Recursive generation of higher-order terms in the Magnus expansion

S. Klarsfeld and J. A. Oteo
Division de Physique Théorique, Institut de Physique Nucléaire, F-91406 Orsay CEDEX, France
(Received 11 July 1988; revised manuscript received 24 October 1988)

Several methods for systematically calculating higher-order terms in the Magnus expansion of the time-displacement operator are discussed from a unified point of view. It is shown that a quadratic recursive scheme recently introduced in the average Hamiltonian formalism of NMR spectroscopy can be extended to other cases, including the original multiple commutator approach developed by Magnus [Commun. Pure Appl. Math. 7, 649 (1954)].

I. INTRODUCTION

The unitary time-displacement operator $U=U(t,0)$ for a quantum system with Hamiltonian $H=H(t)$ satisfies the Schrödinger equation

$$\frac{\partial}{\partial t}U=\tilde{H}U \quad (\tilde{H}=H/i\hbar) , \tag{1.1}$$

with the initial condition $U=1$ at $t=0$. Equation (1.1) is easily solved by iteration, with $1/\hbar$ as a natural ordering parameter (this is equivalent to perturbation theory). Let us assume U expanded as

$$U=1+\sum_{n=1}^{\infty}P_n, \quad P_n\sim(1/\hbar)^n , \tag{1.2}$$

where $P_n=0$ at $t=0$. Substituting into Eq. (1.1) and comparing terms of equal orders, one finds

$$\frac{\partial}{\partial t}P_1=\tilde{H}, \quad \frac{\partial}{\partial t}P_n=\tilde{H}P_{n-1} \quad (n\geq 2) , \tag{1.3}$$

whence

$$P_n=P_n(t)=\int_0^t dt_1\cdots\int_0^{t_{n-1}}dt_n\tilde{H}_1\cdots\tilde{H}_n ,$$
$$\tilde{H}_i=\tilde{H}(t_i) . \tag{1.4}$$

All this is well known, but was repeated here for further reference, and as an illustration of a general technique used below.

If the Hamiltonian does not depend on time, Eq. (1.4) readily yields $P_n=(t\tilde{H})^n/n!$ and the summation in Eq. (1.2) can be done in closed form, giving $U=\exp(t\tilde{H})$. Magnus[1] has shown that under certain conditions an exponential representation of U, viz.,

$$U=e^{\Omega}=1+\sum_{k=1}^{\infty}\frac{1}{k!}\Omega^k , \tag{1.5}$$

can be found also in the case of a time-dependent Hamiltonian. The operator $\Omega=\Omega(t)$ is expressed formally as a series expansion similar to Eq. (1.2):

$$\Omega=\sum_{n=1}^{\infty}\Omega_n, \quad \Omega_n\sim(1/\hbar)^n , \tag{1.6}$$

with $\Omega_n=0$ at $t=0$. To first order Eq. (1.5) gives $U\simeq 1+\Omega_1$, so that Ω_1 clearly coincides with P_1. The following terms in Eq. (1.6) were obtained by an iterative process which makes apparent a nested commutator structure of increasing complexity. Compact and symmetric formulas of this type have been derived up to fourth order[2] (see Appendix). Milfeld and Wyatt, who used the Magnus expansion to study the behavior of molecular systems in intense laser fields,[3] have given alternative expressions through fifth order, but in a less symmetrical form. The Magnus expansion became rapidly popular and has already been used in a variety of time-dependent problems: semiclassical atomic collision theory,[4–7] multiphoton excitation of molecules,[8] multiple Coulomb excitation of nuclei,[9] pulsed magnetic resonance spectra,[10,11] spectral line broadening,[12] infrared divergences in QED,[13] to quote just a few.

For some of the applications mentioned above,[3,4,8,10,11] and more generally in order to investigate the convergence of the expansion,[14,15] it is of interest to develop systematic procedures for generating higher-order terms in Eq. (1.6). In Sec. II we present in a simplified form the generator method recently proposed by Burum.[16] Originally this method was formulated for the specific needs of high-resolution NMR spectroscopy in terms of average Hamiltonians. Here we adopt a more standard form of time-dependent quantum mechanics, which should help make things clearer.

An interesting alternative is provided by a method subsequently introduced by Salzman,[17] who apparently was not aware of Burum's work. For completeness we include a simple derivation of Salzman's formulas in Sec. III. Although the latter have a rather transparent structure, the rapid increase with order of the number and complexity of terms in the operator Ω_n appears as a serious hindrance in the numerical treatment of problems that involve more than two states.[18] As will be seen, it is straightforward to extend the generator idea here in order to circumvent this drawback by a recursive process. Finally, in Sec. IV a similar treatment is applied in a specific form to the original Magnus approach, in which Ω is expressed in terms of multiple commutators.

II. BURUM'S METHOD

The two infinite expansions in Eqs. (1.2) and (1.5) are assumed to represent the same operator U. With due account of Eq. (1.6) we identify terms of the same order in $1/\hbar$ to get

$$P_1=\Omega_1 ,$$
$$P_2=\Omega_2+\frac{1}{2!}\Omega_1^2 , \tag{2.1}$$
$$P_3=\Omega_3+\frac{1}{2!}(\Omega_1\Omega_2+\Omega_2\Omega_1)+\frac{1}{3!}\Omega_1^3, \ldots .$$

The general term can be written as

$$\Omega_n=P_n-\sum_{k=2}^{n}\frac{1}{k!}Q_n^{(k)} \quad (n\geq 2) , \tag{2.2}$$

where

$$Q_n^{(k)}=\sum\Omega_{i_1}\cdots\Omega_{i_k} \quad (i_1+\cdots+i_k=n) . \tag{2.3}$$

Notice that subscripts indicate the order with respect to $1/\hbar$, while superscripts represent the number of factors in each product. Thus the summation in Eq. (2.3) extends over all possible products of k operators Ω_i (in general, noncommuting), such that the overall order of each term is equal to n. Equation (2.1) [or (2.2)] is the starting point in Burum's method.

By regrouping terms in Eq. (2.3) we get

$$\begin{aligned}Q_n^{(k)}=&\Omega_1\sum_{i_2+\cdots+i_k=n-1}\Omega_{i_2}\cdots\Omega_{i_k}\\&+\Omega_2\sum_{i_2+\cdots+i_k=n-2}\Omega_{i_2}\cdots\Omega_{i_k}\\&+\cdots+\Omega_{n-k+1}\sum_{i_2+\cdots+i_k=k-1}\Omega_{i_2}\cdots\Omega_{i_k} .\end{aligned} \tag{2.4}$$

Each of the remaining sums is indeed a lower-order Q operator formed with products of $k-1$ factors Ω_i. Therefore we can rewrite Eq. (2.4) as

$$\begin{aligned}&Q_n^{(k)}=\sum_{m=1}^{n-k+1}Q_m^{(1)}Q_{n-m}^{(k-1)} \quad (2\leq k\leq n) ,\\&Q_n^{(1)}=\Omega_n, \quad Q_n^{(n)}=\Omega_1^n .\end{aligned} \tag{2.5}$$

Equation (2.5) is what Burum called "the Magnus expansion generator." Together with Eq. (2.2) it offers a convenient basis for computing Ω_n. For a given n only the nth order perturbative contribution P_n must be calculated explicitly, while the rest is obtained recursively from preceding Ω_m's ($m<n$).

Other generators may be easily produced by ordering terms in Eq. (2.3) in a different way. For instance,

$$\begin{aligned}Q_n^{(k)}=&\Omega_1^2\sum_{i_3+\cdots+i_k=n-2}\Omega_{i_3}\cdots\Omega_{i_k}\\&+(\Omega_1\Omega_2+\Omega_2\Omega_1)\sum_{i_3+\cdots+i_k=n-3}\Omega_{i_3}\cdots\Omega_{i_k}\\&+\cdots ,\end{aligned}$$

leads to

$$Q_n^{(k)}=\sum_{m=2}^{n-k+2}Q_m^{(2)}Q_{n-m}^{(k-2)} \quad (3\leq k\leq n) . \tag{2.6}$$

In practice, however, the form in Eq. (2.5) has been found to be the most useful.

III. SALZMAN'S METHOD

In his paper Salzman used a rather lengthy induction procedure in order to solve Eq. (2.1) for the "unknown" quantities Ω_n in terms of the "known" perturbation operators P_m. Instead, we simply notice here that formally the Magnus operator can be defined also by $\Omega=\log[1+(U-1)]$. From Eqs. (1.2) and (1.6) we then have

$$\sum_{n=1}^{\infty}\Omega_n=\log\left[1+\sum_{n=1}^{\infty}P_n\right] . \tag{3.1}$$

Taking into account the Taylor expansion of the function $\log(1+z)$ we further obtain

$$\sum_n\Omega_n=\sum_i P_i-\tfrac{1}{2}\sum_{i,j}P_iP_j+\tfrac{1}{3}\sum_{i,j,k}P_iP_jP_k+\cdots . \tag{3.2}$$

The above equation immediately yields Ω_n in terms of the P_k's ($k\leq n$) if we collect all terms of order $(1/\hbar)^n$ in the right-hand side. In this way one has successively,

$$\begin{aligned}&\Omega_1=P_1 ,\\&\Omega_2=P_2-\tfrac{1}{2}P_1^2 ,\\&\Omega_3=P_3-\tfrac{1}{2}(P_1P_2+P_2P_1)+\tfrac{1}{3}P_1^3, \cdots ,\end{aligned} \tag{3.3}$$

which are precisely Salzman's formulas. It is clear that Eq. (3.3) is nothing but the inverse of the system given above in Eq. (2.1). Since the two systems have a similar structure it is an easy matter to introduce a generator for Eq. (3.3) as in Burum's case. To this end we write the general Magnus term of order n in the form

$$\Omega_n=P_n-\sum_{k=2}^{n}\frac{(-1)^k}{k}R_n^{(k)} \quad (n\geq 2) , \tag{3.4}$$

where

$$R_n^{(k)}=\sum P_{i_1}P_{i_2}\cdots P_{i_k} \quad (i_1+\cdots+i_k=n) . \tag{3.5}$$

Proceeding as in Eq. (2.4) one readily gets the quadratic recursion formula

$$\begin{aligned}&R_n^{(k)}=\sum_{m=1}^{n-k+1}R_m^{(1)}R_{n-m}^{(k-1)} \quad (2\leq k\leq n) ,\\&R_n^{(1)}=P_n, \quad R_n^{(n)}=P_1^n .\end{aligned} \tag{3.6}$$

Equation (3.6) represents the Magnus expansion generator in Salzman's approach. The obvious advantage of the latter over Burum's method is that it provides an explicit expression of the nth order Magnus approximant Ω_n in terms of perturbation theory operators [notice, however, that the presence of inverse factorials in Eq. (2.2) might have in turn beneficial effects in numerical calculations]. More general recursive schemes, similar to Eq. (2.6), are valid here too, but do not seem of much practical interest.

Finally, we should like to recall that the term P_n in

Eqs. (2.2) and (3.4) is actually obtained by iteration, as shown in Sec. I. Thus from Eq. (1.3) one has

$$P_n=\int_0^t dt'\tilde{H}(t')P_{n-1}(t')\approx\sum_q w_q\tilde{H}(t_q)P_{n-1}(t_q)\ , \tag{3.7}$$

where the w_q's are weights for some conveniently chosen quadrature formula. The problem therefore reduces once again to evaluating a sum over products of two operators. As a prerequisite for this, one must, of course, store intermediate-time results at each stage.

IV. THE COMMUTATOR APPROACH

Unlike the two methods described above, the older derivations of the Magnus expansion[1,2,9,19] proceeded directly from the Schrödinger equation (1.1) without any reference to the perturbative solution. This led to the following differential equation satisfied by $\Omega(t)$:

$$\dot{\Omega}=\sum_{k=0}^{\infty}\frac{B_k}{k!}\{\Omega^k,\tilde{H}\}\ . \tag{4.1}$$

Here the dot indicates the time derivative, the curly brackets denote a multiple commutator with Ω entering k times:

$$\{\Omega^k,\tilde{H}\}=[\Omega,[\cdots[\Omega,\tilde{H}]\cdots]],\quad \{\Omega^0,\tilde{H}\}=\tilde{H} \tag{4.2}$$

and the B_k's are Bernoulli numbers[20] (in particular, $B_{2m+1}=0$ for $m>0$). Substituting the expansion of Eq. (1.6) into Eq. (4.1) and equating terms of the same order one finds

$$\dot{\Omega}_1=\tilde{H},\quad \dot{\Omega}_n=\sum_{k=1}^{n-1}\frac{B_k}{k!}S_n^{(k)}\quad (n\geq 2)\ , \tag{4.3}$$

where

$$S_n^{(k)}=\sum[\Omega_{i_1},[\cdots[\Omega_{i_k},\tilde{H}]\cdots]] \qquad (i_1+\cdots+i_k=n-1)\ . \tag{4.4}$$

Notice that in the last equation the order of $\tilde{H}$ has been explicitly reckoned, whereas k represents the number of Ω's.

It is easy to see that the newly defined operators $S_n^{(k)}$ can again be calculated recursively. The recurrence relations are now given by

$$\begin{aligned} &S_n^{(k)}=\sum_{m=1}^{n-k}[\Omega_m,S_{n-m}^{(k-1)}],\quad (2\leq k\leq n-1)\ ,\\ &S_n^{(1)}=[\Omega_{n-1},\tilde{H}],\quad S_n^{(n-1)}=\{\Omega_1^{n-1},\tilde{H}\}\ . \end{aligned} \tag{4.5}$$

Other forms [e.g., similar to Eq. (2.6)] seem to be prohibited by the presence of commutators.

This, of course, is not the end of the story, since the final result is reached only after integrating over t. Thus from Eq. (4.3) one obtains

$$\Omega_1=\int_0^t dt'\tilde{H}(t'),\quad \Omega_n=\sum_{k=1}^{n-1}\frac{B_k}{k!}\int_0^t dt'S_n^{(k)}(t')\quad (n\geq 2)\ , \tag{4.6}$$

which is the counterpart of Eq. (3.7). However, in this case the whole recursive scheme must be carried out for some set of intermediate times $0<t_q<t$.

V. DISCUSSION AND CONCLUSIONS

We have shown that the first two methods exposed are based on systems of equations which are indeed inverse to each other. Burum's method gives Ω_n, basically, in terms of P_n and of lower-order Ω_k's, while Salzman's method handles only perturbative contributions. In view of Eqs. (2.1) and (3.3) it is easy to understand that these two methods are completely equivalent. On the other hand, they both clearly emphasize the Magnus expansion as a rearrangement of the perturbation expansion.

Properly speaking, Eqs. (2.5) and (3.6) are generators not for Ω_n but for the difference Ω_n-P_n (incidentally, it is just this difference that ensures that the unitarity property $U^\dagger U=UU^\dagger=1$ is satisfied to each order of the Magnus expansion). Similarly, in the third method, Eq. (4.5) is actually a generator for the time derivative of Ω_n. The chief advantage of these equations stems from the fact that they involve only products of two operators (matrices). This should greatly facilitate numerical and algebraical calculations of higher-order contributions in the case of multistate systems. However, whatever method is employed, some additional time integrations are needed, which requires that provision should be made of intermediate-time results at each order.

ACKNOWLEDGMENTS

One of the authors (J.A.O.) thanks the Division de Physique Théorique de l'Institut de Physique Nucléaire for its hospitality, and the Ministerio de Educación y Ciencia (Spain) for financial support under the program MEC/MRES. The Division de Physique Théorique is a "Unité de Recherche des Universités Paris 11 et Paris 6 Associée au CNRS."

APPENDIX

For the reader's convenience we reproduce below the compact time-ordered expressions of the first four terms in the Magnus expansion as derived by Wilcox:[2]

$$\Omega_1(t)=\int_0^t dt_1\tilde{H}_1\ , \tag{A1}$$

$$\Omega_2(t)=\tfrac{1}{2}\int_0^t dt_1\int_0^{t_1}dt_2[\tilde{H}_1,\tilde{H}_2]\ , \tag{A2}$$

$$\Omega_3(t)=\tfrac{1}{6}\int_0^t dt_1\int_0^{t_1}dt_2\int_0^{t_2}dt_3\{[\tilde{H}_1,[\tilde{H}_2,\tilde{H}_3]]+[[\tilde{H}_1,\tilde{H}_2],\tilde{H}_3]\}\ , \tag{A3}$$

$$\Omega_4(t)=\tfrac{1}{12}\int_0^t dt_1\int_0^{t_1} dt_2\int_0^{t_2} dt_3\int_0^{t_3} dt_4\{[[[\tilde{H}_1,\tilde{H}_2],\tilde{H}_3],\tilde{H}_4]+[\tilde{H}_1,[[\tilde{H}_2,\tilde{H}_3],\tilde{H}_4]] +[\tilde{H}_1,[\tilde{H}_2,[\tilde{H}_3,\tilde{H}_4]]]+[\tilde{H}_2,[\tilde{H}_3,[\tilde{H}_4,\tilde{H}_1]]]\} . \tag{A4}$$

Other equivalent forms are easily worked out by using the Jacobi identity for double commutators. Notice that similar formulas given in Ref. 19, and reproduced in Ref. 21, are flawed by a number of misprints (in particular, the integrand of the fourth-order term is incomplete).

[1]W. Magnus, Commun. Pure Appl. Math. **7**, 649 (1954).
[2]R. M. Wilcox, J. Math. Phys. **8**, 962 (1967).
[3]K. F. Milfeld and R. E. Wyatt, Phys. Rev. A **27**, 72 (1983).
[4]D. Baye and P. H. Heenen, J. Phys. B **6**, 105 (1973); **6**, 1255 (1973).
[5]J. Eichler, Phys. Rev. A **15**, 1856 (1977).
[6]U. Wille, Z. Phys. A **308**, 3 (1982).
[7]H. A. Hyman, Phys. Rev. A **31**, 2142 (1985).
[8]I. Schek, J. Jortner, and M. L. Sage, Chem. Phys. **59**, 11 (1981).
[9]D. W. Robinson, Helv. Phys. Acta **36**, 140 (1963).
[10]W. A. B. Evans, Ann. Phys. **48**, 72 (1968).
[11]J. S. Waugh, J. Magn. Reson. **50**, 30 (1982).
[12]W. A. Cady, J. Chem. Phys. **60**, 3318 (1974).
[13]H. D. Dahmen, B. Scholz, and F. Steiner, Nucl. Phys. B **202**, 365 (1982).
[14]M. M. Maricq, J. Chem. Phys. **85**, 5647 (1987).
[15]W. R. Salzman, Phys. Rev. A **36**, 5074 (1987).
[16]D. P. Burum, Phys. Rev. B **24**, 3684 (1981).
[17]W. R. Salzman, J. Chem. Phys. **82**, 822 (1985); **85**, 4605 (1986).
[18]G. Jolicard and G. D. Billing, Chem. Phys. **104**, 357 (1986).
[19]P. Pechucas and J. C. Light, J. Chem. Phys. **44**, 3897 (1966).
[20]*Handbook of Mathematical Functions*, edited by M. A. Abramowitz and I. A. Stegun (Dover, New York, 1965).
[21]G. Dattoli, J. Gallardo, and A. Torre, J. Math. Phys. **27**, 772 (1986).