Available online at www.sciencedirect.com
ScienceDirect
Discrete Mathematics 307 (2007) 2979–2992
DISCRETE MATHEMATICS
www.elsevier.com/locate/disc

# Counting labeled general cubic graphs

Gab-Byung Chae[a], Edgar M. Palmer[b], Robert W. Robinson[c]

[a]Department of Mathematics, Yonsei University, Wonju, Korea 220-710, Republic of Korea
[b]Department of Mathematics, Michigan State University, East Lansing, MI 48823, USA
[c]Computer Science Department, University of Georgia, Athens, GA 30602-7404, USA

Received 5 October 2005; received in revised form 6 December 2006; accepted 10 March 2007
Available online 15 March 2007

**Abstract**

Recurrence relations are derived for the numbers of labeled 3-regular graphs with given connectivity, order, number of double edges, and number of loops. This work builds on methods previously developed by Read, Wormald, Palmer, and Robinson.


*MSC:* 05A15

*Keywords:* General cubic graphs; Labeled enumeration; Exponential generating functions; Connectivity; Recurrence relations

## 1. Introduction

Enumeration problems for cubic (i.e., 3-regular) graphs have a long history [4], and have been studied by chemists [1] as well as mathematicians. In his dissertation [7], Read derived recurrence relations for the numbers of connected labeled general cubic graphs by a reduction technique which we discuss further below. His aim was to deduce recurrences for the numbers of labeled connected simple cubic graphs and the numbers of unrestricted labeled simple cubic graphs. These were later reported in a paper [8] which omitted many of the algebraic details. Read's recurrences were equivalent to a non-linear second order differential equation satisfied by the exponential generating function (egf) for the labeled connected simple cubic graphs, and a linear second order differential equation satisfied by the egf for unrestricted labeled simple cubic graphs. Wormald [12] applied reductions to enumerate labeled simple cubic graphs without having to treat arbitrary general cubic graphs. He found differential equations for counting labeled $k$-connected simple cubic graphs for $k = 0, 1, 2$, and 3. For each $k$ he derived a recurrence relation and used it to calculate the numbers for order up to 30. These results appeared in his dissertation [11].

More recently Palmer, Read, and Robinson found a recurrence relation for the number of labeled claw-free cubic graphs. They derived a linear partial differential equation based on removing a simple edge which is satisfied by the egf of labeled general cubic graphs [6, Eq. (1)], and mentioned that it could be used to derive a recurrence relation for the number $g(s, d, l)$ of labeled general cubic graphs with no triple edges having $s$ simple edges, $d$ double edges and $l$ loops. In the present paper this is carried out by extracting coefficients from their differential equation. Then the logarithmic derivative is treated in the same way to provide a recurrence relation for the corresponding number $g_1(s, d, l)$ of labeled connected general cubic graphs. Next, the method which Wormald [12] developed to count labeled 2-connected simple

*E-mail addresses:* rivendell@yonsei.ac.kr (G.-B. Chae), palmer@math.msu.edu (E.M. Palmer), rwr@cs.uga.edu (R.W. Robinson).

0012-365X/$ - see front matter 
doi:10.1016/j.disc.2007.03.011

cubic graphs is generalized to allow for double edges. Again this is based on removing a simple edge, yielding a pde for the egf and a corresponding recurrence relation for the number $g_2(s, d)$ of labeled 2-connected general cubic graphs. These recurrences are used to calculate numbers of labeled general cubic graphs which are $k$-connected for $k = 0$, 1, and 2. Note that 3-connected general cubic graphs can contain no loops or multiple edges, so these are just the 3-connected simple cubic graphs counted by Wormald [12]. The reader is referred to [5, Chapter 1] for an introduction to the techniques essential for counting labeled graphs, including the use of egf's.

We also derive alternative sets of recurrences for the numbers of labeled general cubic graphs which are $k$-connected for $k = 0$, 1, and 2. These are based on removing loops and double edges, which give linear recurrences even when $k = 1$ or 2. Because of this the alternative sets of recurrences are asymptotically more efficient when $k = 1$ or 2. Our alternative approach is similar to that taken by Read in Chapter 3 of his dissertation [7, pp. 34–54], where simple edge deletion was only treated for simple cubic graphs. The major difference, which added complexity to Read's derivation, was that he maintained an extra enumeration parameter for trumpets, which are subgraphs on three vertices containing one double edge and two simple edges. Another difference is that his reductions were all applied in the connected case. His objective was to find recurrences for counting simple graphs, so for the unrestricted case (0-connected) a recurrence was found only for simple cubic graphs.

## 2. General cubic graphs

Let $G(x, y, w) = \sum_{s,d,l} g(s, d, l)x^s y^d w^l/(2n)!$ be the egf of general cubic graphs. The first and second order partial derivatives of $G(x, y, w)$ are denoted in the usual way. For example, $G_x$ is the partial derivative of $G(x, y, w)$ with respect to $x$. Furthermore, $G_x$ is the egf for labeled cubic graphs which are rooted at a simple edge but the root edge is not represented by a factor of $x$.

Palmer et al. [6] derived a partial differential equation involving these egf's by applying a reduction operation which removes the root edge. This operation is performed on a cubic graph $H$ in the following way. Suppose $u$ and $v$ are the vertices of the root edge. Let $u_1$ and $u_2$ be the other neighbors of $u$, while $v_1$ and $v_2$ are the other neighbors of $v$. Now we remove from $H$ the vertices $u$ and $v$ and edges incident with them. Then we add the new edges $u_1u_2$ and $v_1v_2$, which become new root edges. Thus the degrees of $u_1$, $u_2$, $v_1$, and $v_2$ are preserved. However, there are many possibilities for the types of new root edges that may result. Each of the two new edges could be a simple edge, part of a double or triple edge, an ordinary loop, or a *pointless loop*, which is a loop without point, depending on how the vertices $u_1$, $u_2$, $v_1$, and $v_2$ were originally related. There are 17 types of new root pairs, which can be seen based on the following observations. First, if $u$ has an incident ordinary loop, a pointless root loop results from deleting the root edge $uv$ from $H$. Second, if $u$ has an incident double edge, an ordinary root loop at $u$ is created by the reduction. Third, if $u$ has two incident simple edges $uu_1$ and $uu_2$, then the reduction gives rise to a simple root edge if there was no edge $u_1u_2$ in $H$, a double root edge if there was an edge $u_1u_2$ in $H$, or a triple root edge if there was an double edge $u_1u_2$ in $H$. These observations also apply at the other vertex $v$ of the root edge.

However, among the new roots a pointless root loop or a triple root edge is not allowed as a component of a cubic graph. Therefore any such components are dropped and the above operations convert $H$ to another cubic graph having 2, 4 or 6 fewer vertices than $H$ and 2, 1, or 0 root edges. The egf was found for each of the 17 types of rooted graph, leading to the following partial differential equation [6, Eq. (1)]:

$$
\begin{aligned}
G_x = {} & \left(\frac{w^2}{2} + \frac{x^5}{4} + \frac{x^2yw}{2} + \frac{x^4y^2}{8}\right) G \\
& + \left(x^2w + \frac{x^4y}{2}\right) G_x + \left(\frac{x^4}{2} + x^3w + \frac{x^5y}{2}\right) G_y \\
& + \left(yw + \frac{x^2y^2}{2}\right) G_w + \frac{x^4}{2} G_{xx} + x^5 G_{xy} \\
& + x^2yG_{xw} + \frac{x^6}{2} G_{yy} + x^3yG_{yw} + \frac{y^2}{2} G_{ww}.
\end{aligned} \tag{1}
$$

Every non-empty cubic graph without triple edges must contain at least one simple edge. Therefore we assume $s > 0$ and extract the coefficient of $x^{s-1}y^d w^l/(2n)!$ from both sides of Eq. (1), giving the following recurrence relation for the number of labeled cubic graphs in which the only boundary conditions we need are $g(0,0,0)=1$ and $g(s,d,l)=0$ if $s<1$, $d<0$, or $l<0$.

$$\begin{aligned} g(s,d,l) = \frac{1}{s}\Bigg\{ &\binom{2n}{2} g(s-1,d,l-2) + (6+12d)\binom{2n}{4} g(s-6,d,l) \\ &+ 12\binom{2n}{4} g(s-3.d-1,l-1) + 90\binom{2n}{6} g(s-5,d-2,l) \\ &+ 2(s-2)\binom{2n}{2} g(s-2,d,l-1) + 12(s-4)\binom{2n}{4} g(s-4,d-1,l) \\ &+ \binom{2n}{2}((d+1)+2(s-5)(d+1))g(s-5,d+1,l) \\ &+ 2(d+1)\binom{2n}{2} g(s-4,d+1,l-1) + 2l\binom{2n}{2} g(s-1,d-1,l) \\ &+ 12(l+1)\binom{2n}{4} g(s-3,d-2,l+1) + (s-3)(s-4)\binom{2n}{2} g(s-3,d,l) \\ &+ 2(s-2)(l+1)\binom{2n}{2} g(s-2,d-1,l+1) \\ &+ (d+2)(d+1)\binom{2n}{2} g(s-7,d+2,l) \\ &+ 2d(l+1)\binom{2n}{2} g(s-4,d,l+1) \\ &+ (l+2)(l+1)\binom{2n}{2} g(s-1,d-2,l+2)\Bigg\}. \end{aligned} \tag{2}$$

Since the recurrence relation (2) requires a bounded number of arithmetic operations to calculate $g(s,d,l)$ (independently of $s$, $d$, and $l$) it is seen that all values for order up to $2n$ can be computed with $O(n^3)$ arithmetic operations in total.

An alternative to the recurrence relation (2) can be obtained from a known recurrence for simple cubic graphs combined with recurrences based on operations which remove a loop and contract a double edge. Let $q_n$ denote the number of labeled simple cubic graphs of order $2n$. Then [12, Eq. (2.6)] takes the form

$$\begin{aligned} q_{n+1} = {} & (2n+1)(3n^2+5n)q_n - \binom{2n+1}{3} q_{n-1} \\ & - 20\binom{2n+1}{5}(9n^2-36n+38)q_{n-2} - 6\times 7!\binom{2n+1}{8} q_{n-3} \\ & - 6\times 7!\binom{2n+1}{9}(3n-14)q_{s-4} + 330\times 7!\binom{2n+1}{11} q_{n-5}, \end{aligned} \tag{3}$$

which holds for all $n\geqslant 0$ with boundary conditions $q_0=1$ and $q_n=0$ whenever $n<0$. The removal operation for a given loop removes it along with its vertex and its adjacent simple edge, then smooths out the vertex of degree 2 at the other end of the simple edge. The order is reduced by 2, and the smoothing produces a new edge which must be (or belong to) a simple edge, a double edge, a normal loop, a pointless loop, or a triple edge. A pointless loop is obtained if the loop chosen for removal belongs to a *dumbbell*, which is an order 2 connected component consisting of two loops joined by a simple edge. A triple edge is obtained when the chosen loop belongs to a *wine glass*, which is an order 4 component containing a loop and a double edge. In terms of the egf $G(x,y,w)$ and its first order partial derivatives, the choice of a loop followed by its removal gives the equation

$$G_w = x^3G_x + x^4G_y + xyG_w + \left(xw + \frac{x^3y}{2}\right)G, \tag{4}$$

which is [6, Eq. (3)]. Now set $y = 0$ and for $l \geqslant 1$ extract the coefficient of $x^s w^{l-1}/(2n)!$ from both sides of Eq. (4), giving the recurrence

$$g(s, 0, l) = \frac{2}{l}\binom{2n}{2}\{(s-2)g(s-2, 0, l-1) + g(s-4, 1, l-1) + g(s-1, 0, l-2)\}, \tag{5}$$

which holds for $l \geqslant 1$ and $s \equiv -l \pmod 3$.

The contraction operation for a given double edge contracts it to a vertex of degree 2, which it then smooths out. Again the order is reduced by 2, and the smoothing produces a new edge which must be (or belong to) a simple edge, a double edge, a normal loop, or a triple edge. Note that a pointless loop would have to come from a triple edge, which has been excluded by definition. A triple edge is obtained when the chosen double edge belongs to an order 4 component containing two double edges, called a *drum*. In terms of the egf $G(x, y, w)$ and its first order partial derivatives, the choice of a double edge followed by its contraction gives the equation

$$G_y = x^2 G_x + x^3 G_y + \frac{x^2}{2} G_w + \frac{x^2 y}{2} G, \tag{6}$$

which is [6, Eq. (2)]. For $d \geqslant 1$ extract the coefficient of $x^s y^{d-1} w^l/(2n)!$ from both sides of Eq. (6) to obtain the recurrence

$$\begin{aligned} g(s, d, l) = \frac{1}{d}\binom{2n}{2}\{&2(s-1)g(s-1, d-1, l) + 2dg(s-3, d, l) \\ &+ (l+1)g(s-2, d-1, l+1) + (2n-2)(2n-3)g(s-2, d-2, l)\}, \end{aligned} \tag{7}$$

which holds for $d \geqslant 1$ and $s \equiv d - l \pmod 3$.

One can now calculate $g(3m, 0, 0) = q_m$ from relation (3) by induction on $m$, then $g(3m-l, 0, l)$ from relation (5) by induction on $l$, and finally $g(3m-2d-l, d, l)$ from relation (7) by induction on $d$. With this alternate approach all of the values for order up to $2n$ can be computed with $O(n^3)$ arithmetic operations. This is the same growth rate as for calculation based on relation (2).

In `Maple` the alternate approach runs about twice as fast as the first approach. For connected and 2-connected cubic graphs it will be seen in the next two sections that the alternate approach leads to more significant improvements in calculation efficiency.

## 3. Connected general cubic graphs

Eq. (1) can be converted to a partial differential equation whose formal solution is the egf for the number of connected cubic graphs by the substitution $G(x, y, w) = e^{G_1(x,y,w)}$, where $G_1(x, y, w)$ is the egf for connected cubic graphs, i.e., $G_1(x, y, w) = \sum_{s,d,l} g_1(s, d, l) x^s y^d w^l/(2n)!$. This substitution followed by dividing through by $G(x, y, w)$ gives

$$\begin{aligned} (G_1)_x = &\left(\frac{w^2}{2} + \frac{x^5}{4} + \frac{x^2yw}{2} + \frac{x^4y^2}{8}\right) \\ &+ \left(x^2w + \frac{x^4y}{2}\right)(G_1)_x + \left(\frac{x^4}{2} + x^3w + \frac{x^5y}{2}\right)(G_1)_y \\ &+ \left(yw + \frac{x^2y^2}{2}\right)(G_1)_w + \frac{x^4}{2}(G_1)_{xx} + x^5(G_1)_{xy} \\ &+ x^2y(G_1)_{xw} + \frac{x^6}{2}(G_1)_{yy} + x^3y(G_1)_{yw} + \frac{y^2}{2}(G_1)_{ww} \\ &+ \frac{x^4}{2}(G_1)_x(G_1)_x + x^5(G_1)_x(G_1)_y + x^2y(G_1)_x(G_1)_w \\ &+ \frac{x^6}{2}(G_1)_y(G_1)_y + x^3y(G_1)_y(G_1)_w + \frac{y^2}{2}(G_1)_w(G_1)_w. \end{aligned} \tag{8}$$

As we did for Eq. (1), we can find a recurrence relation for the numbers of connected cubic graphs by extracting the coefficient of $x^{s-1}y^d w^l/(2n)!$ from both sides of (8):

$$
\begin{aligned}
g_1(s,d,l) = \frac{1}{s}\Bigg\{ & 2(s-2)\binom{2n}{2} g_1(s-2,d,l-1) + 12(s-4)\binom{2n}{4} g_1(s-4,d-1,l) \\
& + (d+1)(2s-9)\binom{2n}{2} g_1(s-5,d+1,l) \\
& + 2(d+1)\binom{2n}{2} g_1(s-4,d+1,l-1) + 12d\binom{2n}{4} g_1(s-6,d,l) \\
& + 2l\binom{2n}{2} g_1(s-1,d-1,l) + 12(l+1)\binom{2n}{4} g_1(s-3,d-2,l+1) \\
& + (s-3)(s-4)\binom{2n}{2} g_1(s-3,d,l) \\
& + 2(s-2)(l+1)\binom{2n}{2} g_1(s-2,d-1,l+1) \\
& + (d+1)(d+2)\binom{2n}{2} g_1(s-7,d+2,l) \\
& + 2d(l+1)\binom{2n}{2} g_1(s-4,d,l+1) \\
& + (l+1)(l+2)\binom{2n}{2} g_1(s-1,d-2,l+2)\Bigg\} \\
& + \frac{(2n)!}{2s}\Bigg\{ \sum_{i,j,k}^{s-3,d,l} \frac{i g_1(i,j,k)(s-3-i) g_1(s-3-i,d-j,l-k)}{(m_{i,j,k})!\cdot(m_{s-3-i,d-j,l-k})!} \\
& + \sum_{i,j,k}^{s-5,d+1,l} \frac{2i g_1(i,j,k)(d+1-j) g_1(s-5-i,d+1-j,l-k)}{(m_{i,j,k})!\cdot(m_{s-5-i,d+1-j,l-k})!} \\
& + \sum_{i,j,k}^{s-2,d-1,l+1} \frac{2i g_1(i,j,k)(l+1-k) g_1(s-2-i,d-1-j,l+1-k)}{(m_{i,j,k})!\cdot(m_{s-2-i,d-1-j,l+1-k})!} \\
& + \sum_{i,j,k}^{s-7,d+2,l} \frac{j g_1(i,j,k)(d+2-j) g_1(s-7-i,d+2-j,l-k)}{(m_{i,j,k})!\cdot(m_{s-7-i,d+2-j,l-k})!} \\
& + \sum_{i,j,k}^{s-4,d,l+1} \frac{2j g_1(i,j,k)(l+1-k) g_1(s-4-i,d-j,l+1-k)}{(m_{i,j,k})!\cdot(m_{s-4-i,d-j,l+1-k})!} \\
& + \sum_{i,j,k}^{s-1,d-2,l+2} \frac{k g_1(i,j,k)(l+2-k) g_1(s-1-i,d-2-j,l+2-k)}{(m_{i,j,k})!\cdot(m_{s-1-i,d-2-j,l+2-k})!}\Bigg\},
\end{aligned} \tag{9}
$$

where $m_{i,j,k} = (2i+4j+2k)/3$ and $s>0$.

This recurrence relation is supported by the boundary conditions $g_1(1,0,2)=1$, $g_1(6,0,0)=1$, $g_1(3,1,1)=12$, $g_1(5,2,0)=270$, and $g_1(s,d,l)=0$ if $s<1$, $d<0$, or $l<0$. The non-zero boundary conditions are determined by the first four terms on the right side of Eq. (8).

The triple sums lead to $O(n^3)$ arithmetic operations to calculate $g_1(s,d,l)$. Thus to compute all values for order up to $2n$ using relation (9) takes $O(n^6)$ arithmetic operations in total. The increased complexity of $O(n^6)$ compared with $O(n^3)$ obtained for the 0-connected numbers in the previous section comes from the non-linearity of Eq. (8), which in turn is due to the fact that removing a simple edge may not preserve 1-connectivity.

We now derive an alternative to the recurrence relation (9) which reduces the complexity of the overall calculation from $O(n^6)$ to $O(n^3)$ arithmetic operations. It is obtained in the same way that an alternative to relation (2) was found in the previous section. Let $r_n$ satisfy the initial conditions $r_0=0$, $r_1=0$, $r_2=1$ and the recurrence relation

$$r_n = 3nr_{n-1} + 4r_{n-2} + 2r_{n-3} + \sum_{i=2}^{n-3} r_i(r_{n-1-i} - 2r_{n-2-i} - 2r_{n-3-i}) \tag{10}$$

for all $n \geqslant 3$. Then from [12, Section 3] the numbers of labeled connected simple cubic graphs are given by

$$g_1(3n,0,0) = \frac{(2n)!}{3n2^n}(r_n - 2r_{n-1} - 2r_{n-2}) \tag{11}$$

for all $n \geqslant 2$. The operations defined in the previous section for removing a loop or contracting a double edge both preserve connectedness. Therefore when applied to connected cubic graphs these two operations give rise to egf equations which are very similar to (4) and (6), and in particular are still linear:

$$(G_1)_w = x^3(G_1)_x + x^4(G_1)_y + xy(G_1)_w + xw + \frac{x^3y}{2}, \tag{12}$$

$$(G_1)_y = x^2(G_1)_x + x^3(G_1)_y + \frac{x^2}{2}(G_1)_w + \frac{x^2y}{2}. \tag{13}$$

Now set $y=0$ and for $l \geqslant 1$ extract the coefficient of $x^s w^{l-1}/(2n)!$ from both sides of Eq. (12), giving the recurrence

$$g_1(s,0,l) = \frac{2}{l}\binom{2n}{2}\{(s-2)g_1(s-2,0,l-1) + g_1(s-4,1,l-1)\}, \tag{14}$$

which holds for $l \geqslant 1$ and $s \equiv -l \pmod 3$ except that $g_1(1,0,2)=1$ (corresponding to the dumbbell term $xw$).

For $d \geqslant 1$ extract the coefficient of $x^s y^{d-1} w^l/(2n)!$ from both sides of Eq. (13) to obtain the recurrence

$$\begin{aligned} g_1(s,d,l) = \frac{1}{d}\binom{2n}{2}\{&2(s-1)g_1(s-1,d-1,l) + 2dg_1(s-3,d,l) \\ &+ (l+1)g_1(s-2,d-1,l+1)\}, \end{aligned} \tag{15}$$

which holds for $d \geqslant 1$ and $s \equiv d-l \pmod 3$ except that $g_1(2,2,0)=6$ (corresponding to the drum term $x^2y/2$).

One can now compute $r_m$ from relation (10) by induction on $m$, allowing $g_1(3m,0,0)$ to be calculated on the basis of relation (11) for $m \geqslant 2$. Of course $g_1(s,0,0)=0$ if $s<6$ or if $s$ is not divisible by 3. Then $g_1(3m-l,0,l)$ is determined from relation (14) by induction on $l$, and finally $g_1(3m-2d-l,d,l)$ from relation (15) by induction on $d$. With this alternate approach all of the values for order up to $2n$ can be computed with $O(n^3)$ arithmetic operations. This is much faster asymptotically that the $O(n^6)$ operations needed to calculate the same values on the basis of the single recurrence relation (9).

In `Maple` the alternate approach runs very much more quickly even for small orders. The `Maple` calculations and conjectures which they suggest or support are discussed in the penultimate section.

## 4. 2-connected general cubic graphs

To find the numbers of 2-connected cubic graphs, we use an approach different from that of previous sections. Following Wormald [12] we begin with graphs which are cubic except for one or two vertices of degree 2. Since we modify and extend Wormald's method for simple cubic graphs to general cubic graphs, we will use his terminology.

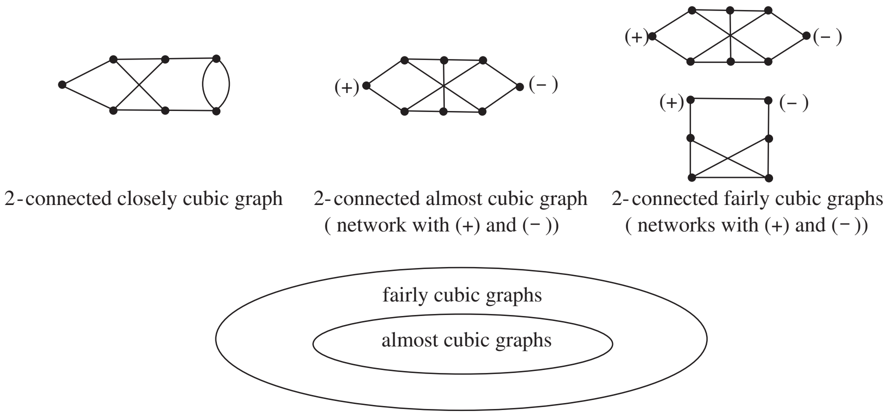


Fig. 1. Types of 2-connected graphs and networks.

A *closely cubic* graph is a graph in which just one vertex is of degree 2 and the rest are of degree 3. A *fairly cubic* graph is a graph in which two vertices are of degree 2 and the rest are of degree 3. An *almost cubic* graph is a fairly cubic graph in which the two vertices of degree 2 are non-adjacent. A *special almost cubic graph* is an almost cubic graph which is not 2-connected but becomes 2-connected after joining the two vertices of degree two. A *network* is a graph in which one vertex is distinguished as a positive pole $(+)$ and a second vertex is distinguished as a negative pole $(-)$. A *special almost cubic network* is a special almost cubic graph in which the two vertices of degree 2 are distinguished as a positive pole and a negative pole. An *almost cubic network* and a *fairly cubic network* are defined similarly (see Fig. 1).

Let $G_2(x, y)$ be the egf $G_2(x, y) = \sum_{s,d} g_2(s, d)x^s y^d/(2n)!$ where $g_2(s, d)$ is the number of 2-connected labeled cubic graphs with $s$ simple edges, $d$ double edges and order $2n = (2s + 4d)/3$. The loop parameter is absent here because 2-connected cubic graphs have no loops. Let $C(x, y)$ be the egf for the number $c(s, d)$ of 2-connected closely cubic graphs, where the order is $2n-1=(2s+4d+1)/3$. For fairly cubic graphs the order is $2n=(2s+4d+2)/3$ and we define egf's $F(x, y)$, $A(x, y)$ and $B(x, y)$ for the numbers $f(s, d)$ of all 2-connected fairly cubic graphs, $a(s, d)$ of 2-connected almost cubic graphs and $b(s, d)$ of special almost cubic networks, respectively. The next task is to find five relationships among the numbers of the graphs above and derive a recurrence relation for the number $g_2(s, d)$ of 2-connected labeled cubic graphs. We begin with definitions of some basic graph operations that are useful in relating the five types of graphs just defined. The *removal* of a vertex from a graph is the operation which removes the vertex and all incident edges. The *suppression* of a vertex $v$ of degree 2 consists of removing $v$ and joining the two vertices formerly adjacent to $v$ by a new edge.

The first relationship comes from removing a simple edge from a 2-connected cubic graph, which produces a 2-connected almost cubic graph or a special almost cubic graph. The latter has connectivity 1 (see Fig. 2). There are $s$ ways to choose a simple edge to remove. Hence we have

$$s \cdot g_2(s, d) = a(s-1, d) + b(s-1, d)/2.$$

Equivalently,

$$(G_2)_x = A + B/2. \tag{16}$$

Next, consider the operation of removing the vertex of degree 2 from a 2-connected closely cubic graph, which produces two vertices of degree 2 (see Fig. 3). That means we will be left with a 2-connected fairly cubic graph if the resulting graph is still 2-connected, or a special almost cubic graph if it has connectivity 1. But there is an extra term needed, because a 2-connected closely cubic graph which has one double edge and two simple edges on three vertices (following Read [8] we call this a *trumpet*) can be converted into a graph with one double edge on two vertices. The latter graph does not belong to any of the classes of graphs established above. The inverse operation is to add a new vertex to a 2-connected fairly cubic graph or a special almost cubic graph to produce $(2n-1)$ closely cubic graphs.

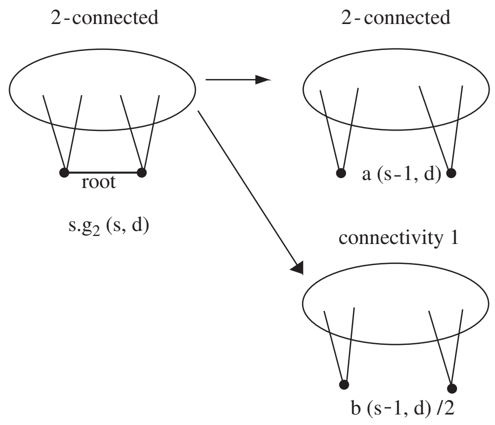


Fig. 2. Conversion of 2-connected cubic graphs rooted at a simple edge.

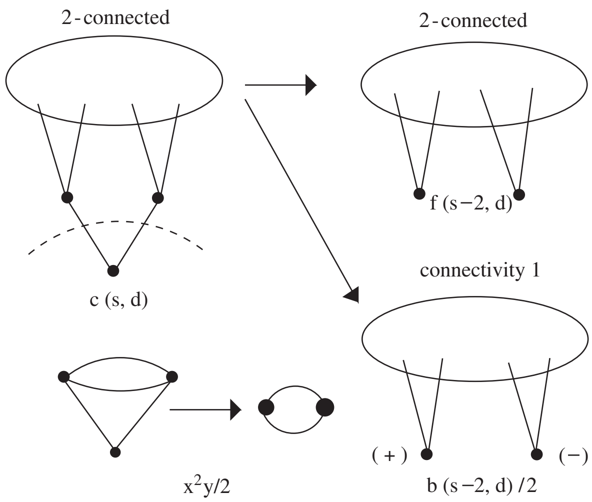


Fig. 3. Conversion of 2-connected closely cubic graphs.

The factor of $(2n-1)$ is the number of ways to label the new vertex. Therefore we have $c(s,d)=(2n-1)f(s-2,d)+(2n-1)b(s-2,d)/2$, for $(s,d)\neq(2,1)$. Then the relationship between the numbers of these graphs in egf form is

$$C=x^2F+\frac{x^2}{2}B+\frac{x^2y}{2}, \tag{17}$$

where the egf $x^2y/2$ is for the trumpet.

The next task is to find a relationship between the 2-connected fairly cubic graphs and other graphs (see Fig. 4). The 2-connected fairly cubic graphs consist of 2-connected almost cubic graphs and the graphs which have the two vertices of degree 2 adjacent to each other. From the latter we remove the two vertices of degree 2 and all incident edges. The resulting graph is a 2-connected fairly cubic graph or a special almost cubic graph depending on its connectivity. Again we have to add an extra term corresponding to the fairly cubic graphs which consist of three simple edges and one double edge on four vertices. These have $x^3y/2$ as egf. The removal of two adjacent vertices of degree 2 reduces the number of simple edges by 3. Hence we have $f(s,d)=a(s,d)+(2n)(2n-1)f(s-3,d)+(2n)(2n-1)b(s-3,d)/2$ for $(s,d)\neq(3,1)$.

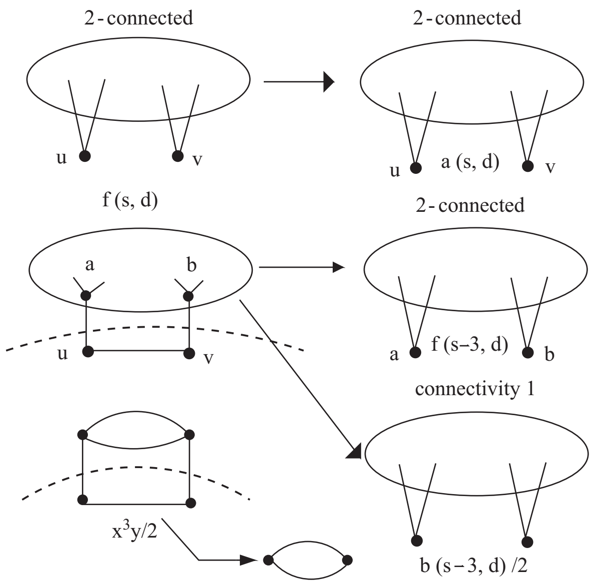


Fig. 4. Conversion of 2-connected fairly cubic graphs.

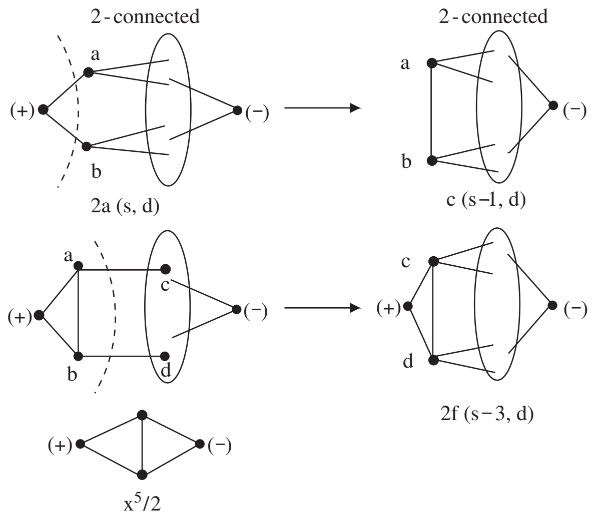


Fig. 5. Conversion of 2-connected almost cubic networks.

The relationship between the numbers of these graphs in egf form is

$$F = A + x^3 F + \frac{x^3}{2} B + \frac{x^3 y}{2}. \tag{18}$$

Next we will convert 2-connected almost cubic networks to 2-connected closely cubic graphs or 2-connected fairly cubic networks by suppressing the positive pole $(+)$ if its neighbors are not adjacent or else suppressing the neighbors of $(+)$ if they are adjacent (see Fig. 5). In the first case, the suppression operation gives us a 2-connected closely cubic graph with exactly one fewer simple edges and the same number of double edges. In the second case let $u$ and $v$ be the neighbors of $(+)$ and suppose that there is no other vertex which is adjacent to both of them. By removing the vertices $(+)$, $u$ and $v$, we have a graph which has two vertices, say $w_1$ and $w_2$, of degree 2, which were adjacent

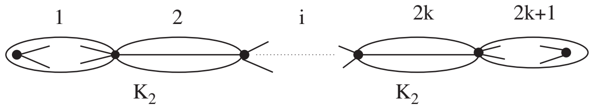


Fig. 6. Special almost cubic network.

to $u$ and $v$, respectively. Now adding a new positive pole (+) to this graph by joining it to $w_1$ and $w_2$ results in a 2-connected fairly cubic network. But if some vertex $z$ other than (+) is adjacent to both $u$ and $v$, then $z=(-)$ since otherwise $z$ would be a cut-vertex separating the two poles. Hence the network must have $(s,d)=(5,0)$ and there are exactly 12 of these. These graphs contribute $x^5/2$ to the egf for $2A$. Collecting these observations we have $2a(s,d)=2n(s-3)c(s-1,d)+2n(2n-1)2f(s-3,d)$, for $(s,d)\neq(5,0)$. The corresponding relation among egf's is

$$2A = x^2C_x - 2xC + 2x^3F + \frac{x^5}{2}. \tag{19}$$

To find a relationship between special almost cubic networks and the other graphs, consider a special almost cubic network as a sequence of at least two blocks, say $G_1,\ldots,G_k$ for some integer $k\geqslant 2$. Note that each $G_i$ is a block, because this graph must become 2-connected after joining the two poles (see Fig. 6). We number the blocks so that $G_1$ contains the positive pole and $G_k$ contains the negative pole. The intersection of each pair of consecutive blocks must be a cut vertex. All vertices other than the poles must have degree 3. Hence all cut vertices have degree 3, so their neighbors belong to consecutive blocks. Thus the cut vertices consist of $v_i\colon 1\leqslant i<k$ where $v_i$ is the cut vertex which belongs to $G_i$ and $G_{i+1}$. That means $v_i$ has degree 2 in $G_i$ and degree 1 1n $G_{i+1}$ or *vice versa*. But if $v_i$ is of degree one in $G_i$, then $G_i$ must be isomorphic to $K_2$ or else it would not be a block. We conclude that $G_i$ is isomorphic to $K_2$ if $i$ is even and is a 2-connected fairly cubic graph if $i$ is odd. Also $k$ must be odd (see [13]).

In all, the egf of a special cubic graph is the product of the egf's of its blocks $G_i$ for $i=1,\ldots,k$, because they do not share any edge. There are two possibilities for assigning poles to a fairly cubic graph, so when they are considered as networks their contribution to the egf of $G_i$ when $i$ is odd is $2F$. But in that case $G_i$ might be the graph with 1 double edge on two vertices, which does not belong to any of our graph categories. So we have to include the monomial $y$ in the egf for the fairly cubic networks, which we now see is $2F+y$. Then the egf for the special almost cubic networks with $2m$ cut-vertices and $2m+1$ blocks is $[(2F+y)x]^m(2F+y)$, where the factor of $x$ accounts for considering $K_2$ as a network. It follows that

$$B = \sum_{m=1}^{\infty}(2F+y)^{m+1}\cdot x^m = \frac{x(2F+y)^2}{1-x(2F+y)}. \tag{20}$$

The five equations (16), …, (20) along with the partial derivatives with respect to $x$ of all except (19) can be solved for $(G_2)_x$ and $(G_2)_{xx}$, giving

$$\begin{aligned}(G_2)_x &= (x^5-x^8)(G_2)_x(G_2)_{xx}\\ &\quad+\frac{1}{2}(x^4-2x^7+x^{10}+x^5y-x^8y)(G_2)_{xx}+(2x^4+x^7)(G_2)_x(G_2)_x\\ &\quad+\frac{1}{2}(8x^3-6x^6-x^9+x^{12}+2xy-2x^4y+8x^7y-2x^{10}y)(G_2)_x\\ &\quad+\frac{1}{4}x^5-\frac{3}{4}x^8+\frac{3}{4}x^{11}-\frac{1}{4}x^{14}+\frac{3}{2}x^6y-\frac{9}{4}x^9y+\frac{3}{4}x^{12}y+\frac{1}{2}xy^2\\ &\quad-x^4y^2+\frac{7}{4}x^7y^2-\frac{1}{2}x^{10}y^2.\end{aligned} \tag{21}$$

As usual we can find a recurrence relation for the numbers of 2-connected cubic graphs by extracting the coefficient of $x^{s-1}y^d/(2n)!$ from both sides of Eq. (21):

$$\begin{aligned} g_2(s,d) = \frac{1}{s}\Bigg\{ & 8(s-3)\binom{2n}{2} g_2(s-3,d) - 72(s-6)\binom{2n}{4} g_2(s-6,d) \\ & - 360(s-9)\binom{2n}{6} g_2(s-9,d) + 20,160(s-12)\binom{2n}{8} g_2(s-12,d) \\ & + 2(s-1)\binom{2n}{2} g_2(s-1,d-1) - 24(s-4)\binom{2n}{4} g_2(s-4,d-1) \\ & + 2880(s-7)\binom{2n}{6} g_2(s-7,d-1) - 8!(s-10)\binom{2n}{8} g_2(s-10,d-1) \\ & + (s-3)(s-4)\binom{2n}{2} g_2(s-3,d) - 24(s-6)(s-7)\binom{2n}{4} g_2(s-6,d) \\ & + 360(s-9)(s-10)\binom{2n}{6} g_2(s-9,d) + 12(s-4)(s-5)\binom{2n}{4} g_2(s-4,d-1) \\ & - 360(s-7)(s-8)\binom{2n}{6} g_2(s-7,d-1)\Bigg\} \\ & + \frac{(2n)!}{s}\Bigg\{ 2\sum_{i,j}^{s-3,d} \frac{i g_2(i,j)(s-3-i) g_2(s-3-i,d-j)}{(m_{i,j})!\cdot(m_{s-3-i,d-j})!} \\ & + \sum_{i,j}^{s-6,d} \frac{i g_2(i,j)(s-6-i) g_2(s-6-i,d-j)}{(m_{i,j})!\cdot(m_{s-6-i,d-j})!} \\ & + \sum_{i,j}^{s-3,d} \frac{i g_2(i,j)(s-3-i)(s-4-i) g_2(s-3-i,d-j)}{(m_{i,j})!\cdot(m_{s-3-i,d-j})!} \\ & - \sum_{i,j}^{s-6,d} \frac{i g_2(i,j)(s-6-i)(s-7-i) g_2(s-6-i,d-j)}{(m_{i,j})!\cdot(m_{s-6-i,d-j})!}\Bigg\}, \end{aligned} \tag{22}$$

where $m_{i,j}=(2i+4j)/3$. This relation is supported by the boundary conditions $g_2(6,0)=1$, $g_2(9,0)=70$, $g_2(12,0)=19,320$, $g_2(15,0)=11,052,720$, $g_2(7,1)=180$, $g_2(10,1)=45,360$, $g_2(13,1)=24,948,000$, $g_2(2,2)=6$, $g_2(5,2)=180$, $g_2(8,2)=45,360$, $g_2(11,2)=24,494,400$ and $g_2(s,d)=0$ if $s<2$ or $d<0$. The non-zero boundary conditions are determined by the last 11 terms on the right side of Eq. (21).

The double sums lead to $O(n^2)$ arithmetic operations to calculate $g_2(s,d)$. Thus to compute all values for order up to $2n$ using relation (22) takes $O(n^4)$ arithmetic operations in total.

An alternative to the recurrence relation (22) can be obtained in the same way that alternatives to relations (2) and (9) were found in the previous two sections. Let $t_n$ satisfy the initial conditions $t_1=0$, $t_2=1$ and the recurrence relation

$$t_n = 3nt_{n-1} + 2t_{n-2} + (3n-1)\sum_{i=2}^{n-3} t_i t_{n-1-i} \tag{23}$$

for all $n \geqslant 3$. Then from [12, Section 3] the numbers of labeled connected simple cubic graphs are given by

$$g_2(3n,0) = \frac{(2n)!}{3n2^n}(t_n - 2t_{n-1}) \tag{24}$$

for all $n \geqslant 2$.

The contraction operation for a double edge used in the previous two sections preserves 2-connectedness. Therefore when applied to 2-connected cubic graphs this operation gives rise to an egf equation which is very similar to (13), and is again linear:

$$(G_2)_y = x^2(G_2)_x + x^3(G_2)_y + \frac{x^2 y}{2}. \tag{25}$$

Now for $d \geqslant 1$ extract the coefficient of $x^s y^{d-1}/(2n)!$ from both sides of Eq. (25) to obtain the recurrence

$$g_2(s,d) = 2\binom{2n}{2}\left\{\frac{s-1}{d} g_2(s-1,d-1) + g_2(s-3,d)\right\}, \tag{26}$$

which holds for $d \geqslant 1$ and $s \equiv d \pmod 3$ except that $g_2(2,2) = 6$ (corresponding to the drum term $x^2 y/2$).

One can now compute $t_m$ from relation (23) by induction on $m$, allowing $g_2(3m, 0)$ to be calculated on the basis of relation (24) for $m \geqslant 2$. Of course $g_2(s, 0) = 0$ if $s < 6$ or if $s$ is not divisible by 3. Finally, $g_2(3m - 2d, d)$ is determined from relation (26) by induction on $d$. With this alternate approach all of the values for order up to $2n$ can be computed with $O(n^2)$ arithmetic operations. This is much faster asymptotically that the $O(n^4)$ operations needed to calculate the same values on the basis of the single recurrence relation (22).

In `Maple` the alternate approach runs very much more quickly even for small orders. The `Maple` calculations and conjectures which they suggest or support are discussed in the next section.

## 5. Calculations and conjectures

In Sections 2, 3 and 4 asymptotic estimates (up to a constant factor) are given for the numbers of arithmetic operations needed to calculate $g(s, d, l)$, $g_1(s, d, l)$ and $g_2(s, d)$ based on different sets of recurrence relations. These estimates are presented in terms of $n$, where $2n$ is the maximum order of graph for which numbers are to be determined. Observed times for computations carried out in `Maple` (see [10]) grow more quickly as a function of $n$ than the number of arithmetic operations. Two factors which together probably account for this phenomenon are increases in the CPU time for multiplications due to growth in the lengths of the numbers, and increases in memory access times due to growth in the amount of data stored and retrieved.

To estimate CPU time we can restrict our attention to multiplication operations, since those take longer than additions or subtractions and for the recurrences being solved are just as frequent (up to a constant factor). Division operations are infrequent, so can be ignored for an asymptotic analysis. The largest of the numbers being computed can be seen to have length $O(n \log n)$ by the main theorem of [2]. The length, say in bytes, of an integer is proportional to its logarithm to some fixed base. Recurrence (9) requires $O(n^6)$ products in which two factors have length $O(n \log n)$. All other factors are easily seen to have length $O(\log n)$. The standard algorithm for multiplication takes time proportional to the product of the lengths of the factors, giving an asymptotic estimate of $O(n^8 \log^2 n)$ for the CPU time needed to solve (9) for all values of $g_1(s, d, l)$ for orders up to $2n$. Similarly, the CPU time needed to solve (22) for all values of $g_2(s, d)$ for orders up to $2n$ is $O(n^6 \log^2 n)$.

All products in the linear recurrences contain at most one factor of length $O(n \log n)$, the rest again having lengths $O(\log n)$. Thus all values of $g(s, d, l)$ for orders up to $2n$ can be calculated in CPU time $O(n^4 \log^2 n)$ either from (2) or from (3), (5) and (7). Also it can be seen that all values of $g_1(s, d, l)$ for orders up to $2n$ can be calculated in CPU time $O(n^4 \log^2 n)$ on the basis of (10), (11), (14) and (15). The first of these is non-linear, with $O(n^2)$ products taking time $O(n^2 \log^2 n)$ each, the second needs only $O(n)$ products of the same sort, and the other two are linear recurrences, with $O(n^3)$ products taking time $O(n \log n)$ each. Finally, all values of $g_2(s, d)$ for orders up to $2n$ can be calculated in CPU time $O(n^4 \log^2 n)$ on the basis of (23), (24) and (26). The time is dominated by the first of these recurrences, which is non-linear as in the previous case.

To store all values of $g(s, d, l)$ or $g_1(s, d, l)$ for all orders up to $2n$ entails that $O(n^3)$ numbers be stored, with lengths $O(n \log n)$ as noted above. Thus the total data storage space needed is $O(n^4 \log n)$. Similarly, to store all of the $g_2(s, d)$ for orders up to $2n$ takes $O(n^3 \log n)$ for storage space. As $n$ increases, then, much of the data is forced down in the memory hierarchy and access times are thereby increased. Access times to the several levels of cache memory and to blocks of disk data are strongly dependent on locality of reference. Data access patterns depend on the implementation of `Maple` as well as the coding of the recurrence relations, so we do not attempt a quantitative prediction of average access time as a function of $n$. However, our experiments show that the increase in memory access times due to increased total memory used can be quite substantial, suggesting that the number of stored values should be kept to a minimum. The linear recurrences in the previous sections are all of small fixed depth, so that calculations of order $2n$ terms require only terms of the previous one, two or three orders. Thus if the lower order terms are not needed for some other purpose, the linear recurrence calculations can reduce their storage requirements by a factor of $\Theta(n)$ without needing to recalculate any of the terms. In this way the recurrences for $g(s, d, l)$ can be solved for all orders up to $2n$ using just $O(n^3 \log n)$ memory. Similarly it can be seen that all values of $g_1(s, d, l)$ for orders up to $2n$ can be calculated using memory $O(n^3 \log n)$ on the basis of (10), (11), (14) and (15), and that all values of $g_2(s, d)$ for orders up to $2n$ can be calculated using memory $O(n^2 \log n)$ on the basis of (23), (24), and (26).

We implemented space-efficient versions of the linear recurrences in `Maple`, enabling calculation (but not simultaneous storage) of all numbers $g(s, d, l)$ for order $2n \leqslant 800$, all $g_1(s, d, l)$ for order $2n \leqslant 1000$, and all $g_2(s, d)$ for order $2n \leqslant 10,000$.

It is readily observed that for fixed order 6, 8 or 10 and fixed $s$ the values of $g(s, d, l)$ form a unimodal sequence as a function of $d$, or equivalently as a function of $l$ in view of the relation $n = s + 2d + l$. The above computations were used to check that this unimodality property holds for all orders $6 \leqslant 2n \leqslant 800$. Unimodality also seems to hold for the other five sequences which can be formed from $g(s, d, l)$ by fixing two of the parameters $n, s, d, l$. For $n$ and $d$ fixed and for $n$ and $l$ fixed unimodality has been verified for $6 \leqslant 2n \leqslant 800$. For the other three cases unimodality has been checked for $6 \leqslant 2n \leqslant 300$. Note that monotone sequences are considered to be unimodal. On the basis of the computational evidence we conjecture that in all six cases unimodality holds for all $6 \leqslant 2n$. In addition we conjecture that it is strictly increasing as a function of $n$ when $s$ and $l$ are constant and when $d$ and $l$ are constant.

We make the same conjectures for $g_1(s, d, l)$, having verified them computationally over the same range of parameters except for extending it to orders $6 \leqslant 2n \leqslant 1000$ in the three cases for which $n$ is fixed. For $g_2(s, d)$ we conjecture that the sequence is unimodal when $n \geqslant 6$ is fixed, and is strictly increasing as a function of $n \geqslant 6$ when $s$ or $d$ is fixed. These conjectures have been verified computationally for fixed order $2n \leqslant 10,000$, and for order $2n \leqslant 1000$ in the other two cases.

For fixed order $2n$ we can predict the values of $d$ and $l$ for which the maximum value of $g(s, d, l)$, $g_1(s, d, l)$, and $g_2(s, d)$ is attained, even though there are asymptotic ties. We conjecture that for order $2n \geqslant 10$ the maximum value of $g(s, d, l)$ is for $d = 1$ and $l = 2$ uniquely; this has been verified for $2n \leqslant 800$. For $g_1(s, d, l)$ and fixed order $2n \geqslant 6$ we conjecture that the maximum is at $d = 2$ and $l = 1$ uniquely; this has been verified for $2n \leqslant 1000$. And for $g_2(s, d)$ with fixed order $2n \geqslant 6$ we conjecture that the maximum is attained when $d = 1$, uniquely if $2n \geqslant 10$; this has been verified for order $2n \leqslant 10,000$. On the other hand it is known [3] that $g(3n - 3, 1, 1)$, $g(3n - 4, 1, 2)$, $g(3n - 5, 2, 1)$, $g(3n - 6, 2, 2)$, $g_1(3n - 3, 1, 1)$, $g_1(3n - 4, 1, 2)$, $g_1(3n - 5, 2, 1)$ and $g_1(3n - 6, 2, 2)$ are all asymptotically equal and that $g_2(3n - 2, 1)$ and $g_2(3n - 4, 2)$ are asymptotically equal.

## 6. Related results

Clearly a 3-connected cubic graph cannot contain double edges. Therefore, 3-connected cubic graphs are precisely the 3-connected simple cubic graphs. An egf equation for 3-connected cubic graphs was found by Wormald [12, Section 5]. This led to the recurrence relation

$$u_n = (3n - 2)\left(u_{n-1} + \sum_{i=2}^{n-2} u_i u_{n-i}\right) \tag{27}$$

for $n \geqslant 3$ with the boundary condition $u_2 = 1$, where the number $g_3(3n)$ of 3-connected cubic graphs with $3n$ (simple) edges is given by

$$g_3(3n) = \frac{(2n)!}{3n2^n} u_n$$

for $n \geqslant 2$. Of course $g_3(s) = 0$ if $s < 6$ or $s$ is not divisible by 3. Tables can be found in [11].

Palmer et al. [6] counted labeled simple claw-free cubic graphs by using expansion and dilation operations. Our results together with [6] will be used to find the number of $k$-connected claw-free simple cubic graphs for $k = 1, 2,$

and 3. We also plan to investigate the enumeration problem for 4-regular general graphs which are $k$-connected for $k = 0, 1, 2, 3$ and 4 (see [9]).

An extended preliminary version of this paper is available on our web sites which contains tables and some identities for the numbers of general cubic graphs with given connectivity (http://rg.yonsei.ac.kr/∼chae/ or http://www.cs.uga.edu/∼rwr/).

## Acknowledgments

We are grateful to the referees for their comments on the paper.

## References

[1] A.T. Balaban, Chemical graphs. VIII. Valence isomerism and general cubic graphs, Rev. Roumaine Chim. 15 (1970) 463–486.
[2] E.A. Bender, E.R. Canfield, The asymptotic number of labeled graphs with given degree sequences, J. Combin. Theory Ser. A 24 (1978) 296–307.
[3] G.-B. Chae, Enumeration of general cubic graphs, Doctoral Thesis, Michigan State University, East Lansing, MI, 2001.
[4] H. Gropp, Enumeration of regular graphs 100 years ago, Discrete Math. 101 (1992) 73–85.
[5] F. Harary, E.M. Palmer, Graphical Enumeration, Academic Press, New York, 1973.
[6] E.M. Palmer, R.C. Read, R.W. Robinson, Counting claw-free cubic graphs, SIAM J. Discrete Math. 16 (2002) 65–73.
[7] R.C. Read, Some enumeration problems in graph theory, Doctoral Thesis, University of London, 1958.
[8] R.C. Read, Some unusual enumeration problems, Ann. New York Acad. Sci. 175 (1970) 314–326.
[9] R.C. Read, N.C. Wormald, Number of labeled 4-regular graphs, J. Graph Theory 4 (1980) 203–212.
[10] D. Redfern, The Maple Handbook: Maple V Release 4, Springer, New York, 1996.
[11] N.C. Wormald, Some problems in the enumeration of labelled graphs, Doctoral Thesis University of Newcastle, Callaghan, NSW, Australia, 1978.
[12] N.C. Wormald, Enumeration of labelled graphs II: cubic graphs with a given connectivity, J. London Math. Soc. ( 2) 20 (1979) 1–7.
[13] N.C. Wormald, E.M. Wright, The exponential generating function of labelled blocks, Discrete Math. 25 (1979) 93–96.