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Computing the Permanental Polynomial of the High Level Fullerene C_{70} with High Precision

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Abstract

The permanental polynomial of IPR fullerene $C_{70}(D_{5h})$ is computed with quadruple precision arithmetic based on sparse graph on PC in acceptable time. The computing adopts 128 bits to store one float and works well for C_{70}, while the largest fullerene computed before is C_{60}, which can be easily obtained now. Some properties of the coefficients and zeroes of the permanental polynomials of IPR fullerenes C_{60} and C_{70} are also investigated. Computational results show the quadruple precision method can handle permanental polynomial of C_{70} and even larger fullerenes, which are of interest in applications.

1 Introduction

The permanental polynomial of a graph is of interest in chemical graph theory [1–5]. It is defined as follows:

$$\pi(G,\lambda) = per(\lambda I - A) = \sum_{k=0}^{n} b_k \lambda^{n-k}\,, \tag{1}$$

where A is the adjacency matrix of a graph G with n vertices, and I is the identity matrix of order n. Here $per(A)$ denotes the permanent of the matrix A, which is defined as

$$per(A) = \sum_{\sigma\in\Lambda_n} \prod_{i=1}^{n} a_{i\sigma(i)}\,, \tag{2}$$

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where Λ_n denotes the set of all permutations of {1,2,...,n}.

It can be traced back to 1981 that the permanental polynomial was considered in chemistry. Kasum et al. [6] investigated the properties of the permanental polynomial and demonstrated its relations to the structure of conjugated molecules. Computing the permanental polynomial of a graph is based on the computation of the permanent of the adjacency matrix of the graph. For a graph with n vertices, its permanental polynomial can be computed by $n/2 + 1$ permanents of $n \times n$ matrices and an $(n + 1)$-element FFT [7]. Evaluating the permanent of a matrix is proved to be a #P-complete problem in counting [8]. Even for one 3-regular matrix,which is with 3 nonzero entries in each row and column, computing its permanent is still a #P-complete problem [9]. Thus,the permanental polynomial of a graph is much harder in computation. The research on the graph polynomial was limited by the difficulty in its calculation for a long time. Over the last decade, this situation has changed with some efficient algorithms were proposed [5, 7, 10]. Cash investigated the properties of coefficients and zeroes by all fullerenes $C_{\leq 36}$ [11]. Then all the permanental polynomials of fullerenes $C_{\leq 50}$ were computed and some new properties were discovered [12]. Recently, a novel algorithm based on graph bisection for permanent of sparse graph was proposed [13]. The algorithm increases the computable scale of permanent for a sparse graph. However, it is also difficult to compute the permanental polynomial of larger sparse graph $C_n(n \geq 60)$ because of the double precision limitation.

Quadruple precision algorithm named as QPA is proposed in this paper to improve the ability of computation of the permanental polynomials. The idea of the method is simply based on the Fast Fourier Transformation (FFT) based method [7] and graph bisection based method [13]. It is possible to compute C_{70} and even larger fullerenes, which are of interest in many real-world applications.

The plan of this paper is the following. We give the quadruple precision algorithm(QPA) detail in section 2. The permanental polynomial for IPR fullerene C_{70} is given in section 3. The Properties of permanental polynomial of C_{60} and C_{70} are discussed in section 4. Finally some conclusions are given in Section 5.

2 Quadruple Precision Algorithm

2.1 Analysis of Computational Precision

The coefficients of a permanental polynomial are all integers, while inverse Fourier transformation gives output in real numbers. The rounded part of the FFT shows the computational precision to some extent. Let $round(x)$ be the integer which is the nearest to x and cof_C_n be the coefficients vector of C_n derived from FFT directly. The measure of the computational precision is shown as follows [7, 12].

$$error = \max_{1 \le k \le n+1} \mid round(cof\_C_n(k)) - cof\_C_n(k) \mid$$

Table 1 shows the double precision for FFT based method is not fit to compute the

Table 1: The error trend of the computational precision with double precision [7]

Fullerene	C_{20}	$C_{30}(C_{2\nu})$	$C_{40}(C1)$	$C_{50}(D_{5h})$
Error	4.37×10^{-11}	3.44×10^{-8}	1.49×10^{-5}	1.76×10^{-3}
Fullerene	$C_{52}(D_2)$	$C_{54}(D_3)$	$C_{56}(T_d)$	
Error	1.47×10^{-2}	8.16×10^{-2}	1.44×10^{-1}	

permanental polynomial of fullerene when the number of vertices $n > 56$.

2.2 The Quadruple Precision Algorithm

For handling the double precision limitation, in this paper we adapt fortran 95 as programming language and quadruple precision(128 bits) to compute the permanental polynomial of lager fullerene $C_{70}(D_{5h})$. It works well for the permanental polynomial of C_{70} and is promising to compute larger fullerenes. The high precision algorithm based on the graph bisection named as quadruple precision algorithm(**QPA**), is given as follows.

Algorithm QPA(Quadruple Precision Algorithm)

Input: A - an $n \times n$ 0-1 valued matrix.

Output: $(a_0, a_1, ..., a_n)$- the coefficients of $per(xI - A)$.

Step1: Let $\omega_{n+1} = e^{(-2\pi i)/(n+1)}$ be the $(n+1)$-th root of unity,

take $x_j = \omega_{n+1}^j (j = 0, 1, \cdots, n)$;

Step2: Computing $p_j = per(x_j I - A)$ for $j = 0, 1, \cdots, n$ by sparse permanent algorithm based on graph bisection(SP) [13];

Step3: Do inverse Fourier transform for $(p_0, p_1, \cdots, p_n)$ to get a^{IFFT};

Step4: $(a_0, a_1, \cdots, a_n) = \text{ANINT}(a^{IFFT})$.

Notes: The function ANINT(x) in the algorithm gives the integer that is closest to x; When compute $w_{n+1}^j (j = 0, 1, \cdots, n)$, take quadruple precision(128 bits) for π in step 1; Also adopt the same computational precision in step 2, 3, 4; Thus each function in the algorithm **QPA** must support the quadruple precision computation.

3 The Permanental Polynomial of $C_{70}(D_{5h})$

The result of permanental polynomial for buckminsterfullerene $C_{60}(I_h)$ was reported in [10]. It was achieved with intensive parallel computation. Using the High precision algorithm QPA, the permanental polynomial of IPR fullerene C_{60} can be easily obtained, and $C_{70}(D_{5h})$ is computed within acceptable time by PC. All numerical experiments in this paper are carried on an Intel Core i3 530(2930 MHz) with fortran 95 as the programing language. The coefficients of permanental polynomial of C_{70} are listed in Table 2.

In order to test the validity of the numerical results, the following three identify equations are applied,

$$per(I - A) = \sum_{i=0}^{n} a_i\,, \quad per(I + A) = \sum_{i=0}^{n} |a_i|\,, \quad per(2I - A) = \sum_{i=0}^{n} 2^i a_i\ .$$

For $C_{70}(D_{5h})$, the following equations holds:

$$per(I - A) = 425433425553580224, \quad \sum_{i=0}^{70} a_i = 425433425553580224;$$

$$per(I + A) = 3218848356932962496, \quad \sum_{i=0}^{70} |a_i| = 3218848356932962496;$$

$$per(2I - A) = 418584157483919600049622590200 = \sum_{i=0}^{70} 2^i a_i;$$

Computational results show that the coefficients of $C_{70}(D_{5h})$ obtained in this paper satisfy all of the equations. Table 3 shows the maximal errors of all C_n for $30 \le n \le 70$ and it shows very good performance for these fullerenes under the quadruple precision(128 bits). Permanental polynomials of lager fullerenes are promising to be obtained by the algorithm QPA.

Table 2: Coefficients of Permanental Polynomial of $C_{70}(D_{5h})$

power	coef	power	coef	power	coef
70	1	46	107008896432105	22	245494060539318985
69	0	45	-31722152142120	21	-199166020371411200
68	105	44	432795553705505	20	196878885263740003
67	0	43	-151016962132240	19	-155405515524027020
66	5250	42	1515742026255585	18	136830096741982390
65	-24	41	-613608311508140	17	-103153821051548260
64	166440	40	4610947639946519	16	81515675892315300
63	-2280	39	-2136939063152860	15	-57641574176393540
62	3758505	38	12214184625928020	14	40942439191026055
61	-102840	37	-6397962553436280	13	-26652478906287780
60	64388193	36	28232606977943430	12	16913747932999775
59	-2932200	35	-16501764332321040	11	-9920622582303100
58	870306935	34	5704584764816845 5	10	5539521700416647
57	-59361780	33	-3671151040750090 0	9	-2847465406090760
56	9530743885	32	1009169223775396 75	8	1360966721130985
55	-908688556	31	-7048837320088678 0	7	-589194336437960
54	86172442035	30	1565165004766352 26	6	230106708406160
53	-10936700360	29	-1168162740064889 20	5	-78766376928844
52	652299617065	28	2130434075652601 40	4	23162102035020
51	-106254055960	27	-1670283393571037 20	3	-5584320116600
50	4177691243662	26	2546296278965095 40	2	1044505555260
49	-848953954160	25	-2058831094429534 72	1	-134101348480
48	22821827937180	24	2671178346054737 80	0	9193937544
47	-5654832819880	23	-2184790467985530 80		

4 Properties of Permanental Polynomial of C_{70}

4.1 The Properties of Coefficients

Some relations between the coefficients of characteristic polynomial and permanental polynomial are presented by Gutman [14] and Chou et al [15]. In this section, several relations between the coefficients of the permanental and characteristic polynomials of $C_{70}(D_{5h})$ are also observed. Let G be the $C_{70}(D_{5h})$ graph. The characteristic polynomial of the adjacency matrix A of fullerene $C_{70}(D_{5h})$ is defined as follows.

$$\phi(G,\lambda) = det(\lambda I - A) \tag{3}$$

In parallel to Eq.(2), we write it in the coefficient form

$$\phi(G,\lambda) = \sum_{k=0}^{n} a_k \lambda^{n-k} \ . \tag{4}$$

For $k = 0, 1, \cdots, 9$, $|a_k| = |b_k|$. $a_{10} = 64388193$ and $b_{10} = -64387665$, so $|b_{10}| < a_{10}$ is satisfied. Moreover, it is shown that $|a_k| = |b_k|$ for the first few k's and $|a_k| < |b_k|$ for

Table 3: The trend of the computational precision with n

Fullerene	$C_{30}(C_{2\nu})$	$C_{40}(D_{2h})$	$C_{44}(T)$	$C_{50}(D_{5h})$
error	4.2579e-026	3.0300e-023	4.3352e-022	1.4042e-020
Fullerene	$C_{52}(D_2)$	$C_{56}(T_d)$	$C_{60}(I_h)$	$C_{70}(D_{5h})$
error	4.2000e-020	8.3241e-019	1.1277e-017	4.5680e-013

larger k's. Figure 1 shows $ln(|a_k|)$ and $ln(|b_k|)$ of C_{60} and C_{70}. One can see that $ln(|a_k|)$ and $ln(|b_k|)$ are very close before they reach the maximums. There is distinct difference between $ln(|a_k|)$ and $ln(|b_k|)$ when k is larger. This a general conclusion for an IPR fullerene from Theorem 3 by Ivan Gutman and Gordon G. Cash [14].

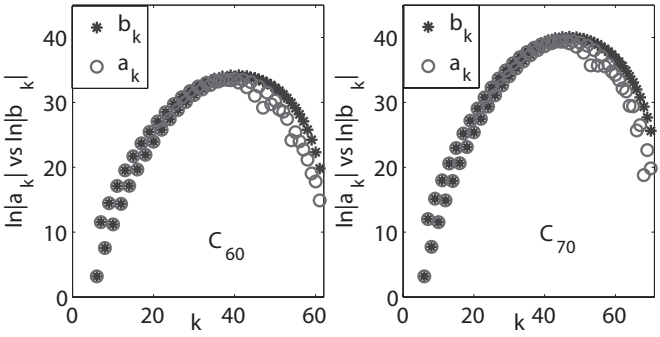

Figure 1: $ln(|a_k|)$ and $ln(|b_k|)$ of C_{60} and C_{70}

Let b_{max} be the largest positive coefficient of the permanental polynomial. The properties of b_{max} were studied by Cash [11] and Tong et al [12]. It was shown that b_{max}'s are very close in an isomer set C_n. Using the data of all fullerenes in $C_{\leq 50}$, a linear regression function of the average values of $\ln(b_{max})$ was given in [12].

$$Y = 0.58463n - 0.95477\,, \qquad r = 0.999991\,, \tag{5}$$

where n is the number of atoms.

The numerical results show that the maximum coefficient of C_{60} is b_{40} and that of C_{70} is b_{46}. The $ln(b_{max})$'s of C_{60} and C_{70} fit the equation (5) also very well. As shown in Table 4, the relative residual errors, $\frac{|Y - ln(b_{max})|}{Y}$, are no more than 0.4%.

Table 4: $ln(a_{max})$ of C_{60} and C_{70}

Fullerene	n	a_{max}	location	$ln(a_{max})$	Y
$C_{60}(I_h)$	60	710621056476228	40	34.1972	34.1230
$C_{70}(D_{5h})$	70	267117834605473780	46	40.1265	39.9693

4.2 The Properties of Zeroes

The following two results were addressed by Cash [11] and confirmed by Tong et al [12].

Property 4.1. *There are $n/2$ independent zeroes for each permanental polynomial. Ten of them are nearly a constant for all isomers in C_n with fixed n, while the remaining $n/2-10$ zeroes vary with structure.*

The ten clustered zeroes that seem to characterize any given isomer sets also vary in a systematic way with molecular size n.

Property 4.2. *The average values of three clusters among the ten are nearly straight lines for each isomer sets C_n as n varies. In all three cases, the order of points on the line is monotonic to the carbon numbers n.*

The $n/2$ independent zeroes of C_{60} and C_{70} are shown in Figure 2. The distributions of the zeroes of the two fullerenes are close, and we also note that the zeroes are all complex with nonzero real and imaginary parts.

The linear equations for the average values of the three zero clusters were given from the data of all fullerenes in $C_{\leq 50}$ [12].

$$cluster(1): \ y = -5.20722x - 2.69918, \quad r = 0.999026 \tag{6}$$

$$cluster(2): \ y = +2.16174x + 2.16390, \quad r = 0.993564 \tag{7}$$

$$cluster(3): \ y = -0.45937x + 2.91265, \quad r = 0.990359 \tag{8}$$

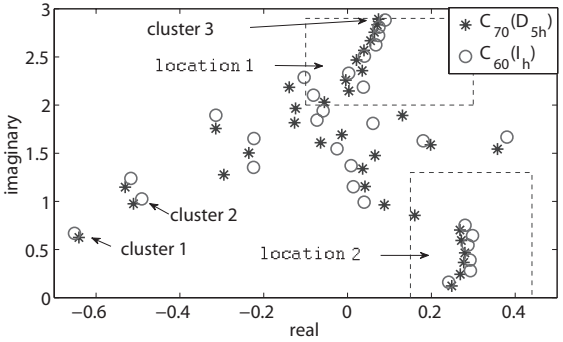

Figure 2: Zeroes of the permanental polynomials of $C_{60}(\circ)$ and $C_{70}(*)$

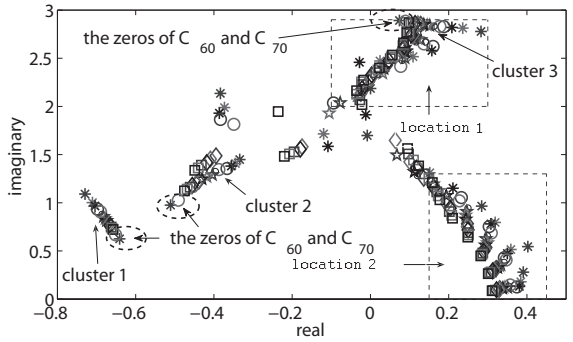

Figure 3: The linear patterns of zeroes

The roots of the permanental polynomials of the fullerenes C_{60} and C_{70} are shown in Figure 2. Because of the demand of precision, the roots can be obtained with symbolic computation from many scientific computation software, such as MATLAB, MAPLE and MATHEMATICA. Since all their roots appear in conjugate pairs, only up-half plane is plotted. Roots of the characteristic polynomials are useful in chemical graphs. As with the coefficients, this may suggest future uses of the roots of the permanental polynomial as well. The zeroes of C_{60} and C_{70}, which are corresponding to the three linear patterns, cluster 1-3, are marked in Figure 2. The average values of the zero clusters for each isomer series from C_{20} to C_{50} are given in Figure 3. The six zeroes, which are associated to C_{60} and C_{70} are also plotted in the Figure 3 and marked by dash ellipses. It is obvious that they fit the equations (6)-(8) very well. The order of points on the line is monotonic to the carbon numbers. The residual errors of the six points are no more than 0.08.

There are more linear patterns were observed in the two locations [12], which are enclosed by 0.15, 0.15+1.3i, 0.42, 0.42+1.3i and -0.1+2i, -0.1+2.9i, 0.3+2i, 0.3+2.9i and marked in Figure 2 and Figure 3. In location 1, there are 8 zeroes of permanental polynomial of $C_{60}(\circ)$ and 10 zeroes of permanental polynomial of $C_{70}(*)$. In the location 2, the numbers of zeroes are 7 and 6 respectively. Almost half of the zeroes of C_{60} and C_{70} are contained in the two locations. These zeroes show the regularity obviously.

5 Conclusions

In this paper, an efficient quadruple precision algorithm(QPA) is proposed for computing the permanental polynomial of fullerenes($n \geq 60$). For fullerene-type graph, the computable scale of permanents and permanental polynomial increases in acceptable time by PC. By the algorithm QPA, the permanental polynomial of fullerene C_{70} is obtained. We find that some of the properties of the permanental polynomials of IPR C_{60} and C_{70} are consistent with those proposed by [11, 12], which are obtained through data of $C_{\leq 36}$ and $C_{\leq 50}$.

With the analysis of the precision trend of the algorithm QPA, it is promising to compute the permanental polynomials of larger fullerenes($n \geq 60$) in bulk. The algorithm is also applicable to other types of chemical graphs. Using the more plentiful data, more work could be done in identifying the relationship of the permanental polynomial to chemical structure and properties. This is one of our future projects.

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