Magnus expansion generator

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A recursion formula for the Magnus expansion is presented which can be used to deduce higher-order terms and to investigate their properties. The application of this formula is illustrated with several examples which were motivated by NMR spectroscopy.

I. INTRODUCTION

The Magnus expansion[1] was originally introduced simply as a series solution to the equation $dY/dT = AY$ of the form $Y(t) = \exp\Omega$, where $A(t)$, $Y(t)$, and $\Omega(t)$ are all linear operators of the real variable t. Although the subject of his paper was essentially mathematical, presenting a continuous form of the Baker-Campbell-Hausdorf formula, Magnus probably recognized some of the possibilites for practical application of his expansion, since he noted that if iA were Hermitian, Y would remain Hermitian even when the series expansion was truncated after an arbitrary number of terms.

It was Evans[2] and Haeberlen and Waugh[3] who first applied the Magnus expansion to NMR, where $A(t)$ was then assumed to be a time-dependent Hamiltonian satisfying periodic and cyclic properties. Since that time, the Magnus expansion has been instrumental in the development of improved techniques in NMR spectroscopy. By applying an appropriately designed rf perturbation to a nuclear spin system a strong, periodic time dependence can be imposed on the internal Hamiltonian in the interaction reference frame. The Magnus expansion then allows this time-varying Hamiltonian to be replaced by an effective, "average" Hamiltonian which is valid for all multiples of the periodic time. Since the nature of the rf perturbation is under the control of the experimentalist, the net result of this procedure is the replacement of the internal Hamiltonian with an averaged term tailored to suit the requirements of the particular experiment.

Improved NMR techniques have been developed in this way which clearly benefit from the elimination of unwanted terms up to fourth order in a Magnus expansion.[4] One of the limitations of the Magnus expansion, however, is that the explicit formula for all terms except the first 3 are so complicated and cumbersome that they are nearly useless in practice. In fact, to our knowledge explicit formulas have only been published for the first four terms.[5]

In this paper we present a recursion formula which facilitates the establishment of theorems for terms of arbitrary order in the Magnus expansion. In the next section the derivation of the Magnus expansion is briefly reviewed in order to clarify the origin of the recursion formula, which we call the Magnus expansion "generator." This formula is introduced in Sec. III, and its use is illustrated in Sec. IV by application in providing five theorems. The first three theorems are not new, but are included to show how the Magnus expansion generator can facilitate their proofs. The last two, however, are new, and deal with cases which may be of interest in a variety of areas.

The choice of the theorems proven in Sec. III, and indeed the overall slant of the presentation given in this paper, was motivated by our experience in NMR spectroscopy, but it is our hope that the basic results presented will be much more generally applicable.

II. MAGNUS EXPANSION

In this section we briefly review the derivation of the Magnus expansion using notation similar to that of Haeberlen.[6]

We wish to find a solution of the operator differential equation

$$\frac{dU(t)}{dt} = -i\mathscr{H}(t)U(t), \quad U(0)=1 \tag{1}$$

in the form of an exponential,

$$U(t) = \exp\{-it\overline{\mathscr{H}}(t)\} \ . \tag{2}$$

In particular, we wish to find $\overline{\mathscr{H}}(t_c)$ at a particular time t_c. We begin by dividing t_c into n intervals each of length τ, $t_0=0<t_1<t_2\cdots<t_n=t_c$, and define $\mathscr{H}'(t)$, a stepwise time-dependent approximation to $\mathscr{H}(t)$, by

$$\mathscr{H}'(t)\equiv\mathscr{H}_j=\mathscr{H}(t_j),\ \ t_{j-1}\le t<t_j \tag{3}$$

clearly,

$$\lim_{n\to\infty}\mathscr{H}'(t)=\mathscr{H}(t) \tag{4}$$

and similarly, for the solution $U'(t)$ of the differential equation

$$\frac{dU'(t)}{dt}=-i\mathscr{H}'(t)U'(t),\ \ U'(0)=1 \tag{5}$$

we have

$$\lim_{n\to\infty}U'(t_c)=U(t_c)\ . \tag{6}$$

But $U'(t_c)$ is given by

$$U'(t_c)=\prod_{j=1}^{n}\exp\{-i\mathscr{H}_j\tau\}\ , \tag{7}$$

where the exponentials in the product are ordered with larger values of j to the left. By making n sufficiently large, we can ensure that $\mathscr{H}_j\tau<<1$ for all j, so that the exponentials in Eq. (7) can be expanded into monotonically converging series:

$$U'(t_c)=\prod_{j=1}^{n}\left\{\sum_{k=0}^{\infty}\frac{(-i\tau)^k}{k!}(\mathscr{H}_j)^k\right\}\ . \tag{8}$$

The terms in Eq. (8) can be regrouped to give

$$\begin{aligned}U'(t_c)&=1+\frac{-i\tau}{1!}\{\mathscr{H}_1+\mathscr{H}_2+\cdots+\mathscr{H}_n\}\\&\quad+\frac{(-i\tau)^2}{2!}\{\mathscr{H}_1^2+\mathscr{H}_2^2+\cdots\\&\qquad+2\mathscr{H}_2\mathscr{H}_1+\cdots\}\\&\quad+\cdots\\&=1-it_c\sum_{j=0}^{\infty}\overline{h}_n^{(j)}(t_c)\ ,\end{aligned} \tag{9}$$

where

$$\begin{aligned}\overline{h}_n^{(0)}&\equiv\frac{\tau}{t_c}\{\mathscr{H}_1+\mathscr{H}_2+\cdots+\mathscr{H}_n\}\ ,\\\overline{h}_n^{(1)}&\equiv\frac{-i\tau^2}{2t_c}\{\mathscr{H}_1^2+\mathscr{H}_2^2+\cdots2\mathscr{H}_2\mathscr{H}_1+\cdots\}\ ,\end{aligned}$$

etc. (10)

It can be shown with a little algebra[6] that

$$\lim_{n\to\infty}\overline{h}_n^{(j)}(t_c)=\overline{h}^{(j)}(t_c)\ , \tag{11}$$

where the reduced average Hamiltonian term $\overline{h}^{(j)}$ is given by a multiple integral of our original function $\mathscr{H}(t)$ (Ref. 4):

$$\overline{h}^{(j)}(t_c)=\frac{(-i)^j}{t_c}\int_0^{t_c}dt_{j+1}\int_0^{t_{j+1}}dt_j\cdots\int_0^{t_2}dt_1\mathscr{H}(t_{j+1})\mathscr{H}(t_j)\cdots\mathscr{H}(t_1)\ . \tag{12}$$

Taking the limit $n\to\infty$, we have

$$U(t_c)=1-it_c\sum_{j=0}^{\infty}\overline{h}^{(j)}(t_c)\ . \tag{13}$$

But we would like to have $U(t_c)$ in terms of an exponential operator,

$$U(t_c)=\exp\{-it_c\overline{\mathscr{H}}(t_c)\}\ , \tag{14}$$

where the full average average Hamiltonian, $\overline{\mathscr{H}}(t_c)$, is given by a converging series of terms

$$\overline{\mathscr{H}}(t_c)=\overline{\mathscr{H}}^{(0)}(t_c)+\overline{\mathscr{H}}^{(1)}(t_c)+\cdots\ . \tag{15}$$

[For simplicity, we will usually write $\overline{\mathscr{H}}^{(j)}$ instead of $\overline{\mathscr{H}}^{(j)}(t_c)$.] Expanding the exponential in Eq. (14), we obtain

$$U(t_c)=\sum_{j=0}^{\infty}\frac{(-it_c)^j}{j!}\times(\overline{\mathscr{H}}^{(0)}+\overline{\mathscr{H}}^{(1)}+\overline{\mathscr{H}}^{(2)}+\cdots)^j\ . \tag{16}$$

Assuming that $\overline{\mathscr{H}}^{(j)}$ and $\overline{h}^{(j)}$ are both of order $j+1$ in the two expansions for $U(t_c)$ we obtain by comparing Eqs. (13) and (16)

$$\begin{aligned}\overline{h}^{(0)}&=\overline{\mathscr{H}}^{(0)}\ ,\\\overline{h}^{(1)}&=\overline{\mathscr{H}}^{(1)}\frac{-it_c}{2}(\overline{\mathscr{H}}^{(0)})^2\ ,\\\overline{h}^{(2)}&=\overline{\mathscr{H}}^{(2)}\frac{-it_c}{2!}(\overline{\mathscr{H}}^{(1)}\overline{\mathscr{H}}^{(0)}+\overline{\mathscr{H}}^{(0)}\overline{\mathscr{H}}^{(1)})\\&\quad-\frac{t_c^2}{3!}(\overline{\mathscr{H}}^{(0)})^3\ ,\end{aligned} \tag{17}$$

etc., and, in general,

$$\overline{h}^{(j)} = \sum_{k=1}^{j+1} \frac{(-it_c)^{-1}}{k!} H_k^j \ , \tag{18}$$

where the mixed term H_k^j is defined[6] as the sum of *all* ordered products of k terms of the full average Hamiltonian for which the product is of order $j + 1$. Since H_1^j is simply $\overline{\mathscr{H}}^{(j)}$, it is clear that

$$\overline{\mathscr{H}}^{(j)}(t_c) = \overline{h}^{(j)}(t_c) - \sum_{k=2}^{j+1} \frac{(-it_c)^{k-1}}{k!} H_k^j(t_c) \ , \quad j = 1,2,\ldots \ . \tag{19}$$

From Eq. (19) and the definition of $\overline{h}^{(j)}(t_c)$ given in Eq. (12), one finds that[1-3,5,6]

$$\overline{\mathscr{H}}^{(0)} = \frac{1}{t_c} \int_0^{t_c} dt_1 \mathscr{H}(t_1) \ ,$$

$$\overline{\mathscr{H}}^{(1)} = \frac{-i}{2t_c} \int_0^{t_c} dt_2 \int_0^{t_2} dt_2 [\mathscr{H}(t_2), \mathscr{H}(t_1)] \ , \tag{20}$$

and

$$\overline{\mathscr{H}}^{(2)} = \frac{-1}{6t_c} \int_0^{t_c} dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 (\{ \mathscr{H}(t_3), [\mathscr{H}(t_2), \mathscr{H}(t_1)] \} + \{ \mathscr{H}(t_1), [\mathscr{H}(t_2), \mathscr{H}(t_3)] \}) \ .$$

Note that the notation has been defined in such a way that the terms $\overline{h}^{(j)}$, H_k^j, and $\overline{\mathscr{H}}^{(j)}$ are all assumed to be of order $j + 1$ in $\| \mathscr{H} \| t_c$. Thus $\overline{\mathscr{H}}^{(0)}$ is first order, $\overline{h}^{(1)}$ is second order, etc.

III. GENERATOR

As was stated in the Introduction, the explicit formulas for the terms $\overline{\mathscr{H}}^{(j)}$ of the full average Hamiltonian are exceedingly cumbersome for $j \geq 4$. However, we showed in the last section, Eq. (19), that $\overline{\mathscr{H}}^{(j)}$ is given by the reduced average Hamiltonian term, $\overline{h}^{(j)}$, for which we do have a simple formula valid for all j, plus a sum over mixed terms H_k^j. In this section we derive a recursion formula for H_k^j: the Magnus expansion generator.

The mixed term H_k^j was defined in the last section as the sum of all ordered products of k terms from the full average Hamiltonian for which the product is of order $j + 1$. As was stated previously,

$$H_1^{(j)} = \overline{\mathscr{H}}^{(j)} \ . \tag{21}$$

For $k \geq 2$, each ordered product of k terms in H_k^j can be divided into a single term, $\overline{\mathscr{H}}^{(l)}$, and a product of $k - 1$ terms which is of order $j - l$, where $0 \leq l \leq j - k + 1$. In fact, for each $0 \leq l \leq j - k + 1$, H_k^j will contain the product of $\overline{\mathscr{H}}^{(l)} = H_1^l$ and all possible ordered products of $k - 1$ terms for which the product is of order $j - l$. This can be written

$$H_k^j = \sum_{l=0}^{j-k+1} H_1^l H_{k-1}^{j-l-1} \ . \tag{22}$$

Equation (22) is already the special form of the Magnus expansion generator which we have found most useful. However, it is worthwhile to proceed a few steps further. For $k \geq 3$ each product of k in H_k^j can be divided into a product of two terms of total order $l + 1$, $1 \leq l \leq j - k + 2$, and a product of $k - 2$ terms of total order $j - l$. Since H_k^j must contain all such combinations, we have

$$H_k^j = \sum_{l=1}^{j-k+2} H_2^l H_{k-2}^{j-l-1} \ , \ k \geq 2 \ . \tag{23}$$

Continuing this line of reasoning, we find in general that

$$H_k^j = \sum_{l=m-1}^{j-k+m} H_m^l H_{k-m}^{j-l-1} \ , \ k \geq m \geq 1 \ . \tag{24}$$

Equation (24) is the Magnus expansion generator in its general form.

We have found the triangle shown in Fig. 1 helpful for visualizing the properties of the mixed terms H_k^j. In each square of the triangle all possible sums of k integers whose total is $j + 1$ are listed with the integers arranged in all possible orders. Each integer i represents the full average Hamiltonian term $\overline{\mathscr{H}}^{(i-1)}$, so that a sum of integers in the triangle indicates multiplication of the corresponding average Hamiltonian terms. The mixed term H_k^j is then given by the sum of all the products of terms indicated in the $(j + 1, k)$ square of the triangle. For example, in the $j + 1 = 4$, $k = 2$ square we find the following set of sums: $\{ 1 + 3, 3 + 1, 2 + 2 \}$. This tells us that H_2^3 is given by

$$H_2^3 = \overline{\mathscr{H}}^{(0)} \overline{\mathscr{H}}^{(2)} + \overline{\mathscr{H}}^{(2)} \overline{\mathscr{H}}^{(0)} + \overline{\mathscr{H}}^{(1)} \overline{\mathscr{H}}^{(1)} \ . \tag{25}$$

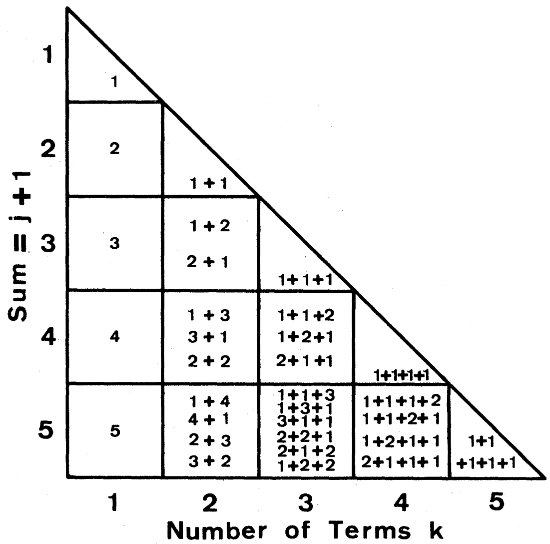

FIG. 1. H_k^j triangle. This triangle, shown here for $j+1 \leq 5$ and $k \leq 5$, is helpful for visualizing properties of the mixed average Hamiltonian H_k^j and of the Magnus-expansion-generator recursion formula. Each square contains all possible sums of k integers which total $j+1$, arranged in all possible orders. Each integer i represents the full average Hamiltonian term $\overline{\mathscr{H}}^{(i-1)}$, and a sum of integers indicates the product of the corresponding average Hamiltonian terms. The mixed term H_k^j is then given by the sum of all products of k average Hamiltonian terms indicated in the $(j+1,k)$ square of the triangle.

The Magnus expansion generator [Eq. (24)] can be verified by inspection of Fig. 1 for $j+1 \leq 5$, $k \leq 5$. For example, the sums in the $j+1=5$, $k=4$ square of the triangle may be generated by combining the sum $1+1$ in the $j+1=2$, $k=2$ square with the two sums in the $j+1=3$, $k=2$ square to obtain $1+1+1+2$ and $1+1+2+1$ and then reversing the order of combination to obtain $1+2+1+1$ and $2+1+1+1$. This process corresponds to setting $m=2$ in the generator [Eq. (24)] to obtain

$$H_4^4 = H_2^1 H_2^2 + H_2^2 H_2^1 \quad . \tag{26}$$

The same mixed term can also be obtained by combining squares with $k=1$ and $k=3$. This corresponds to setting $m=1$ in Eq. (24):

$$H_4^4 = H_1^0 H_3^3 + H_1^1 H_3^2 \quad . \tag{27}$$

The third possibility is to set $m=3$ in Eq. (24), which leads to

$$H_4^4 = H_3^2 H_1^1 + H_3^3 H_1^0 \quad . \tag{28}$$

By combining the Magnus expansion generator in its special form, Eq. (22), with Eq. (19) we obtain an expression for $\overline{\mathscr{H}}^{(j)}$ in terms of $\overline{h}^{(j)}$ and lower-order mixed terms

$$\overline{\mathscr{H}}^{(j)} = \overline{h}^{(j)} - \sum_{k=2}^{j+1} \sum_{l=0}^{j-k+1} \frac{(-it_c)^{k-1}}{k!} \overline{\mathscr{H}}^{(l)} H_{k-l}^{j-l-1} \; , \qquad j = 1,2,\ldots \; , \tag{29}$$

where Eq. (21) has also been used.

It would of course be possible to derive other recursion formulas for H_k^j in terms of products of three or more lower-order terms, but we have not yet found any need for such a formula, and so we will not pursue the possiblity in this paper.

IV. APPLICATIONS OF THE MAGNUS EXPANSION GENERATOR

In this section we present five theorems, primarily for the purpose of demonstrating how the Magnus expansion generator can be useful in verifying properties of the Magnus expansion. As stated in the Introduction, the first three theorems are, in fact, well-known properties which have been proven elsewhere[6–9] either by different arguments or, in some cases, along the same lines as here but in less specific terms. The last two theorems are new, and were motivated by our work in pulsed NMR spectroscopy.

A. Vanishing low-order terms

Theorem 1: (Refs. 6 and 7). If $\overline{\mathscr{H}}^{(l)}=0$ for all $l \leq m$, then $\overline{\mathscr{H}}^{(j)} = \overline{h}^{(j)}$ for all $j \leq 2m+2$. This can be restated

$$\overline{\mathscr{H}}^{(j)} = \overline{h}^{(j)} \text{ if } \overline{\mathscr{H}}^{(l)} = 0, \text{ for all } \begin{cases} l \leq \dfrac{j-1}{2}, j \text{ odd} \\ l \leq \dfrac{j}{2} - 1, j \text{ even} \, . \end{cases} \tag{30}$$

Our assumption and Eq. (21) tell us that

$$H_1^l = 0, \; l \leq m \quad . \tag{31}$$

We see from the special form of the Magnus expansion generator [Eq. (22)] that

$$H_2^l = \sum_{k=1}^{l} \overline{\mathscr{H}}^{(k-1)} \overline{\mathscr{H}}^{(l-k)} \quad . \tag{32}$$

For a nonzero result we need $(k-1)$ and $(l-k)$ both greater than m. This implies that

$$H_2^l = 0, \quad l \leq 2m+2 \ . \tag{33}$$

Using Eq. (22) again we see that

$$H_3^l = \sum_{k=1}^{l-1} \overline{\mathscr{H}}^{(k-1)} H_2^{l-k} \ . \tag{34}$$

For a nonzero result we need $(k-1) > m$ and $(l-k) > 2m+2$, which implies that

$$H_3^l = 0, \quad l \leq 3m+4 \tag{35}$$

and, in general,

$$H_n^l = 0, \quad l \leq (m+2)n - 2 \ . \tag{36}$$

Clearly, the lowest-order nonzero term, other than $H_1^{m+1} = \overline{\mathscr{H}}^{(m+1)}$, will be H_2^{2m+3}. According to Eq. (19) the theorem is therefore proved, since we have

$$H_k^j = 0, \quad k \geq 2, \ j \leq 2m+2 \ . \tag{37}$$

The validity of this theorem can almost be seen by inspection of Fig. 1.

B. Antisymmetric Hamiltonian

Theorem 2: (Ref. 6). If $H(t)$ is antisymmetric, that is if $\mathscr{H}(t_c - t) = -\mathscr{H}(t)$, then $\overline{\mathscr{H}}^{(j)}(t_c) = 0$ for all j.

The theorem is easily demonstrated for $j = 0$ using the formula for $\overline{\mathscr{H}}^{(0)}$ given by Eq. (20). Now we shall assume that $\overline{\mathscr{H}}^{(j)} = 0$ for $j \leq m$, and show that $\overline{\mathscr{H}}^{(m+1)} = 0$, thereby proving the theorem by induction.

From theorem 1 we know that

$$\overline{\mathscr{H}}^{(m+1)} = \overline{h}^{(m+1)} = \frac{(-i)^{m+1}}{t_c} \int_0^{t_c} dt_{m+2} \int_0^{t_{m+2}} dt_{m+1} \cdots \int_0^{t_2} dt_1 \mathscr{H}(t_{m+2}) \cdots \mathscr{H}(t_1) \ , \tag{38}$$

where the definition of $\overline{h}^{(k)}$ given in Eq. (12) has been used. If we now make the change of variables $t'_{m+2} \equiv t_c - t_{m+2}$ and use the fact that $\mathscr{H}(t_c - t_{m+2}) = -\mathscr{H}(t_{m+2})$, we find that

$$\overline{h}^{(m+1)} = -\overline{h}^{(m+1)} = 0 \ , \tag{39}$$

which completes the proof.

C. Symmetric Hamiltonian

Theorem 3: (Refs. 8 and 9). If $\mathscr{H}(t)$ is symmetric, that is if $\mathscr{H}(t_c - t) = \mathscr{H}(t)$, then $\overline{\mathscr{H}}^{(j)}(t_c) = 0$ for all odd j.

The Magnus expansion is only concerned with $\mathscr{H}(t)$ as it is defined over the interval $0 \leq t \leq t_c$. However, for convenience we may assume that $\mathscr{H}(-t) = \mathscr{H}(t_c - t)$. Then we can consider $\overline{\mathscr{H}}^{(j)}(-t_c)$ and its component parts $\overline{h}^{(j)}(-t_c)$ and $H_k^j(-t_c)$. According to the definition given in Eq. (12),

$$\overline{h}^{(j)}(-t_c) = \frac{(-i)^{j+1}}{t_c} \int_0^{-t_c} dt_{j+1} \cdots \int_0^{t_2} dt_1 \mathscr{H}(t_{j+1}) \cdots \mathscr{H}(t_1) \ . \tag{40}$$

Making the substitution $t'_l = -t_l$, and recalling that $\mathscr{H}(-t'_l) = \mathscr{H}(t_c - t'_l) = \mathscr{H}(t'_l)$ since $\mathscr{H}(t)$ is symmetric, we obtain

$$\overline{h}^{(j)}(-t_c) = (-1)^{j+1} \frac{(-i)^{j+1}}{t_c} \int_0^{t_c} t_{j+1} \cdots \int_0^{t_2} dt_1 \mathscr{H}(t_{j+1}) \cdots \mathscr{H}(t_1) = (-1)^j \overline{h}^{(j)}(t_c) \ . \tag{41}$$

Now we wish to prove a similar relationship for $\mathscr{H}_k^j$. From the explicit formulas for $\overline{\mathscr{H}}^{(0)} = H_1^0$ and $\overline{\mathscr{H}}^{(1)} = H_1^1$ in Eq. (20), it is easy to show that

$$H_1^{(0)}(-t_c) = H_1^{(0)}(t_c) \ , \quad H_1^1(-t_c) = -H_1^1(t_c) \ . \tag{42}$$

Assume that $H_1^j(-t_c)=(-1)^j H_1^j(t_c)$ for $j\le m$. Then we can use the Magnus expansion generator in its special form [Eq. (22)] to show that

$$\begin{aligned} H_2^j(-t_c) &= \sum_{l=0}^{j-1} H_1^l(-t_c) H_1^{j-l-1}(t_c) \\ &= (-1)^{j-1} H_2^j(t_c),\ j\le m\ , \end{aligned} \tag{43}$$

and thus, by repeating the process,

$$H_k^j(-t_c)=(-1)^{j-k+1}H_k^j(t_c),\ j\le m\ . \tag{44}$$

Inserting Eqs. (41) and (44) into the basic formula for $\overline{\mathscr{H}}^{(j)}$, Eq. (19), we obtain

$$\begin{aligned} \overline{\mathscr{H}}^{(j)}(-t_c) &= \overline{h}^{(j)}(-t_c) - \sum_{k=2}^{j+1} \frac{(it_c)^{k-1}}{k!} H_k^j(-t_c) \\ &= (-1)^j \left[\overline{h}^{(j)}(t_c) - \sum_{k=2}^{j+1} \frac{(it_c)^{k-1}}{k!} (-1)^{k-1} H_k^j(t_c) \right] \\ &= (-1)^j \overline{\mathscr{H}}^{(j)}(t_c)\ . \end{aligned} \tag{45}$$

The proof is now completed[9] by realizing that, since $\mathscr{H}(-t)=\mathscr{H}(t)$, it must be true that the time development operators are also equal

$$U(-t_c)=U(t_c)\ , \tag{46}$$

and, therefore,

$$\begin{aligned} \sum_{j=0}^{\infty} \overline{\mathscr{H}}^{(j)}(-t_c) &= \sum_{j=0}^{\infty} \overline{\mathscr{H}}^{(j)}(t_c) \\ &= \sum_{j=0}^{\infty} (-1)^j \overline{\mathscr{H}}^{(j)}(t_c)\ . \end{aligned} \tag{47}$$

This can only be true if $\overline{\mathscr{H}}^{(j)}$ vanishes for all odd j.

D. Decoupling

If the interval t_c is divided into two parts, $0<t_1<t_c$, then the Magnus expansion can be carried out over each subinterval as well as over the entire interval t_c. This results in

$$\overline{\mathscr{H}}_1=\sum_{j=0}^{\infty}\overline{\mathscr{H}}_1^{(j)}\ ,\quad \overline{\mathscr{H}}_2=\sum_{k=0}^{\infty}\overline{\mathscr{H}}_2^{(k)}\ , \tag{48}$$

where

$$\begin{aligned} \overline{\mathscr{H}}_1^{(0)} &= \frac{1}{t_{c1}}\int_0^{t_1}\mathscr{H}(t)\,dt\ , \\ \overline{\mathscr{H}}_2^{(0)} &= \frac{1}{t_{c2}}\int_{t_1}^{t_c}\mathscr{H}(t)\,dt\ , \end{aligned} \tag{49}$$

etc., and

$$t_{c1}=t_1,\ t_{c2}=t_c-t_1\ . \tag{50}$$

A term in the Magnus expansion $\overline{\mathscr{H}}^{(j)}$ is said to decouple if

$$\overline{\mathscr{H}}^{(j)}=\frac{1}{t_c}(t_{c1}\overline{\mathscr{H}}_1^{(j)}+t_{c2}\overline{\mathscr{H}}_2^{(j)})\ . \tag{51}$$

It was shown previously[4] for reduced average Hamiltonian terms that if $\overline{h}^{(l)}=0$ for all $l\le m$, $\overline{h}^{(j)}$ decouples for all $j\le 2m+2$. From theorem 1, it should be clear that $\overline{\mathscr{H}}^{(j)}$ decouples under the same conditions, i.e., if $\overline{\mathscr{H}}^{(l)}=0$ for all $l\le m$.

Evans[2] makes the following statement near the end of his classic paper on average Hamiltonian theory, speaking of multiple-pulse NMR experiments: "suppose we have cycles (or subcycles) of pulses, over each of which the zeroth Magnus term vanishes identically, then it may be shown rigorously that the sum of the whole Magnus expansion after an integer number of cycles (or subcycles) is the algebraic sum of the Magnus expansions evaluated for each cycle (or subcycle) considered singly." In other words, he claims that $\overline{\mathscr{H}}_1^{(0)}=\overline{\mathscr{H}}_2^{(0)}=0$ is enough to ensure that $\overline{\mathscr{H}}^{(j)}$ decouples for all j. Although Evan's statement is certainly true for a series of identical intervals, or "cycles," it does not hold for arbitrary subintervals, or "subcycles." In order to demonstrate this fact, we prove the following theorem.

Theorem 4: If a time interval t_c is divided into two subintervals, $0\le t_1\le t_c$, with $t_{c1}\equiv t_1$ and $t_{c2}\equiv t_c-t_1$, and if $\overline{\mathscr{H}}_1^{(0)}=\overline{\mathscr{H}}_1^{(0)}=0$, then $\overline{\mathscr{H}}^{(3)}$ decouples if and only if $\overline{\mathscr{H}}_1^{(1)}$ and $\overline{\mathscr{H}}_2^{(1)}$ commute.

The formula for $\overline{\mathscr{H}}^{(3)}$ is readily obtained from Eq. (19):

$$\overline{\mathscr{H}}^{(3)}=\overline{h}^{(3)}+\frac{it_c}{2}H_2^3+\frac{t_c^2}{6}H_3^3-\frac{it_c^3}{24}H_4^3\ . \tag{52}$$

Since $\overline{\mathscr{H}}^{(0)}=0$, we find by setting $m=0$ in Eq. (36) that $H_3^3=H_4^3=0$. From the special case of the Magnus expansion generator given in Eq. (32), we see that

$$H_2^3=\overline{\mathscr{H}}^{(0)}\overline{\mathscr{H}}^{(2)}+\overline{\mathscr{H}}^{(1)}\overline{\mathscr{H}}^{(1)}+\overline{\mathscr{H}}^{(2)}\overline{\mathscr{H}}^{(0)}=(\overline{\mathscr{H}}^{(1)})^2 \ , \tag{53}$$

so that

$$\overline{\mathscr{H}}^{(3)}=\overline{h}^{(3)}+\frac{it_c}{2}(\overline{\mathscr{H}}^{(1)})^2 \ . \tag{54}$$

Because $\overline{\mathscr{H}}_1^{(0)}=\overline{\mathscr{H}}_2^{(0)}=0$, formulas similar to Eq. (54) apply to $\overline{\mathscr{H}}_1^{(3)}$ and $\overline{\mathscr{H}}_2^{(3)}$. From the definition of $\overline{h}^{(j)}$, Eq. (12), we see that[4]

$$\begin{aligned}\overline{h}^{(3)}&=\frac{-i}{t_c}\int_0^{t_c}dt_4\int_0^{t_4}dt_3\int_0^{t_3}dt_2\int_0^{t_2}dt_1\mathscr{H}(t_4)\mathscr{H}(t_3)\mathscr{H}(t_2)\mathscr{H}(t_1)\\&=\frac{-i}{t_c}\int_0^{t_{c1}}dt_4\int_0^{t_4}dt_3\int_0^{t_3}dt_2\int_0^{t_2}dt_1\mathscr{H}(t_4)\mathscr{H}(t_3)\mathscr{H}(t_2)\mathscr{H}(t_1)\\&\quad+\frac{-i}{t_c}\left[\int_{t_{c1}}^{t_c}dt_4\mathscr{H}(t_4)\right]\int_0^{t_{c1}}dt_3\int_0^{t_3}dt_2\int_0^{t_2}dt_1\mathscr{H}(t_3)\mathscr{H}(t_2)\mathscr{H}(t_1)+\cdots\\&=t_c^{-1}[t_{c1}\overline{h}_1^{(3)}+t_{c2}\overline{h}_2^{(3)}-it_{c1}t_{c2}(\overline{h}_2^{(0)}\overline{h}_1^{(2)}+\overline{h}_2^{(1)}\overline{h}_1^{(1)}+\overline{h}_2^{(2)}\overline{h}_1^{(0)})] \ .\end{aligned}\tag{55}$$

But since $\overline{h}_1^{(0)}=\overline{h}_2^{(0)}=0$, we have

$$\overline{h}^{(3)}=t_c^{-1}(t_{c1}\overline{h}_1^{(3)}+t_{c2}\overline{h}_2^{(3)}-it_{c1}t_{c2}\overline{h}_2^{(1)}\overline{h}_1^{(1)}) \ . \tag{56}$$

Since $\overline{\mathscr{H}}^{(0)}=0$, $\overline{\mathscr{H}}^{(1)}=\overline{h}^{(1)}$ and we find by an argument similar to that given above that

$$\overline{h}^{(1)}=t_c^{-1}(t_{c1}\overline{h}_1^{(1)}+t_{c2}\overline{h}_2^{(1)}) \ . \tag{57}$$

Inserting Eqs. (56) and (57) into Eq. (54), we obtain finally

$$\begin{aligned}\overline{\mathscr{H}}^{(3)}&=t_c^{-1}\left[t_{c1}\overline{h}_1^{(3)}+t_{c2}\overline{h}_2^{(3)}-it_{c1}t_{c2}\overline{h}_2^{(1)}\overline{h}_1^{(1)}+\frac{i}{2}(t_{c1}\overline{h}_1^{(1)}+t_{c2}\overline{h}_2^{(1)})^2\right]\\&=t_c^{-1}\left[t_{c1}\left[\overline{h}_1^{(3)}+\frac{it_{c1}}{2}(\overline{h}^{(1)})^2\right]+t_{c2}\left[\overline{h}_2^{(3)}+\frac{it_{c2}}{2}(\overline{h}^{(2)})^2\right]+\frac{it_{c1}t_{c2}}{2}[\overline{h}_1^{(1)},\overline{h}_2^{(1)}]\right]\\&=t_c^{-1}\left[t_{c1}\overline{\mathscr{H}}_1^{(3)}+t_{c2}\overline{\mathscr{H}}_2^{(3)}+\frac{it_{c1}t_{c2}}{2}[\overline{\mathscr{H}}_1^{(1)},\overline{\mathscr{H}}_2^{(1)}]\right] \ ,\end{aligned}\tag{58}$$

where, in the last step, Eq. (54) has been used for $\overline{\mathscr{H}}_1^{(3)}$ and $\overline{\mathscr{H}}_2^{(3)}$, and the fact that $\overline{h}_1^{(1)}=\overline{\mathscr{H}}_1^{(1)}$ and $\overline{h}_2^{(1)}=\overline{\mathscr{H}}_2^{(1)}$ has been utilized.

E. Averaging by a time-independent interaction

Theorem 5: If $\mathscr{H}(t)=\exp\{i\mathscr{H}_Lt\}\mathscr{H}_s\times\exp\{-i\mathscr{H}_Lt\}$, *where* $\mathscr{H}_L$ *and* $\mathscr{H}_S$ *are both time independent and* $\mathscr{H}(t_c)=\mathscr{H}(0)=\mathscr{H}_S$, *then*

$$[\mathscr{H}_L,\overline{\mathscr{H}}^{(j)}(t_c)]=[\overline{\mathscr{H}}^{(j-1)}(t_c),\mathscr{H}_S] \ . \tag{59}$$

This theorem is of importance when a time-independent Hamiltonian consists of a large part, $\mathscr{H}_L$, and a smaller part $\mathscr{H}_S$, and the Magnus expansion is to be applied in the interaction representation in order to characterize the averaging effect of $\mathscr{H}_L$ on $\mathscr{H}_S$. The commutation relations of $\mathscr{H}_L$ and $\overline{\mathscr{H}}^{(j)}(t_c)$ are important, since

$$\begin{aligned}U(t_c)&=\exp\{-i(\mathscr{H}_L+\mathscr{H}_S)t_c\}\\&=\exp\{-i\mathscr{H}_Lt_c\}\exp\{-it_c\overline{\mathscr{H}}(t_c)\}\end{aligned}\tag{60}$$

and if, after truncation, we have $[\mathscr{H}_L,\overline{\mathscr{H}}]=0$ we can write

$$U(t_c)=\exp\{-i(\mathscr{H}_L+\overline{\mathscr{H}})t_c\} \ , \tag{61}$$

which represents the replacement of $\mathscr{H}_S$ by $\overline{\mathscr{H}}$.

We begin the proof of theorem 5 with a lemma.

Lemma 1: If $\mathscr{H}(t) = \exp\{ i\mathscr{H}_L t \}\mathscr{H}_S \exp\{ -i\mathscr{H}_L t \}$, $\mathscr{H}_L$ and $\mathscr{H}_S$ both time independent, then for $j \geq 1$

$$[\mathscr{H}_L, \bar{h}^{(j)}(t_c)] = \bar{h}^{(j-1)}(t_c)\mathscr{H}_S - \mathscr{H}(t_c)\bar{h}^{(j-1)}(t_c) \ . \tag{62}$$

We begin by noting the following property of commutators:

$$[A, BCDE \cdots]\ [A,B]CDE \cdots + B[A,C]DE \cdots + BC[A,D]E \cdots + \cdots \ . \tag{63}$$

Using the definition of $\bar{h}^{(j)}$ given in Eq. (12), we find that

$$[\mathscr{H}_L, \bar{h}^{(j)}] = \frac{(-i)^j}{t_c} \sum_{l=1}^{j+1} \int_0^{t_c} dt_{j+1} \cdots \int_0^{t_2} dt_1 \times \{ \mathscr{H}(t_{J+1}) \cdots \mathscr{H}(t_{l+1})[\mathscr{H}_L, \mathscr{H}(t_l)]\mathscr{H}(t_l - 1) \cdots \mathscr{H}(t_1) \} \ . \tag{64}$$

Changing the order of integration in each term of the sum, we obtain

$$[\mathscr{H}_L, \bar{h}^{(j)}] = \frac{(-i)^j}{t_c} \sum_{l=1}^{j+1} \int_0^{t_c} dt_{j+1} \cdots \int_0^{t_{l+2}} dt_{l+1} \int_0^{t_{l+1}} dt_{l-1} \cdots \int_0^{t_2} t_1 \times \left[\mathscr{H}(t_{j+1}) \cdots \mathscr{H}(t_{l+1}) \left[\int_{t_{l-1}}^{t_{l+1}} dt_l [\mathscr{H}_L, \mathscr{H}(t_l)] \right] \mathscr{H}(t_{l-1}) \cdots \mathscr{H}(t_1) \right] \ . \tag{65}$$

But

$$\int_{t_A}^{t_B} dt\, [\mathscr{H}_L, \mathscr{H}(t)] = \int_{t_A}^{t_B} dt\, [\mathscr{H}_L \exp(i\mathscr{H}_L t)\mathscr{H}_S \exp(-i\mathscr{H}_L t) - \exp(i\mathscr{H}_L t)\mathscr{H}_S \mathscr{H}_L \exp(-i\mathscr{H}_L t)]$$
$$= -i[\mathscr{H}(t_B) - \mathscr{H}(t_A)] \ . \tag{66}$$

Inserting Eq. (66) into Eq. (65), we then have

$$[\mathscr{H}_L, \bar{h}^{(j)}] = \frac{(-i)^{j+1}}{t_c} \sum_{l=1}^{j+1} \int_0^{t_c} dt_{j+1} \cdots \int_0^{t_{l+2}} dt_{l+1} \int_0^{t_{l+1}} dt_{l-1} \cdots \int_0^{t_2} dt_1 \times \{ \mathscr{H}(t_{j+1}) \cdots \mathscr{H}(t_{l+1})[\mathscr{H}(t_{l+1}) - \mathscr{H}(t_{l-1})]\mathscr{H}(t_{l-1}) \cdots \mathscr{H}(t_1) \} \ , \tag{67}$$

where we can define $t_0 \equiv 0$ and $t_{k+2} \equiv t_c$. Most of the terms in the summation cancel each other, leaving only the first and last terms. Relabeling the indices leads to

$$[\mathscr{H}_L, \bar{h}^{(j)}] = \frac{(-i)^{j+1}}{t_c} \mathscr{H}(t_c) \int_0^{t_c} dt_j \cdots \int_0^{t_c} dt_1 \mathscr{H}(t_j) \cdots \mathscr{H}(t_1)$$
$$- \frac{(-i)^{j+1}}{t_c} \int_0^{t_c} dt_j \cdots \int_0^{t_2} dt_1 \mathscr{H}(t_j) \cdots \mathscr{H}(t_1)\mathscr{H}(0)$$
$$= \bar{h}^{(j-1)}\mathscr{H}_S - \mathscr{H}(t_c)\bar{h}^{(j-1)} \ . \tag{68}$$

For our theorem we have assumed that $\mathscr{H}(t_c) = \mathscr{H}_S$, which leads to

$$[\mathscr{H}_L, \bar{h}^{(j)}] = [\bar{h}^{(j-1)}, \mathscr{H}_S] \ . \tag{69}$$

Using Eq. (66) and the definition of $\bar{\mathscr{H}}^{(0)}$ given in Eq. (20), we see that

$$[\mathscr{H}_L, \bar{\mathscr{H}}^{(0)}] = t_c^{-1} \int_0^{t_c} [\mathscr{H}_L, \mathscr{H}(t)]dt = -i[\mathscr{H}(t_c) - \mathscr{H}(0)] = 0 \ . \tag{70}$$

From Eq. (19) we find that

$$[\mathscr{H}_L,\overline{\mathscr{H}}^{(1)}]=[\mathscr{H}_L,\overline{h}^{(1)}]+\frac{it_c}{2}[\mathscr{H}_L,\mathscr{H}_2^1] \quad . \tag{71}$$

But the special case of the Magnus expansion generator, Eq. (32) tells us that

$$H_2^1=(\overline{\mathscr{H}}^{(1)})^2 \quad . \tag{72}$$

Equations (69)–(72) then lead to

$$[\mathscr{H}_L,\overline{\mathscr{H}}^{(1)}]=[\overline{\mathscr{H}}^{(0)},\mathscr{H}_S] \quad . \tag{73}$$

Having shown that the theorem is true for $j=1$, we now assume that it is true for $j\leq m$ and prove that it is also true for $j=m+1$. Simultaneously, we must also show that the theorem holds for H_k^j when $j\geq 1$ and $k\leq j+1$. From the special case of the Magnus expansion generator, Eq. (32), we see that

$$H_2^2=\overline{\mathscr{H}}^{(0)}\overline{\mathscr{H}}^{(1)}+\overline{\mathscr{H}}^{(1)}\overline{\mathscr{H}}^{(0)} \quad . \tag{74}$$

Combining this with Eqs. (63), (70), and (73) gives

$$\begin{aligned}[\mathscr{H}_L,H_2^2]&=\overline{\mathscr{H}}^{(0)}[\mathscr{H}_L,\overline{\mathscr{H}}^{(1)}]+[\mathscr{H}_L,\overline{\mathscr{H}}^{(1)}]\overline{\mathscr{H}}^{(0)}\\&=\overline{\mathscr{H}}^{(0)}[\overline{\mathscr{H}}^{(0)},\mathscr{H}_S]+[\overline{\mathscr{H}}^{(0)},\mathscr{H}_S]\overline{\mathscr{H}}^{(0)}\\&=[(\overline{\mathscr{H}}^{(0)})^2,H_S]\\&=[H_2^1,\mathscr{H}_S] \quad .\end{aligned} \tag{75}$$

Now assume that the theorem holds for $j\leq m$ separately for $\overline{\mathscr{H}}^{(j)}$ and H_k^j for all $k\leq j+1$. Since $H_{j+1}^j=(\overline{\mathscr{H}}^{(0)})^{j+1}$, we see that $\mathscr{H}_L$ commutes with H_{j+1}^j. From Eq. (29) we have

$$[\mathscr{H}_L,\overline{\mathscr{H}}^{(m+1)}]=[\mathscr{H}_L,\overline{h}^{(m+1)}]-\sum_{k=2}^{m+2}\sum_{l=0}^{m-k+2}\frac{(-it_c)^{k-1}}{k!}([\mathscr{H}_L,\overline{\mathscr{H}}^{(l)}]H_{k-1}^{m-l}+\overline{\mathscr{H}}^{(l)}[\mathscr{H}_L,H_{k-1}^{m-l}]) \quad . \tag{76}$$

Since both (l) and $(m-l)\leq m$ over the entire summation, we can use our lemma and assumptions to obtain

$$\begin{aligned}[\mathscr{H}_L,\overline{\mathscr{H}}^{(m+1)}]&=[\overline{h}^{(m)},\mathscr{H}_S]-\sum_{k=2}^{m+2}\sum_{l=1}^{m-k+2}\frac{(-it_c)^{k-1}}{k!}[\overline{\mathscr{H}}^{(l-1)},\mathscr{H}_S]H_{k-1}^{m-l}-\sum_{k=2}^{m+2}\sum_{l=0}^{m-k+1}\overline{\mathscr{H}}^{(l)}[H_{k-1}^{m-l-1},\mathscr{H}_S]\\&=[\overline{h}^{(m)},\mathscr{H}_S]-\sum_{k=2}^{m+2}\sum_{l=0}^{m-k+1}[\overline{\mathscr{H}}^{(l)}H_{k-1}^{m-l-1},\mathscr{H}_S]\\&=[\overline{\mathscr{H}}^{(m)},\mathscr{H}_S] \quad .\end{aligned} \tag{77}$$

This completes the proof.

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