Explicit Formula for the Generating Series of Diagonal 3D Rook Paths

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Joint article in preparation with Alin Bostan, Mark van Hoeij, and Lucien Pech

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Supported in part by the

August 15, 2010, DZ 60 (in honor of Doron Zeilberger’s 60th birthday), Tianjin (China)
Diagonal 3D Rook Paths

Problem
Determine the number $a_n$ of paths from $(0, 0, 0)$ to $(n, n, n)$ that use positive multiples of $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$.

A144045 in Sloane’s EIS (since 2008)
1, 6, 222, 9918, 486924, 25267236, 1359631776, 75059524392, 4223303759148, ...

Conjecture by Erickson, Fernando, and Tran (201?)

$$
2n^2(n - 1)a_n - (n - 1)(121n^2 - 91n - 6)a_{n-1}
- (n - 2)(475n^2 - 2512n + 2829)a_{n-2}
+ 18(n - 3)(97n^2 - 519n + 702)a_{n-3}
- 1152(n - 3)(n - 4)^2a_{n-4} = 0,
\text{ for } n \geq 4.
$$
Our Contributions

1. Proof of the 4th-order recurrence. There is even 3rd-order recurrence:

\[
192n^2(35n + 88)(n + 1)a_n - (n + 1)(11305n^3 + 59889n^2 + 100586n + 54864)a_{n+1} + (n + 2)(4655n^3 + 30114n^2 + 63493n + 43362)a_{n+2} - 2(n + 2)(35n + 53)(n + 3)^2a_{n+3} = 0, \quad \text{for } n \geq 0.
\]

2. Explicit form for the enumerative generating series:

\[
G(x) = 1 + 6 \cdot \int_0^x \frac{2F_1\left(\frac{1}{3}, \frac{2}{3} \left| \frac{27w(2-3w)}{(1-4w)^3} \right. \right)}{(1 - 4w)(1 - 64w)} dw.
\]

3. New, simpler proof of the asymptotic formula:

\[
a_n \sim \frac{9\sqrt{3}}{40\pi} \cdot \frac{64^n}{n}.
\]
Remark: The 2D Case is Easy

A051708: 1, 2, 14, 106, 838, 6802, 56190, 470010, ...
(In the EIS since 1999.)

Generating series is algebraic:

\[
\frac{1 - x}{2\sqrt{1 - 10x + 9x^2}} + \frac{1}{2}.
\]
Generating series for the number $r_{i,j,k}$ of paths that end at $(i, j, k)$

$$f(s, t, u) := \left(1 - \sum_{n \geq 1} s^n - \sum_{n \geq 1} t^n - \sum_{n \geq 1} u^n\right)^{-1}$$

$$= \frac{(1 - s)(1 - t)(1 - u)}{1 - 2(s + t + u) + 3(st + tu + us) - 4stu} \in \mathbb{Q}[[s, t, u]].$$

Diagonal representation

$$G(x) = \text{Diag}(f) = \sum_{n \geq 0} r_{n,n,n}x^n \in \mathbb{Q}[[x]].$$
Lemma (Lipshitz, 1988)

After setting

\[ F := \frac{1}{st} f \left( \frac{s}{t}, \frac{t}{s}, \frac{x}{t} \right), \]

if \( P(x, \partial_x) \) satisfies

\[ P(F) = \frac{\partial S}{\partial s} + \frac{\partial T}{\partial t} \]

for some \( S, T \in \mathbb{Q}(x, s, t) \), then \( P(\text{Diag}(f)) = 0 \).

Proof: In a \( \mathbb{Q}[x, s, t]\langle \partial_x, \partial_s, \partial_t \rangle \)-module of suitable formal power series,

\[ P(\text{Diag}(f)) = P([s^{-1}t^{-1}] F) = [s^{-1}t^{-1}] P(F) = 0. \]
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Remaining problem

Compute such \( P, S, \) and \( T \).
Lipshitz’s Approach: Counting Dimensions

Method

1. Find annihilator $L(x, \partial_x, \partial_s, \partial_t)$ of $F$.
2. Write $L = P(x, \partial_x) + \partial_s A(x, \partial_x, \partial_s, \partial_t) + \partial_t B(x, \partial_x, \partial_s, \partial_t)$ (modifying $L$ to ensure $P \neq 0$ if needed).
3. Return $P, S := A(F)$, and $T := B(F)$.

Note: $P(F), S, T \in \mathbb{Q}[x, s, t, q^{-1}]$ if $F = p/q$.

Existence of $L$

$$x^i \partial_x^j \partial_s^k \partial_t^\ell (F) \rightarrow q^{-(N+1)} x^i s^j t^k$$

$$0 \leq i + j + k + \ell \leq N \quad 0 \leq i \leq 2N + 1, \ 0 \leq j, k \leq 3N + 2$$

$$\binom{N+4}{4} \sim N^4/24 \quad 18(N + 1)^3 \sim 18N^3$$

$N \geq 425$ ensures a relation, but linear algebra in dimension $> 10^9$!

Refined bound (better filtration + predicting zeros): still $> 1.6 \cdot 10^6$!!
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Algorithm is useless in practice.
Larger and larger classes of inputs

1. hypergeometric, \(q\)-hypergeometric, bibasic, \ldots\) (DZ, Koornwinder, Paule, Riese, Schorn, 1990–)

2. hyperexponential (Almkvist–DZ, 1990)

3. D-finite (FC, 2000; Koutschan, 2010)

4. Abel-type (Majewicz, 1996); Stirling-type (Kauers, 2007); Bernoulli and Euler type (Chen–Sun, 2008)

5. beyond D-finite (FC–Kauers–Salvy, 2009)

6. in difference fields (Schneider, 200?–)

7. symmetric functions (FC–Mishna–Salvy, 2002, 2005)

Complexity point of view

Polynomial time algorithm for bivariate rational functions (Bostan, Chen, FC, Li, 2010)
Pech’s Maple implementation of Chyzak’s generalized algorithm to D-finite functions (2000) finds:

\[ P = P_2 \partial_x, \quad S = \frac{(s-t) \cdot U}{2st \cdot q_1^2 \cdot \text{disc}_t(q_1)}, \quad T = \frac{t \cdot V}{2xs^2(3s-2)^2 \cdot q_1^3 \cdot \text{disc}_t(q_1)^2}, \]

where

\[ P_2 = x(x-1)(64x-1)(3x-2)(6x+1)\partial_x^2 \]
\[ + (4608x^4 - 6372x^3 + 813x^2 + 514x - 4)\partial_x \]
\[ + 4(576x^3 - 801x^2 - 108x + 74), \]

\[ q_1 = q/(st), \quad \text{deg}_{x,s,t} U = (5, 8, 3), \quad \text{deg}_{x,s,t} V = (9, 17, 5). \]
One variable less: simplified key equation

For $F \in \mathbb{Q}(u, v)$, find $P(u, \partial_u)$ and $S \in \mathbb{Q}(u, v)$ such that $P(F) = \frac{\partial S}{\partial v}$.

Algorithm (simplified)

For $r = 0, 1, 2, \ldots$:
1. set $P = \eta_r(u)\partial_u^r + \cdots + \eta_0(u)$ for undertermined $\eta_i \in \mathbb{Q}(u)$;
2. set $S = \phi(u, v)F$ for undertermined $\phi \in \mathbb{Q}(u, v)$;
3. derive first-order ODE on $\phi$;
4. solve by a variant of Abramov’s decision algorithm;
5. if solvable, output $(P, S)$, else loop.

Original A & Z’s algorithm

$F$ and $S$ are hyperexponential; solving uses this specific feature.
Creative Telescoping (2): Chyzak’s D-Finite Case

Definition

\( F(u, v) \) is D-finite if there exists a finite maximal set of derivatives \( \partial_u^a \partial_v^b(F) \) that are linearly independent over \( \mathbb{Q}(u, v) \).

Algorithm (Chyzak, 2000)

Adapt A & Z’s algorithm (simplified) by:

1. Fix a set of \((a, b)\) from the definition and change the ansatz into

\[
S = \sum_{(a, b)} \phi_{a,b}(u, v) \partial_u^a \partial_v^b(F).
\]

2. Equation on \( \phi \) is replaced with a system of coupled ODE’s on the \( \phi_{a,b} \)’s.

3. Solved by uncoupling or a direct approach.

Remark: The \((a, b)\)’s can be obtained by a Gröbner-basis calculation.
A Failure and a Cure

Key equation: Solve for $P(x, \partial_x)$ and rational functions $S$ and $T$

$$P(F) = \frac{\partial S}{\partial s} + \frac{\partial T}{\partial t}.$$ 

Obstruction

Even for rational $F$, no algorithm is known to solve the ansatz

$$P(F(s, t, x)) = \frac{\partial}{\partial s} (\phi_1(s, t, x)F) + \frac{\partial}{\partial t} (\phi_2(s, t, x)F).$$
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A Salvaging Observation

In A & Z, dependency of $P$ in a single derivation $\partial_u$ is inessential. Extended ansatz (Chyzak, 2000):

$$P = \sum_{0 \leq i+j \leq r} \eta_{i,j}(u_1, u_2) \partial_{u_1}^i \partial_{u_2}^j$$

for undetermined $\eta_{i,j} \in \mathbb{Q}(u_1, u_2)$. 

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Creative Telescoping (3): Iterated Chyzak Algorithm
with the “UFO” finish for non-natural boundaries

1. Extended A & Z algorithm for the rational function $F(s, x, t) \rightarrow$

$$P^{(\alpha)}(s, x, \partial_s, \partial_x)(F) = \frac{\partial}{\partial t} \left( \phi^{(\alpha)}(s, t, x)F \right).$$

2. Chyzak’s algorithm for $\hat{F}(s, x)$ annihilated by all $P^{(\alpha)} \rightarrow$

$$P(x, \partial_x)(\hat{F}) = \frac{\partial}{\partial s} \left( Q(s, x, \partial_s, \partial_x)(\hat{F}) \right).$$
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1. Extended A & Z algorithm for the rational function $F(s, x, t) \rightarrow$

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2. Chyzak’s algorithm for $\hat{F}(s, x)$ annihilated by all $P^{(\alpha)} \rightarrow$

   $$P(x, \partial_x)(\hat{F}) = \frac{\partial}{\partial s} \left( Q(s, x, \partial_s, \partial_x)(\hat{F}') \right).$$

3. Obtain operators $L^{(\alpha)}(s, x, \partial_s, \partial_x)$ satisfying

   $$P(x, \partial_x) - \partial_s Q(s, x, \partial_s, \partial_x) = \sum_{\alpha} L^{(\alpha)}(s, x, \partial_s, \partial_x)P^{(\alpha)}(s, x, \partial_s, \partial_x)$$

   by non-commutative multivariate division.

4. A solution $(P, S, T)$ of the key equation is given upon setting

   $$S := Q(s, x, \partial_s, \partial_x)(F) \quad \text{and} \quad T := \sum_{\alpha} L^{(\alpha)}(s, x, \partial_s, \partial_x)(\phi^{(\alpha)}(s, t, x)F).$$
Fourth-order conjectured recurrence

Proved classically from the differential operator $P$.

Third-order recurrence

1. Observe that $-1/6$ is an apparent singularity of $P$.
2. The differential operator of order 4 provides a second fourth-order recurrence.
3. Elimination of $a_{n+4}$ yields the announced third-order recurrence.

Variant: Guess it, then show it has the same solution as the fourth-order one.
General speculation of Dwork’s (about nilpotent $p$-curvature) applies to $P_2$: $\partial_x(\text{Diag}(f))$ is likely to be of the form

$$(r_0 y + r_1 y') \cdot \exp\left(\int r \right) \text{ for } y = 2F_1\left(\begin{array}{c} a \\ b \\ c \end{array} \mid f \right)$$

where $a, b, c \in \mathbb{Q}$ and $r, r_0, r_1, f \in \mathbb{Q}(x)$.

**Principles for determining $y$**

1. $f$ must transfer the location and behaviour at the singularities of the Gauss ODE to those of $P_2$.
2. “Exponent difference” (attached to each singular point) is a natural guide to $f$.
3. For the Gauss hypergeometric function:

$$\left( e_0, e_1, e_\infty \right) = \left( \pm(1 - c), \pm(c - a - b), \pm(a - b) \right).$$
Solution in Explicit Form: Calculations

1. First candidate: \((e_0, e_1, e_\infty) = (0, 1/3, 0)\) and
   \[
   f = 1 - \frac{(4x - 1)^3}{(x - 1)^2(64x - 1)} = -\frac{81x(x - 2/3)}{64(x - 1)^2(x - 1/64)}.
   \]

2. Optimized candidate: \((e_0, e_1, e_\infty) = (1, 1, 1/3)\) and
   \[
   \bar{f} = \frac{f}{1 - f} = \frac{27x(2 - 3x)}{(1 - 4x)^3}.
   \]

3. \((a, b, c) = (1/3, 2/3, 2)\).

4. Identification: \(r = r_1 = 0\) and \(r_0 = \frac{6}{(1 - 4x)(1 - 64x)}\).

5. Taking initial conditions into account:

   \[
   G(x) = 1 + 6 \cdot \int_0^x \frac{x \, 2F_1\left(\begin{array}{c}1/3, 2/3 \\ 2 \end{array}\right)_2 \frac{27w(2 - 3w)}{(1 - 4w)^3}}{(1 - 4w)(1 - 64w)} \, dw.
   \]
Asymptotic Expression for $a_n$

Recall: $\partial_x (\text{Diag}(f)) = \frac{6 \cdot 2F_1\left(\frac{1/3}{2}, \frac{2/3}{2} \Bigg| \frac{27x(2-3x)}{(1-4x)^3} \right)}{(1 - 4x)(1 - 64x)}$.

Dominant singularity is $1/64$, with residue $r = \frac{6}{(1 - \frac{4}{64})} \cdot 2F_1\left(\frac{1/3}{2}, \frac{2/3}{2} \Bigg| \frac{27/64(2 - \frac{3}{64})}{(1 - \frac{4}{64})^3} \right) = \frac{32}{5} \cdot 2F_1\left(\frac{1/3}{2}, \frac{2/3}{2} \Bigg| 1 \right) = \frac{72\sqrt{3}}{5\pi}$.

Thus: $a_n \sim \frac{1}{64n} (r \cdot 64^n) = \frac{9\sqrt{3}}{40\pi} \cdot \frac{64^n}{n} \simeq 0.124 \cdot 64^n$. 
Asymptotic Expression for $a_n$

Recall: $\partial_x(\text{Diag}(f)) = \frac{6 \cdot _2F_1\left(\begin{array}{cc}1/3 & 2/3 \\ 2 & \end{array}\middle| \frac{27x(2-3x)}{(1-4x)^3}\right)}{(1 - 4x)(1 - 64x)}$.

Dominant singularity is $1/64$, with residue $r = \frac{6}{(1 - \frac{4}{64})} \cdot _2F_1\left(\begin{array}{cc}1/3 & 2/3 \\ 2 & \end{array}\middle| \frac{27}{64}(2 - \frac{3}{64}) \right) = \frac{32}{5} \cdot _2F_1\left(\begin{array}{cc}1/3 & 2/3 \\ 2 & \end{array}\middle| 1\right) = \frac{72\sqrt{3}}{5\pi}$.

Thus: $a_n \sim \frac{1}{64n}(r 64^n) = \frac{9\sqrt{3}}{40\pi} \cdot \frac{64^n}{n} \sim 0.124 \cdot 64^n$.

This avoids general multivariate asymptotics à la Raichev and Wilson.
Concluding remarks

1. Series is D-finite but not algebraic.
2. Beukers communicated a derivation by differential forms, leading to a similar but different representation.
3. 3D queens paths is a challenge: order 6, degree 71, only guessed.
4. Apply same technique to all nearest-neighbour types of walks (in progress, same authors + Kauers).
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Happy Birthday Doron!
\[
F := \frac{(s-t)(-1+s)(t-x)}{st(-st + 2s^2t + 2t^2 + 2xs - 3s^2t - 3xt - 3xs^2 + 4xs)}
\]

(1)

\[
P, S, T := \text{op(Mgfun:-creative_telescoping}(F, x::\text{diff}, [s::\text{diff}, t::\text{diff}])):
\]

(2)

\[
P := \text{collect(DEtools[de2diffop](P, _F(x), [dx,x]), dx, factor)};
\]

(3)

\[
S := \text{eval}(S, _f = \text{unapply}(F, x, s, t)):
\]

(4)

\[
T := \text{eval}(T, _f = \text{unapply}(F, x, s, t)):
\]

(5)

\[
normal(\text{eval}(P, _F(x) = F) - \text{diff}(S, s) - \text{diff}(T, t));
\]

(6)
\[ S := \text{factor}(S); \]
\[ T := \text{factor}(T); \]
\[ q := \text{factor}(\text{denom}(F)); \]
\[ q := s t \left(-s t + 2 s^2 t + 2 x s - 3 s t^2 - 3 x t - 3 x s^2 + 4 x s t\right) \]
\[ q1 := q/s/t; \]
\[ \text{disc} := \text{factor}(\text{discrim}(q1, t)); \]
\[ \text{disc} := \left(-16 x s^2 + 24 x s - 9 x - 4 s^2 + 4 s^3 + s\right) (s - x) \]
\[ U := 2 * s*t * q1^2 * \text{disc} * S / (s-t); \]
\[ V := 2 * x * s^2 * q1^3 * \text{disc}^2 * (3*s-2)^2 * T / t; \]
\[ \text{map2}(|\text{degree}|, q1, [x,s,t]); \]
\[ \text{map2}(|\text{degree}|, U, [x,s,t]); \]
\[ \text{map2}(|\text{degree}|, V, [x,s,t]); \]
\[ \text{map2}(|\text{degree}|, P, [x,dx]); \]
\[ \text{collect}(P_, \{\_F, \text{diff}\}, \text{factor}); \]
\[ \text{rec4} := \text{gfun}[\text{diffeqtorec}](\% , \_F(x), u(n)); \]
\[ \text{Alg} := \text{Ore_algebra}[\text{diff_algebra}](\{dx, x\}); \]
\[ \text{dxP} := \text{Ore_algebra}[\text{skew_product}](dx, P, \text{Alg}); \]
\[ \text{eval}(\text{dxP}, x=-1/6); \]
\[ 828 \, dx - 105 \, dx^2 \quad (17) \]

\[ > \text{eval(P, x=-1/6)}; \]
\[ - \frac{1225}{36} \, dx^2 + \frac{805}{3} \, dx \quad (18) \]

\[ > \text{normal(\%\%/\%)}; \]
\[ \frac{108}{35} \quad (19) \]

\[ > \text{collect((35*dxP - 108*P) / (6*x+1), dx, factor);} \]
\[ 35 \, (x - 1) \, (64 \, x - 1) \, (3 \, x - 2) \, x \, dx^3 - 6 \, (x - 1) \, (3456 \, x^3 - 12438 \, x^2 + 4621 \, x - 35) \, dx^3 \]
\[ + \left( -82944 \, x^3 + 249480 \, x^2 - 186414 \, x + 28782 \right) \, dx^2 + \left( -41472 \, x^2 + 104904 \, x \right. \]
\[ - 47088 \right) \, dx \quad (20) \]

\[ > \text{Ore_algebra[applyop]}(\%, \_F(x), \text{Alg}); \]
\[ (-41472 \, x^2 + 104904 \, x - 47088) \left( \frac{d}{dx} - F(x) \right) - 6 \, (x - 1) \, (3456 \, x^3 - 12438 \, x^2 + 4621 \, x \]
\[ - 35) \left( \frac{d^3}{dx^3} - F(x) \right) + \left( -82944 \, x^3 + 249480 \, x^2 - 186414 \, x + 28782 \right) \left( \frac{d^2}{dx^2} - F(x) \right) \]
\[ + 35 \, (x - 1) \, (64 \, x - 1) \, (3 \, x - 2) \, x \left( \frac{d^4}{dx^4} - F(x) \right) \quad (21) \]

\[ > \text{gfun[diffeqtorec]}(\%, \_F(x), \text{u(n)}); \]
\[ (-20736 \, n^2 - 20736 \, n^3) \, \text{u}(n) + \left( 272460 \, n + 104904 + 242760 \, n^2 + 81924 \, n^3 \right. \]
\[ + 6720 \, n^4 \right) \, \text{u}(n + 1) + \left( -788428 \, n - 467004 - 482171 \, n^2 - 124964 \, n^3 \right. \]
\[ - 11305 \, n^4 \right) \, \text{u}(n + 2) + \left( 247603 \, n^2 + 479136 \, n + 340308 + 55866 \, n^3 + 4655 \, n^4 \right) \, \text{u}(n \]
\[ + 3) + \left( -910 \, n^3 - 4340 \, n^2 - 8960 \, n - 6720 - 70 \, n^4 \right) \, \text{u}(n + 4) \quad (22) \]

\[ > \text{rec4bis := collect(\%, \text{u}, \text{factor});} \]
\[ \text{rec4bis} := -20736 \, n^2 (n + 1) \, \text{u}(n) + 12 \, (n + 1) \left( 560 \, n^3 + 6267 \, n^2 + 13963 \, n + 8742 \right) \, \text{u}(n \]
\[ + 1) - (n + 2) \left( 11305 \, n^3 + 102354 \, n^2 + 277463 \, n + 233502 \right) \, \text{u}(n + 2) + (n + 3) \, (n \]
\[ + 2) \left( 4655 \, n^2 + 32591 \, n + 56718 \right) \, \text{u}(n + 3) - 70 \, (n + 3) \, (n + 2) \, (n + 4)^2 \, \text{u}(n + 4) \quad (23) \]

\[ > \text{solve(rec4, u(n+4));} \]
\[ \frac{1}{2} \left( -1152 \, u(n) \, n^2 - 1152 \, u(n) \, n^3 + 7830 \, u(n + 1) \, n + 3204 \, u(n \]
\[ + 1) + 6372 \, u(n + 1) \, n^2 + 1746 \, u(n + 1) \, n^3 - 2957 \, u(n + 2) \, n - 762 \, u(n + 2) \]
\[ - 2238 \, u(n + 2) \, n^2 - 475 \, u(n + 2) \, n^3 - 4197 \, u(n + 3) \, n - 4698 \, u(n + 3) \]
\[ - 1240 \, u(n + 3) \, n^2 - 121 \, u(n + 3) \, n^3 \right) \quad (24) \]

\[ > \text{solve(rec4bis, u(n+4));} \]
\[ \frac{1}{70} \left( -20736 \, u(n) \, n^3 - 20736 \, u(n) \, n^2 + 272460 \, u(n + 1) \, n \right. \]
\[ n + 1) + 72564 \, u(n + 1) \, n^2 + 2238 \, u(n + 1) \, n^3 - 5281 \, u(n + 2) \, n - 672 \, u(n + 2) \]
\[ - 1500 \, u(n + 2) \, n^2 - 300 \, u(n + 2) \, n^3 - 4197 \, u(n + 3) \, n - 9390 \, u(n + 3) \]
\[ - 1330 \, u(n + 3) \, n^2 - 121 \, u(n + 3) \, n^3 \right) \quad (25) \]
+ 104904 u(n + 1) + 242760 u(n + 1) n^2 + 81924 u(n + 1) n^3 + 6720 u(n + 1) n^4
- 788428 u(n + 2) n - 467004 u(n + 2) - 482171 u(n + 2) n^2 - 124964 u(n + 2) n^3
- 11305 u(n + 2) n^4 + 247603 u(n + 3) n^2 + 479136 u(n + 3) n + 340308 u(n + 3)
+ 55866 u(n + 3) n^3 + 4655 u(n + 3) n^4)

> collect(numer(normal(%%-%)/3), u, factor);
192 n^2 (35 n + 88) \(n + 1\) u(n) - (n + 1) (11305 n^3 + 59889 n^2 + 100586 n
+ 54864) u(n + 1) + (n + 2) (4655 n^3 + 30114 n^2 + 63493 n + 43362) u(n + 2)
- 2 (n + 2) (35 n + 53) (n + 3)^2 u(n + 3)