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Properties of higher-order Trotter formulas

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We investigate higher-order Trotter formulas which converge more rapidly towards the continuum than the usual version. We derive a formula which is convergent up to fourth order in the discretization parameter. We test this formulation by applying it to the path integral treatment of the quantum mechanical harmonic oscillator and to a quantum statistical toy model. Some problems inherent in this approach are pointed out.

1. Introduction

In many cases of practical interest involving functional integration it is necessary or unavoidable to do the calculations explicitly with the discrete version of the path integral. This necessity arises if the legitimacy of the limiting procedure is dubious as is the case, e.g., in derivations of the Fokker–Planck equation from path integral representations of the heatbath where the well-known problem of operator ordering notoriously manifests itself [1]. Also dealing with the discrete version is unavoidable if calculations are to be performed by the computer as in Monte Carlo simulations [2]. It is therefore highly desirable to have discrete formulations of the path integral that approximate the continuous case to a high degree of accuracy, and various attempts in this direction have been published in the last years (for a review see, e.g., ref. [3]).

One way to improve the convergence of the discrete path integral is to work with better approximations of the short time propagator. Since quantum effects are effectively suppressed for short times, this can be achieved by using a semiclassical expansion of the Wigner–Kirkwood type [4]. Rederiving the first terms of this expansion such an approach was first proposed by Makri and Miller [5]. Recently precisely the same method has been rediscovered and extended to curved manifolds [6]. Another promising possibility is to apply variational approximations to the short time propagator [7]. Other approaches based on the Fourier decomposition of path integrals are described in a recent review by Doll et al. [8].

The Trotter formula [9,10] provides an elegant way to derive the path integral representation of a quantum mechanical system and another suitable way to look for improved discretization schemes. The underlying mathematics being quite general, corresponding low-order discretization schemes have also been discussed in the context of classical physics (for electromagnetic pulse propagation, see, e.g., ref. [11]). Generalized Trotter formulas proposed by Suzuki [12] considerably improve the convergence of the discretized path integral and have successfully been used in Monte Carlo applications [13,14]. A disadvantage of these generalized Trotter formulas, however, is that they involve higher commutators of the operators. In this paper we also investigate an approach to find more sophisticated versions of Trotter formulas which, however, are independent of the commutator. Outlining this approach in section 2 we find an improved Trotter formula which is convergent up to fourth order in the discretization parameter. In section 3 we use this formula to derive a more rapidly converging discrete formulation of the path integral. The rate of convergence is explicitly demonstrated in section 4 by specializing to the harmonic oscillator potential. In section 5 we consider a quantum statistical toy model and show that better convergence can be gained also in this field. Although the approach investigated here is feasible in principle it is nonetheless marred by difficulties which arise in practical applications and are discussed in section 6.

2. Higher-order Trotter formulas

Trotter's well-known formula in its simplest version states that for any two non-commuting operators A and B the following identity holds (for technical details see ref. [10]),

$$e^{A+B} = \lim_{N\to\infty} (e^{A/N} e^{B/N})^N . \qquad (1)$$

Clearly, for finite N the error on the r.h.s. of this equation is of order $1/N$, and a symmetrization of the decomposition like $e^{A/2N}e^{B/N}e^{A/2N}$ yields an error of order $1/N^2$.

The idea of the approach that we are investigating here is that the error introduced by the splitting of the exponential may further be reduced by working with a decomposition like

$$e^{\alpha_1 A/N} e^{\beta_1 B/N} e^{\alpha_2 A/N} e^{\beta_2 B/N} \ldots ,$$

where some freedom is gained to adjust the coefficients. More specifically we expand $e^{(A+B)/N}$ and

$$e^{\alpha_1 A/N} e^{\beta_1 B/N} e^{\alpha_2 A/N} e^{\beta_2 B/N} \ldots$$

in powers of $1/N$ and try to adjust the coefficients α_j, β_j under the obvious constraint that $\sum_j \alpha_j = \sum_j \beta_j = 1$. For the simple decomposition $e^{A/N}e^{B/N}$ used in (1) we see that there is no freedom to adjust any coefficient at all, whereas the symmetrized version has one free coefficient which is uniquely determined to be $\frac{1}{2}$ to equate the terms of order $1/N^2$ [#1]. Proceeding in this way (see table 1) we find that a decomposition of four exponentials yields the needed coefficient non-uniquely but does not yet allow one to equate the cubic terms. Convergence up to third order may eventually be achieved by starting with a decomposition of five exponentials. The coefficients in this case are uniquely determined and turn out to be complex. Starting with a decomposition of six exponentials a free parameter is gained again in the coefficients but no better convergence may be achieved. Note that in this case one of the α's and one of the β's are always negative no matter what value we take for the free parameter γ.

Since our primary concern in this investigation was to find a rapidly convergent solution which could also easily be used in practical applications we eventually tried a decomposition of seven exponentials and found that

[#1] Note that the convergence of the full Trotter formula for e^{A+B} is trivially reduced by one order compared to the decomposition of $e^{(A+B)/N}$.

Table 1
Coefficients of higher-order Trotter formulas. γ is an arbitrary parameter, and Γ is defined by $\Gamma \equiv [(-12\gamma^3+45\gamma^2-48\gamma+16)/(-12\gamma+9)]^{1/2}$. The order of convergence refers to the decomposition of e^{A+B} as, e.g., in (1), (2).

Number of exponentials	α_1	β_1	α_2	β_2	α_3	β_3	α_4	O
2	1	1						$\frac{1}{N}$
3	$\frac{1}{2}$	1	$\frac{1}{2}$					$\frac{1}{N^2}$
4	$1-\gamma$	$\frac{1}{2\gamma}$	γ	$1-\frac{1}{2\gamma}$				$\frac{1}{N^2}$
5	$\frac{3\pm i\sqrt{3}}{12}$	$\frac{3+i\sqrt{3}}{6}$	$\frac{1}{2}$	$\frac{3\mp i\sqrt{3}}{6}$	$\frac{3\mp i\sqrt{3}}{12}$			$\frac{1}{N^3}$
6	$1-\gamma$	$\frac{1}{2\gamma}\frac{\frac{4}{3}-\gamma\pm\Gamma}{\gamma\pm\Gamma}$	$\frac{\gamma\pm\Gamma}{2}$	$\frac{1}{2}\frac{3-4\gamma}{2-3\gamma}$	$\frac{\gamma\mp\Gamma}{2}$	$1-\frac{1}{2\gamma}\frac{3\gamma-\frac{4}{3}\mp\Gamma}{\gamma\mp\Gamma}$		$\frac{1}{N^3}$
7	$\frac{\beta_1}{2}$	$\frac{1}{2-2^{1/3}}$	$\frac{1-2^{1/3}}{2}\beta_1$	$-2^{1/3}\beta_1$	$\frac{1-2^{1/3}}{2}\beta_1$	$\frac{1}{2-2^{1/3}}$	$\frac{\beta_1}{2}$	$\frac{1}{N^4}$

$$e^{A+B}=(e^{\alpha_1 A/N}e^{\beta_1 B/N}e^{\alpha_2 A/N}e^{\beta_2 B/N}$$
$$\times e^{\alpha_2 A/N}e^{\beta_1 B/N}e^{\alpha_1 A/N})^N+O(1/N^4)\,, \qquad (2)$$

where

$$\beta_1=\frac{1}{2-2^{1/3}}=+1.35...,\quad \beta_2=-2^{1/3}\beta_1=-1.70...,$$
$$\alpha_1=\tfrac{1}{2}\beta_1=+0.67...,\quad \alpha_2=\frac{1-2^{1/3}}{2}\beta_1=-0.17.... \qquad (3)$$

There is also another set of complex coefficients but if we impose the restriction that the coefficients be real this choice of coefficients is furthermore unique. We will now examine the usefulness of this formula in two applications.

3. Convergence of the discretized path integral

Let us briefly recall how the path integral representation of a quantum mechanical system is derived using the Trotter formula. Starting from the time propagator

$$\langle x_b t_b | x_a t_a\rangle$$
$$=\langle x_b|\exp\left[-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)(t_b-t_a)\right]|x_a\rangle \qquad (4)$$

we cut the time interval into short pieces of length $\epsilon\equiv(t_b-t_a)/N$ by inserting $N-1$ complete sets of position eigenstates,

$$\int dx_j\,|x_j\rangle\langle x_j|=1\,.$$

The exponentials of the short time propagators are now split according to Trotter's formula (1),

$$\exp\left[-\frac{i\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)\right]$$
$$\approx\exp\left(-\frac{i\epsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(-\frac{i\epsilon}{\hbar}V(\hat{x})\right) \qquad (5)$$

or, using the symmetrized version,

$$\exp\left[-\frac{i\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)\right]\approx\exp\left(-\frac{i\epsilon}{2\hbar}V(\hat{x})\right)$$
$$\times\exp\left(-\frac{i\epsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(-\frac{i\epsilon}{2\hbar}V(\hat{x})\right). \qquad (6)$$

To proceed we need the matrix elements

$$\langle x_j|\exp\left(-\beta\frac{i\epsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)|x_{j-1}\rangle=\left(\frac{m}{2\pi i\hbar\epsilon\beta}\right)^{1/2}$$
$$\times\exp\left[\frac{im\epsilon}{2\beta\hbar}\left(\frac{x_j-x_{j-1}}{\epsilon}\right)^2\right], \qquad (7)$$

where we have included an arbitrary real constant β the relevance of which will become clear later on, presently we have $\beta=1$. Using (5) and (7) we finally arrive at the path integral representation of (4) as the limit

$$\langle x_b t_b|x_a t_a\rangle=\int \mathscr{D}x\,\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}[\tfrac{1}{2}m\dot{x}^2-V(x)]\,dt\right)$$
$$=\lim_{N\to\infty}\frac{1}{A}\prod_{j=1}^{N-1}\left(\int\frac{dx_j}{A}\right)\exp\left\{\frac{i\epsilon}{\hbar}\sum_{j=1}^{N}\left[\frac{m}{2}\left(\frac{x_j-x_{j-1}}{\epsilon}\right)^2\right.\right.$$
$$\left.\left.-V(x_{j-1})\right]\right\}, \qquad (8)$$

where $A=(2\pi i\hbar\epsilon/m)^{1/2}$ and $x_0\equiv x_a$, $x_N\equiv x_b$.

Clearly, the ordinary path integral given in (8) is accurate only to $O(1/N)$. Using the symmetrized version (6) instead of (5) the discretized action integral in the exponential would contain an additional term $(i\epsilon/2\hbar)[V(x_N)-V(x_0)]$, and the overall convergence of the path integral would be of $O(1/N^2)$. Note that the version with the better convergence is obtained by discretizing the potential in the action integral according to the trapezoidal rule instead of the primitive Riemann sum. The situation is thus quite similar to the convergence behaviour in ordinary numerical integration. For the following argument it is, however, essential to realize that this similarity can at most serve as a heuristic argument. The different convergence behaviour is really a consequence of the better convergence of the Trotter formula in its simple but symmetrized version as pointed out in section 2. The point is now that the modification of the Trotter formula given in eq. (2) allows one to derive a discretization which is even more rapidly convergent. The only difference is that instead of using (5) or (6) the exponentials are approximated by the decomposition according to (2),

$$\exp\left[-\frac{\mathrm{i}\epsilon}{\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)\right]\approx\exp\left(-\alpha_1\frac{\mathrm{i}\epsilon}{\hbar}V\right)$$
$$\times\exp\left(-\beta_1\frac{\mathrm{i}\epsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(-\alpha_2\frac{\mathrm{i}\epsilon}{\hbar}V\right)$$
$$\times\exp\left(-\beta_2\frac{\mathrm{i}\epsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(-\alpha_2\frac{\mathrm{i}\epsilon}{\hbar}V\right)$$
$$\times\exp\left(-\beta_1\frac{\mathrm{i}\epsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(-\alpha_1\frac{\mathrm{i}\epsilon}{\hbar}V\right), \tag{9}$$

with the coefficients α_j, β_j given by (3). Due to the extra exponentials in (9) we will now have to insert $3N-1$ instead of only $N-1$ position eigenstates, i.e. we will have to work with a finer time slicing. This disadvantage will eventually, however, be compensated by the more rapid convergence. Furthermore we will now have to use (7) with $\beta=\beta_1$ respectively β_2. The final result then reads

$$\int\mathscr{D}x\exp\left(\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b}\left[\tfrac{1}{2}m\dot{x}^2-V(x)\right]\mathrm{d}t\right)$$
$$=\frac{1}{A_3}\int\frac{\mathrm{d}x_{3N-1}}{A_2}\int\frac{\mathrm{d}x_{3N-2}}{A_1}$$
$$\times\prod_{j=1}^{N-1}\left(\int\frac{\mathrm{d}x_{3j}}{A_3}\int\frac{\mathrm{d}x_{3j-1}}{A_2}\int\frac{\mathrm{d}x_{3j-2}}{A_1}\right)\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{A}_N\right)$$
$$+\mathrm{O}(1/N^4), \tag{10}$$

where

$$\mathscr{A}_N\equiv\tilde{\epsilon}\sum_{j=1}^{N}\Bigg[-\tilde{\alpha}_1V(x_{3j-3})$$
$$+\frac{m}{2\tilde{\beta}_1}\left(\frac{x_{3j-2}-x_{3j-3}}{\tilde{\epsilon}}\right)^2-\tilde{\alpha}_2V(x_{3j-2})$$
$$+\frac{m}{2\tilde{\beta}_2}\left(\frac{x_{3j-1}-x_{3j-2}}{\tilde{\epsilon}}\right)^2-\tilde{\alpha}_2V(x_{3j-1})$$
$$+\frac{m}{2\tilde{\beta}_1}\left(\frac{x_{3j}-x_{3j-1}}{\tilde{\epsilon}}\right)^2-\tilde{\alpha}_1V(x_{3j})\Bigg] \tag{11}$$

and $\tilde{\epsilon}\equiv\frac{1}{3}\epsilon$, $\tilde{\alpha}_j\equiv3\alpha_j$, $\tilde{\beta}_j\equiv3\beta_j$, $x_0\equiv x_a$, $x_{3N}\equiv x_b$, and $A_1\equiv A_3\equiv(2\pi\mathrm{i}\hbar\tilde{\epsilon}\tilde{\beta}_1/m)^{1/2}$, $A_2\equiv(2\pi\mathrm{i}\hbar\tilde{\epsilon}\tilde{\beta}_2/m)^{1/2}$.

Eqs. (10) and (11) are to be compared with eq. (8). Note that up to this point the treatment is completely independent of the potential. Also note that, although the formula does look quite lengthy at first sight, its content is rather simple. The only difference to (8) is that the sites of the time lattice are periodically decorated with simple, real numerical factors.

The feasibility of this formula shall now be demonstrated by applying it to the harmonic oscillator potential.

4. Application to the harmonic oscillator

Since the purpose of this section is to demonstrate that the discretization of eqs. (10) and (11) does indeed provide an approximation of the continuous path integral accurate to $\mathrm{O}(1/N^4)$ we will take a short cut of the calculation and only look at the "quantum mechanical partition function"

$$\mathscr{Z}_{\mathrm{QM}}\equiv\int\mathrm{d}x\,\langle xt_b|xt_a\rangle\,. \tag{12}$$

Inserting the harmonic oscillator potential $V=\frac{1}{2}m\omega^2x^2$, the additional integration allows us to write [#2]

$$\mathscr{Z}_{\mathrm{QM}}=\lim_{N\to\infty}\prod_{k=1}^{3N}\left(\int\frac{\mathrm{d}x_k}{A_{1,2,3}}\right)\exp\left(\frac{im}{2\hbar\tilde{\epsilon}}(\boldsymbol{x}^{\mathrm{T}}\mathbf{M}\boldsymbol{x})\right)$$
$$=\lim_{N\to\infty}\left(\frac{1}{A_1A_2A_3}\right)^N\left(\frac{2\pi\mathrm{i}\hbar\tilde{\epsilon}}{m}\right)^{3N/2}(\det\mathbf{M})^{-1/2}, \tag{13}$$

where $\boldsymbol{x}^{\mathrm{T}}\equiv(x_1,x_2,\ldots,x_{3N})$, and $\mathbf{M}$ is a $3N\times3N$ matrix of the following structure,

$$\mathbf{M}=\begin{pmatrix} b & d & & & & & c\\ d & b & c & & & & \\ & c & a & c & & & \\ & & c & b & d & & \\ & & & d & \ddots & \ddots & \\ & & & & \ddots & & \\ & & & & & b & c\\ c & & & & & c & a\end{pmatrix}, \tag{14}$$

[#2] To avoid problems with caustics we confine ourselves to the case $\omega(t_b-t_a)<\pi$.

with

$$a=-2\tilde{\alpha}_1(\tilde{\epsilon}\omega)^2+2/\tilde{\beta}_1\,,$$
$$b=-\tilde{\alpha}_2(\tilde{\epsilon}\omega)^2+1/\tilde{\beta}_1+1/\tilde{\beta}_2\,,$$
$$c=-1/\tilde{\beta}_1\,,\quad d=-1/\tilde{\beta}_2\,. \tag{15}$$

The determinant of $\mathbf{M}$ can be found by the following strategy. First we eliminate the entries in the upper right and lower left corner by expanding the determinant. We are then left with the problem of finding the determinant of a tridiagonal $\tilde{N}\times\tilde{N}$ matrix $\tilde{\mathbf{M}}$ with periodically repeated entries. To calculate det $\tilde{\mathbf{M}}$ we define an auxiliary lower triangular $(\tilde{N}+1)\times(\tilde{N}+1)$ matrix

$$\mathbf{W}=\begin{pmatrix} w & & & & & \\ v_1 & u_1 & & & & \\ & v_2 & u_2 & & & \\ & & v_3 & u_3 & & \\ & & & v_1 & u_1 & \\ & & & & \ddots & \ddots \end{pmatrix}, \tag{16}$$

with trivial determinant. We then expand $\det(\mathbf{W}\mathbf{W}^{\mathrm{T}})=w^2\det\mathbf{U}-w^2v_1^2\det\mathbf{U}'$, where $\mathbf{U}$ has the same structure as $\tilde{\mathbf{M}}$. Equating $\tilde{\mathbf{M}}=\mathbf{U}$ we obtain u_i, v_i as functions of a, b, c, d by solving quartic equations. To get rid of $\mathbf{U}'$ we choose $w=1/v_1$ and select two sets of solutions $u_{i\pm}$, $v_{i\pm}$ with $v_{1+}^2\neq v_{1-}^2$. By forming a linear combination we can now express det $\tilde{\mathbf{M}}$ as

$$\det\tilde{\mathbf{M}}=\frac{\det(\mathbf{W}_+\mathbf{W}_+^{\mathrm{T}})-\det(\mathbf{W}_-\mathbf{W}_-^{\mathrm{T}})}{w_+^2-w_-^2}$$

and thus det $\tilde{\mathbf{M}}$ as a function of $u_{i\pm}$, $v_{i\pm}$. We eventually end up with

$$\det\mathbf{M}=-(-c^2d)^N\times4\sin^2(\tfrac{1}{2}N\epsilon\Omega)\,, \tag{17}$$

where

$$\cos(\epsilon\Omega)\equiv\frac{2bc^2-a(b^2-d^2)}{2c^2d}\,. \tag{18}$$

Together with the prefactors in (13) the final result may now be written as

$$\mathscr{Z}^N_{\mathrm{QM}}=\frac{1}{2\mathrm{i}\sin[\frac{1}{2}\Omega(t_\mathrm{b}-t_\mathrm{a})]}\,, \tag{19}$$

which is to be compared with the continuum result

$$\mathscr{Z}_{\mathrm{QM}}=\frac{1}{2\mathrm{i}\sin[\frac{1}{2}\omega(t_\mathrm{b}-t_\mathrm{a})]}\,. \tag{20}$$

To check the convergence behaviour we use definition (15) to express $\cos(\epsilon\Omega)$ given in (18) in terms of the weights α_i, β_i,

$$\begin{aligned}\cos(\epsilon\Omega)&=1-(\epsilon\omega)^2(2\alpha_1\beta_1+\alpha_1\beta_2+2\beta_1\alpha_2+\alpha_2\beta_2)\\&\quad+(\epsilon\omega)^4\beta_1\alpha_2(2\alpha_1\beta_1+2\alpha_1\beta_2+\alpha_2\beta_2)\\&\quad-(\epsilon\omega)^6\alpha_1\beta_1^2\alpha_2^2\beta_2 \qquad (21)\\&=1-\frac{(\epsilon\omega)^2}{2!}+\frac{(\epsilon\omega)^4}{4!}\\&\quad-\left(-\frac{5}{4^{2/3}+4^{1/3}-4}\right)\frac{(\epsilon\omega)^6}{6!}\,. \qquad (22)\end{aligned}$$

In the last line we have finally inserted the explicit values for the weights given in eq. (3). Clearly the discrete frequency Ω agrees with the continuous one up to fourth order in ϵ whereas the usual discretization is correct only up to $\mathrm{O}(\epsilon^2)$ as can readily be seen by inserting $\alpha_1=\frac{1}{2}$, $\beta_1=\frac{1}{2}$, $\alpha_2=\beta_2=0$ into (21).

5. Quantum statistical toy model

The derivation of the path integral as given in the previous two sections does not take over to the Euclidean case which is due to the fact that the Euclidean version of (7) is only valid for positive β whereas β_2 as given in (3) is negative. In the treatment of the harmonic oscillator this problem is reflected by the fact that $\mathbf{M}$ would contain negative eigenvalues which would invalidate a Euclidean version of (13). For this reason we will now discuss the applicability of the higher-order Trotter formula (2) to a quantum statistical toy model which has also been treated in a similar context in ref. [13]. The motivation for this investigation is that in quantum statistical spin models the operators A and B are usually compact and thus one may expect that the above-mentioned problem will not be encountered in these applications.

Consider the single site problem

$$\mathscr{Z}\equiv\mathrm{Tr}\exp(J\sigma_z+\Gamma\sigma_x)\,, \tag{23}$$

where σ are spin-$\frac{1}{2}$ operators. It is a one-line calculation to show that the exact partition function of this simple problem is given by

$$\mathscr{Z}=2\cosh\sqrt{J^2+\Gamma^2}\ . \tag{24}$$

To apply the Trotter formulas we write

$$\mathscr{Z}_N=\mathrm{Tr}\,\mathbf{M}^N\ , \tag{25}$$

where for the usual version $\mathbf{M}$ is given by

$$\mathbf{M}^{(\mathrm{I})}=\mathrm{e}^{(J/N)\sigma_z}\mathrm{e}^{(\Gamma/N)\sigma_x} \tag{26}$$

and for the more rapidly converging version by

$$\mathbf{M}^{(\mathrm{II})}=\mathrm{e}^{\alpha_1(J/N)\sigma_z}\mathrm{e}^{\beta_1(\Gamma/N)\sigma_x}\mathrm{e}^{\alpha_2(J/N)\sigma_z}\mathrm{e}^{\beta_2(\Gamma/N)\sigma_x}\times\mathrm{e}^{\alpha_2(J/N)\sigma_z}\mathrm{e}^{\beta_1(\Gamma/N)\sigma_x}\mathrm{e}^{\alpha_1(J/N)\sigma_z}\ . \tag{27}$$

Note that since $\det\mathbf{M}^N=\det\mathbf{M}=1$ the matrix $\mathbf{M}$ has eigenvalues $\lambda_\pm$ with $\lambda_+\lambda_-=1$ and we can write quite generally

$$\mathscr{Z}_N=2\cosh(N\ln\lambda_+)\equiv 2\cosh\Omega_N\ , \tag{28}$$

with

$$\cosh(\Omega_N/N)\ =\tfrac{1}{2}\,\mathrm{Tr}\,\mathbf{M}\ . \tag{29}$$

Applying the Trotter formula in its ordinary version (1) we now obtain

$$\cosh(\Omega_N^{(\mathrm{I})}/N)=\cosh(J/N)\cosh(\Gamma/N)\ , \tag{30}$$

whereas the sophisticated version (2) yields

$$\begin{aligned}\cosh(\Omega_N^{(\mathrm{II})}/N)&\\ =\cosh(J/N)&\cosh^2(\beta_1\Gamma/N)\cosh(\beta_2\Gamma/N)\\ &+\cosh[2(\alpha_1-\alpha_2)J/N]\sinh^2(\beta_1\Gamma/N)\\ &\times\cosh(\beta_2\Gamma/N)+2\cosh(2\alpha_1J/N)\sinh(\beta_1\Gamma/N)\\ &\times\cosh(\beta_1\Gamma/N)\sinh(\beta_2\Gamma/N)\end{aligned} \tag{31}$$

for arbitrary α_j, β_j. From this we find that the exact partition function is approximated by

$$\begin{aligned}\mathscr{Z}_N^{(\mathrm{II})}=\mathscr{Z}+&\frac{J^2\Gamma^2\sinh\sqrt{J^2+\Gamma^2}}{12\sqrt{J^2+\Gamma^2}}\{6[2\beta_1^2+\beta_2^2\\ &+8(\alpha_1-\alpha_2)^2\beta_1^2+16\beta_1\beta_2\alpha_1^2]-2\}\frac{1}{N^2}\\ &+\mathrm{O}(1/N^4)\ .\end{aligned} \tag{32}$$

For the simple version we put $\beta_1=\frac{1}{2}$, $\beta_2=0$ and obtain

$$\mathscr{Z}_N^{(\mathrm{I})}=\mathscr{Z}+\frac{J^2\Gamma^2\sinh\sqrt{J^2+\Gamma^2}}{3\sqrt{J^2+\Gamma^2}}\frac{1}{N^2}+\mathrm{O}(1/N^4)\ , \tag{33}$$

whereas the coefficients of (3) give as expected

$$\mathscr{Z}_N^{(\mathrm{II})}=\mathscr{Z}+\mathrm{O}(1/N^4)\ . \tag{34}$$

6. Discussion

Higher-order Trotter formulas provide a very general and systematic way to derive discrete approximations of path integrals for quantum mechanical or quantum statistical systems. These discretizations converge more rapidly while being only slightly more complicated than the usual low-order formulation. This has been demonstrated for a version of the Trotter formula which exhibits an increase of the rate of convergence by two orders of magnitude in the discretization parameter. This advantage, however, cannot be readily exploited in Monte Carlo simulations (as was our primary hope when starting this investigation) since a Euclidean version of the more rapidly converging discrete path integral does not exist. This restriction is a consequence of the fact that the negative coefficients of the higher-order Trotter formula imply a negative mode which cannot be integrated out since the range of integration is infinite. The resulting divergences are quite similar to the ones appearing in the treatment of metastable systems. They are of an intrinsic nature since the operators in the path integral are essentially non-compact.

We have therefore investigated quantum statistical spin models where the non-commuting operators of the Trotter formula in contrast are compact. Encouraged by the successful treatment of the quantum statistical toy model which demonstrated that indeed no principal problems are encountered in this case, we then tried to apply the higher-order Trotter formula to the less trivial two-dimensional transverse Ising model. Again, however, the more rapid convergence could not be exploited in numerical computations since in this case some of the local Boltzmann weights turn out to be negative (as it often happens with quantum Monte Carlo formulations) and render the numerics unstable. It is therefore an open problem whether this approach or a modification thereof will be of practical use in this field. Since, however, the Trotter formula in its improved form is still perfectly general it is conceivable that it may be of use in other fields of physics (e.g., laser beam design [11]). In quantum mechanics another application may be found in numerical evaluations of path integrals in real time, a technically challenging problem where considerable progress has been made in the last few years [#3].

[#3] Early attempts to treat this problem are reported in ref. [15]. For a review of the recent development in this field see ref. [3].

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