Chapter 26
A Lower Bound for Graph Energy of Fullerenes

Morteza Faghani, Gyula Y. Katona, Ali Reza Ashrafi, and Fatemeh Koorepazan-Moftakhar

Abstract A molecular graph is a graph in which vertices are atoms and edges are molecular bonds. These graphs are good mathematical models for molecules. Suppose G is a molecular graph with adjacency matrix A. The graph energy G is defined as the sum of the absolute values of the eigenvalues of A. The aim of this chapter is to describe a method for computing energy of fullerenes. We apply this method for computing a lower bound for energy of an infinite class of fullerene graphs with exactly $12n$ vertices. Our method is general and can be extended to other class of fullerene graphs.

26.1 Introduction

All graphs in this chapter are finite, simple, and connected. Suppose G is such a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. The *eigenvalues* of G are defined as the eigenvalues of its adjacency matrix and the set of all eigenvalues is called the *spectrum*, $Spec(G)$, of G. Set $Spec(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. The *graph energy*

M. Faghani
Department of Mathematics, Payam-e Noor University, Tehran, Iran

G.Y. Katona
Department of Computer Science and Information Theory, Budapest University of Technology and Economics, Budapest, Hungary

MTA-ELTE Numerical Analysis and Large Networks, Research Group, Budapest, Hungary

A.R. Ashrafi (✉) • F. Koorepazan-Moftakhar
Department of Nanocomputing, Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-53153, Iran

Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-53153, Iran
e-mail: ashrafi@kashanu.ac.ir

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of G, $\varepsilon(G)$, is defined as $\varepsilon(G) = \sum_{i=1}^{n} |\lambda_i|$ (Gutman 1978, 2012). This graph invariant has some important applications in Hückel theory, and so it has been extensively studied. An extension of this graph invariant was done by Nikiforov (Nikiforov 2007). We refer the interested readers to (Li et al. 2012) for more information on this topic.

Suppose K_n and $K_{n,n}$ denote the complete graph on n vertices and balanced complete bipartite graph on 2n vertices. Define $K(a_n(k))$, $K(b_n(k))$, $K(c_n(k))$, and $K(d_n(k))$ to be graphs obtained from K_n by deleting k edges so that all of them have a common endpoint, by deleting k independent edges, by deleting a complete set of $k(k-1)/2$ mutually incident edges, and by deleting the edges of a k-membered cycle, respectively. In (Gutman and Pavlović 1999), some inequalities among the energies of the above graphs are given, and in Gutman (2001), the connection between the energy and the total electron energy of a class of organic molecules is investigated.

A graph G is called *3-connected*, if there does not exist vertices $x, y \in V(G)$ whose removal disconnects the graph. If all vertices of G have degree 3, then we say G is *cubic*. A *fullerene* graph is a cubic planar and 3-connected graph such that its faces are pentagon and hexagon. Suppose p, h, n, and m are the number of pentagons, hexagons, vertices, and edges of a fullerene graph F, respectively. Then $f = p + h$ and the Euler's theorem implies that $n - m + f = 2$. Since F is cubic, $m = 3n/2$ and since each vertex lies in exactly three faces, $n = (5p + 6h)/3$ and $m = (5p + 6h)/2 = 3/2n$. So $(5p + 6h)\ /3 - (5p + 6h)\ /2 + p + h = 2$. Therefore, $p = 12$, $n = 2h + 20$, and $m = 3h + 30$. We encourage the interested readers to consult the famous book (Fowler and Manolopoulos 2006) for the mathematical properties of this important class of molecular graphs and (Djafari et al. 2013; Koorepazan–Moftakhar et al. 2014) for more information on this topic.

26.2 Algebraic Background

Some of the present authors (Katona and Faghani 2014) applied Ky Fan theorem (Fan 1951) to obtain a lower bound for the graph energy of a sequence of fullerenes. To describe this method, we need some algebraic notions. A matrix $A_{n\times n}$ is called centrosymmetric if $a_{ij} = a_{n-i+1,n-j+1}$, $1 \le i,j \le n$. The mathematical properties of this special class of matrices can be found in (Liu 2003). In Gutman et al (2007), the authors proved that the energy of any n-vertex regular graph G of degree $r > 0$ is greater than or equal to n with equality if and only if every component of G is isomorphic to the complete bipartite graph $K_{r,r}$. If G is triangle- and quadrangle-free, then $\varepsilon(G) \ge nr\ /\ \sqrt{(2r-1)}$. In particular, every n-vertex fullerene F satisfies $1.34n \le \varepsilon(F) \le 1.73n$. In (Katona and Faghani 2014), the authors improved the last inequality. They proved that a particular $10n$-vertex fullerene graph can have a centrosymmetric adjacency matrix. Then by applying the mathematical properties of these matrices and an iterative use of the Key–Fan theorem, a relation between energies of two fullerenes of orders $10 \times 2^k m$ and m, respectively, is provided. They observed that the relation gives a better lower bound to the energy of an n-vertex fullerene than the lower bound $1.34n$, for the special cases that $n = 10 \times 2 \times 5$, $10 \times 2 \times 7$, $10 \times 2 \times 11$, or $10 \times 2 \times 13$. We encourage the interested readers to

consult (Ghorbani et al. 2014) for more information on the energy of this infinite sequence of fullerenes. In this paper, the authors applied the centrosymmetricity of adjacency and PI adjacency matrices to approximate the energy and PI-energy of this class of fullerenes with exactly *10n* vertices. It is noteworthy to mention here that the centrosymmetricity of adjacency matrix of fullerene usually implies the same property for other vertex- or edge-weighted matrices obtained from the adjacency matrix of the fullerene graph under consideration.

Suppose G is a graph and $x, y \in V(G)$. The distance between x and y is defined as the length of a shortest path connecting x and y. The *Wiener index* of G, $W(G)$, is then the sum of all such distances over all pairs of vertices in G. Wiener called this graph invariant, the *path number* (Wiener 1947). It is the oldest distance-based graph invariant applicable in molecular branching. A fullerene graph is said to be *centrosymmetric* if it has a vertex labeling for which its adjacency matrix is centrosymmetric. (Graovac et al. 2011) considered a sequence of centrosymmetric fullerenes and applied this property to obtain exact formula for the Wiener index of the general term of fullerene sequence under consideration. In the mentioned paper, the authors conjectured that all fullerenes are centrosymmetric. In a recent paper (Fowler and Myrvold 2014), this conjecture was disproved; in fact, it proved that most fullerenes are not centrosymmetric. In this paper the necessary and sufficient conditions are stated in terms of the 28 possible fullerene automorphism groups: if the group is C_1 or C_3, the fullerene is not centrosymmetric; for C_{3h}, C_{3v}, or C_s, the fullerene is centrosymmetric unless some vertex is fixed by a mirror plane; for all other groups, the fullerene is centrosymmetric. Briefly, they noticed that most fullerenes have trivial C_1 symmetry group and hence they are not centrosymmetric.

Let J_n be an $n \times n$, $\{0\ ,1\}$ matrix in which an entry is unit if and only if it lies on counterdiagonal of J_n. It is clear that the matrix A is centrosymmetric if and only if $AJ = JA$. The set of all centrosymmetric matrices is denoted by Cen.

Theorem 26.1 (Cantoni and Buter 1976) If $n = 2m$ and $A_{n\times n} \in Cen$, then

$$\mathbf{A} = \begin{pmatrix} \mathrm{B} & \mathrm{J_m C J_m} \\ \mathrm{C} & \mathrm{J_m B J_m} \end{pmatrix}$$

where B and C are $m \times m$ matrices. Moreover, we have,

$$\mathbf{Q^T A Q} = \begin{pmatrix} \mathrm{B - J_m C} & 0 \\ 0 & \mathrm{B + J_m C} \end{pmatrix},$$

where

$$\mathbf{Q} = \frac{\sqrt{2}}{2} \begin{pmatrix} \mathrm{I_m} & \mathrm{I_m} \\ -\mathrm{J_m} & \mathrm{J_m} \end{pmatrix}.$$

Let

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & 0 & 0 & 0 & A_{1m} \\ A_{21} & A_{22} & 0 & 0 & 0 & A_{2m} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ A_{m1} & A_{m2} & 0 & 0 & 0 & A_{mm} \end{pmatrix}$$

be the block form of $A = [a_{i,j}]$, $1 \leq i, j \leq n$, and all blocks are $s \times s$ matrices. The following theorem is useful when the adjacency matrix have a block form (Katona and Faghani 2014):

Theorem 26.2 Let

$$\mathbf{A} = \begin{pmatrix} A_{11} & 0 & 0 & 0 & A_{1m} \\ 0 & 0 & 0 & 0 & A_{2m} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ A_{m1} & 0 & 0 & 0 & A_{mm} \end{pmatrix}$$

be the block form of A. If $m = 2k$ and $A_{i,j}J = JA_{2k-i+1,2k-j+1}$, then A is orthogonally similar to the following block matrix:

$$\begin{pmatrix} \coprod + \Psi \bigcup & o \\ o & \coprod - \Psi \bigcup \end{pmatrix}$$

in which

$$\coprod = \begin{pmatrix} A_{1,1} & 0 & 0 & 0 & A_{1,k} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ A_{k,1} & 0 & 0 & 0 & A_{k,k} \end{pmatrix} \quad \text{and U} = \begin{pmatrix} A_{k+1,1} & 0 & 0 & 0 & A_{k+1,k} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ A_{2k,1} & 0 & 0 & 0 & A_{2k,k} \end{pmatrix}$$

Proof See (Katona and Faghani 2014) for details.

26.3 A Lower Bound for the Energy of C_{12n}

We are now ready to describe our method for an infinite sequence of fullerenes, C_{12n}, with exactly $12n$ carbon atoms, Fig. 26.1. By tedious calculations, we can find a centrosymmetric labeling for the vertices of C_{12n}. The adjacency matrix of the general term of this fullerene series is as follows:

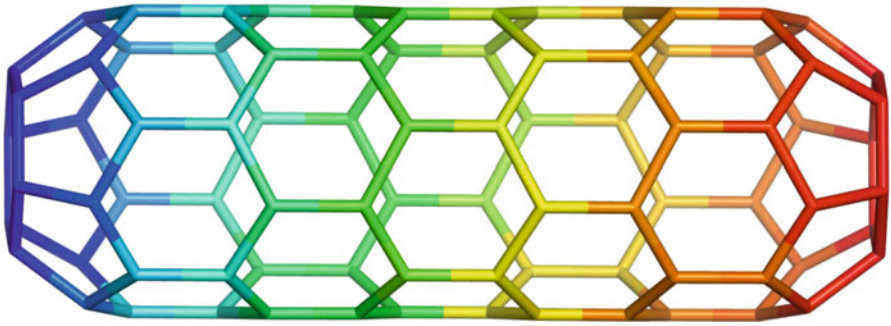

Fig. 26.1 The fullerene C_{12n}, $n = 7$

$$A(C_{12n}) = \begin{pmatrix} X & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix},$$

in which $Q = P^t$ and all blocks are 6×6 matrices given by:

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{p} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{X} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

By Theorem 26.2, we can take the adjacency matrix as follows:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

in which

$$\mathbf{A} = \begin{pmatrix} X & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix} \text{ and}$$

$$\mathbf{D} = \begin{pmatrix} 0 & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0. & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix} \mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0. & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & 0 & 0 \end{pmatrix}$$

$$\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ P & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & 0 & 0 \end{pmatrix}.$$

So, the matrix A (C_{12n}) is similar to the matrix

$$\begin{pmatrix} A + \Psi C & 0 \\ 0 & A - \Psi C \end{pmatrix}.$$

Furthermore,

$$\mathbf{A} + \Psi\mathbf{C} = \begin{pmatrix} X & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & JQ \end{pmatrix}$$

and

$$\mathbf{A}-\Psi\mathbf{C}=\begin{pmatrix} X & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & -JQ \end{pmatrix}.$$

So, $\varepsilon(\mathrm{A}(\mathrm{C}_{12\mathrm{n}}))=\varepsilon(\mathrm{A}+\Psi\mathrm{C})+\varepsilon(\mathrm{A}-\Psi\mathrm{C})$. Notice that

$$(A+\Psi C)+\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & . & . & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & 0 & 0 & 0 & 0 \\ 0 & 0 & . & . & . & . & 0 & X & -JQ \end{pmatrix}$$

$$=\begin{pmatrix} X & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}.$$

This means that we can reduce the order of $A(C_{12n})$ into half such that the centrosymmetricity preserves.

Notice that, $\varepsilon(X-JQ)\approx 7.4641.$ and $\varepsilon(X+JQ)\approx 11.4641.$ By an iterative use of the Key–Fan Theorem, one can prove the following inequality:

Table 26.1 The energy and bounds for some fullerenes

n	k	M	Energy	$2^k\epsilon(A(C_{12m})) - 18.9282(2^k - 1)$.
3	0	3	55.244	55.244
5	0	5	93.174	93.174
6	1	3	112.075	91.5598
7	0	7	130.97	130.97
9	0	9	168.733	168.733
11	0	11	206.481	206.481

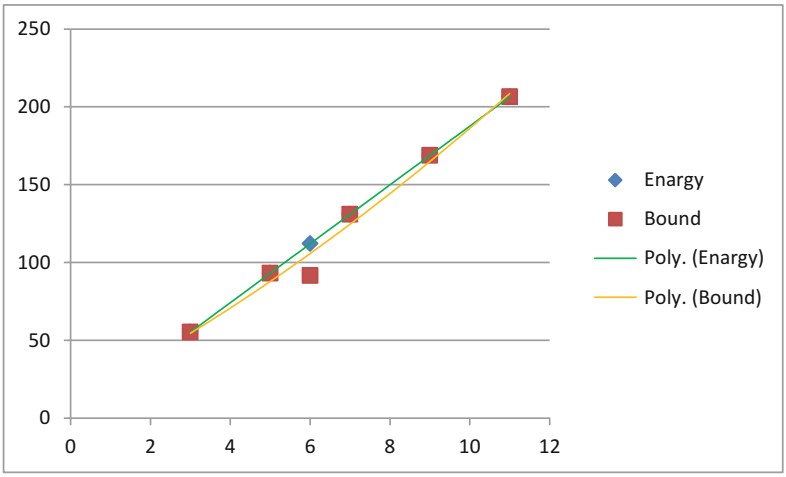

Fig. 26.2 The diagrams for exact and estimated energies

$$\epsilon((A(C_{12n}))) \geq 2\epsilon\left(\begin{pmatrix} X & I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ I & 0 & P & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & Q & 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & . & . & . & 0 & I & 0 & P & 0 \\ 0 & 0 & . & . & . & 0 & Q & 0 & I \\ 0 & 0 & . & . & . & . & 0 & I & X \end{pmatrix}\right) - 18.9282.$$

The right-hand side matrix is again centrosymmetric as its size is half the size of $A(C_{12n})$. So, if n is even, then by repeating the above procedure, we can obtain the following lower bound for the energy of $A(C_{12n})$ as follows:

Theorem 26.3 If $n = 2^k m$ then $\varepsilon(A(C_{12n})) = \varepsilon(A(C_{12(2^k m)})) > 2^k \varepsilon(A(C_{12m})) - 18.9282(2^k - 1)$.

In Table 26.1, the exact values of energy in some cases are compared with our bound. It seems that the bound is good, but it is important to always compare the exact energy with the computed bound. Since the fullerene is a huge molecule, this is an open question that the error is small. In Fig. 26.2, these values are compared in a diagram.

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