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Explicit formulae for the powers of a Schrödinger-like ordinary differential operator

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Abstract. We call $L = \frac{d^r}{dx^r} + u$ a Schrödinger-like differential operator and derive some explicit formulae for the powers or iterations L^n ($n = 1, 2, \dots$) of it.

1. Introduction

It is desirable for several purposes to have an explicit formula for the powers or iterations $L^n = LL \dots L$ (n times) of an ordinary linear differential operator of the simple form

$$L = D^r + u \quad (1)$$

where $D = \frac{d}{dx}$ and $u = u(x)$ is a function. There is one independent variable x , while the number N of dependent variables is arbitrary. Thus, we assume $u = u(x)$ to be $N \times N$ matrix valued. The scalar case is included with $N = 1$. For some low values of r such operators have many mathematical and physical applications. The case $r = 1$ is important since every linear (autonomous) evolution equation can be brought into the form

$$(D + u)y = f. \quad (2)$$

The case $r = 2$ concerns the time-independent one-dimensional Schrödinger operator

$$L = D^2 + u. \quad (3)$$

There is an abundance of applications and ramifications of the latter. In particular, let us mention the relation, via the inverse scattering method, to the Korteweg–de Vries (KdV) equation

$$u_t = 6uu_x + u_{xxx} \quad (4)$$

or, more generally, to the KdV hierarchy of solitonic partial differential equations

$$u_t = \frac{\partial}{\partial x} G_n[u]. \quad (5)$$

The latter admits the Lax representation [1, 2]

$$L_t \equiv [A_n, L] \quad (6)$$

where L is the one-dimensional Schrödinger operator (3) and A_n is a linear differential operator of the order $2n + 1$, the coefficients of which are differential polynomials in u . In particular, we have for $n = 1$

$$A_1 = 4D^3 + 3uD + 3Du \quad (7)$$

and (6) becomes the KdV equation (4).

Since equation (1) generalizes the one-dimensional Schrödinger operator (3), we propose to call it a *Schrödinger-like differential operator* and $u = u(x)$ the *potential*. For $r = 4$ there are also physical applications, for example, in the theory of elasticity. It is a challenge, from a mathematical point of view, to construct an explicit formula for L^n for general r , that is an expression for the coefficients of the linear differential operator L^n . This is what we shall do in this paper. Our investigation is partly inspired by Torriani's paper [3].

2. An explicit formula for L^n

Let us start with some general formulae for the powers of the sum of two linear operators.

Proposition 1. Let $A : V \rightarrow V, B : V \rightarrow V$ be two linear operators acting on a vector space V . There holds

$$(A + B)^n = \sum_{p=0}^n \sum_{n_0, n_1, \dots, n_p} A^{n_0} B A^{n_1} B A^{n_2} \dots B A^{n_p} \quad (8)$$

where the inner sum runs through all integers $n_0 \geq 0, n_1 \geq 0, \dots, n_p \geq 0$ such that $n_0 + n_1 + \dots + n_p = n - p$. For $p = 0$ the inner sum equals, by definition, the single term A^n .

Proof. There is a combinatorial argument behind the above, but we prefer to use a more transparent proof by means of mathematical induction. Let us set $L = A + B$. A simple induction shows

$$L^n = A^n + \sum_{m=1}^n L^{m-1} B A^{n-m}.$$

Initially we take this formula and then insert the following into it

$$L^{m-1} = A^{m-1} + \sum_{m_1=1}^{m-1} L^{m_1-1} B A^{m-1-m_1}.$$

Then into the latter formula we insert

$$L^{m_1-1} = A^{m_1-1} + \sum_{m_2=1}^{m_1-1} L^{m_2-1} B A^{m_1-1-m_2}$$

and so on. In the p th step, we have to treat

$$\sum_{m_0=1}^n \sum_{m_1=1}^{m_0-1} \dots \sum_{m_p=1}^{m_{p-1}-1} L^{m_p-1} B A^{m_{p-1}-1-m_p} B \dots B A^{n-m_0}$$

in order to reduce the powers of L . Owing to the condition

$$1 \leq m_p < m_{p-1} < \dots < m < m_0 \leq n$$

the procedure stops at $p = n - 1$ where

$$m_{n-1} = 1 \quad m_{n-2} = 2, \dots, m_0 = n$$

and we omit the powers of L . Finally, the index transformation

$$n_0 = m_{p-1} \quad n_1 = m_{p-1} - 1 - m_p \quad n_2 = m_{p-2} - 1 - m_{p-1}, \dots, n_p = n - m_0$$

gives the result. \square

Next we apply our formula to $L = A + B \equiv D^r + u$. Multiplication by a function u is notationally identified with u .

Proposition 2. The powers of a Schrödinger-like operator $L = D^r + u$ are given by

$$L^n y = y_{rn} + \sum_{p=1}^n \sum_{n_0, n_1, \dots, n_p} D^{rn_0} (u D^{rn_1} (u D^{rn_2} \dots (u y_{rn_p}))) \quad (9)$$

where the inner sum runs through all integers $n_0 \geq 0, n_1 \geq 0, \dots, n_p \geq 0$ such that $n_0 + n_1 + \dots + n_p = n - p$.

Proof. Insert $A = D^r, B = u$ into (8). □

We now arrive at our main result. We abbreviate $u_k := D^k u$ for $k = 1, 2, \dots, u_0 := u$.

Theorem 1. The n th power of an r th-order Schrödinger-like operator $L = D^r + u$ is given by

$$L^n y = y_{rn} + \sum_{p=1}^n \sum_{k_0, k_1, \dots, k_p} C_{k_1 k_2 \dots k_p} u_{k_1} u_{k_2} \dots u_{k_p} y_{k_0} \quad (10)$$

where the inner sum runs through all integers k_0, k_1, \dots, k_p such that $k_0, k_1, \dots, k_p \geq 0, k_0 + k_1 + \dots + k_p = r(n - p)$, and where the coefficients are equal to

$$C_{k_1, k_2, \dots, k_p} = \sum_{m_0, m_1, \dots, m_p} \binom{rm_0}{k_1} \binom{rm_1 - k_1}{k_2} \binom{rm_2 - k_1 - k_2}{k_3} \dots \binom{rm_p - k_1 - \dots - k_{p-1}}{k_p}. \quad (11)$$

Here the sum runs through all integers m_0, m_1, \dots, m_p such that $0 \leq m_0 \leq m_1 \leq \dots \leq m_p = n - p$.

Proof. We apply the iterated Leibniz rule to (9). Namely in the first step we insert

$$D^{rn_0} (u Z_1) = \sum_{k_1 \geq 0} \binom{rn_0}{k_1} u_{k_1} D^{rn_0 - k_1} Z_1$$

and in the second step we set

$$D^{rn_0 - k_1} Z_1 = D^{r(n_0 + n_1) - k_1} (u Z_2) = \sum_{k_2 \geq 0} \binom{r(n_0 + n_1) - k_1}{k_2} D^{r(n_0 + n_1) - k_1 - k_2} Z_2$$

with suitable abbreviations Z_1, Z_2 , and so on. Note that the sum over $k_1 \geq 0$ effectively ends at $k_1 = rn_0$ and the sum over $k_2 \geq 0$ ends at $k_2 = r(n_0 + n_1) - k_1$, because the binomial coefficients vanish for higher values of k_1 or k_2 . The final step of this mathematical induction reads

$$\begin{aligned} D^{r(n_0 + n_1 + \dots + n_{p-2}) - k_1 - \dots - k_{p-1}} Z_{p-1} &= D^{r(n_0 + \dots + n_{p-1}) - k_1 - \dots - k_{p-1}} (u y_{rn_p}) \\ &= \sum_{k_p \geq 0} \binom{r(n_0 + n_1 + \dots + n_{p-1}) - k_1 - \dots - k_{p-1}}{k_p} u_{k_p} y_{r(n_0 + \dots + n_p) - k_1 - \dots - k_p} \end{aligned}$$

where the sum runs through $0 \leq k_p \leq r(n_0 + n_1 + \cdots + n_{p-1}) - k_1 - \cdots - k_{p-1}$. Here $n_0 + n_1 + \cdots + n_p = n - p$ and we introduce $k_0 := r(n - p) - k_1 - \cdots - k_p$. Hence

$$\begin{aligned} L^n y = y_{rn} + \sum_{p=1}^n \sum_{\substack{n_0, n_1, \dots, n_p \geq 0 \\ n_0 + n_1 + \cdots + n_p = n-p}} \sum_{k_1, k_2, \dots, k_p \geq 0} \binom{rn_0}{k_1} \binom{r(n_0 + n_1) - k_1}{k_2} \\ \times \binom{r(n_0 + n_1 + n_2) - k_1 - k_2}{k_3} \cdots \binom{r(n_0 + \cdots + n_p) - k_1 - \cdots - k_{p-1}}{k_p} \\ \times u_{k_1} u_{k_2} \cdots u_{k_p} y_{k_0}. \end{aligned} \quad (12)$$

Let us introduce the new summation indices

$$m_0 = n_0, m_1 = n_0 + n_1, m_2 = n_0 + n_1 + n_2, \dots, m_p = n_0 + n_1 + \cdots + n_p.$$

They are then subject to

$$0 \leq m_0 \leq m_1 \leq m_2 \leq \cdots \leq m_p = n - p$$

and only to these conditions. Finally, the summation over m_0, m_1, \dots, m_p and the summation over k_1, k_2, \dots, k_p can be interchanged and we arrive at

$$L^n y = y_{rn} + \sum_{p=1}^n \sum_{k_0, k_1, \dots, k_p \geq 0} C_{k_1 k_2 \dots k_p} u_{k_1} u_{k_2} \cdots u_{k_p} y_{k_0} \quad (13)$$

where the coefficients $C_{k_1 k_2 \dots k_p}$ have the accounted form (11). \square

Let us present some of the terms in theorem 1 more explicitly. There holds

$$L^n y = y_{nr} + \sum_{k=0}^{(n-1)r} C_k u_k y_{(n-1)r-k} + \sum_{k_1, k_2=0}^{(n-2)r} C_{k_1 k_2} u_{k_1} u_{k_2} y_{(n-2)r-k_1-k_2} + \cdots + u^n y$$

where the intermediate dots indicate the terms of degree greater than 2 and less than n in u and where

$$\begin{aligned} C_k &= \sum_{m=0}^{n-1} \binom{rm}{k} \equiv \binom{0}{k} + \binom{r}{k} + \cdots + \binom{(n-1)r}{k} \\ C_{k_1 k_2} &= \sum_{m_1=0}^{n-2} \sum_{m_2=0}^{m_1} \binom{rm_2}{k_1} \binom{rm_1 - k_1}{k_2}. \end{aligned}$$

Note that for $p = n$ we have $k_0 = k_1 = \cdots = k_n = 0$ and the single coefficient $C_{00\dots 0} = 1$. The terms of the inner sum of (10) are in one-to-one correspondence with number-theoretical partitions. More precisely, in the general non-commutative case the terms correspond to vectors (k_0, k_1, \dots, k_p) of integers k_0, k_1, \dots, k_p such that

$$k_0, k_1, \dots, k_p \geq 0 \quad \text{and} \quad k_0 + k_1 + \cdots + k_p = r(n - p).$$

Proposition 3. The inner sum over k_0, k_1, \dots, k_p in (10) has exactly $\binom{r(n-p)+p}{p}$ terms.

Proof. The number of ordered partitions of an integer m into s non-negative integers equals, according to textbooks of combinatorics, $\binom{m+s-1}{s-1}$ [4, 5]. Here we insert $m = r(n - p)$, $s = p + 1$. \square

In the special commutative case some terms can be added together to form a new term. The new terms correspond to unordered partition of $r(n - p)$ into $p + 1$ non-negative

integers. Unfortunately, there is no practical closed formula for the number of unordered partitions. Clearly, the total number of terms on the right-hand side of equation (10) equals

$$\sum_{p=0}^n \binom{r(n-p)+p}{p}.$$

Let us specialize our result to $r = 2$, that means present an explicit formula for the powers L^n of the one-dimensional Schrödinger operator $L = D^2 + u$. We find

$$L^n = (D^2 + u)^n = D^{2n} + \sum_{p=1}^n \sum_{k_0, k_1, \dots, k_p} C_{k_1 k_2 \dots k_p} u_{k_1} u_{k_2} \dots u_{k_p} D^{k_0} \quad (14)$$

where

$$C_{k_1 k_2 \dots k_p} = \sum_{m_0, m_1, \dots, m_p} \binom{2m_0}{k_1} \binom{2m_1 - k_1}{k_2} \binom{2m_2 - k_1 - k_2}{k_3} \dots \binom{2m_p - k_1 - \dots - k_{p-1}}{k_p}.$$

The non-negative summation indices are subject to $k_0 + k_1 + \dots + k_p = 2(n - p)$ and $m_0 \leq m_1 \leq \dots \leq m_p = n - p$.

3. An alternative formula for L^n

Schimming [6, 7] derived an explicit formula for the right-hand sides of the KdV hierarchy (5) or (6). He used a special symbolism in order to present a non-recursive expression for the differential polynomials $G_n[u]$ ($n = 1, 2, \dots$). This method also works in our case. Namely, let us abbreviate, as before, the k th derivative of $u = u(x)$ by $u_k = u^{(k)}$ ($k = 0, 1, 2, \dots$) and let us supplement this by the formal definitions

$$u_{-1} = 0, \dots, u_{1-r} = 0 \quad u_{-r} = 1.$$

Furthermore, we set

$$c(k, l) := \binom{k}{l} + \delta_l^{k+r}$$

where the second term is a Kronecker symbol.

Theorem 2. There holds

$$L^n y = \sum_{k_1, k_2, \dots, k_n} \left(\prod_{i=1}^n c(k_{i-1}, k_i) u_{k_{i-1}-k_i} \right) y_{k_n} \quad (15)$$

where the sum runs through the integers k_1, k_2, \dots, k_n such that

$$0 \leq k_i \leq k_{i-1} + r \quad \text{for } i = 1, 2, \dots, n, \quad k_0 = 0.$$

Proof. Let us set here $y_{(n)} := L^n y$. Then

$$y_{n+1} = L y_{(n)} = y_{(n)}^{(r)} + u y_{(n)}$$

$$y_{(n+1)}^{(k)} = y_{(n)}^{(k+r)} + \sum_{l=0}^k \binom{k}{l} u_{k-l} y_{(n)}^{(l)} = \sum_{l=0}^{k+r} c(k, l) u_{k-l} y_{(n)}^{(l)}.$$

Thus, we have some linear recursion equation for the double sequence $(y_{(n)}^{(k)})$ ($n, k = 0, 1, 2, \dots$). This recursion can be solved by means of mathematical induction. The first two steps read

$$\begin{aligned} y_{(n)}^{(k)} &= \sum_{k_1=0}^{k+r} c(k, k_1) u_{k-k_1} y_{(n-1)}^{(k_1)} \\ &= \sum_{k_1=0}^{k+r} \sum_{k_2=0}^{k_1+r} c(k, k_1) c(k_1, k_2) u_{k-k_1} u_{k_1-k_2} y_{(n-2)}^{(k_2)} \end{aligned}$$

and the procedure stops after n steps:

$$y_{(n)}^{(k_0)} = \sum_{k_1=0}^{k_0+r} \dots \sum_{k_n=0}^{k_{n-1}+r} c(k_0, k_1) \dots c(k_{n-1}, k_n) u_{k_0-k_1} \dots u_{k_{n-1}-k_n} y_{(0)}^{(k_n)}.$$

The result follows by some rearrangement and by setting $k_0 = 0$, $y_{(0)}^{(k_n)} = y_{k_n}$, $y_{(n)}^{(0)} = L^n y$. Formula (14) is not as simple as it appears to be, because each coefficient $c(k_{i-1}, k_i)$ involves two or three cases:

$$c(k, l) = \binom{k}{l} \text{ for } l \leq k \quad c(k, l) = 1 \text{ for } l = k + r \quad c(k, l) = 0 \text{ otherwise.}$$

We can rewrite (14) in the form

$$L^n y = \sum_{k=0}^{rn} P_{(n)}^k[u] y_k$$

where

$$P_{(n)}^k[u] = \sum_{k_1, k_2, \dots, k_{n-1}} \left(\prod_{i=1}^n c(k_{i-1}, k_i) u_{k_{i-1}-k_i} \right) \quad k_0 = 0, \quad k_n = k.$$

□

The following might be seen as a curiosity; we mention it for the sake of completeness. Define an infinite matrix $U = (u_{kl})$ for $k, l = 0, 1, 2, \dots$ by

$$u_{kl} = \binom{k}{l} u_{k-1} + \delta_l^{k+r}.$$

Denote the elements of $U^n = UU \dots U$ (n times) by $u_{kl}^{(n)}$. Then

$$P_{(n)}^k[u] = u_{0k}^{(n)}.$$

4. Discussion

Torriani [3] discussed the one-dimensional Schrödinger operator $L = D^2 + u$ in the scalar case. He presented recursion formulae with respect to n for the coefficients $c_{k_1, k_2, \dots, k_p}^{(n)}$ in

$$L^n y = \sum_{p=0}^n \sum_{k_1, k_2, \dots, k_p} c_{k_1, k_2, \dots, k_p}^{(n)} u_{k_1} \dots u_{k_2} \dots u_{k_p} y_{k_0}.$$

We are not able to generalize Torriani's recursion to the general case $L = D^r + u$; we think that our explicit formulae are more useful. Schimming and Rida presented [8] an

explicit formula for the powers L^n of a first-order operator $L = D + u$ in terms of the Bell polynomials $B_n (n = 1, 2, \dots)$. Namely, we showed

$$L^n = \sum_{k=0}^n \binom{n}{k} B_k(u, u', \dots, u^{(n-1)}) D^{n-k}$$

where $B_0 \equiv 1$, $B_1 \equiv y_1$, and

$$B_n(y_1, y_2, \dots, y_n) = \sum_{d=1}^n \sum_{n_2, \dots, n_d=1}^n \binom{n-1}{n_2} \binom{n_2-1}{n_3} \dots \binom{n_{d-1}-1}{n_d} y_{n_d} y_{n_{d-1}-n_d} \dots y_{n_2-n_3} y_{n-n_2}$$

for $n \geq 2$, cf [8] for details.

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