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Moments and asymptotic expansion of derangement polynomials in terms of Touchard polynomials

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Abstract: In this paper we study the polynomial $\widehat{D}_n(x) = n! \sum_{j=0}^n x^j / j!$, which is a variant of derangement polynomials. First we obtain an asymptotic expansion for $\widehat{D}_n(x)$ with coefficients in terms of Touchard polynomials. Then, we compute the moments $\sum_{n=0}^{\infty} (e^x n! - \widehat{D}_n(x))^k$ for any integer $k \geq 1$ and any real $x \in [0, 1)$.

Keywords: Derangement polynomial, Touchard polynomials, Bell numbers. 2020 Mathematics Subject Classification: 05A05, 05A16, 11B73.

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1 Introduction

1.1 Derangement polynomials

A derangement is a permutation that has no fixed points. We denote the number of derangements on a set of cardinality n by D_n . The derangement polynomials are natural extensions of the derangement numbers, mostly admitting D_n in a certain value. These polynomials are defined in several different ways in literature [5, 8, 9, 23, 24, 33, 34], but the most common definition is

$$
D_n(x) = n! \sum_{j=0}^n \frac{(-1)^j}{j!} x^{n-j}.
$$
 (1.1)

This definition appears in the work of Radoux [33, 34], where he studied a Hankel determinant constructed on $D_n(x)$. These polynomials are associated with the number of derangements on a set of cardinality *n* by $D_n = D_n(1)$.

In this paper we consider the following variant of the derangement polynomial, defined for any integer $n \geq 0$ and any real $x \neq 0$ by

$$
\widehat{D}_n(x) = n! \sum_{j=0}^n \frac{x^j}{j!},
$$
\n(1.2)

and for $x = 0$ by $\widehat{D}_n(0) = n!$. As a classical result, Sylvester [39, p. 516] (see also [32, p. 46]) studied the roots of $\widehat{D}_n(x)$ by showing that it has no real zero or one real zero according as n is even or odd. Also, this polynomial is known as derangement function [17, p. 6] and satisfies the following generalized recursive relations

$$
\widehat{D}_n(x) = (x+n)\widehat{D}_{n-1}(x) - x(n-1)\widehat{D}_{n-2}(x) \n= x^n + n\widehat{D}_{n-1}(x),
$$

with initial values $\widehat{D}_0(x) = 1$ and $\widehat{D}_1(x) = x + 1$. Note that $\widehat{D}_n(-1) = D_n$. Also $\widehat{D}_n(0) = n!$, which is indeed the number of permutations of n distinct objects. Moreover $\widehat{D}_n(1) = w_{n+2}$, where w_{n+2} denotes the number of all distinct paths between a specific pair of vertices in a complete graph on $n + 2$ vertices (see [18, 19] and the references given there).

1.2 Asymptotic results

Analytic enumeration concerns with the study of asymptotic behaviour of combinatorial subjects, and making precise the counting formulas in sense of their magnitude. We refer the interested reader to [1, 4, 12, 16, 27, 28, 35, 38] for this topic and around. In this paper we refer to the notion of asymptotic series [13, Section 1.5], due to Poincare. Accordingly, an asymptotic expansion for ´ D_n has been obtained in [20, Theorem 3] by showing that given any positive integer r, for any integer $n \geqslant 1$ we have

$$
D_n = \frac{n!}{e} + \sum_{k=1}^r (-1)^{n+k-1} \frac{B_k}{n^k} + \widetilde{\mathcal{O}}\left(\frac{B_{r+1}}{n^{r+1}}\right),\tag{1.3}
$$

where B_k denotes the k-th Bell number [41, p. 178], and through the paper by $f = \widetilde{\mathcal{O}}(g)$ we mean $|f| \leq q$, providing an explicit version of Bachmann–Landau Big O notation. We refer the interested reader to [11, 14] for more relations between the number of derangements and Bell numbers.

Similar to (1.3), an asymptotic expansion for w_{n+2} has been obtained in [21, Theorem 1.1] by showing that there exist computable constants c_1, \ldots, c_r such that

$$
w_{n+2} = e n! - \sum_{k=1}^{r} \frac{c_k}{n^k} + \widetilde{\mathcal{O}}\left(\frac{e^2 B_{r+1}}{n^{r+1}}\right).
$$
 (1.4)

Dobinski's formula [41, p. 178] concerning the k -th Bell number asserts that

$$
e B_k = \sum_{j=0}^{\infty} \frac{j^k}{j!}.
$$
\n(1.5)

The constants c_k in (1.4) match the k-th term of the sequence A014182 on OEIS [37], and satisfy the following alternating form of Dobinski's formula

$$
\frac{(-1)^k}{e} c_k = \sum_{j=0}^{\infty} (-1)^j \frac{j^k}{j!}.
$$
 (1.6)

Some initial values of c_k is $1, 0, -1, 1, 2, -9, 9, 50, -267, 413$.

In this paper, first we obtain an asymptotic expansion concerning $\widehat{D}_n(x)$ with explicit error term. Our work generalize asymptotic expansions (1.3) and (1.4). More precisely, we prove the following result.

Theorem 1.1. *Given any positive integer* r, for any integer $n \ge 1$ *and any real* $x \ne 0$ *we have the asymptotic expansion*

$$
\widehat{D}_n(x) = e^x n! - x^n \sum_{k=1}^r \frac{(-1)^k}{n^k} T_k(-x) + \widetilde{\mathcal{O}}\left(\frac{|x|^n}{n^{r+1}} e^{x+|x|} T_{r+1}(|x|)\right),\tag{1.7}
$$

where $T_k(x)$ *is the k-th Touchard polynomial.*

Remark 1.1. *The Touchard polynomials* $T_k(x)$ *, studied by Jacques Touchard [40], defined by*

$$
T_k(x) = \sum_{j=0}^k S(k,j)x^j,
$$

where S(k, j) *is the Stirling numbers of the second kind, counting the number of partitions of a set of size* k *into j disjoint non-empty subsets. Thus,* $T_k(x)$ *is a generating function for the finite sequence* $(S(k, j))_{0\leq j\leq k}$ *. We refer the interested reader to [6,7,10,25,30,31,42] and [36, Chapter 5] for the above definition and a remarkable number of properties, including the following identity*

$$
B_k = T_k(1),
$$

and the probabilistic property asserting that if X *is a random variable with a Poisson distribution* with expected value x, then its k-th moment is $E(X^k) = T_k(x)$ (see the second page of [31]). *This leads to the following analogue of Dobinski's formula*

$$
e^x T_k(x) = \sum_{j=0}^{\infty} x^j \frac{j^k}{j!}.
$$
 (1.8)

Note that for $x = 1$ *the relation* (1.8) *coincides with* (1.5)*, and for* $x = -1$ *it coincides with* (1.6)*. More precisely, we have*

$$
c_k = (-1)^k T_k(-1). \tag{1.9}
$$

Moreover, we observe that for $x = -1$ *and* $x = 1$ *the relation* (1.7) *implies* (1.3) *and* (1.4)*, respectively.*

A simple algebraic computation shows that the polynomials $D_n(x)$ and $\hat{D}_n(x)$ are related for any real $x \neq 0$ by the following identities

$$
D_n(x) = x^n \widehat{D}_n\left(-\frac{1}{x}\right), \quad \widehat{D}_n(x) = (-x)^n D_n\left(-\frac{1}{x}\right).
$$
 (1.10)

The above relations allow us to transfer results between $D_n(x)$ and $\widehat{D}_n(x)$. Accordingly, the truth of Theorem 1.1 reads as follows.

Corollary 1.1. Given any positive integer r, for any integer $n \geq 1$ and any real $x \neq 0$ we have *the asymptotic expansion*

$$
D_n(x) = x^n e^{-\frac{1}{x}} n! - (-1)^n \sum_{k=1}^r \frac{(-1)^k}{n^k} T_k\left(\frac{1}{x}\right) + \widetilde{\mathcal{O}}\left(\frac{1}{n^{r+1}} e^{-\frac{1}{x} + \frac{1}{|x|}} T_{r+1}\left(\frac{1}{|x|}\right)\right),
$$

where $D_n(x)$ *is the derangement polynomial defined by* (1.1) *and* $T_k(x)$ *is the k-th Touchard polynomial.*

1.3 Moment results

The moments of the combinatorial differences $D_n - e^{-1}n!$ and $w_{n+2} - e n!$ have been computed in [20, Theorem 2] and [21, Theorem 1.4], respectively. As a generalization, recently in [22] we computed the k-th moments of the difference $D_n(x) - x^n e^{-\frac{1}{x}} n!$ for any real $x > 0$ and each integer $k \ge 1$. Because of the condition $x > 0$ we cannot use the transferring formulas (1.10) to convert the above mentioned moment results in terms of $\widehat{D}_n(x)$. Although, following similar argument as in [20–22] we are able to obtain the following.

Theorem 1.2. *For any integer* $k \ge 1$ *and any real* $x \in [0, 1)$ *we have*

$$
\mathcal{M}_k(x) := \sum_{n=0}^{\infty} \left(e^x n! - \widehat{D}_n(x) \right)^k = e^{kx} \int_0^x \cdots \int_0^x \frac{e^{-(z_1 + \cdots + z_k)}}{1 - z_1 \cdots z_k} d\mathbf{Z},
$$
(1.11)

where **Z** *represents the k*-tuple (z_1, \ldots, z_k) *. More precisely,*

$$
\mathcal{M}_1(x) = e^{x-1} \left(\text{Ei}(1) - \text{Ei}(1-x) \right),\tag{1.12}
$$

where the exponential integral function Ei *[29, Section 6.2] is defined by the Cauchy principal value of the integral*

Also,

$$
\operatorname{Ei}(x) = -\int_{-x}^{\infty} \frac{e^{-z}}{z} dz.
$$

$$
\mathcal{M}_2(x) = 4e^{2x} \int_0^{\frac{x}{2}} \widehat{h}(z) dz,
$$
(1.13)

where

$$
\widehat{h}(z) = \frac{e^{-2z}}{\sqrt{1-z^2}} \tan^{-1} \frac{z}{\sqrt{1-z^2}} + \frac{e^{2z-2x}}{\sqrt{1-(x-z)^2}} \tan^{-1} \frac{z}{\sqrt{1-(x-z)^2}}.
$$

Remark 1.2. *The function* $\mathcal{M}_1(x)$ *defined by* (1.12) *satisfies* $\mathcal{M}_1(0) = 0$ *and* $\lim_{x\to 1^-} \mathcal{M}_1(x) =$ $+\infty$ *. Moreover, it satisfies the differential equation* $\mathcal{M}'_1(x) = \mathcal{M}_1(x) + 1/(1-x)$ *. Thus,* $\mathcal{M}'_1(x) > 0$ for $x \in [0, 1)$.

2 Proofs

2.1 Proof of Theorem 1.1

Let $P(n, j)$ be the number of j-permutations of n objects. We rewrite $\widehat{D}_n(x)$ in terms of $P(n, j)$ as follows

$$
\widehat{D}_n(x) = \sum_{j=0}^n P(n,j)x^{n-j} = x^n \sum_{j=0}^n P(n,j) \left(\frac{1}{x}\right)^j.
$$

Regarding a generating function for the finite sequence $(P(n, j))_{0 \leq j \leq n}$, it is known [21, Theorem 1.3] that for any integer $n \geq 0$ and for each real $x \neq 0$ we have

$$
\sum_{j=0}^{n} P(n,j) x^{j} = (-1)^{n} x^{n} e^{\frac{1}{x}} \int_{-\infty}^{-\frac{1}{x}} t^{n} e^{t} dt.
$$
 (2.1)

Replacing x by $\frac{1}{x}$, and changing the variable $t \to -t$ in the last integral, we deduce that

$$
\widehat{D}_n(x) = e^x \Gamma(n+1, x),
$$

where $\Gamma(\alpha, z)$ is the incomplete gamma function (see [29, Chapter 8] and [41, p. 1473]) defined by

$$
\Gamma(\alpha, z) = \int_z^{\infty} t^{\alpha - 1} e^{-t} dt.
$$

Note that $n! = \int_0^\infty t^n e^{-t} dt$. Thus,

$$
\widehat{D}_n(x) = e^x n! - \mathcal{R}_n(x),\tag{2.2}
$$

where $\mathcal{R}_n(x) = e^x \mathcal{I}_n(x)$ with

$$
\mathcal{I}_n(x) = \int_0^x t^n e^{-t} dt.
$$

The rest of proof is to obtain an asymptotic for $\mathcal{I}_n(x)$. Following an argument similar to the proofs of [20, Theorem 3] and [21, Theorem 1.1] we have

$$
\mathcal{I}_n(x) = \int_0^x t^n \sum_{j=0}^\infty \frac{(-t)^j}{j!} \, \mathrm{d}t = \sum_{j=0}^\infty \frac{(-1)^j}{j!} \int_0^x t^{n+j} \, \mathrm{d}t = \sum_{j=0}^\infty \frac{(-1)^j x^{n+j+1}}{j!(n+j+1)}.
$$

We split the last sum by using the following simple but useful identity, which is valid for any real c and positive integer r, provided $n + c \neq 0$,

$$
\frac{1}{n+c} = \sum_{k=1}^{r} (-1)^{k-1} \frac{c^{k-1}}{n^k} + \frac{(-1)^r}{n+c} \left(\frac{c}{n}\right)^r.
$$

Since $n > 0$, taking $c = j + 1$ with $j \ge 0$ fulfills the above condition. Thus,

$$
\sum_{j=0}^{\infty} \frac{(-1)^j x^{n+j+1}}{j!(n+j+1)} = \sum_{j=0}^{\infty} \sum_{k=1}^r \frac{(-1)^{k-1}}{n^k} \frac{(-1)^j (j+1)^{k-1}}{j!} x^{n+j+1} + (-1)^r \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(n+j+1)} \left(\frac{j+1}{n}\right)^r x^{n+j+1}.
$$

Therefore,

$$
\mathcal{I}_n(x) = \sum_{k=1}^r \frac{(-1)^{k-1} x^n}{n^k} \sum_{j=0}^\infty \frac{(-1)^j (j+1)^{k-1}}{j!} x^{j+1} + \frac{(-1)^r x^n}{n^r} \sum_{j=0}^\infty \frac{(-1)^j (j+1)^r}{j!(n+j+1)} x^{j+1}.
$$

Note that Touchard polynomials are hidden in hear of the inner sum, because

$$
\sum_{j=0}^{\infty} \frac{(-1)^j (j+1)^{k-1}}{j!} x^{j+1} = \sum_{j=0}^{\infty} (-1)^j \frac{(j+1)^k}{(j+1)!} x^{j+1} = \sum_{j=1}^{\infty} (-1)^{j-1} \frac{j^k}{j!} x^j
$$

$$
= -\sum_{j=1}^{\infty} (-x)^j \frac{j^k}{j!} = -\sum_{j=0}^{\infty} (-x)^j \frac{j^k}{j!} = -e^{-x} T_k(-x).
$$

Also, we have

$$
\left|\sum_{j=0}^{\infty} \frac{(-1)^j (j+1)^r}{j!(n+j+1)} x^{j+1}\right| \leq \sum_{j=0}^{\infty} \frac{(j+1)^r}{j!(n+j+1)} |x|^{j+1} < \frac{1}{n} \sum_{j=0}^{\infty} \frac{(j+1)^r}{j!} |x|^{j+1}.
$$

Note that

$$
\sum_{j=0}^{\infty} \frac{(j+1)^r}{j!} |x|^{j+1} = \sum_{j=0}^{\infty} \frac{(j+1)^{r+1}}{(j+1)!} |x|^{j+1} = \sum_{j=1}^{\infty} \frac{j^{r+1}}{j!} |x|^j = \sum_{j=0}^{\infty} \frac{j^{r+1}}{j!} |x|^j.
$$

Thus, we get

$$
\left|\sum_{j=0}^{\infty} \frac{(-1)^j (j+1)^r}{j!(n+j+1)} x^{j+1}\right| < \frac{1}{n} \sum_{j=0}^{\infty} \frac{j^{r+1}}{j!} |x|^j = \frac{1}{n} e^{|x|} T_{r+1}(|x|).
$$

Considering the above estimates we deduce that

$$
\mathcal{R}_n(x) = x^n \sum_{k=1}^r \frac{(-1)^k}{n^k} T_k(-x) + \widetilde{\mathcal{O}}\left(\frac{|x|^n}{n^{r+1}} e^{x+|x|} T_{r+1}(|x|)\right).
$$
 (2.3)

This completes the proof of Theorem 1.1. \Box

Remark 2.1. *We may rewrite* $\mathcal{I}_n(x)$ *in terms of the (second) incomplete gamma function [29, Chapter 8] defined by*

$$
\gamma(\alpha, z) = \int_0^z t^{\alpha - 1} e^{-t} dt \qquad (\Re(\alpha) > 0).
$$

Moreover, in the proof of (2.3) *we may take* $n > -1$ *any arbitrary real. Thus, from* (2.3) *we deduce that*

$$
\mathcal{I}_n(x) = \gamma(n+1, x) = \frac{x^n}{e^x} \sum_{k=1}^r \frac{(-1)^k}{n^k} T_k(-x) + \widetilde{\mathcal{O}}\left(\frac{|x|^n}{n^{r+1}} e^{|x|} T_{r+1}(|x|)\right).
$$

For more related expansions see [29, Section 8.7].

2.2 Proof of Theorem 1.2

We conclude from (2.2) that

$$
\mathcal{M}_k(x) = \sum_{n=0}^{\infty} \left(e^x \int_0^x t^n e^{-t} dt \right)^k = e^{kx} \lim_{N \to \infty} \sum_{n=0}^N \left(\int_0^x t^n e^{-t} dt \right)^k.
$$

By using Fubini's theorem [3, Theorem 5.32] we deduce that

$$
\mathcal{M}_k(x) = e^{kx} \lim_{N \to \infty} \sum_{n=0}^N \prod_{j=1}^k \left(\int_0^x z_j^n e^{-z_j} dz_j \right)
$$

\n
$$
= e^{kx} \lim_{N \to \infty} \sum_{n=0}^N \int_0^x \cdots \int_0^x \prod_{j=1}^k (z_j^n e^{-z_j}) d\mathbf{Z}
$$

\n
$$
= e^{kx} \lim_{N \to \infty} \int_0^x \cdots \int_0^x e^{-(z_1 + \cdots + z_k)} \sum_{n=0}^N (z_1 \cdots z_k)^n d\mathbf{Z}
$$

\n
$$
= e^{kx} \lim_{N \to \infty} \int_0^x \cdots \int_0^x e^{-(z_1 + \cdots + z_k)} \left(\frac{1 - (z_1 \cdots z_k)^{N+1}}{1 - z_1 \cdots z_k} \right) d\mathbf{Z}.
$$

Now we use the bounded convergence theorem [3, Theorem 3.26] to interchange the limit and multiple integral in the last relation. Since $\lim_{N\to\infty} (z_1 \cdots z_k)^{N+1} = 0$, we obtain (1.11).

For $k = 1$, the relation (1.11) reads as follows

$$
\mathcal{M}_1(x) = e^x \int_0^x \frac{e^{-t}}{1-t} dt.
$$

To evaluate the last integral we apply the change of variable $-z = 1 - t$, satisfying $t = 1 + z$ and $dt = dz$. Therefore

$$
\int_0^x \frac{e^{-t}}{1-t} dt = \int_{-1}^{x-1} \frac{e^{-1-z}}{-z} dz = e^{-1} \left(- \int_{-1}^{-(1-x)} \frac{e^{-z}}{z} dz \right) = e^{-1} \left(Ei(1) - Ei(1-x) \right).
$$

This gives (1.12).

For $k = 2$, the relation (1.11) reads as follows

$$
\mathcal{M}_2(x) = e^{2x} \int_0^x \int_0^x \frac{e^{-(z_1+z_2)}}{1-z_1z_2} dA_{z_1,z_2}.
$$

We denote the last double integral by $\mathcal J$. To compute $\mathcal J$ we follow an argument due to LeVeque [26], which has been described by Aigner and Ziegler in [2, Chapter 9]. Accordingly, we apply the change of coordinates by letting $u = (z_2 + z_1)/2$ and $v = (z_2 - z_1)/2$. We get the new domain of integration from old domain by first rotating it by -45° and then shrinking it by a factor of $\sqrt{2}$. This new domain of integration and the function to be integrated are symmetric with respect to the *u*-axis. Also, $dA_{z_1,z_2} = 2dA_{u,v}$. Therefore,

$$
\mathcal{J} = 4 \int_0^{\frac{x}{2}} \int_0^u \frac{e^{-2u}}{1 - u^2 + v^2} dv du + 4 \int_{\frac{x}{2}}^x \int_0^{x-u} \frac{e^{-2u}}{1 - u^2 + v^2} dv du
$$

=
$$
4 \int_0^{\frac{x}{2}} \frac{e^{-2u}}{\sqrt{1 - u^2}} \tan^{-1} \frac{u}{\sqrt{1 - u^2}} du + 4 \int_{\frac{x}{2}}^x \frac{e^{-2u}}{\sqrt{1 - u^2}} \tan^{-1} \frac{x - u}{\sqrt{1 - u^2}} du.
$$

By letting $z = x - u$ in the last integral and simplifying we obtain (1.13), hence concluding the proof. \Box

3 Conclusion

The idea of representing combinatorial numbers by integrals is a fruitful one, first done for generalized derangements by Even and Gillis [15]. By generalized derangements we mean the problem of redistributing elements of sets (boxes) of given sizes n_1, n_2, \ldots, n_k in such a way that nothing stays in the set (box) it originally occupied. Recently, the second author of the present paper, obtained integral representations for D_n , the number of derangements on a set of cardinality n, and w_{n+2} , the number of all distinct paths between a specific pair of vertices in a complete graph on $n + 2$ vertices, as follows

$$
D_n = \frac{n!}{e} + \sum_{k=1}^r (-1)^{n+k-1} \frac{B_k}{n^k} + \widetilde{\mathcal{O}}\left(\frac{B_{r+1}}{n^{r+1}}\right), \text{ and } w_{n+2} = e n! - \sum_{k=1}^r \frac{c_k}{n^k} + \widetilde{\mathcal{O}}\left(\frac{e^2 B_{r+1}}{n^{r+1}}\right),
$$

where B_k denotes the k-th Bell number, c_k is the sequence A014182 on OEIS [37], and by $f = \mathcal{O}(q)$ we mean $|f| \leq q$. Motivated by gathering the above asymptotic relations, in this paper we consider the following variant of the derangement polynomial, defined for any integer $n \geq 0$ and any real $x \neq 0$ by

$$
\widehat{D}_n(x) = n! \sum_{j=0}^n \frac{x^j}{j!}.
$$

Hence, $\widehat{D}_n(-1) = D_n$ and $\widehat{D}_n(1) = w_{n+2}$. We show that given any positive integer r, for any integer $n \geq 1$ and any real $x \neq 0$ we have

$$
\widehat{D}_n(x) = e^x n! - x^n \sum_{k=1}^r \frac{(-1)^k}{n^k} T_k(-x) + \widetilde{\mathcal{O}}\left(\frac{|x|^n}{n^{r+1}} e^{x+|x|} T_{r+1}(|x|)\right),
$$

where $T_k(x)$ is the k-th Touchard polynomial, admitting $B_k = T_k(1)$ and $c_k = (-1)^k T_k(-1)$. Moreover, we study the moments of the difference $e^x n! - \tilde{D}_n(x)$, by showing that for any integer $k \geq 1$ and any real $x \in [0, 1)$ we have

$$
\mathcal{M}_k(x) := \sum_{n=0}^{\infty} \left(e^x n! - \widehat{D}_n(x) \right)^k = e^{kx} \int_0^x \cdots \int_0^x \frac{e^{-(z_1 + \cdots + z_k)}}{1 - z_1 \cdots z_k} d\mathbf{Z},
$$

where Z represents the k-tuple (z_1, \ldots, z_k) . More precisely, $\mathcal{M}_1(x) = e^{x-1}$ (Ei(1) – Ei(1 – x)), where Ei denotes the exponential integral function, and

$$
\mathcal{M}_2(x) = 4e^{2x} \int_0^{\frac{x}{2}} \left(\frac{e^{-2z}}{\sqrt{1-z^2}} \tan^{-1} \frac{z}{\sqrt{1-z^2}} + \frac{e^{2z-2x}}{\sqrt{1-(x-z)^2}} \tan^{-1} \frac{z}{\sqrt{1-(x-z)^2}} \right) dz.
$$

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