Projection operator based expansion of the evolution operator

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Abstract

The not necessarily unitary evolution operator of a finite dimensional quantum system is studied with the help of a projection operators technique. Applying this approach to the Schrödinger equation allows the derivation of an alternative expression for the evolution operator, which differs from the traditional chronological exponent. An appropriate choice of projection operators results in the possibility of studying the diagonal and non-diagonal elements of the evolution operator separately. The suggested expression implies a particular form of perturbation expansion, which leads to a new formula for the short time dynamics. The new kind of perturbation expansion can be used to improve the accuracy of the usual chronological exponent significantly. The evolution operator for any arbitrary time can be efficiently recovered using the semigroup properties. The method is illustrated by two examples, namely the dynamics of a three-level system in two nonresonant laser fields and the calculation of the partition function of a finite XY-spin chain.

Keywords: evolution operator, projection operators, perturbation expansion

1. Introduction

The evolution operator is the most fundamental object in quantum mechanics, in the sense that the time dynamics of any quantum object can be defined through the action of the evolution operator. Equations for the evolution operator often represent a system of linear differential equations. In general, such equations cannot be solved analytically, and are usually studied with the help of approximations. Most approaches are actually some modification of perturbation expansion for the evolution operator, which describe only the short time behaviour. Typical examples are the Dyson series \(^1\), different variants of geometrical
integrators, such as the Magnus [2, 3], Fer or Wilcox [4] methods, and the exponential splitting method [5]. The long-time dynamics are traditionally recovered with the help of the Lie–Trotter formula [6] or its analogues [7], or, alternatively, the Feynman path integrals [8].

An alternative way to study the evolution operator is direct numerical integration. There is a vast number of different numerical algorithms [9, 10] which may be used for an investigation of the evolution operator. In many applications, the direct numerical integration using high-performance algorithms is preferable to the perturbation approach. Nevertheless, in cases when one is interested only in some part of the evolution operator, for example, in the calculation of a partition function, which is directly connected with the evolution operator due to the Wick rotation [11], the numerical methods do not give much of an advantage. In particular, this problem is crucial in higher dimensions. It is evident that none of the abovementioned methods allows the extraction of the necessary elements without calculation of the full evolution operator.

In this paper, we study the evolution operator with the help of projection operators. Using the projection operators we split the Schrödinger equation for the evolution operator into two parts and study each part separately. The study of these parts is performed with the help of a procedure which is an analogue of the important time-convolutionless technique in the theory of open quantum systems [12]. Moving to the simplest possible form of the method we concretise the projection operator, which extracts the diagonal part of the evolution operator. In this case, the system for the diagonal elements decomposes into a set of independent linear differential equations and can be solved analytically. The full evolution operator is represented as a product of two matrices, one of which is diagonal and can be studied separately. We consider this expression as a starting point for the development of a particular form of perturbation theory. Interestingly, the new perturbation expansion allows improvement of the results following from the usual chronological exponent of the corresponding order. The perturbation expansion up to the second order approximates the short time dynamics of the evolution operator. This approximation can be used for recovering the evolution operator using the semigroup property of the evolution operator iteratively. The technique is illustrated with the examples of the dynamics of a three-level system in two non-resonant laser fields and the calculation of the partition function for the finite XY-spin chain.

The paper is organised as follows. In section 2 we discuss the general properties of the evolution operator. Section 3 deals with the projection operator technique in the context of the evolution operator problem. In this section we derive in details our most important result equation (15) and, moreover, discuss the new form of perturbation expansion. We qualitatively compare different forms of perturbation expansions with the suggested one. The suggested formalism is applied to two concrete physical systems in section 4. We conclude in section 5.

2. Evolution operator

The evolution operator satisfies the Schrödinger evolution equation

\[ \dot{U} = -iHU, \]  

(1)

with the initial condition \( U(t_0, t_0) = I, \) where \( H \) is the system Hamiltonian, which is not necessarily hermitian, and \( I \) is the identity operator (we set \( \hbar = 1 \)). The formal solution of the Schrödinger equation can be written in the form of the so-called chronological exponent or time-ordered product.
\( U(t, t_0) = \exp \left[ -i \int_{t_0}^{t} H(s) ds \right] \)

\[
= I + \sum_{n=1}^{\infty} ( -i )^n \int_{t_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2 \cdots \int_{t_0}^{s_{n-1}} ds_n H(s_1) H(s_2) \cdots H(s_n). \quad (2)
\]

We also need an inverse evolution operator. Note that the evolution operator may not be unitary for non-hermitian Hamiltonians. The inverse evolution operator is governed by the following equation

\( \dot{U}^{-1} = iU^{-1}H. \quad (3) \)

The solution of the above equation can be expressed through the antichronological exponent

\( \dot{U}^{-1}(t, t_0) = \exp \left[ i \int_{t_0}^{t} H(s) ds \right] \)

\[
= I + \sum_{n=1}^{\infty} i^n \int_{t_0}^{t} ds_1 \int_{t_0}^{s_1} ds_2 \cdots \int_{t_0}^{s_{n-1}} ds_n H(s_1) H(s_2) \cdots H(s_n). \quad (4)
\]

The evolution operator possesses the semi-group property

\( U(t, t_0) = U(t, s) U(s, t_0), \quad (5) \)

which is the basis of different approximation techniques, such as the Lie–Trotter–Kato formula \([6]\) and the Chernoff theorem \([7]\).

### 3. Projection operator techniques

Let us introduce the pair of projection operators \( P = P^2 \) and \( Q = Q^2 \) with the following properties: (i) \( PQ = QP = 0 \); (ii) \( P + Q = I \); and (iii) \( \frac{d}{dt} P = P \frac{d}{dt} \). In the above expressions \( I \) is the identity operator and \( t \) is time. A specific form for projection operator will be discussed later. Now, we let the projection operators act on both sides of the Schrödinger equation (1) to derive

\[
P \dot{U} = -iPH(P + Q)U, \quad (6)
\]

\[
Q \dot{U} = -iQH(P + Q)U. \quad (7)
\]

The formal solution of equation (7) is

\[
QU = \tilde{G}(t, t_0) QI - i \int_{t_0}^{t} ds \tilde{G}(t, s) QHPU(s, t_0), \quad (8)
\]

where we introduce \( \tilde{G}(t, s) = \exp \left\{ -i \int_{t_0}^{t} ds' \tilde{G}(t', s) \right\} \).

Substituting (8) for (6) leads to the integro-differential equation of the form

\[
P \dot{U} = -iPHPU - iPH \left\{ \tilde{G}(t, t_0) QI - i \int_{t_0}^{t} ds \tilde{G}(t, s) QHPU(s, t_0) \right\}. \quad (9)
\]

The evolution operator is defined by the solution of equations (8)–(9) and has the obvious form, namely, \( U = PPU + QU \). The technique used in deriving equations (8)–(9) is analogue to the famous Nakajima–Zwanzig projection operator technique in the theory of open quantum systems \([12–14]\). Notice that equations (8)–(9) are absolutely equivalent to the initial Schrödinger equation (1). At the same time, the specific choice of projection operators may
simplify an investigation of the evolution operator. An obvious advantage of the approach is that the equations (8)–(9) allow the reduction of the number of equations in the system (1).

Because the above theory, in fact, does not lead to a new perturbation expansion, let us continue the formal transformation as it is usually done in the time-convolutionless projection operator technique [12]. We substitute the identity

\[ U(t, t_0) = \frac{1}{\mathcal{P}} U(t, t_0) \mathcal{Q} U(t, t_0) \]

where the inverse operator is understood as an antichronological exponent (4), into equation (8) and after some algebra we get

\[ \mathcal{Q} U(t, t_0) = [I - \Sigma(t)]^{-1} (\Sigma(t) \mathcal{P} U(t, t_0) + \mathcal{G}(t, t_0) \mathcal{Q} I) \]  \hspace{1cm} (10)

where we introduced the superoperator

\[ \Sigma(t) = -i \int_{t_0}^{t} ds \mathcal{G}(t, s) \mathcal{Q} H(s) \mathcal{P} U^{-1}(t, s) \].

From equations (6) and (10) we finally find

\[ \mathcal{P} \dot{U}(t, t_0) = \mathcal{K}(t) \mathcal{P} U(t, t_0) + \mathcal{I}(t) \mathcal{Q} I \] \hspace{1cm} (11)

In the above equation \( \mathcal{K}(t) = -i \mathcal{P} H(t) [I - \Sigma(t)]^{-1} \mathcal{P} \) and \( \mathcal{I}(t) = -i \mathcal{P} H(t) [I - \Sigma(t)]^{-1} \mathcal{G}(t, t_0) \mathcal{Q} \). All the above expressions are exact and valid for any projection operator. Notice, that equations (8)–(11) can be used to obtain an alternative expression for the evolution operator.

3.1. Specific form of projection operators and alternative expression for the evolution operator

We choose a specific form of projection operators and study equations (10) and (11) more precisely. Firstly, we divide the evolution operator into two parts, namely, the diagonal part and the non-diagonal part. The projection operator which extracts the diagonal part has the following form

\[ \mathcal{P} A = \sum_{i} \text{tr}(AE_{ii})E_{ii} \] \hspace{1cm} (12)

and the additional projection operator is

\[ \mathcal{Q} A = (I - \mathcal{P}) A \] \hspace{1cm} (13)

where \( E_{ij} \) is a \( n \times n \) matrix with only one unit in the intersection of \( i \)th row and \( j \)th column and 0 elsewhere.

Such a choice of the projection operators allows us to drop off terms proportional to \( \mathcal{Q} I \) in equations (10) and (11), because they are equal to zero.

Secondly, we transform the system Hamiltonian to get rid of the diagonal elements

\[ H_{I}(t) = \exp \left[ i \int_{t_0}^{t} \mathcal{P} H(s) ds \right] \mathcal{Q} H(t) \exp \left[ -i \int_{t_0}^{t} \mathcal{P} H(s) ds \right] \] \hspace{1cm} (14)

The above transformation is equivalent to transition to the interaction picture with respect to the Hamiltonian \( H_{I}(t) = \mathcal{P} H(t) \). The total evolution operator is a product

\[ U(t, t_0) = \exp \left[ -i \int_{t_0}^{t} \mathcal{P} H(s) ds \right] \exp \left[ -i \int_{t_0}^{t} H_{I}(s) ds \right] = U_{0}(t, t_0) U_{I}(t, t_0) \]

where \( U_{I}(t, t_0) \) satisfies the Schrödinger equation (1) with the Hamiltonian \( H_{I}(t) \), and \( U_{0}(t, t_0) \) satisfies the Schrödinger equation (1) with the Hamiltonian \( H_{0}(t) \). This can be proved by the direct substitution of the total evolution operator in the Schrödinger equation (1). Notice that the operator \( U_{0}(t, t_0) = \exp \left[ -i \int_{t_0}^{t} \mathcal{P} H(s) ds \right] \) can always be found in the exact analytical form. Now it can be checked that for the projection operators (12) and (13) the following relations hold

\[ \mathcal{P} H_{I}(t) \mathcal{P} = 0, \mathcal{Q} I = 0, \text{ and } \mathcal{P} I = I. \]
Below we will show that the transformation \((14)\) allows the reduction of the number of terms in the perturbation expansions of the operator \(U_\ell(t, t_0)\) and, thus, simplifies the study of a quantum systems with the help of the suggested method.

Equation \((11)\) with the projection operators \((12)\) and \((13)\) actually represents a homogeneous system of \(n\) uncoupled differential equations of the first order. Such a system can be easily solved in quadratures and the solution has the form \(\mathcal{P}U_\ell(t, t_0) = \exp\left[\int_{t_0}^t \mathcal{K}(s) ds\right]I\).

The solution of equation \((11)\) after substitution for \((10)\) gives the following expression for the full evolution operator \(U_\ell(t, t_0) = \mathcal{P}U_\ell(t, t_0) + QU_\ell(t, t_0)\)

\[
U_\ell(t, t_0) = \exp\left[\int_{t_0}^t \mathcal{K}(s) ds\right]I + \left[1 - \Sigma(t)\right]^{-1}\Sigma(t)\exp\left[\int_{t_0}^t \mathcal{K}(s) ds\right]I
= \left[1 - \Sigma(t)\right]^{-1}\exp\left[\int_{t_0}^t \mathcal{K}(s) ds\right]I.
\]

The expression \((15)\) is the main result of this paper. Notice that the right-hand side of equation \((15)\) is the superoperator which acts on the identity operator. At the same time, the exponent is actually a diagonal matrix and the superoperator \([I - \Sigma(t)]^{-1}\) acts trivially on this matrix. Thus, the expression \((15)\) represents the product of two matrices, namely the diagonal matrix \(\exp\left[\int_{t_0}^t ds\mathcal{K}(s) ds\right]I\) and the matrix \(([I - \Sigma(t)]^{-1}I)\). In other words one can calculate the two matrices independently and then multiply them. At the same time, the exact calculation of the right-hand side of equation \((15)\) already implies the knowledge of the inverse evolution operator. Moreover, even if the inverse operator is known this calculation is not a trivial task. Nevertheless, equation \((15)\) is the basis for an alternative form of the perturbation expansion, which we will develop in the next section.

3.2. Perturbation expansion for the evolution operator

Suppose that the Hamiltonian in \((1)\) depends on some perturbation parameter \(\alpha\). From the explicit form of the superoperator \(\mathcal{K}(t) = -i\mathcal{P}H(t)[I - \Sigma(t)]^{-1}\mathcal{P}\) it is obvious that the perturbation expansion is completely determined by the expansion of \([I - \Sigma(t)]^{-1} = \sum_{j=0}^\infty \Sigma(t)^j = \sum_j (\sum_{j=0}^\infty (\alpha^j \Sigma_j(t))^j \approx I + \alpha \Sigma_1(t) + \alpha^2 (\Sigma_1(t)^2 + \Sigma_2(t)) + O(\alpha^3)\).

Here we suppose that the superoperator \([I - \Sigma]^{-1}\) exists and can be expanded in a geometric series. Notice, that the superoperator \(\Sigma(t)\) consists both of the chronological exponent \(\mathcal{G}(t, s) = \exp\left\{-i \int_s^t \mathcal{Q}H(t') dt'\right\}\), and of the antichronological exponent \(U^{-1}(t, t_0) = \exp\left[i \int_{t_0}^t \mathcal{H}(s) ds\right]\). Thus, the perturbation expansion has no well defined time-ordering. Using the explicit expression for \(\Sigma(t)\) one can find that

\[
\Sigma_1(t) = -i \int_{t_0}^t \mathcal{Q}H(s) \mathcal{P}ds,
\]

which immediately gives \(\Sigma_1(t)^2 = 0\), due to the identity \(\mathcal{Q}\mathcal{P} = 0\), and

\[
\Sigma_2(t) = -i \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 (\mathcal{Q}H(t_1) \mathcal{Q}H(t_2) \mathcal{P} - \mathcal{Q}H(t_2) \mathcal{Q}H(t_1))\mathcal{P}.
\]

Now, to simplify the second order term we may get rid of the diagonal elements of the Hamiltonian, by using the transformation \((14)\). In other words, we transform the Hamiltonian
to the interacting picture. Notice, that this transformation simplifies the method. In the interaction picture the identity $\mathcal{P}H(t)\mathcal{P} = 0$ can be easily proven and the second term in equation (17) can be put equal to zero. The resulting expressions for the superoperator $\mathcal{K}(t)$ up to the second order is

$$\mathcal{K}(t) = -\int_{t_0}^t ds \mathcal{P}H(t)H(s)\mathcal{P} + O(\alpha^3),$$

(18)

$$[I - \Sigma(t)]^{-1} = I - i \int_{t_0}^t ds \mathcal{P}H(s)\mathcal{P} - \int_{t_0}^t ds \int_{t_0}^s ds_1 \mathcal{P}H(s)H(s_1)\mathcal{P} + O(\alpha^3).$$

(19)

The general term of the $n$th order may be found using a method similar to the cumulant expansion for stochastic differential equations suggested by van Kampen in [15]. The resulting expression for $\mathcal{K}_n(t)$ has the following form

$$\mathcal{K}_n(t) = (-i)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-2}} dt_{n-1} \times \sum (-1)^q \mathcal{P}H(t) ... H(t_i)\mathcal{P}H(t_j) ... H(t_k)\mathcal{P}H(t_l) ... H(t_m)\mathcal{P} ... \mathcal{P},$$

(20)

where the right-hand side is defined as follows [12]. First, one writes down a string of the form $\mathcal{P}H ... \mathcal{P}$ with $n$ factors of $H$ in between two $\mathcal{P}$s. Next, one inserts an arbitrary number of factors $\mathcal{P}$ between the $H$s such that at least one $H$ stands between two successive $\mathcal{P}$ factors. The resulting expression is multiplied by a factor $(-1)^q$ and all $H$s are furnished with a time argument: the first one is always $H(t)$. The remaining $H$s carry any permutation of the time arguments $t_i, t_2, \ldots, t_{n-1}$ with the only restriction that the time arguments in between two successive $\mathcal{P}$s must be ordered chronologically. Finally, the resulting expression is obtained by a summation over all possible insertions of $\mathcal{P}$ factors and over all allowed distributions of the time arguments.

The same procedure can be used to obtain the expansion of $[I - \Sigma(t)]^{-1}$, if we remember that $\mathcal{K}(t) = -i \mathcal{P}H(t)(I - \Sigma(t))^{-1}\mathcal{P}$, i.e., $\mathcal{K}_n(t) = -i \mathcal{P}H(t)\Sigma_{n-1}(t)\mathcal{P}$.

The above perturbation expansions is alternative to the Dyson series. Nevertheless, the difference between the two expansions can be understood from the explicit form of the superoperators, which consists of both chronological and anti-chronological exponents. Thus, the expansion of equation (15) does not have well defined chronological ordering, opposite to the Dyson series. Below we compare the two expansions for concrete examples.

3.3. Scheme of recovery of the evolution operator

The equation (15) with superoperators (18)–(19) reproduces the short time form of the evolution operator $U(t, t_0)$, where $\alpha (t - t_0) \ll 1$. To recover the evolution operator for any time we act in the spirit of the famous Lie–Trotter theory, namely, divide the time interval $[0, t]$ into $N$ subintervals. Using the semigroup property of the evolution operator (5) we can write

$$U(t, t_0) = U(t = t_N, t_{N-1})U(t_{N-1}, t_{N-2}) \ldots U(t_1, t_0).$$

(21)

Each operator $U(t_0, t_{i-1})$ is defined with the help of equations (15), (18) and (19). Now, we indicate an interesting iterative expression, which allows us to speed up the calculation...
The iterative scheme requires only one matrix multiplication per iteration. Moreover, the $U(t_N, t_{N-1})$ is a continuous operator on the time interval $[t_N, t_{N-1}]$. Thus, the iterative scheme (22) gives a continuous expression for the evolution operator.

The equation (15) is an identity and formally fulfilled for infinite dimensional systems. At the same time, calculation of the evolution operator for high dimensional systems with this expression is extremely difficult. Nevertheless, the same remark is correct for calculation of the usual truncated Dyson series or other approximation techniques.

3.4. Comparison with other expansions

There exists several different types of expansions which are used in various applications. The Dyson series [1] is probably the most typical one, and is just a time ordered product

$$U(t, t_0) = \exp \left[ -i \int_{t_0}^{t} H(t') dt' \right].$$

It can be easily proved that the Nakajima–Zwanzig projection operator technique leads exactly to the Dyson series for the full evolution operator independently of the concrete form of a projection operator. In contrast, local in time forms of the projection technique consist of both chronological and anti-chronological exponents and, thus, have no well defined time ordering. This fact makes equation (15) absolutely different from the Dyson series, where the time ordering is well defined. This can already be seen from the second order perturbation term (17).

Another common type of expansion is the Magnus series [4]. The Magnus series has the following general form

$$U(t, t_0) = \exp[M(t, t_0)],$$

where $M(t, t_0) = \sum_{n=1}^{\infty} M_n(t, t_0) \approx -i \int_{t_0}^{t} H(s) ds - \int_{t_0}^{t} ds [H(s_1), H(s)] + \cdots$. The explicit form of the general $W_n$ can be found in [4]. The expansion (24) has a big advantage, namely, it preserves the main characteristic of the exact solution $U(t, t_0)$, for example unitarity, in any order of the perturbation expansion. None of the expansions (15) or (23) has such a property. It is clear that Magnus expansion does not coincide with the expansion (15) in any perturbation order. Similarly, equation (15) differs from any others type of geometrical integrators, such as the Fer or Wilcox methods [4]. Nevertheless, notice that the explicit calculation of the operator exponent in (24) (and similar methods) is associated with huge difficulties and can be done only approximately in most cases. This fact nullifies any advantages of the method in concrete applications. Neither expansion (15) nor (23) have such a problem.

4. Examples

4.1. Three level $\Lambda$-system in two non-resonant laser fields

The interaction Hamiltonian of the model in the interaction pictures is

$$H(t) = \Omega_1(t) E_{32} + \Omega_2(t) E_{31} + \text{h.c.},$$

where the $E_{ij}$ have been introduced earlier, $\Omega_i(t) = \Omega_i \exp[\omega_i t]$, and $\Omega_i$, $\omega_i$, are, respectively, the Rabi frequency of the $i$th external field and the detuning of the laser field frequency from the atomic transition frequency.
The direct calculation of equation (18)–(19) gives

\[
\exp \left[ - \int_{t_0}^{t} \mathcal{K}(t) \, dt \right] = \exp \left[ E_{23}(f_1^* + f_2^*) + E_{23}f_1 + E_{11}f_2 \right]
\]

(26)

\[
[I - \Sigma(t)]^{-1} = I - i \int_{t_0}^{t} ds \, H(s) - \Omega_2 \Omega_2 (gE_{23} + \text{h.c.}),
\]

(27)

where \( f_1(t, t_0) = -\Omega_2^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} ds \exp [i(s - t') \omega_i] \) and \( g(t, t_0) = \int_{t_0}^{t} dt_0 \int_{0}^{t} ds \exp [-i\hbar \omega_1 + i\omega_2 s]. \) All the integrals in the above expressions are easily calculated and the approximate evolution operator given by equation (15) and (21). Thus, the perturbation expression for the evolution operator, given by the suggested method, is equal to

\[
U(t, t_0) = \begin{pmatrix}
    e^{\mathcal{U}(t, t_0)} & -e^{\mathcal{U}(t, t_0)} \Omega_2 \Omega_2 g^* (t, t_0) & -i\hbar^2 (t, t_0) e^{\mathcal{U}(t, t_0)} - e^{\mathcal{U}(t, t_0)} \Omega_2 \Omega_2 g (t, t_0) \\
    -e^{\mathcal{U}(t, t_0)} g (t, t_0) \Omega_2 \Omega_2 & e^{\mathcal{U}(t, t_0)} & -i\hbar^2 (t, t_0) e^{\mathcal{U}(t, t_0)} \\
    -i\omega_1 (t_0) h_2 (t, t_0) & -i\hbar (t, t_0) e^{\mathcal{U}(t, t_0)} & e^{\mathcal{U}(t, t_0)} \end{pmatrix}
\]

(28)

where

\[
h_1(t, t_0) = \int_{t_0}^{t} \Omega_i (s) \, ds = \frac{-i\Omega_i (e^{i\omega_i t} - e^{i\omega_i t_0})}{\omega_i}.
\]

(29)

For comparison we also calculate the second order Dyson expansion

\[
U(t, t_0) \approx I + i \int_{t_0}^{t} ds \, H(s) - \int_{t_0}^{t} dt' \int_{t_0}^{t'} ds \, H(t') H(s).
\]

The explicit form is
Even in this example one can clearly see that resulting expressions differ significantly. The results of the calculation for the population of the ground state $|1\rangle$ from initial state $|\psi(0)\rangle = |1\rangle$, i.e. $|\langle 1|U(t, 0)|1\rangle|^2$, are presented in figure 1. In the same figure we plot also the ‘exact’ result following from the numerical solution of the Schrödinger equation with Hamiltonian (25) and the result of the standard second order approximation of the evolution operator (30) with iterative procedure (21). The time step of the iterative procedure was $\Omega_2 t = 0.1$ and figure 1 shows the result from 150 to 200 iterations. As one can see both the iterative procedures reproduce the exact dynamics quite accurately, even for such a large time step, but the perturbation formula equation (15) works better, in this particular example. At the same time, the deviations from the exact solution have different signs for the iterative schemes. This fact allows us to say that the approximation with the help of equation (15) are not equivalent to the standard perturbation expansion and can be considered as an alternative to traditional approximation schemes. It is interesting that the last fact allows the improvement of both the approximations just by averaging the resulting expressions. The average value of the two approximation schemes is also presented in figure 1 and one can see that the averaging really gives more accurate results.

4.2. Partition function of a finite XY-spin chain

In this paragraph we consider another interesting application of the above theory. Let us calculate the partition function $Z = \text{Tr} \exp[-\beta H]$, where $\beta$ is the inverse temperature of a finite dimensional XY-spin chain. The Hamiltonian of the system is
\[ H = A \sum_{i}^{N} (\sigma_{i}^{+} \sigma_{i+1}^{-} + \sigma_{i}^{-} \sigma_{i+1}^{+}), \]  

(31)

where \( A \) is the constant of the spin–spin interaction, \( \sigma_{\pm} \) are the usual Pauli matrices and \( N \) is number of sites in the chain. We also assume the periodic boundary conditions.

To apply the above theory let us notice that formally \( \exp[-\beta H] = U(-i \beta) \), so, the calculation of the partition function is equivalent to the calculation of the evolution operator with pure imaginary time. Also, one has to keep only the diagonal part of the evolution operator. The diagonal part of the evolution operator gives the expression \( \exp \left[ \int_{0}^{\beta} K(s) ds \right] \) and can be calculated with any accuracy.

The Hamiltonian (31) does not have non-zero diagonal elements. Thus, the second order approximation of the partition function is \( \text{Tr} \exp[\beta^2 H^2/2] \). In particular, for the spin chain consisting of ten sites the second order approximation gives

\[ Z_{\text{TCL}} = 8 \exp \left[ \frac{5(A\beta)^2}{2} \right] \cosh \left( \frac{(A\beta)^2}{2} \right) (44 \cosh ((A\beta)^2) + \cosh (2(A\beta)^2) + 83), \]  

(32)

while the traditional second order approximation \( Z = \text{Tr}(I + \beta^2/2H^2) \) gives

\[ Z_{\text{Dyson}} = 1024 + 2560(A\beta)^2. \]  

(33)

The comparison of the approximation results with the exact partition function is presented in figure 2. It is clearly seen that equation (32) reproduces the partition function for small \( A\beta \) better than the corresponding result from equation (33). The deviations of the both methods from the exact result again have different signs. We plot also the average value \( 1/2(Z_{\text{TCL}} + Z_{\text{Dyson}}) \) in figure 2. The average value of the two methods improves the results.

5. Conclusions

In this paper, we study an evolution operator with the help of the projection operator technique. Applied to the Schrödinger equation, the procedure, which is an analogue to the famous time-convolutionless projection technique in the theory of open quantum systems and statistical physics, leads to the alternative expression (15) for the evolution operator. This expression can be considered as the starting point for a systematic perturbative investigation of the evolution operator. The resulting perturbative expression differs from the one derived by cutting off the chronological exponent and any other perturbation expansions. The approximated evolution operator can be used to recover the full evolution operator in the spirit of the Lie–Trotter formula through the iterative procedure (22). The iterative procedure can be considered as a numerical scheme for the simulation of a wide class of linear differential systems. The deviation of the iterative scheme from the exact result seems to have a different sign in comparison with the using of the truncated chronological exponent and simple averaging of the two approximations improves the results. The interesting feature of the suggested technique is the possibility of studying independently the diagonal elements of the evolution operator, which are given by the solution of equation (11). This feature may be very useful for the calculation of the partition function \( Z = \text{Tr} \exp[-\beta H] \), which is formally derived by substitution \( t \to -i \beta \) for the evolution operator.
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