah^2 \sigma^x/12}, \quad (2.4)$$

because this simplifies the calculation and the result for g_4 without affecting its correctness up to fourth order in τ . The results for the different approximants of the partition function may be summarized as follows:

TABLE I. The free energy of the spin- $\frac{1}{2}$ model $H = -h\sigma^z - a\sigma^x$ obtained from (2.5) using (2.7) ($F_m^{(1)}$), (2.8) ($F_m^{(2)}$), (2.9) ($F_m^{(3)}$), and (2.10) ($F_m^{(4)}$) as a function of the number of time slices m . The free energy $\bar{F}_m^{(4)}$ is obtained by interchanging A and B . The inverse temperature $\beta = 1$, $h = 1$, and $a = 2$.

m	$F_m^{(1)}$	$F_m^{(2)}$	$F_m^{(3)}$	$F_m^{(4)}$	$\bar{F}_m^{(4)}$
1	-2.4519	-1.0714	0.0000	-3.3477	-3.0049
2	-2.3136	-2.4211	-1.9327	-2.3060	-2.2878
3	-2.2784	-2.3538	-2.1616	-2.2581	-2.2550
4	-2.2652	-2.3130	-2.2180	-2.2507	-2.2498
5	-2.2589	-2.2911	-2.2350	-2.2487	-2.2484
6	-2.2554	-2.2784	-2.2413	-2.2481	-2.2479
7	-2.2533	-2.2704	-2.2441	-2.2478	-2.2477
8	-2.2520	-2.2652	-2.2455	-2.2476	-2.2476
9	-2.2510	-2.2615	-2.2462	-2.2475	-2.2475
10	-2.2503	-2.2589	-2.2466	-2.2475	-2.2475
12	-2.2494	-2.2554	-2.2470	-2.2475	-2.2475
14	-2.2489	-2.2533	-2.2472	-2.2474	-2.2474
16	-2.2486	-2.2520	-2.2473	-2.2474	-2.2474
24	-2.2479	-2.2494	-2.2474	-2.2474	-2.2474
32	-2.2477	-2.2486	-2.2474	-2.2474	-2.2474
64	-2.2475	-2.2477	-2.2474	-2.2474	-2.2474
128	-2.2474	-2.2475	-2.2474	-2.2474	-2.2474
∞	-2.2474	-2.2474	-2.2474	-2.2474	-2.2474

TABLE II. The energies $E_m^{(1)}, E_m^{(4)}$ and the specific heats $C_m^{(1)}, C_m^{(4)}, \hat{C}_m^{(4)}$ of the spin- $\frac{1}{2}$ model $H = -h\sigma^z - a\sigma^x$ as a function of the number of time slices m . The inverse temperature $\beta=1$, $h=1$, and $a=2$.

m	$E_m^{(1)}$	$E_m^{(4)}$	$C_m^{(1)}$	$C_m^{(4)}$	$\hat{C}_m^{(4)}$
1	-2.6896	-6.9972	0.7026	14.0756	-43.9606
2	-2.3780	-2.4191	0.5432	1.3944	-0.8520
3	-2.2790	-2.2072	0.3952	0.3768	0.1284
4	-2.2398	-2.1837	0.3266	0.2498	0.2315
5	-2.2208	-2.1805	0.2914	0.2241	0.2456
6	-2.2102	-2.1806	0.2714	0.2180	0.2450
7	-2.2038	-2.1813	0.2590	0.2169	0.2420
8	-2.1995	-2.1820	0.2508	0.2172	0.2389
9	-2.1966	-2.1826	0.2451	0.2178	0.2364
10	-2.1945	-2.1830	0.2411	0.2185	0.2343
12	-2.1918	-2.1837	0.2357	0.2196	0.2313
14	-2.1902	-2.1842	0.2324	0.2205	0.2294
16	-2.1891	-2.1845	0.2303	0.2211	0.2280
24	-2.1871	-2.1851	0.2264	0.2223	0.2255
32	-2.1864	-2.1853	0.2251	0.2227	0.2246
64	-2.1858	-2.1855	0.2238	0.2232	0.2236
128	-2.1856	-2.1855	0.2234	0.2233	0.2234
∞	-2.1856	-2.1856	0.2233	0.2233	0.2233

$$Z_m^{(\alpha)} = (\lambda_+^{(\alpha)})^m + (\lambda_-^{(\alpha)})^m, \quad (2.5)$$

$$\lambda_{\pm}^{(\alpha)} = X^{(\alpha)} \pm [(X^{(\alpha)})^2 - 1]^{1/2}, \quad (2.6)$$

$$X^{(1)} = \cosh(\tau h) \cosh(\tau a), \quad (2.7)$$

$$X^{(2)} = \cosh(\tau h) \cosh(\tau a) \cos(\tau^2 h a) + \sinh(\tau h) \sinh(\tau a) \sin(\tau^2 h a), \quad (2.8)$$

$$X^{(3)} = \cosh \left[\tau h \left(1 - \frac{4\tau^2 a^2}{3} \right) \right] \cosh \left[\tau a \left(1 + \frac{2\tau^2 h^2}{3} \right) \right] \cos(\tau^2 h a) \\ + \sinh \left[\tau h \left(1 - \frac{4\tau^2 a^2}{3} \right) \right] \sinh \left[\tau a \left(1 - \frac{2\tau^2 h^2}{3} \right) \right] \sin(\tau^2 h a), \quad (2.9)$$

$$X^{(4)} = \cosh(\tau h) \cosh \left[\frac{\tau^3 a^2 h}{3} \right] \cosh \left[\tau a \left(1 + \frac{\tau^2 h^2}{6} \right) \right] - \sinh(\tau h) \sinh \left[\frac{\tau^3 a^2 h}{3} \right]. \quad (2.10)$$

From the above results for $Z_m^{(\alpha)}$ the approximants $F_m^{(\alpha)} \equiv -(1/\beta) \ln Z_m^{(\alpha)}$ for the free energy, $E_m^{(\alpha)} \equiv -(\partial/\partial\beta)Z_m^{(\alpha)}$ for the energy, and $C_m^{(\alpha)} \equiv -\beta^2(\partial/\partial\beta)E_m^{(\alpha)}$ for the specific heat may be obtained in a straightforward manner.

Results for $F_m^{(\alpha)}$, for $\beta=1$, $h=1$, and $a=2$ are displayed in Table I. As might be expected from our discussion in Sec. I, $F_m^{(2)}$ does not yield any improvement compared to $F_m^{(1)}$. The results of the simplest approximation are even slightly better. Going to higher approximants, the rate of convergence rapidly increases and our results demonstrate that it is possible to obtain good estimates of the free energy even for small m values. The approximant $\tilde{F}_m^{(4)}$ corresponds to an $F_m^{(4)}$ where we have interchanged the role of A and B . This choice for A and B yields better results and this is generally true for $a > h$ whereas for $a < h$ our first choice is better. This clearly demonstrates that the choice of the representation and the way of partitioning the Hamiltonian are related and a careful examination of the different possibilities is necessary. In Table II we show

some results for the energy and specific heat approximants. Whereas $C_m^{(4)}$ is obtained in the usual manner by taking derivatives of $Z_m^{(4)}$, we calculated $\hat{C}_m^{(4)}$ using the identity $C = \beta^2(\langle H^2 \rangle - \langle H \rangle^2)$, which gives

$$\hat{C}_m^{(4)} = \beta^2[h^2 + a^2 - (E_m^{(4)})^2]. \quad (2.11)$$

As the specific heat is essentially a second derivative with respect to β of the partition function it is understandable that especially for this quantity the gain in accuracy when using higher approximants is considerable. When m is sufficiently large the energy and free-energy approximants converge to the exact value from below. It is important to note that for small m values the energy is smaller than the free energy which is of course an unphysical result. This indicates that in order to get meaningful results one should go to higher m values. For most applications the Trotter formula is used in combination with the Monte Carlo simulation technique. The Monte Carlo techniques used in recent work^{5-9,13} are not suited to calculate the

TABLE III. The free energy $F_m^{(1)}$, energy $E_m^{(1)}$, and specific heat $C_m^{(1)}$ of the harmonic oscillator as a function of the number of time slices. The inverse temperature $\beta=5$ and the oscillator frequency $\omega=1$. For small m the free energy is larger than the thermal energy.

m	$F_m^{(1)}$	$E_m^{(1)}$	$C_m^{(1)}$
1	0.3219	0.2000	1.0000
2	0.4160	0.3220	1.1338
3	0.4530	0.3923	0.9630
4	0.4703	0.4316	0.7692
5	0.4796	0.4545	0.6198
6	0.4850	0.4687	0.5134
7	0.4884	0.4779	0.4380
8	0.4907	0.4842	0.3838
9	0.4923	0.4887	0.3439
10	0.4935	0.4920	0.3139
12	0.4951	0.4964	0.2729
14	0.4960	0.4991	0.2470
16	0.4966	0.5008	0.2298
24	0.4977	0.5041	0.1975
32	0.4981	0.5053	0.1859
64	0.4985	0.5064	0.1746
128	0.4986	0.5067	0.1717
∞	0.4986	0.5068	0.1707

free energy.¹⁴ This is probably the reason that this anomaly was not noted before. It shows however that using the Trotter formula without studying the convergence as a function of m may lead to erroneous and unphysical conclusions.

III. HARMONIC OSCILLATOR

As a second model we consider a single harmonic oscillator $H=A+B$ with $A=\omega^2x^2/2$ and $B=p^2/2$. For C_2 and C_3 we obtain

TABLE IV. The free energy $F_m^{(4)}$, energy $E_m^{(4)}$, and specific heat $C_m^{(4)}$ of the harmonic oscillator as a function of the number of time slices. The inverse temperature $\beta=5$ and the oscillation frequency $\omega=1$. The approximation (3.5) is only meaningful if $\beta\omega/m < 1$.

m	$F_m^{(4)}$	$E_m^{(4)}$	$C_m^{(4)}$
5	0.4888	0.4571	1.2055
6	0.4940	0.4834	0.6473
7	0.4961	0.4943	0.4227
8	0.4972	0.4995	0.3168
9	0.4977	0.5023	0.2613
10	0.4981	0.5038	0.2299
12	0.4984	0.5054	0.1992
14	0.4985	0.5060	0.1860
16	0.4986	0.5063	0.1797
24	0.4986	0.5067	0.1725
32	0.4986	0.5068	0.1713
64	0.4986	0.5068	0.1708
128	0.4986	0.5068	0.1707
∞	0.4986	0.5068	0.1707

$$C_2 = -i\omega^2(xp + px)/4, \tag{3.1}$$

$$C_3 = \omega^2(2p^2 - \omega^2x^2)/6. \tag{3.2}$$

The approximants $Z_m^{(\alpha)}$ are calculated in the coordinate representation, using the well-known relation

$$\langle x | e^{-a^2p^2/2} | x' \rangle = (2\pi a^2)^{-1/2} e^{-(x-x')^2/2a^2}. \tag{3.3}$$

In contrast to the spin model, the non-Hermiticity of C_2 now complicates the expressions in such a way that a calculation of $Z_m^{(2)}$ and $Z_m^{(3)}$ seems to be out of the question. Consequently the practical value of non-Hermitian approximants like those given by Eqs. (1.5) and (1.6) may be rather doubtful. The evaluation of $Z_m^{(4)}$ however is straightforward in principle, though tedious. We find

$$Z_m^{(4)} = \left\{ 2\pi\tau \left[1 + \frac{\psi}{3} \right] \left[1 - \frac{\psi^2}{12} \left[1 + \frac{\psi}{3} \right] \right] \right\}^{-m/2} \times \int \prod_{j=1}^m dx_j e^{-S(\{x_j\})}, \tag{3.4a}$$

where

$$S(\{x_j\}) = 2\tau^{-1} \left[\frac{\psi}{2} + \left[1 + \frac{\psi}{3} \right]^{-1} \right] \sum_{j=1}^m x_j^2 - \tau^{-1} \left[1 + \frac{\psi}{3} \right]^{-1} \left[1 - \frac{\psi^2}{12} \left[1 + \frac{\psi}{3} \right] \right]^{-1} \times \sum_{j=1}^m (x_j^2 + x_j x_{j+1}), \tag{3.4b}$$

where $\psi = \omega^2\tau^2/2$. The m -dimensional integral (3.4) can be evaluated by performing a Fourier transformation with respect to the imaginary-time variable j . The final result reads

$$Z_m^{(4)} = 2^{-m/2} \prod_{k=1}^m \left[1 - \cos \left[\frac{2\pi k}{m} \right] + \psi \left[1 + \frac{\psi}{6} - \frac{5\psi^2}{36} - \frac{\psi^3}{18} - \frac{\psi^4}{108} \right] \right]^{-1/2}. \tag{3.5}$$

The expression for $Z_m^{(1)}$ is obtained by retaining in Eq. (3.5) only the term linear in ψ . Some results are given in Tables III and IV. Concerning convergence properties we may draw the same conclusions as for the spin model. For small m values we again observe that the energy approximants are lower than the free-energy approximants. From Eq. (3.5) we see that the argument of the square root can become negative for large values of ψ , and therefore the lowest m values do not appear in Table IV. Obviously this is no limitation whatsoever because useful results can only be expected for $\omega\tau < 1$.

IV. ANHARMONIC OSCILLATOR

As a nontrivial example we consider the one-dimensional motion of a particle moving in an arbitrary potential $V(x)$. Choosing $A=V(x)$ and $B=p^2/2$ we have

$$C_3 = f + p^2 g + gp^2, \quad (4.1a)$$

$$f = \frac{1}{12} [V^{(4)} - 2(V^{(1)})^2], \quad (4.1b)$$

$$\langle x | e^{-\tau p^2/4} f e^{-\tau p^2/4} | y \rangle = \langle x | e^{-\tau p^2/2} | y \rangle \left[\frac{2}{\pi\tau} \right]^{1/2} \int_{-\infty}^{\infty} dz f(z) \exp \left[-\frac{2}{\tau} \left[z - \frac{x+y}{2} \right]^2 \right], \quad (4.2a)$$

$$\langle x | e^{-\tau p^2/4} (p^2 g + gp^2) e^{-\tau p^2/4} | y \rangle = -4 \frac{\partial}{\partial \tau} \langle x | e^{-\tau p^2/4} g e^{-\tau p^2/4} | y \rangle, \quad (4.2b)$$

leads to an analytic expression for $\langle x | g_4(A, B) | y \rangle$ in terms of the coordinates x and y only, provided that the integrations in (4.2) can be carried out analytically. Obviously this is the case for the most commonly used potentials such as polynomials, exponentials, and trigonometric functions of the position operator. The approximant $Z_m^{(4)}$ then reads

$$Z_m^{(4)} = \left[\frac{1}{2\pi\tau} \right]^{m/2} \int \left[\prod_{j=1}^m dx_j \right] e^{-S_m^{(1)}} \times \prod_{j=1}^m F(x_j, x_{j+1}), \quad (4.3a)$$

where

$$S_m^{(1)} = \sum_{j=1}^m \left[\frac{1}{2\tau} (x_j - x_{j+1})^2 + \tau V(x_j) \right]. \quad (4.3b)$$

Obviously the form of $F(x_j, x_{j+1})$ depends on the choice of V and we reobtain the simplest approximant $Z_m^{(1)}$ by replacing $F(x_j, x_{j+1})$ by 1. In contrast to the examples treated in the previous sections it is very difficult, if not impossible to evaluate (4.3) analytically unless the potential is harmonic. However, we can calculate estimators for the thermodynamic functions by using the standard Monte Carlo method.¹⁴ To demonstrate that this is possible we have done some simulations for the case of a double-well potential $V(x) = -2x^2 + x^4/2$. In Fig. 1 we compare the energy as obtained from the simple approximant [$F(x_j, x_{j+1}) = 1$] and (4.3) for $\beta = 5$. We also calculated the (numerically) exact result for the energy, $E(\beta = 5) = -0.7997$, by using the exact eigenvalues of the Hamiltonian.¹⁵ From Fig. 1 we conclude that $E_m^{(4)}$ converges much faster than $E_m^{(1)}$. The additional CPU (central processing unit) time needed to calculate the last factor in (4.3a) is only a small fraction of the total CPU time for simulating $Z_m^{(1)}$, and therefore use of the more complicated form (4.3a) leads to an important reduction of the CPU time. In the case of Monte Carlo simulations of quantum systems the use of the higher approximants has an even more interesting advantage. It is well known that

$$g = \frac{1}{6} V^{(2)}. \quad (4.1c)$$

For the explicit evaluation of the matrix element $\langle x | g_4(A, B) | y \rangle$ we replace $\exp(-\tau^3 C_3/4)$ by $1 - \tau^3 C_3/4$ in (1.11). The resulting modified form for $g_4(A, B)$ is correct up to the same order in τ as the original result (1.11) and thus *a priori* it is an equally good approximant. Assuming that $f=f(x)$ and $g=g(x)$ straightforward application of the identities

the statistical errors on the kinetic energy grow rapidly when going to higher m values, because the kinetic energy is obtained as $1/\tau$ minus a quantity which is of the same order of magnitude and which has a statistical error because it is gotten by Monte Carlo sampling.¹² Thus the fact that for the higher approximants smaller m values are sufficient automatically leads to a reduction of the statistical errors.

V. CONCLUSIONS

We have used the generalized Trotter formula to obtain systematic approximants for the thermodynamic functions of quantum systems and we studied their conver-

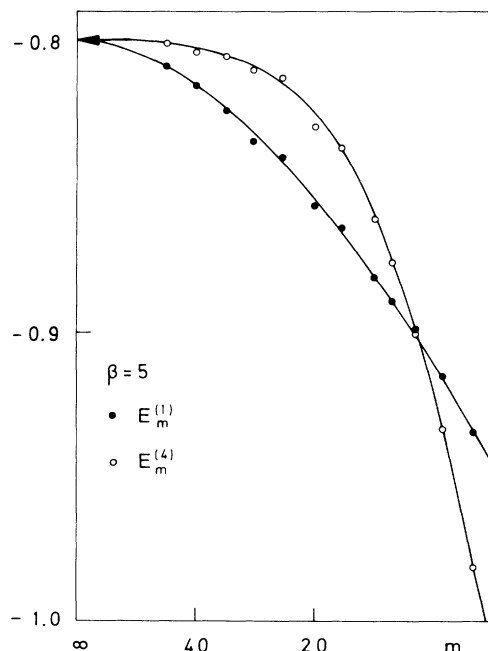


FIG. 1. Simple ($E_m^{(1)}$) and improved ($E_m^{(4)}$) approximants to the energy of a particle in a double-well potential as a function of the inverse of the number of imaginary time slices ($1/m$). Arrow denotes the exact result for the energy at the inverse temperature $\beta = 5$. Solid lines are guides to the eye only.

gence. We found it especially fruitful to construct Hermitian approximants because this simplifies calculations without affecting the convergence rate. Also a good choice of decomposing the Hamiltonian and the choice of the representation may affect the complexity of the calculations and the convergence. We demonstrated that the use of the Trotter formula without a careful study of its convergence as a function of m , may lead to unphysical results. Whereas up to now, for the study of many-particle systems the Trotter formula was only used in its simplest form, our analysis shows that using better ap-

proximants can improve the results considerably, or equivalently in the case of a Monte Carlo approach it may reduce the number of "time slices" m and thus the amount of computer time needed to get equally good results.

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