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Nonlinear operators and their propagators

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Mathematical physicists are familiar with a large set of tools designed for dealing with linear operators, which are so common in both the classical and quantum theories; but many of those tools are useless with nonlinear equations of motion. In this work a general algebra and calculus is developed for working with nonlinear operators: The basic new tool being the “slash product,” defined by $A(1 + \epsilon B) = A + \epsilon A/B + O(\epsilon^2)$. For a generic time development equation, the propagator is constructed and then there follows the formal version of time dependent perturbation theory, in remarkable similarity to the linear situation. A nonperturbative approximation scheme capable of producing high accuracy computations, previously developed for linear operators, is shown to be applicable as well in the nonlinear domain. A number of auxiliary mathematical properties and examples are given. © 1997 American Institute of Physics. [S0022-2488(97)03301-X]

I. INTRODUCTION

Physicists are familiar with a large set of mathematical tools for dealing with linear operators. This comes mostly from work in quantum theory but also shows up in classical theory. However, when it comes to nonlinear equations of motion, most of those familiar tools are useless. There are a few specific nonlinear equations that have been studied and solved; and with many others one commonly resorts to a forcible “linearization.” In the domain of numerical computations only low order approximation techniques are known for general nonlinear equations.¹

In this paper we develop a general algebra and calculus for nonlinear operators, with the starting definitions given in Sec. II. The basic new tool is the “slash product” of two operators, A/B , defined by $A(1 + \epsilon B) = A + \epsilon A/B + O(\epsilon^2)$. This quantity has a number of interesting properties which are explored in Secs. III and IV. For a generic time development equation, the propagator is constructed in Sec. V and then in Sec. VI there follows the formal version of time dependent perturbation theory, in remarkable similarity to the linear situation. Section VII explores how the further machinery of quantum theory might look if it were not a linear theory. In Sec. VIII a nonperturbative approximation scheme capable of producing high accuracy computations, previously developed for linear operators, is shown to be applicable as well in the nonlinear domain. A number of auxiliary mathematical results are given in four Appendices.

II. GENERAL PROPERTIES

A nonlinear operator A acts on some input quantity ψ transforming it into an output quantity ϕ ,

$$\phi = A\psi. \quad (1)$$

One might use the alternative notation $\phi = A(\psi)$ to emphasize that the operator A acts on ψ like a function and not by mere multiplication, which is the mode of a linear operator; but we shall have other uses for parentheses and would prefer to avoid this confusion.

Operators A, B, C, \dots (I shall use capital letters for operators) can act in sequence, giving us multiplication which is associative but not commutative.

$$ABC\psi = A(B(C(\psi))). \quad (2)$$

Assuming that the quantities ψ, ϕ can be added and multiplied by ordinary numbers (denoted by lower case letters a, b, c, \dots) we have addition of operators which is associative and commutative

$$A = B + C = C + B; \quad (3)$$

and we have scalar multiplication on the left, $A = bC$, which is not the same as Cb . The symbols 1 and 0 play dual roles, as the unit and null operators as well as ordinary numbers.

The distributive law holds on one side,

$$(A + B)C = AC + BC \quad (4)$$

but not on the other side,

$$A(B + C) \neq AB + AC. \quad (5)$$

However, assuming some continuity in the set of operators, we can define a generalized derivative, which will allow us to do some things with expressions of the sort given in (5). In the limit of $\epsilon \rightarrow 0$,

$$A(B + \epsilon C) = AB + \epsilon \{A, B, C\} + O(\epsilon^2). \quad (6)$$

III. THE SLASH PRODUCT

A simpler definition of this generalized derivative is the following:

$$A(1 + \epsilon B) = A + \epsilon A/B + O(\epsilon^2). \quad (7)$$

This new operator A/B —called the “slash product of A and B ”—will be the most useful tool in the analysis that follows. Assuming that the operator B in (6) has an inverse, we can identify

$$\{A, B, C\} = (A/CB^{-1})B. \quad (8)$$

If we use the representation of the operators as functions, as in (2), then we see that $A/B\psi = 1/\epsilon(A(\psi + \epsilon B(\psi)) - A(\psi)) = A'(\psi)B(\psi)$.

A most important property of the slash product is that it is linear in both of its arguments. Linearity in the first argument,

$$(aA + bB)/C = aA/C + bB/C, \quad (9)$$

follows directly from (4) and (7). Scaling in the second argument for real numbers b ,

$$A/bB = bA/B \quad (10)$$

follows from scaling the parameter ϵ in the definition (7). And linearity in the second argument,

$$A/(B + C) = A/B + A/C, \quad (11)$$

can be shown as follows:

$$\begin{aligned}
A(1 + \epsilon B + \epsilon C) &= A + \epsilon A/(B + C) + O(\epsilon^2) = A(1 + \epsilon C)(1 + \epsilon B) + O(\epsilon^2) \\
&= (A + \epsilon A/C)(1 + \epsilon B) + O(\epsilon^2) = A(1 + \epsilon B) + \epsilon A/C(1 + \epsilon B) + O(\epsilon^2) \\
&= A + \epsilon A/B + \epsilon A/C + O(\epsilon^2).
\end{aligned} \tag{12}$$

Note that there is no ambiguity in writing, as in (10) above, bA/B to mean $b(A/B)$. In fact, if L is a linear operator (of which ordinary numbers are a special case) then, $(LA/B) = L(A/B)$ can be written as LA/B . Also, for linear operators L , we note that $L/B = LB$; thus slash products become ordinary products when we have all linear operators. Be aware, however, that A/L is not equal to AL , and in particular $A/1$ is not equal to A , unless A is linear. Considering the null operator 0 , the statement $A0=0$ is a restriction upon the class of nonlinear operators A which we shall study; but the equations $0A=0/A=A/0=0$ are true in any case.

In general I shall write ABC/DEF without parentheses to mean $(ABC)/(DEF)$; but parentheses are required to specify other things, such as $(A/B)C$ or multiple slash products such as $A/(B/C)$ —which is not the same as $(A/B)/C$ —etc. Note, however, that multiple slash products are linear in each one of their factors, regardless of how the parentheses are drawn. In expressions like $1/2$ or $t^n/n!$ which do not involve any operators, the $/$ symbol means ordinary division.

Another important property is found from the following calculation. Here we assume that the operator B has an inverse; and \cdots means $O(\epsilon^2)$.

$$\begin{aligned}
AB(1 + \epsilon C) &= AB + \epsilon(AB)/C + \cdots = A(B(1 + \epsilon C)) = A(B + \epsilon B/C + \cdots) \\
&= A(1 + \epsilon(B/C)B^{-1} + \cdots)B = (A + \epsilon A/C_B + \cdots)B.
\end{aligned} \tag{13}$$

Here, we have introduced the important definition

$$C_B \equiv (B/C)B^{-1}, \tag{14}$$

which is the generalization of a similarity transformation. One readily shows that $(C_B)_D = C_{DB}$; and the new identity for the slash product is,

$$(AB)/C = (A/C_B)B. \tag{15}$$

Although multiple slash products are not associative, I shall use the notation $A/B/C/\cdots/Z$ to mean the particular order $(\cdots((A/B)/C)/\cdots)/Z$. In addition, I shall use a shorthand notation for this multiple slash product of a single operator:

$$A^{\wedge n} \equiv A/A/A/\cdots/A \quad (n \text{ factors } A) \tag{16}$$

where

$$A^{\wedge 1} = A = 1/A \quad \text{and} \quad A^{\wedge 0} = 1 \tag{17}$$

make this consistent with

$$A^{\wedge n+1} = A^{\wedge n}/A. \tag{18}$$

IV. FURTHER PROPERTIES OF /

We can define higher order slash products by continuing the expansion in Eq. (7)

$$A(1 + \epsilon B) = A + \epsilon A/B + (1/2)\epsilon^2 A//B + O(\epsilon^3). \tag{19}$$

As shown in Appendix A, these higher terms may be reduced to multiple applications of the single slash product; for example,

$$A//B = (A/B)/B - A/(B/B). \quad (20)$$

The expression $A//B$ (which vanishes if A is a linear operator) is linear in the first argument A , but is more complicated (quadratic) in the second argument B . The calculation in Appendix A also leads us to the identity,

$$(A/B)/C - A/(B/C) = (A/C)/B - A/(C/B). \quad (21)$$

Suppose that F and G are two operators that depend on some parameter λ and we write $F' = dF/d\lambda$. Now calculate the derivative of the product,

$$\begin{aligned} (FG)' &= 1/\epsilon((F + \epsilon F')(G + \epsilon G') - FG) = 1/\epsilon(FG + \epsilon(F/G'G^{-1})G + \epsilon F'G - FG + O(\epsilon^2)) \\ &= F'G + (F/G'G^{-1})G = \{F'F^{-1} + (G'G^{-1})_F\}FG. \end{aligned} \quad (22)$$

In the special case where F is a linear operator, the $/$ can be dropped and (22) reads like the usual rule for the derivative of a product; but this result is more general. An interesting special case of (22) is when F is taken to be the operator inverse of G

$$G^{-1'} = -G^{-1}/G'G^{-1}. \quad (23)$$

Extending equation (22) we have

$$(FGH)' = \{F'F^{-1} + (G'G^{-1})_F + ((H'H^{-1})_G)_F\}FGH. \quad (22a)$$

Using the identity $(C_B)_{B^{-1}} = C$, one can deduce an inversion formula for the slash product

$$\text{If } A = B/C, \quad \text{then } C = (B^{-1}/AB^{-1})B. \quad (24)$$

V. PROPAGATORS

Problems of interest concern differential equations of the form

$$\frac{d\psi}{dt} = A\psi, \quad (25)$$

where $\psi = \psi(t)$ but we assume for the moment that the nonlinear operator A is independent of t . Solutions of this equation are given in terms of some operator $E(A, t)$, which we call the propagator for A

$$\psi(t) = E(A, t)\psi(0). \quad (26)$$

The propagator should obey the composition law

$$E(A, t_1)E(A, t_2) = E(A, t_1 + t_2) \quad (27)$$

and we have

$$E(A, 0) = 1. \quad (28)$$

There is also a scaling law, implied by the structure of Eq. (25),

$$E(aA, t) = E(A, at). \quad (29)$$

In the special case where A is a linear operator, $E(A, t)$ is just the exponential function of argument tA .

For a simple example, consider the nonlinear operator $A\psi = p\psi^q$. The differential equation (25) is readily solved and we get this formula for the propagator

$$E(A,t)\psi = [\psi^{1-q} + tp(1-q)]^{1/(1-q)}. \quad (30)$$

In what follows we shall assume that a power series expansion exists for the propagator, at least for sufficiently small values of t . The basic operator equation, writing d_t for d/dt , is

$$d_t E(A,t) = AE(A,t) \quad (31)$$

so that the power series starts as $1 + tA + \dots$. To see what the later terms look like, take another derivative of (31). Writing E for $E(A,t)$ and using (22)

$$d_t^2 E = d_t(AE) = (A/(d_t E)E^{-1})E = (A/A)E = A^2 E. \quad (32)$$

Repeating this procedure any number of times, then taking the limit $t=0$, yields the terms in the infinite power series.

$$E(A,t) = \sum t^n/n! A^n. \quad (33)$$

It is interesting to take the derivative of this power series.

$$d_t E(A,t) = \sum n t^{n-1}/n! A^n = \sum t^n/n! A^{n+1} = E(A,t)/A, \quad (34)$$

where we have used the linear property of the slash product. Thus we have the special identity for propagators

$$AE(A,t) = E(A,t)/A, \quad (35)$$

which is not easily verified by multiplying A times the series (33).

Now consider the general case when the operator A is time dependent.

$$d_t \psi(t) = A(t)\psi(t). \quad (36)$$

The propagator must now be given two time variables

$$\psi(t_2) = E(A;t_2, t_1)\psi(t_1), \quad (37)$$

where

$$E(A;t, t) = 1. \quad (38)$$

Taking the derivative of (37) with respect to t_2 yields the equation

$$d/dt_2 E(A;t_2, t_1) = A(t_2)E(A;t_2, t_1) \quad (39)$$

while taking the derivative of (37) with respect to t_1 yields

$$d/dt_1 E(A;t_2, t_1) = -E(A;t_2, t_1)/A(t_1). \quad (40)$$

With these two equations, one can now prove the general group property

$$E(A;t_3, t_2)E(A;t_2, t_1) = E(A;t_3, t_1) \quad (41)$$

as follows: Take the derivative of the expression on the left hand side of (41) with respect to t_2 and, using both (39) and (40), show that the result is 0; then, since this product is independent of the value of t_2 , one can set $t_2 = t_1$, and the right hand side of (41) is obtained.

The power series solution for the propagator is easily constructed by using Eq. (40)

$$E(A; t, t_0) = \sum \int dt_1 \cdots \int dt_n \Theta A(t_n)/A(t_{n-1})/\cdots/A(t_2)/A(t_1), \quad (42)$$

where the symbol Θ selects the region of the n -dimensional integration space for which

$$t_0 \leq t_1 \leq t_2 \leq \cdots \leq t_{n-1} \leq t_n \leq t \quad (\text{assuming that } t_0 \leq t). \quad (43)$$

This result reverts to (33) when A is independent of the time. One might give this series (42) the symbolic name $T/\exp(\int^t dt' A(t'))$, where $T/$ is read, "time ordered slash products."

VI. PERTURBATION THEORY

We consider the equation

$$\frac{d\psi}{dt} = A\psi + B\psi; \quad (44)$$

and assuming we know the propagator $E(A; t_2, t_1)$ we want to study the full propagator $E(A+B; t_2, t_1)$, expanded in a power series in the small operator B . We start with the decomposition

$$E(A+B; t_2, t_1) = U(t_2, t_1)E(A; t_2, t_1) \quad (45)$$

introducing the operator U ; and we take the time derivative d/dt_1 and use (40), assuming A is time-independent, to arrive finally at

$$d/dt_1 U(t_2, t_1) = -U(t_2, t_1)/B_E(t_2, t_1) \quad (46)$$

where I use the shorthand: $B_E(t_2, t_1) = (E(A; t_2, t_1)/B(t_1))E^{-1}(A; t_2, t_1)$. This would be called the "perturbation operator in the interaction representation."

Equation (46) is of the form of (40) and so we can write the power series analog of (42) to obtain the result

$$U(t, t_0) = \sum \int dt_1 \cdots \int dt_n \Theta B_E(t, t_n)/B_E(t, t_{n-1})/\cdots/B_E(t, t_2)/B_E(t, t_1), \quad (47)$$

Further manipulation of the terms in (47) allows one to rewrite this result as follows:

$$\begin{aligned} E(A+B; t, t_0) = & \sum \int dt_1 \cdots \int dt_n \Theta ((\cdots((E(A; t, t_n)/B(t_n)) \\ & \times E(A; t_n, t_{n-1})/B(t_{n-1}))E(A; t_{n-1}, t_{n-2})/\cdots)E(A; t_2, t_1)/B(t_1))E(A; t_1, t_0) \end{aligned} \quad (48)$$

which provides the familiar interpretation of a sequence of interactions (B) connected by propagators (E , derived from A).

One more thing of interest is a power series for B_E , when both A and B are time-independent

$$B_E = (E/B)E^{-1} = \sum t^n/n! S_n. \quad (49)$$

A direct computation, similar to those done earlier, yields the result

$$d_t B_E = A/B_E - B_E/A; \quad (50)$$

and thus, using once more the linear properties of the slash product,

$$S_n = A/S_{n-1} - S_{n-1}/A \equiv [A/S_{n-1}] \quad (51)$$

defining the ‘‘slash commutator.’’ The series for B_E then has the familiar form with repeated commutators

$$S_0 = B,$$

$$S_1 = [A/B] = A/B - B/A,$$

$$S_2 = [A/[A/B]] = A/(A/B) - A/(B/A) - (A/B)/A + (B/A)/A. \quad (52)$$

Using the identity (21) one can rewrite the last line of (52) as $(A/A)/B - 2(A/B)/A + (B/A)/A$. One also has a Jacobi identity for the general $[A/[B/C]]$.

VII. FURTHER MACHINERY OF QUANTUM MECHANICS

Suppose we consider a Schrodinger equation

$$i d_t \Psi = H \Psi, \quad (53)$$

where H is a general nonlinear operator. The wave function Ψ depends on the time t as well as the coordinate variables x and perhaps other variables. Equation (53) will have a propagator $E = E(-iH, t)$, which we use (formally) to construct the Heisenberg picture, in which the coordinates and other variables become time dependent. If F is any function or operator made up from these variables in the Schrodinger picture, then we construct the Heisenberg representation of this F as follows:

$$F_E = (E/F)E^{-1} \quad (54)$$

and calculate

$$d_t F_E = -iH/F_E + F_E/iH = [-iH/F_E]. \quad (55)$$

If U is some symmetry operator, with the infinitesimal form $U = 1 + \epsilon S$, then its application to some general operator A can be considered in two forms, each of which has the group property:

$$U A U^{-1} = A + \epsilon(SA - A/S) + \dots \quad (56)$$

or

$$(U/A)U^{-1} = A + \epsilon[S/A] + \dots. \quad (57)$$

For more, see Appendix D.

In order to get stationary states, one needs to put some kind of restriction upon the operator H : It should be time independent and Hermitian in the linear case. So much of the usual machinery of quantum mechanics depends upon this linearity, we should not expect too much in the nonlinear case; but several results can be carried over.

The first thing we require, even for a nonstationary state, is conservation of total probability. We shall keep the usual definition that $\Psi^*\Psi$ is the probability density for this complex time-dependent wave function, which is defined on some set of coordinates we shall refer to simply as x . We require,

$$\int \Psi^*\Psi \, dx = 1 \quad (58)$$

and calculate

$$i d_t \int \Psi^*\Psi \, dx = 0 = \int \Psi^*(H\Psi) \, dx - \int (H\Psi)^*\Psi \, dx. \quad (59)$$

This is our condition on H for any stationary state.

For example, the following nonlinear Hamiltonian satisfies this condition:

$$H = H_L + A, \quad \text{and} \quad A\Psi = f(\Psi^*\Psi)\Psi, \quad (60)$$

where H_L is a linear operator, Hermitian in the usual sense, and f is a real function of its argument. With this model (60) put into the time-dependent equation (53), one can separate out the time dependence in the usual manner, $\Psi = \exp(-i\omega t)\psi$, and get the time-independent (non-linear) Schrodinger equation,

$$H_L\psi + f(\psi^*\psi)\psi = \omega\psi. \quad (61)$$

If we add the normalization condition $\int \psi^*\psi \, dx = 1$, then this is an eigenvalue problem—although not a linear one.

For example, the equation

$$-\frac{d^2\psi}{dx^2} + a\psi(\psi^*\psi)^q = \omega\psi \quad (62)$$

has an eigenfunction of the form $\psi = c(\operatorname{sech}(bx))^p$. Actually, a family of such solutions can be gotten from this one by translation and boosting; a state moving with velocity v has frequency $\omega + 1/4v^2$, thus giving what looks like a “rest energy” as the result of an eigenvalue problem.

Variational principles may also be constructed for equations like (61).

$$J[\psi, \psi^*] = \int dx \{ \psi^* H_L \psi + g(\psi^*\psi) \} - \lambda \left\{ \int dx \psi^* \psi - 1 \right\} \quad (63)$$

is stationary about solutions of (61), if $f = g'$ and $\lambda = \omega$. Note that the stationary value of J is not ω .

VIII. THE PRODUCT APPROXIMATION FOR A COMPLICATED PROPAGATOR

A typical problem of interest looks like the following differential equation, which involves two operators, linear or nonlinear, but assumed time independent

$$d_t \psi = A\psi + B\psi = (A + B)\psi. \quad (64)$$

Neither A nor B is assumed to be small enough to allow a perturbation solution; but we do assume that we can construct and use the separate propagators $E(A,t)$ and $E(B,t)$. Our objective is to construct accurate approximations to the propagator $E(A+B, \delta)$, where δ is a small but not infinitesimal time interval. We shall start by looking at the first few terms of the power series expansion

$$\begin{aligned} E(A+B, \delta) &= 1 + \delta(A+B) + (1/2) \delta^2(A+B)/(A+B) + O(\delta^3) \\ &= 1 + \delta A + \delta B + (1/2) \delta^2(A/A + A/B + B/A + B/B) + O(\delta^3). \end{aligned} \quad (65)$$

A first step, as is commonly done with linear operators,² is to construct a symmetric product of the separate propagators $E(A, \delta)$ and $E(B, \delta)$

$$R(A, B, \delta) = E(A, \delta/2)E(B, \delta)E(A, \delta/2). \quad (66)$$

Using the expansions and the computational rules given above, we find that

$$R(A, B, \delta) = E(A+B, \delta) + O(\delta^3). \quad (67)$$

This is our first major result: Formula (66) uses three steps with the individual propagators to approximate the complete propagator to second order accuracy.

The best way to study, and then remove, the higher order differences between the exact and approximate propagators is not to continue with the power series expansions of the exact propagators E , but rather to represent the quantity R as the exact propagator for some new operator X

$$R(A, B, \delta) = E(X, \delta), \quad (68)$$

where X depends on A , B and δ ; and there will be an expansion,

$$X(A, B, \delta) = X_1(A, B) + \delta X_2(A, B) + \delta^2 X_3(A, B) + \dots \quad (69)$$

which can be determined, term by term, from any given series expansion for R . What follows is a generalization of results previously derived for linear operators by M. Suzuki.³

Making use of the results found in Appendix B, one can readily calculate: $X_2=0$ and $X_3 = -(1/24)[(A+2B)/[A/B]]$. But we do not really need to carry out such calculations, as the following simple arguments suffice.

Clearly $X_1(A, B) = A+B$; and each term X_m will first appear in the power series for R at order δ^m . The symmetric construction of R guarantees the exact relation

$$R(A, B, \delta)R(A, B, -\delta) = 1 \quad (70)$$

from which we infer that

$$X(A, B, -\delta) = X(A, B, \delta). \quad (71)$$

Thus half of the terms in (69) disappear (we already knew this for $m=2$)

$$X = X_1 + \delta^2 X_3 + \delta^4 X_5 + \dots \quad (72)$$

Now we proceed to build on these results to get higher order accuracy, following the general scheme used previously for linear operators. First, the given differential equation may have any number of operators.

$$d_t \psi = \sum \psi, \quad \sum = A+B+C+\dots+Z. \quad (73)$$

The technique given in the standard literature for computing with such a general problem is good only to first order in the time interval δ .⁴ Our second order approximation for the propagator $E(\Sigma, \delta)$ is

$$R(\delta) = E(A, \delta/2)E(B, \delta/2) \cdots E(Z, \delta) \cdots E(B, \delta/2)E(A, \delta/2) \quad (74)$$

which we can represent as $E(\Sigma + \delta^2 X_3 + \delta^4 X_5 + \dots, \delta)$.

Now we seek to eliminate the X_3 terms by constructing the product

$$\Omega_3(\delta) = R(\beta\delta)R(\gamma\delta)R(\beta\delta) \quad (75)$$

with certain values of the numbers β and γ . For this analysis we need to expand the propagator (where A and B are any operators)

$$\begin{aligned} E(A + \epsilon B, \delta) &= E(A, \delta) + \epsilon \delta B + O(\epsilon^2, \epsilon \delta^2) \\ &= (1 + \epsilon \delta B + O(\epsilon^2, \epsilon \delta^2))E(A, \delta) \\ &= E(A, \delta)(1 + \epsilon \delta B + O(\epsilon^2, \epsilon \delta^2)). \end{aligned} \quad (76)$$

Note here that we are expanding in both ϵ and δ independently. That is, we are extracting not the complete derivative of $E(A + \epsilon B, \delta)$, but only the leading term of that derivative expanded in a power series in δ .

Now we are ready to calculate the product of two ‘close’ propagators

$$\begin{aligned} E(A + \epsilon_1 B, \delta_1)E(A + \epsilon_2 B, \delta_2) \\ &= E(A, \delta_1)E(A, \delta_2)(1 + \epsilon_1 \delta_1 B + \cdots)(1 + \epsilon_2 \delta_2 B + \cdots) \\ &= E(A, \delta_1 + \delta_2)(1 + (\epsilon_1 \delta_1 + \epsilon_2 \delta_2)B + \cdots) \end{aligned} \quad (77)$$

where \cdots means next higher order terms in δ as well as ϵ .

Proceeding in this manner we calculate

$$\Omega_3(\delta) = E(\Sigma, (2\beta + \gamma)\delta)(1 + (2\beta^3 + \gamma^3)\delta^3 X_3 + O(\delta^4)). \quad (78)$$

Finally, we fix the free parameters with the conditions

$$2\beta + \gamma = 1 \quad \text{and} \quad 2\beta^3 + \gamma^3 = 0 \quad (79)$$

and we have the fourth order accurate approximation:

$$\Omega_3(\delta) = E(\Sigma + O(\delta^4), \delta). \quad (80)$$

Again, the symmetric construction gives us $\Omega_3(\delta)\Omega_3(-\delta) = 1$ and makes the error go down not one but two orders in δ . I have programmed numerical computations of the time-dependent nonlinear Schrödinger equation (in one space dimension) and found great improvements in accuracy and efficiency by using this fourth order method.

We can now proceed systematically to eliminate the higher order error, two orders in δ at each step. Thus to sixth order accuracy,

$$\Omega_9(\delta) = \Omega_3(\beta\delta)\Omega_3(\gamma\delta)\Omega_3(\beta\delta) = E(\Sigma + O(\delta^6), \delta), \quad (81)$$

where these new coefficients are determined by

$$2\beta + \gamma = 1 \quad \text{and} \quad 2\beta^5 + \gamma^5 = 0. \quad (82)$$

These results are identical in form with those previously derived for linear operators.³

The foregoing analysis was based upon the assumption that the separate operators A, B, \dots , allowed us to obtain and use their exact individual propagators $E(A, \delta)$, etc. Looking back, we see that we can work with considerably less. The key is in the construction of $R(\delta)$, Eq. (74), and its subsequent use, Eq. (75) *et seq.*

There are really only two simple requirements:

$$R(\delta) = 1 + \delta \Sigma + O(\delta^2) \quad \text{and} \quad R(\delta)R(-\delta) = 1; \quad (83)$$

once these two requirements are met, all the higher order accuracy of the Ω_s will follow.

One simple approximation for any propagator is

$$E(A, \delta) \approx (1 - (\delta/2)A)^{-1}(1 + (\delta/2)A) \quad (84)$$

and this may be substituted in (74) without loss of accuracy. One can go even farther. For example, with two operators, one may use

$$R(A, B, \delta) = (1 - (\delta/2)A)^{-1}E(B, \delta)(1 + (\delta/2)A) \quad (85)$$

or

$$R(A, B, \delta) = (1 - (\delta/2)A)^{-1}(1 - (\delta/2)B)^{-1}(1 + (\delta/2)B)(1 + (\delta/2)A). \quad (86)$$

APPENDIX A: HIGHER ORDER SLASH PRODUCTS

Here, we shall look at the higher terms in the expansion

$$A(1 + \epsilon B) = A + \epsilon A/B + (1/2)\epsilon^2 A//B + (1/6)\epsilon^3 A///B + \dots \quad (A1)$$

Start by expanding the following product in one way.

$$\begin{aligned} A(1 + \epsilon B)(1 + \epsilon C) &= A\{1 + \epsilon C + \epsilon B(1 + \epsilon C)\} \\ &= A(1 + \epsilon C + \epsilon B + \epsilon^2 B/C + (1/2)\epsilon^3 B//C + \dots) \\ &= A + \epsilon A/(C + B + \epsilon B/C + (1/2)\epsilon^2 B//C) \\ &\quad + (1/2)\epsilon^2 A//(C + B + \epsilon B/C) + (1/6)\epsilon^3 A///(C + B) + \dots \quad (A2) \end{aligned}$$

And now expand it another way.

$$\begin{aligned} A(1 + \epsilon B)(1 + \epsilon C) &= \{A + \epsilon A/B + (1/2)\epsilon^2 A//B + (1/6)\epsilon^3 A///B + \dots\}(1 + \epsilon C) \\ &= A + \epsilon A/C + (1/2)\epsilon^2 A//C + (1/6)\epsilon^3 A///C + \epsilon A/B \\ &\quad + (1/2)\epsilon^2 A//B + (1/6)\epsilon^3 A///B + \epsilon^2(A/B)/C + (1/2)\epsilon^3(A/B)//C \\ &\quad + (1/2)\epsilon^3(A//B)/C + \dots \quad (A3) \end{aligned}$$

Next we compare expressions order by order in powers of ϵ . The zeroth and first order terms are familiar. In second order we find

$$A/(B/C) + (1/2)A//(B + C) = (1/2)A//C + (1/2)A//B + (A/B)/C. \quad (A4)$$

Setting $C = xB$, where x is a variable number

$$xA/(B/B) + (1/2)(1 + x)^2 A//B = (1/2)x^2 A//B + (1/2)A//B + x(A/B)/B. \quad (A5)$$

Then, choosing $x = -1$, we get the first result

$$A//B = (A/B)/B - A/(B/B), \quad (\text{A6})$$

and also, substituting back in (A4), we get the identity

$$(A/B)/C - A/(B/C) = (A/C)/B - A/(C/B). \quad (\text{A7})$$

Now, going on to third order terms in a similar fashion, we find

$$\begin{aligned} & A/(B//C) + (A/(C+B))/(B/C) + (A/(B/C))/(C+B) \\ & - A/((C+B)/(B/C)) - A/((B/C)/(C+B)) + (1/3)A///(C+B) \\ & = (1/3)A///C + (1/3)A///B + (A/B)//C + (A//B)/C. \end{aligned} \quad (\text{A8})$$

Again, setting $C = xB$, we get

$$\begin{aligned} & x^2 A/(B//B) + x(1+x)(A/B)/(B/B) + x(1+x)(A/(B/B))/B - x(1+x)A/(B/(B/B)) \\ & - x(1+x)A/((B/B)/B) + (1/3)(1+x)^3 A///B \\ & = (1/3)x^3 A///B + (1/3)A///B + x^2(A/B)//B + x(A//B)/B. \end{aligned} \quad (\text{A9})$$

Choosing $x = -1$, yields the identity (not really new)

$$A/(B//B) = (A/B)//B - (A//B)/B. \quad (\text{A10})$$

And substituting this back in the previous equation finally yields

$$\begin{aligned} A///B &= A/(B/(B/B)) + A/((B/B)/B) + ((A/B)/B)/B - 2(A/(B/B))/B - (A/B)/(B/B) \\ &= ((A/B)/B)/B + 2A/((B/B)/B) - 3(A/(B/B))/B. \end{aligned} \quad (\text{A11})$$

If we use the representation of the operators as functions, then, starting from $A/B\psi = A'(\psi)B(\psi)$, we find

$$A//B\psi = A''(\psi)B(\psi)B(\psi), \quad (\text{A12})$$

$$A///B\psi = A'''(\psi)B(\psi)B(\psi)B(\psi). \quad (\text{A13})$$

APPENDIX B: FORMULAS WITH THE EXPONENTIAL

If $X(t)$ is a linear operator depending on a parameter t , then an important formula is this, involving the t -derivative of the exponential function of X

$$e^{-X} d_t e^X = \int_0^1 ds e^{-sX} (d_t X) e^{sX}. \quad (\text{B1})$$

Here, we shall derive the analogous formula for a general nonlinear operator $X = X(t)$ and our nonlinear version of the exponential function,

$$E(X) = 1 + X + (1/2)X/X + (1/6)X/X/X + \dots = \sum_n 1/n!(X)^{n-1}X, \quad (\text{B2})$$

where I use the convention, noted after Eq. (15) that the repeated slash products are grouped with the left-hand factors most interior.

Take the t derivative of (B2), which is easy because of the linear properties of the slash products

$$d_t E(X) = \sum_n \sum_{m < n} 1/n! (X/) ^m (d_t X) (/X)^{n-m-1} \quad (\text{B3})$$

$$= \int_0^1 ds \sum_n \sum_m s^m / m! (1-s)^n / n! (X/) ^m (d_t X) (/X)^n. \quad (\text{B4})$$

Now the infinite sum over m can be carried out because the terms $(X/) ^m$ sit at the interior of all the multiple slash products

$$d_t E(X) = \int_0^1 ds \sum_n (1-s)^n / n! E(sX) (/d_t X) (/X)^n. \quad (\text{B5})$$

In order to collapse the sum over n , we shall need another general formula

$$\sum_n 1/n! B (/A)^n = B E(A). \quad (\text{B6})$$

This may be proved by replacing A by tA and then taking the derivative with respect to t . For the special case $B=A$, this is equation (35).

Thus we have our result, generalizing (B1)

$$d_t E(X) = \int_0^1 ds (E(sX) (/d_t X)) E(-sX) E(X). \quad (\text{B7})$$

And, following the results given after equation (49), we can write

$$(d_t E(X)) E(-X) = \sum_n 1/(n+1)! ([X/] ^n (d_t X))^n \quad (\text{B8})$$

in terms of the repeated slash commutators.

Several useful results may be obtained from the above formulas. First, we can show the generalization of the famous Baker–Campbell–Hausdorff theorem for the product of exponentials of operators

$$E(tA) E(tB) = E(X(t)) \quad (\text{B9})$$

with $X(t) = tX_1 + t^2X_2 + t^3X_3 + \dots$ and X_1 obviously $= A + B$. Taking the t derivative of Eq. (B9), using (22) and (49)–(51) for the left hand side and using (B8) for the right hand side we can equate coefficients of each power of t . Then we see that each of the higher order X 's is expressed in terms of slash commutators built up from the operators A and B . When we let the operators be linear, then the slash-commutators become ordinary commutators and $E(A)$ becomes the ordinary exponential. Thus, the algebraic structure of this theorem is identical in the case of nonlinear operators to what it is for linear operators. We find

$$X_1 = A + B; \quad X_2 = 1/2[A/B]; \quad X_3 = 1/12[(A-B)/[A/B]]; \quad \text{etc.} \quad (\text{B10})$$

And from this it follows that, if $[A/B]=0$, then

$$E(A) E(B) = E(A+B) = E(B) E(A).$$

A second result is obtained by considering the symmetric product,

$$W(t) = E(tA)E(tB)E(tA) = E(X(t)). \quad (\text{B11})$$

Since $W(-t)W(t) = 1$, we conclude that

$$X(t) = tX_1 + t^3X_3 + t^5X_5 + \dots \quad (\text{B12})$$

To determine the X 's we again calculate the t derivative of W , using now Eq. (22a), and we get,

$$(d_t W(t))W(-t) = 2A + B - t^2/2[(A+B)/[A/B]] + \dots \quad (\text{B13})$$

Then we again use (B8) and, comparing terms, find the results

$$X_1 = 2A + B \quad \text{and} \quad X_3 = -1/6[(A+B)/[A/B]]. \quad (\text{B14})$$

A third new result follows from Eq. (B6)

$$BE(A) = E(A_B)B, \quad (\text{B15})$$

which I leave for the reader to verify. If one replaces the operator B by the operator $E(B)$, then one has

$$E(B)E(A)E(B)^{-1} = E(A'), \quad (\text{B16})$$

where

$$A' = A_{E(B)} = (E(B)/A)E(B)^{-1} = \sum_n 1/n!([B/A]^n A)^n. \quad (\text{B17})$$

This reads as the generalized relation between elements of a Lie Group and the corresponding Lie algebra. The exponential e^A of a linear operator is replaced by $E(A)$ for the nonlinear operator; and the usual commutator used in the Lie algebra is replaced by the slash commutator.

An alternative representation for $E(X)$ is the limit, N going to infinity, of $(1 + 1/N X)^N$; and some previous results are readily derived from this.

While many of the above relations involving $E(A)$ could be called trivial in the case of linear operators, this author finds it remarkable that they hold true in the case of general nonlinear operators.

APPENDIX C: SOME OTHER INFINITE SERIES

Here, we shall look at some other infinite series of operators. First, let's find the expansion for the operator

$$V = V(t) = (1 - tA)^{-1} = \sum t^n V_n(A). \quad (\text{C1})$$

Taking the derivative d/dt and using equation (23) we find

$$d_t V = V/A V = (1/t)V/(V-1) = \sum nt^{n-1}V_n. \quad (\text{C2})$$

Substituting (C1) into (C2) and equating like powers of t , we find the relation

$$V_n = 1/(n-1) \sum_{0 < m < n} V_m / V_{n-m}. \quad (\text{C3})$$

Starting with $V_0=1$ and $V_1=A$, we thus find

$$\begin{aligned} V_2 &= A/A, & V_3 &= 1/2(A/A)/A + 1/2A/(A/A), \\ V_4 &= (1/3)\{V_1/V_3 + V_2/V_2 + V_3/V_1\}, \text{etc.} \end{aligned} \quad (\text{C4})$$

The general term $V_n(A)$ is a linear combination of all the distinct ways of writing the multiple slash products of n factors A . To verify this last statement, note that Eq. (C3) provides the necessary step in the proof by induction. The number of such terms in each V_n is equal to

$$2(-4)^{n-1}(1/2)!/[n!(1/2-n)!].$$

The above result can be used in connection with the general equation (A1),

$$A(1+tB) = \sum t^n/n! A^n B, \quad (\text{C5})$$

where $A^0 B = A$, $A^1 B = A/B$, $A^2 B = A//B$, etc. Take the t -derivative of Eq. (C5) and get:

$$\begin{aligned} \sum [t^{n-1}/(n-1)!] A^n B &= (1/t) \{A/[1-(1+tB)^{-1}]\} (1+tB) \\ &= -(1/t) \left\{ \sum_{m>0} (-t)^m A/V_m(B) \right\} (1+tB). \end{aligned} \quad (\text{C6})$$

Using (C5) once again, and equating like powers of t , we find the result

$$A^n B = - \sum_{m>0} [(n-1)!(-1)^m/(n-m)!] (A/V_m(B))^{n-m} B. \quad (\text{C7})$$

With this we can recursively derive former results, (A6) and (A11), and go on to higher orders, for example,

$$A///B = -6A/V_4 + 6(A/V_3)/B - 3(A/V_2)//B + (A/V_1)///B. \quad (\text{C8})$$

For another exercise, consider the infinite series

$$G(A,p) = \sum 1/p^{n+1} A^n. \quad (\text{C9})$$

If we were dealing with linear operators, this would be the same as the first series (C1), but in general it is different. This series $G(A,p)$ would arise, for example, if one took the Laplace transform of the propagator $E(A,t)$ given by Eq. (33). One can readily derive the algebraic identity,

$$pG(A,p) - G(A,p)/A = 1. \quad (\text{C10})$$

This is not something one can readily “solve” for G ; however, this equation is immediately amenable to perturbation theory. If we replace A by $A + \lambda B$, where λ is a small parameter, and we expand

$$G(A + \lambda B, p) = \sum \lambda^n G_n,$$

then we get the relations

$$pG_0 - G_0/A = 1, \quad pG_n - G_n/A = G_{n-1}/B. \quad (C11)$$

Still another variation involves a quantity, denoted by $A^{\sim n}$, which is the sum of all distinct ways of writing the multiple slash products of n factors A . This is similar to the quantity $V_n(A)$ considered above, but with all numerical coefficients equal to 1. Starting with $A^{\sim 1} = A$, we have the recursion formula

$$A^{\sim n} = \sum_{0 < m < n} A^{\sim m} / A^{\sim n-m}. \quad (C12)$$

Consider now the infinite sum

$$Y = \sum_{n > 0} A^{\sim n}. \quad (C13)$$

This satisfies the equation,

$$Y/Y = Y - A \quad (C14)$$

so we have found one solution to the general ‘‘quadratic equation’’ involving nonlinear operators and slash products. The other solution (which does not go to zero when A vanishes) is more complicated; it is not equal to $1 - Y$.

APPENDIX D: SYMMETRY OPERATORS

This concerns symmetry and invariance in the dynamical nonlinear equations. Let U be some operator that produces a transformation of the coordinates or the functions ψ

$$\psi' = U\psi, \quad (D1)$$

where we have an original equation of motion

$$d_t \psi = A\psi. \quad (D2)$$

Let us calculate

$$d_t \psi' = (1/\epsilon) \{ U(\psi + \epsilon d_t \psi) - U\psi \} = (1/\epsilon) \{ U(1 + \epsilon A)\psi - U\psi \} = (U/A)\psi = (U/A)U^{-1}\psi'. \quad (D3)$$

Thus in order for U to be called a symmetry operation the equation for the transformed function ψ' should be identical in form to the original equation for ψ . That is, we require the dynamical operator A to obey the invariance equation

$$(U/A)U^{-1} = A. \quad (D4)$$

If U is a linear operator, this looks like the familiar rule (without the slash) but in general this is different.

Suppose the dynamical equation has not just one operator A but a sum of operators, say $A + B$, each of which individually satisfies the requirement (D4). One can then readily prove that $(U/(A+B))U^{-1} = A + B$. But note that this would not be so without the presence of the slash symbol, unless U is a linear operator.

¹W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd ed. (Cambridge University Press, Cambridge, 1992), Chap. 19.

²See, for example, Paul DeVries, *A First Course in Computational Physics* (Wiley, New York, 1994), "The Pseudo-Spectral Method," p. 380.

³M. Suzuki, *Phys. Lett. A* **146**, 319 (1990); see also Z. Tsuboi and M. Suzuki, *Int. J. Mod. Phys. B* **9**, 3241 (1995), and other references given in these papers.

⁴Reference 1, p. 856, "Operator Splitting Methods Generally," equations (19.3.20).