Proc. Indian Acad. Sci. (Chem. Sci.), Vol. 102, No. 1, February 1990, pp. 51–64.


# Topological solution of algebraic eigenvalue problem

KALI KINKAR DATTA
Department of Chemistry, Burdwan Raj College, Burdwan 713 104, India

MS received 30 March 1989; revised 24 October 1989

**Abstract.** A simple graph theoretical algorithm for simultaneous determination of eigenfunctions, eigenvalues and characteristic polynomials of real symmetric matrices has been developed. The method starts with representing the matrix $\mathbf{A}-\lambda\mathbf{I}$, where $\mathbf{I}$ is an unit matrix of the size of $\mathbf{A}$, by an undirected weighted graph ($G$) and an assumed set of eigenfunctions. Conditions necessary to disconnect one vertex completely from $G$ are then developed. The method does not require any property related to the geometrical symmetry group of the graph and is applicable even to matrices containing a number of multiple eigenvalues.

**Keywords.** Undirected graph; binary operator; characteristic polynomial; eigenvalues; eigenfunctions.

## 1. Introduction

The background theory of the algebraic eigenvalue problem has been known for many years. There are standard techniques for diagonalising a hermitian matrix (Jacobi 1846; Givens 1958; Householder 1958, 1964) which are widely used in computer programs for quantum chemical calculations. During the last two decades, graph theory (GT) has drawn much attention from theoretical chemists (see, for example, Gutman and Polansky 1986, and references cited therein) because it pictorially and easily gives much important chemical information about molecules whose conventional structural formulae are their molecular graphs. In the field of eigenvalue problems it has been successful in two ways; (a) by constructing characteristic polynomials (CP) (for example, Sachs 1962, 1963, Mallion *et al* 1974, Hosoya 1972, El Basil 1984, and others) and cofactors (Kassman 1985; Mukherjee and Datta 1989) of various elements of $|\mathbf{A}-\gamma\mathbf{I}|$, (b) by block diagonalising the adjacency matrices of symmetric undirected graphs (McClelland 1974, 1982; Hall 1977; King 1977; D'Amato 1979; Datta and Mukherjee 1988) by splitting them into smaller disconnected subgraphs.

The aim of the present communication is to translate the algebraic eigenvalue problem into the language and formalism of graph theory. A general real symmetric matrix $\mathbf{A}=[a_{ij}]$ is given and $\mathbf{I}$ is a unit matrix of the size of $\mathbf{A}$. In order to have a mapping of the matrix $\mathbf{A}-\lambda\mathbf{I}$ onto an undirected weighted graph $G$ we imagine a binary operator $\hat{A}$ defined over the set of basis functions $\{\phi_i\}$, $i=1$ to $n$, such that

$$\phi_r^2=\langle\phi_r|\hat{A}|\phi_r\rangle=-\lambda+a_{rr},\quad r=1 \text{ to } n,$$

and

$$\phi_i\phi_j=\langle\phi_i|\hat{A}|\phi_j\rangle=a_{ij},\quad i,j=1 \text{ to } n \text{ but } i\neq j. \tag{1}$$

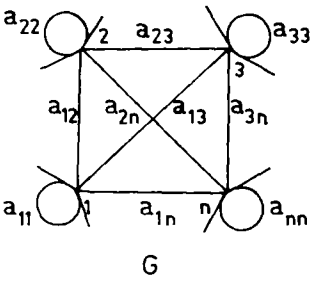


**Figure 1.** Graphical representation of a section of the matrix $\mathbf{A}-\lambda\mathbf{I}$.

Here $a_{rr}$ is the $r$th diagonal element, $a_{ij}$ the $(ij)$ off-diagonal element and $\lambda$ is an eigenvalue of $\mathbf{A}$. In $G$, $a_{rr}$ and $a_{ij}$ are respectively the weights of the $r$th vertex and the edge connecting the vertices $i$ and $j$. With such notations the characteristic matrix can be represented by

$$\mathbf{A}-\lambda\mathbf{I}=[\phi_i\phi_j]_{n\times n}, \tag{2}$$

where $\phi_i\phi_i=\phi_i^2$ and $\phi_i\phi_j=\phi_j\phi_i$. The graph $(G)$ representing above matrix is shown in figure 1.

Now on the basis of a pictorial algorithm we construct a set of new basis functions $\{\psi_i\}$, each of which is a linear combination of $\phi_i$'s, and form the requisite number of equations correlating the components $(x)$ of a desired eigenvector in such a way that one vertex labelled $r$ is completely disconnected from $G$ under the operation of $\hat{A}$. After such detachment or factorisation has been made, the method provides means of obtaining a complete description of the remaining factor graph. For matrices with multiple eigenvalues, the present algorithm can be applied in two alternative ways. This has been discussed in connection with examples 3 and 4 below.

## 2. Algorithm

The steps (a–d) described below are to be followed consecutively.

*Step (a)*: The graph $G$ of the matrix $\mathbf{A}-\lambda\mathbf{I}$ is redrawn as $\bar{G}$, omitting the vertex loops and edge weights (for the sake of clarity of the diagram) as shown in figure 2. Now enclosing only one vertex labelled $r$ (arbitrarily chosen) we draw a circle and join all the other vertices $(i)$ outside the circle to it. If $i$ is not already joined to $r$, a dotted line or arc is used for the purpose. The solid or dotted line or arc connecting the vertex pair $(r, i)$ is marked by $x_i$. The inner side of the circle is marked $(+)$ve and the outer side $(-)$ve.

*Step (b)*: On the basis function $\phi_r$ representing the vertex $r$, every other basis function $\phi_i$ is superimposed additively with the respective multiplicative factor $x_i$, and a new function $\psi_r$ is constructed,

$$\Psi_r=\sum_{i=1}^{n} x_i\phi_i, \quad x_r=1, \tag{3}$$

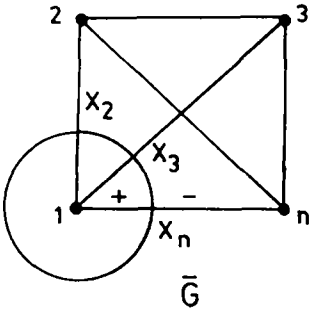


**Figure 2.** Simplified representation of $G$: step (a) of the algorithm.

to represent vertex $r$. On the basis function $\phi_i$ outside the circle, $\phi_r$ is superimposed subtractively with a multiplicative factor $x_i$. Thus the vertex labelled $i$ is to be represented by the new function,

$$\Psi_i = \phi_i - x_i\phi_r. \tag{3a}$$

*Step* (*c*): We next construct $n-1$ equations

$$\langle \Psi_r | \hat{A} | \Psi_i \rangle = 0, \tag{4}$$

using (1) and substitute

$$\lambda = \sum_{i=1}^{n} x_i a_{ir}, \tag{5}$$

in each of them. (4) and (5) constitutes a set of $n$ equations

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}, \tag{6}$$

correlating $\lambda$ and $n-1$ unknown components ($x$) of the column vector x where

$$\mathbf{x}^T = (x_1, x_2, \ldots, x_{r-1}, 1, x_{r+1}, \ldots, x_n). \tag{7}$$

Substituting for $x_i$ a function of $\lambda$ such as

$$x_i = A_{si}/A_{sr}, \tag{8}$$

in the equation obtained from the $s$th row of (6) we obtain an equation whose left side directly gives the CP of $G$. Here $A_{si}$ is the cofactor of the $(si)$ element of $\det(\mathbf{A} - \lambda\mathbf{I})$. It can be obtained by the elimination method using the $n-1$ remaining equations of (6) or directly from $G$ by the graph theoretical method.

*Step* (*d*): The characteristic equation thus obtained is solved by the Newton-Raphson process. From each distinct eigenvalue $\lambda$ one set of solutions for $\{x_i\}$ is obtained by using (5) and (4) or taking the help of (8). Substitution of these values for $x_i$ in (3) gives one eigenfunction $\Psi$ after normalisation.

It is possible to have cases where the use of (6) and (8) is not necessary. The set of equations (4) may either be completely solvable for $\{x_i\}$ after reduction to a polynomial equation in one variable (example 2) or a good number of solutions can

be obtained by inspection (example 3). In these cases we do not generally obtain CP and $\lambda$. The latter can be obtained from the normalised eigenfunction $\Psi$ by using

$$\langle \Psi | \hat{A} | \Psi \rangle = 0, \tag{9}$$

In case of complete graphs and some graphs possessing high geometrical symmetry and multiple eigenvalues two methods of repeated application of the same process as described in example 3 may be feasible for evaluation of the complete set of eigenfunctions.

## 3. Illustrations

*Example* 1: The matrix $\mathbf{A}_1$ shown here is a representative of cases containing no geometrical symmetry and having distinct eigenvalues.

$$\mathbf{A}_1 = \begin{bmatrix} 1 & 2 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 1 \\ 0 & 2 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \end{bmatrix}$$

The graph $G_1$, shown in figure 3a, is the diagramatic representation of $\mathbf{A}_1 - \lambda\mathbf{I}$. It is drawn by using (1).

Following step (a) of the algorithm, we draw $\bar{G}_1$ and enclose the pendent vertext 1 (a vertex connected by a single edge) within the circle. This is shown in figure 3b. According to (3) and (3a) taking $x_1 = 1$ the new eigenfunctions representing vertices $1, 2, \ldots, 5$ are

$$\begin{aligned} \Psi_1 &= \phi_1 + x_2\phi_2 + x_3\phi_3 + x_4\phi_4 + x_5\phi_5, \\ \Psi_2 &= \phi_2 - x_2\phi_1, \\ \Psi_3 &= \phi_3 - x_3\phi_1, \\ \Psi_4 &= \phi_4 - x_4\phi_1, \\ \Psi_5 &= \phi_5 - x_5\phi_1. \end{aligned} \tag{10}$$

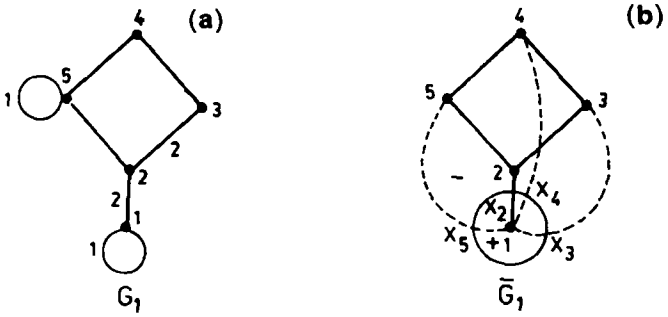


**Figure 3.** (a) Graphical representation of the matrix $\mathbf{A}_1 - \lambda\mathbf{I}$. (b) Simplified diagram of $G_1$: step (a) of the algorithm.

To disconnect vertex 1 completely from $\bar{G}_1$, we use (4) and have the following four equations for $i = 2, 3, 4$ and 5 respectively.

$$\begin{aligned} &2 + 2x_3 + x_5 - x_2\lambda = 0, \\ &2x_2 + x_4 - x_3\lambda = 0, \\ &x_3 + x_5 - x_4\lambda = 0, \\ \text{and} \quad &x_2 + x_4 + x_5 - x_5\lambda = 0. \end{aligned} \tag{11}$$

Here we use $\lambda = 1 + 2x_2$ from (5).

If we enclose vertex 1 within the circle and construct the set of equations (4) in the order $i = 2, 3, \ldots, n$ as shown in (11) the result of elimination at various stages starting from the bottom and ascending upwards can be formulated by

$$x_k = (-1)^{(k-s)} \frac{\sum_{i=1}^{s} x_i |a_{pq}|}{|a_{lm}|}, \tag{12}$$

where $k$ and $s$ are integers, $k > s$; $p = 1, s+1, s+2, \ldots, n$ but $p \neq k$. Each of $q, l$ and $m$ can assume the values $s+1, s+2, \ldots, n$; $a_{ij}$ is the $(ij)$th element of the determinant $(\mathbf{A} - \gamma\mathbf{I})$ and the symbol '$\|$' indicates a determinant of order $n - s$.

Thus taking $k = 4$ and $s = 3$ we have

$$\begin{aligned} p &= 1, \not{4}, 5, \quad \text{for } i = 1, \\ &= 2, \not{4}, 5, \quad \text{for } i = 2, \quad \text{since } p \neq 4 \\ &= 3, \not{4}, 5, \quad \text{for } i = 3, \end{aligned}$$

each of $q, l$ and $m = 4$ and 5 and $x_1 = 1$.

$$\therefore x_4 = (-1)^{(4-3)} \frac{x_1 \begin{vmatrix} a_{14} & a_{15} \\ a_{54} & a_{55} \end{vmatrix} + x_2 \begin{vmatrix} a_{24} & a_{25} \\ a_{54} & a_{55} \end{vmatrix} + x_3 \begin{vmatrix} a_{34} & a_{35} \\ a_{54} & a_{55} \end{vmatrix}}{\begin{vmatrix} a_{44} & a_{45} \\ a_{54} & a_{55} \end{vmatrix}}$$

$$= -\frac{1 \begin{vmatrix} 0 & 0 \\ 1 & -\lambda+1 \end{vmatrix} + x_2 \begin{vmatrix} 0 & 1 \\ 1 & -\lambda+1 \end{vmatrix} + x_3 \begin{vmatrix} 1 & 0 \\ 1 & -\lambda+1 \end{vmatrix}}{\begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda+1 \end{vmatrix}},$$

Similarly taking $k = 5$ and $s = 2$ we have $p = 1, 3, 4, \not{5}$ for $i = 1$, $p = 2, 3, 4, \not{5}$ for $i = 2$ and $q, 1$ and $m = 3, 4, 5$ giving

$$x_5 = x_2(\lambda^2 + 1)/(\lambda^3 - \lambda^2 - 2\lambda + 1).$$

The closed formula (12) will be useful to overcome ambiguity about the factors to be cancelled in various steps during the process of elimination. Since the task of elimination is laborious (particularly for large graphs) one may determine CP and cofactors directly by the GT method and then by using (8) obtain $\{x_i\}$.

For the matrix $\mathbf{A}_1$, we have

$$-\lambda^5 + 2\lambda^4 + 10\lambda^3 - 16\lambda^2 - 4\lambda + 5 = 0, \tag{13}$$

whose left hand side is $|\mathbf{A} - \lambda\mathbf{I}|$. Now we solve (13) by the Newton–Raphson method and five distinct values of $\lambda$, giving the eigenvalues, are 3·4913, 1·5398, 0·5292, −0·5922 and −2·9680. Table 1 shows the eigenvalues and the corresponding values of $x_i$. Using these $x_i$'s normalised eigenfunctions can be obtained from (3).

For simple linear chains ($L_n$, with vertices labelled consecutively) containing no vertex and edge weights the present method applied to vertex 1 arrives at an expression for $x_i$ ($i = 3$ to $n$) in the form of a polynomial in $x_2$ (as $x_1 = 1$) which is the same as $(-1)^{i-1}$ times the CP of a linear chain containing $i-1$ vertices. Evaluation of $x_i$ ($i = 3$ to $n$) for the $r$th eigenvalue ($\lambda_r$) can then be made by putting $x_2 = \lambda_r$ in each of these polynomials. Thus, for $L_n$,

$$x_1 = 1,$$
$$x_2 = \lambda_r,$$
$$x_3 = P(L_2; x_2) = x_2^2 - 1 = \lambda_r^2 - 1,$$
$$x_4 = P(L_3; x_2) = x_2^3 - 2x_2 = \lambda_r^3 - 2\lambda_r \text{ etc.}$$

*Example* 2: Here we consider the graph $G_2$ and enclose vertex 1 of $\bar{G}_2$ as shown in figures 4a and 4b respectively in order to disconnect it. We have selected this in order to give evidence in support of the fact stated in §2, step (d). The matrix $\mathbf{A}_2$ from which we obtain $G_2$ is

$$\mathbf{A}_2 = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}.$$

Applying steps (b) and (c) of the algorithm successively and then from (4) we obtain the conditions

$$\begin{aligned} 1 + x_2 + x_3 - x_2(x_2 + x_4) &= 0, \\ x_2 + 2x_3 + x_4 - x_3(x_2 + x_4) &= 0, \\ 1 + x_3 - x_4(x_2 + x_4) &= 0, \end{aligned} \tag{14a}$$

**Table 1.** Eigenvalues ($\lambda$) of $\mathbf{A}_1$ and corresponding solution sets $\{x_i\}$ obtained from (11).

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ |
|---|---|---|---|---|---|
| 3·4913 | 1 | 1·2456 | 0·8376 | 0·4329 | 0·6737 |
| 1·5398 | 1 | 0·2699 | −0·2235 | −0·8839 | −1·1375 |
| 0·5292 | 1 | −0·2354 | −1·8544 | −0·5105 | 1·5843 |
| −0·5922 | 1 | −0·7961 | −0·4336 | 1·8490 | −0·6613 |
| −2·9680 | 1 | −1·9840 | 1·5970 | −0·7721 | 0·6946 |

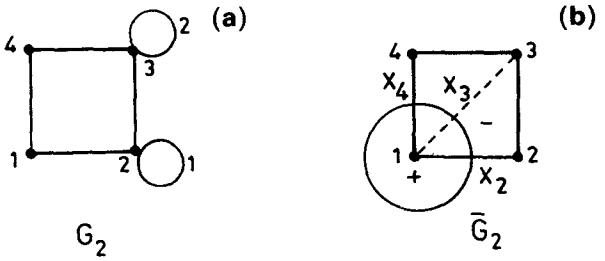


**Figure 4.** (a) Graphical representation of the matrix $\mathbf{A}_2 - \lambda\mathbf{I}$. (b) Simplified diagram of $G_2$: step (a) of the algorithm.

**Table 2.** The solution sets $\{x_i\}$, normalised eigenfunctions ($\psi$) and eigenvalues ($\lambda$) of $\mathbf{A}_2$.

| | | | | Coefficients of eigenfunctions $= \sum_{i=1}^{4} c_i\phi_i$ | | | | |
|---|---|---|---|---|---|---|---|---|
| $x_1$ | $x_2$ | $x_3$ | $x_4$ | $C_1$ | $C_2$ | $C_3$ | $C_4$ | $\lambda$ |
| 1 | 1 | −1 | 0 | $1/\sqrt{3}$ | $1/\sqrt{3}$ | $-1/\sqrt{3}$ | 0 | 1 |
| 1 | 1·8414 | 2·8414 | 1·2447 | 0·2671 | 0·4919 | 0·7590 | 0·3325 | 3·0861 |
| 1 | −0·5691 | 0·4309 | −0·9450 | 0·6451 | −0·3672 | 0·2780 | −0·6097 | −1·5141 |
| 1 | −1·2723 | −0·2723 | 1·7003 | 0·4232 | −0·5384 | −0·1152 | 0·7195 | 0·4280 |

where the substitution (5) i.e., $\lambda = x_2 + x_4$ has not been used.

After simplification from (14a) a polynomial equation in one variable ($x_2$) given by

$$3x_2^4 - 3x_2^3 - 8x_2^2 + 4x_2 + 4 = 0, \tag{14b}$$

is obtained.

The left hand side of (14b) is not same as the CP of $\mathbf{A}_2$. The values of $x_i$'s, normalised eigenfunctions and corresponding eigenvalues calculated by using (9) are shown in table 2. This verifies that the set of equations (4) are the necessary conditions to be satisfied by each set of values of $\{x_i\}$ which is able to disconnect one vertex $r$ although without using (5) we may fail to evaluate such sets.

*Example* 3: *Cyclobutadiene.* Applying HMO formalism to this molecule we obtain matrix $\mathbf{A}_3$. Graph $G_3$, representing $\mathbf{A}_3 - \lambda\mathbf{I}$ is shown in figure 5a.

$$\mathbf{A}_3 = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}.$$

It belongs to the $D_{4h}$ point group and contains multiple eigenvalues. Group theory and very recently graph theory (McClelland 1974, 1982; Datta and Mukherjee 1988) provide most convenient methods for solving the problem. Still we consider the case in order to describe how repeated application of the present process can bring out a complete solution of the problem.

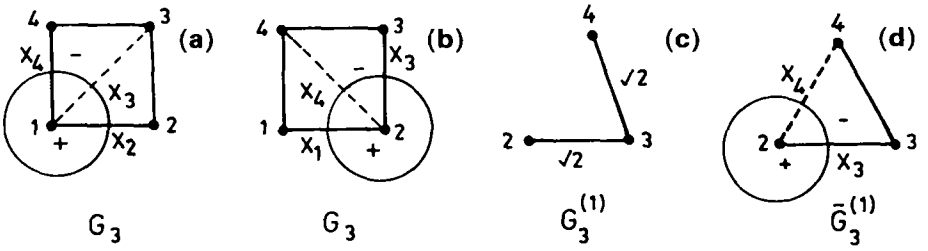


**Figure 5.** (**a**) Cyclobutadiene graph: vertex 1 is enclosed within the circle. (**b**) Cyclobutadiene graph with vertex 2 enclosed: method 1. (**c**) Reduced graph of cyclobutadiene: vertex 1 is disconnected. (**d**) Simplified diagram of $G_3^{(1)}$ with vertex 2 enclosed.

Enclosing vertex 1 within the circle and following steps (b) and (c) of the algorithm we obtain from (4) three equations correlating $x_2, x_3$ and $x_4$. From these and without using the substitution (5) three sets of solutions given by $(x_2, x_3, x_4) = (0, -1, 0), (1, 1, 1)$ and $(-1, 1, -1)$ are easily available by inspection. Substituting the values from each set in (3), only three normalised eigenfunctions $[1/\sqrt{2}(\phi_1 - \phi_3), 1/2(\phi_1 + \phi_2 + \phi_3 + \phi_4)$ and $1/2(\phi_1 - \phi_2 + \phi_3 - \phi_4)]$ respectively and none of the eigenvalues are obtained. The respective eigenvalues 0, 2, and $-2$ are calculated by using (9) in the following way.

For the first normalised eigenfunction $\Psi_1^2 = 0$ gives

$$1/2(\phi_1^2 - 2\phi_1\phi_3 + \phi_3^2) = 0$$

or,

$$1/2(-\lambda + 0 - 2 \times 0 - \lambda + 0) = 0$$

or,

$$\lambda = 0.$$

We can use each of the solution sets $(x_2, x_3, x_4)$ to disconnect vertex 1. Each will give one eigenfunction and the corresponding eigenvalue. In order to obtain all the eigenfunctions and eigenvalues, two methods of repeated application are described below.

*Method* 1: The first application of the algorithm described above, where the whole process has been designed to disconnect vertex $r$ by enclosing it within the circle, can produce only those eigenfunctions in each of which the contribution of $\phi_r$ is nonzero. A second application of the same; enclosing any other vertex of $G$, must therefore give results of which some are already obtained and some in which $\phi_r$ is absent. Such applications can be continued until a proper collection of results of these constitutes the whole set required.

In this example we enclose vertex 2, as shown in figure 5b, and following the description in step (2) construct the new eigenfunctions

$$\begin{aligned} \Psi_2 &= x_1\phi_1 + \phi_2 + x_3\phi_3 + x_4\phi_4, \\ \Psi_1 &= \phi_1 - x_1\phi_2, \\ \Psi_3 &= \phi_3 - x_3\phi_2, \\ \Psi_4 &= \phi_4 - x_4\phi_2, \end{aligned} \tag{15}$$

making $\langle \Psi_2 | \hat{A} | \Psi_i \rangle = 0$ $(i = 1, 3, 4)$, and thus in the usual manner we obtain three sets

of solutions given by $(x_1, x_3, x_4) = (0, 0, -1)$, $(1, 1, 1)$ and $(-1, -1, 1)$. The normalised eigenfunctions are $1/\sqrt{2}(\phi_2 - \phi_4)$, $1/2(\phi_2 + \phi_1 + \phi_3 + \phi_4)$ and $1/2(\phi_2 - \phi_1 - \phi_3 + \phi_4)$ respectively of which only the first one is found to be new. This, along with the three previously obtained, constitutes the whole set of solutions required.

*Method* 2: From the set of solutions ($x_i$'s) obtained after the first application and giving conditions for disconnecting vertex $r$, one set denoted by $\{x_i\}_{ac}$ is suitably chosen to obtain normalised $\Psi_r$ and the corresponding eigenvalue ($ac$ – acceptable). Now a new graph $G^{(1)}$ of reduced size is drawn by omitting the vertex $r$ and representing the other vertices $\{i\}$ by the new normalised basis functions $\{\Psi_i\}$; in computing these new bases, the set $\{x_i\}_{ac}$ is to be used. The reduced graph $G^{(1)}$ has the pecularity that its edge weight may involve $\lambda$. Now we have to repeat the same technique on $G^{(1)}$ and the same process should be continued until all required solutions are available.

In this example we chose $\{x_i\}_{ac} = (x_2, x_3, x_4)_{ac} = (0, -1, 0)$ by trial. Then following (3) and (3a) we have normalised basis functions for the factorised graph as,

$$\Psi_1 = 1/\sqrt{2}(\phi_1 - \phi_3), \quad \lambda_1 = 0,$$
$$\Psi_2 = (\phi_2 - x_2\phi_1) = \phi_2,$$
$$\Psi_3 = 1/\sqrt{2}(\phi_3 + \phi_1) \text{ and } \Psi_4 = \phi_4.$$

Now taking $\Psi_2$, $\Psi_3$ and $\Psi_4$ as new bases we draw the graph $G_3^{(1)}$ shown in figure 5c and concentrate on vertex 2 of its simplified diagram shown in figure 5d. The weights of edges and vertices of $G_3^{(1)}$ are calculated following (1) as shown below.

$$\Psi_2\Psi_3 = (1/\sqrt{2})\phi_2(\phi_3 + \phi_1) = (1/\sqrt{2})(1 + 1) = \sqrt{2}$$
$$\Psi_2\Psi_4 = \phi_2\phi_4 = 0, \quad \Psi_3\Psi_4 = \sqrt{2}.$$
$$\Psi_3^2 = \tfrac{1}{2}(\phi_3^2 + \phi_1^2 + 2\phi_3\phi_1) = \tfrac{1}{2}(-\lambda + 0 - \lambda + 0 + 2 \times 0)$$
$$= -\lambda,$$
$$\Psi_2^2 = \Psi_3^2 = -\lambda.$$

For disconnecting vertex 2 of $\bar{G}_3^{(1)}$ we construct new functions $\{\Psi'\}$ as before

$$\Psi'_2 = \Psi_2 + x'_3\Psi_3 + x'_4\Psi_4,$$
$$\Psi'_3 = \Psi_3 - x'_3\Psi_2, \tag{16}$$
$$\Psi'_4 = \Psi_4 - x'_4\Psi_2.$$

Then from $\Psi'_2\Psi'_3 = 0$ and $\Psi'_2\Psi'_4 = 0$ one has respectively.

$$1 + x'_4 - x'^2_3 = 0,$$
$$x'_3 - x'_3x'_4 = 0,$$

which are solvable for $x'_3$ and $x'_4$ as $(x'_3, x'_4) = (0, -1)$, $(\sqrt{2}, 1)$ and $(-\sqrt{2}, 1)$. These solutions yield three required eigenfunctions and eigenvalues as

$$(1/\sqrt{2})(\Psi_2 - \Psi_4) = (1/\sqrt{2})(\phi_2 - \phi_4), \quad \lambda_2 = 0 \text{ for } x'_3 = 0, \quad x'_4 = -1,$$

$$\tfrac{1}{2}(\Psi_2+\sqrt{2}\Psi_3+\Psi_4)=\tfrac{1}{2}(\phi_1+\phi_2+\phi_3+\phi_4), \quad \lambda_3=2 \text{ for } x'_3=\sqrt{2}, \quad x'_4=1,$$

$$\tfrac{1}{2}(\Psi_2-\sqrt{2}\Psi_3+\Psi_4)=\tfrac{1}{2}(\phi_2-\phi_3-\phi_1+\phi_4), \quad \lambda_4=-2 \text{ for}$$

$$x'_3=-\sqrt{2}, \quad x'_4=1.$$

These, along with $(1/\sqrt{2})(\phi_1-\phi_3)$, $\lambda_1=0$, construct the whole set required.

*Example* 4: *Complete graph.* The graph-spectrum of an unweighted complete graph $K_n$ with $n$ vertices contains an eigenvalue $n-1$ and the eigenvalue $-1$ appears with $(n-1)$-fold degeneracy. This is a typical example of multiple eigenvalue problem for which the well-known cofactor method is unable to yield more than two eigenfunctions. We have chosen this example to illustrate how the aforementioned technique of repeated application can yield solutions expressible by a closed formula for such graphs. Figure 6a represents an unweighted complete graph $K_6$. Following method (1) described in example 3 it is easy to verify that the algorithm applied to any vertex $r$ of $K_n$ yields a set of equations correlating the $x_i$'s which can be reduced to the form

$$x_i=x_n, \quad i\neq r \text{ because } x_r=1,$$

and

$$1+(n-2)x_i-(n-1)x_i^2=0.$$

Therefore, each time we have two solution sets–

First set: $x_i=1$, for all $i$

Second set: $x_r=1$, $x_i=-[1/(n-1)]$ $(i\neq r)$.

Let us choose the vertex labels $r=1,2,\ldots,n$ successively. The first solution set for $r=1$ gives

$$\Psi_1=\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\phi_i \quad \text{and } \lambda_1=n-1, \tag{17a}$$

In each of the successive applications from $r=2$ to $n$ we have found that the first solution set gives a result which is the same as that above. We therefore reject that

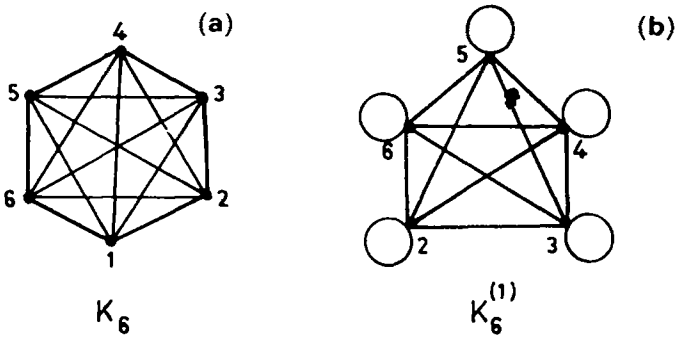


**Figure 6.** (**a**) Unweighted complete graph with six vertices. (**b**) Reduced graph obtained from $K_6$: vertex 1 is absent.

and accept only the second solution set. The eigenfunction thus obtained after enclosing vertex $r$ is

$$\Psi_r = \frac{1}{[n(n-1)]^{\frac{1}{2}}}\left[(n-1)\phi_r - \sum_{i\neq r}\phi_i\right], \quad \lambda_r = -1, \quad r = 2 \text{ to } n. \tag{17b}$$

Putting $r = 2, 3, \ldots, n$ we have $n-1$ eigenfunctions from (17b) which are not pairwise orthogonal. They are orthogonalised by Schmidt's process (see, for example, Joshi 1980) to produce new eigenfunctions representable by the closed formula.

$$\Psi_r = \frac{1}{[(n-r+1)(n-r+2)]^{\frac{1}{2}}}\left[(n-r+1)\phi_{r-1} - \sum_{i=r}^{n}\phi_i\right], \quad r = 2 \text{ to } n, \tag{17c}$$

Thus (17a) and (17c) form the complete set of eigenfunctions for $K_n$.

Following the description given in method (2) of example 3 we have first disconnected vertex 1 and taking $(x_2, x_3, \ldots, x_n)_{ac.} = (1, 1, \ldots, 1)$ calculated the reduced graph $K_n^{(1)}$. Starting from $K_6$, as an example, the reduced graph $K_6^{(1)}$ is shown in figure 6b. Thus we obtain one eigenfunction (17a) and the corresponding eigenvalue. The basis functions representing vertices of $K_n^{(1)}$ are given by

$$\Psi_i = (1/\sqrt{2})(\phi_i - \phi_1), \quad i = 2 \text{ to } n.$$

Using these bases we have found that the weights of each vertex and edge of $K_n^{(1)}$ would be $-1$ and $-\frac{1}{2}(\lambda+1)$, respectively. These are indicated by vertex loops and thick edges in $K_6^{(1)}$. The following is the description of the important steps of second application leading to two solutions for disconnecting the vertex 2 (keeping the condition of vertex 1 unchanged) of $K_6^{(1)}$.

$$\begin{aligned}\Psi'_2 &= \Psi_2 + x'_3\Psi_3 + x'_4\Psi_4 + x'_5\Psi_5 + x'_6\Psi_6\\ \Psi'_i &= \Psi_i - x'_i\Psi_2, \quad i = 3, 4, 5 \text{ and } 6.\end{aligned} \tag{18}$$

By $\Psi'_2\Psi'_i = 0$ and suppressing the factor $-\frac{1}{2}(\lambda+1)$ from each we have the equations

$$\begin{aligned}&1 + x'_4 + x'_5 + x'_6 - x'_3\Sigma x'_i = 0,\\ &1 + x'_3 + x'_5 + x'_6 - x'_4\Sigma x'_i = 0,\\ &1 + x'_3 + x'_4 + x'_6 - x'_5\Sigma x'_i = 0, \quad i = 3 \text{ to } 6,\\ &1 + x'_3 + x'_4 + x'_5 - x'_6\Sigma x'_i = 0,\end{aligned}$$

from which one finds $x'_3 = x'_4 = x'_5 = x'_6$ and $x'_3 = 1, -\frac{1}{4}$. The acceptable solution set is

$$\{x'_i\}_{ac.} = (1, 1, 1, 1)$$

Then from (18) we have

$$\Psi'_2 = (1/\sqrt{30})(5\phi_1 - \phi_2 - \phi_3 - \phi_4 - \phi_5 - \phi_6), \quad \lambda_2 = -1.$$

The collection of such results obtained after successive applications of the method to $K_n^{(2)}$, $K_n^{(3)}$ etc, is found to be pairwise orthogonal and the same as those given in (17a) and (17c).

## 4. Proof

We have used the transformation matrix

$$\mathbf{M}=\begin{bmatrix} 1 & 0\cdots 0 & -x_1 & 0\cdots 0 \\ 0 & 1\cdots 0 & -x_2 & 0\cdots 0 \\ \cdots & \cdots\ \cdots & \cdots & \cdots\ \cdots \\ \cdots & \cdots\ \cdots & \cdots & \cdots\ \cdots \\ 0 & 0\quad 1 & -x_{r-1} & 0\cdots 0 \\ x_1 & x_2\cdots x_{r-1} & 1 & x_{r+1}\cdots x_n \\ \cdots & \cdots\ \cdots & \cdots & \cdots\ \cdots \\ 0 & 0\cdots 0 & -x_n & 0\cdots 1 \end{bmatrix}, \tag{19}$$

It is easy to verify that the $r$th row (or column) vertor of $\mathbf{M}$ is orthogonal to every other row (or column), $\det \mathbf{M} = 1 + \sum_{i\neq r} x_i^2$, and that the matrix obtained by suppressing the $r$th row and column is a unit matrix. The matrix $\mathbf{M}$ is the necessary transformation $\mathbf{\Psi} = \mathbf{M\Phi}$ for linear combinations given explicitely in (3) and 3(a). $\mathbf{\Psi}$ and $\mathbf{\Phi}$ are two similar column vectors and $\mathbf{\Phi}^T = (\phi_1, \phi_2, \ldots, \phi_n)$.

The whole process described in the algorithm is equivalent to transformation $\mathbf{M(A-\lambda I)M}^T$, and according to notations used in (2) it is easy to verify that

$$\mathbf{M(A-\lambda I)M}^T = \mathbf{M}\begin{bmatrix} \phi_1^2 & \phi_1\phi_2 & \cdots & \phi_1\phi_n \\ \phi_2\phi_1 & \phi_2^2 & \cdots & \phi_2\phi_n \\ \cdots & \cdots & & \cdots \\ \cdots & \cdots & & \cdots \\ \phi_n\phi_1 & \phi_n\phi_2 & \cdots & \phi_n^2 \end{bmatrix}\mathbf{M}^T$$

$$= \begin{bmatrix} \psi_1^2 & \psi_1\psi_2 & \cdots & \cdots & \psi_1\psi_n \\ \psi_2\psi_1 & \psi_2^2 & \cdots & \cdots & \psi_2\psi_n \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \psi_n\psi_1 & \psi_n\psi_2 & \cdots & \cdots & \psi_n^2 \end{bmatrix}$$

with $\psi_i\psi_j = \psi_j\psi_i$. The values of $x_1, x_2, \ldots, x_n$ are so chosen that the last matrix takes the form

$$\begin{bmatrix} \psi_1^2 & \cdots & \psi_1\psi_{r-1} & 0 & \psi_1\psi_{r+1} & \cdots & \psi_1\psi_n \\ \psi_2\psi_1 & \cdots & \psi_2\psi_{r-1} & 0 & \psi_2\psi_{r+1} & \cdots & \psi_2\psi_n \\ \cdots & & \cdots & \cdots & \cdots & & \cdots \\ \psi_{r-1}\psi_1 & \cdots & \psi_{r-1}^2 & 0 & \psi_{r-1}\psi_{r+1} & & \psi_{r-1}\psi_n \\ 0 & \cdots & 0 & \psi_r^2 & 0 & \cdots & 0 \\ \psi_{r+1}\psi_1 & \cdots & \psi_{r+1}\psi_{r-1} & 0 & \psi_{r+1}^2 & \cdots & \psi_{r+1}\psi_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \psi_n\psi_1 & \cdots & \psi_n\psi_{r-1} & 0 & \psi_n\psi_{r+1} & \cdots & \psi_n^2 \end{bmatrix}$$

where, $\det \mathbf{M(A-\lambda I)M}^T = (\det \mathbf{M})^2 \det(\mathbf{A}-\lambda\mathbf{I})$. Therefore the matrix equation $\mathbf{A}-\gamma\mathbf{I}=\mathbf{0}$ implies

$$\mathbf{M(A-\lambda I)M}^T = \mathbf{0}.$$

Hence $[\psi_r^2] = \mathbf{0}$ and

$$\begin{bmatrix} \psi_1^2 & \cdots & \psi_1\psi_{r-1} & \psi_1\psi_{r+1} & \cdots & \psi_1\psi_n \\ \psi_2\psi_1 & \cdots & \psi_2\psi_{r-1} & \psi_2\psi_{r+1} & \cdots & \psi_2\psi_n \\ \cdots & & \cdots & \cdots & & \cdots \\ \psi_{r-1}\psi_1 & \cdots & \psi_{r-1}^2 & \psi_{r-1}\psi_{r+1} & \cdots & \psi_{r-1}\psi_n \\ \psi_{r+1}\psi_1 & \cdots & \psi_{r+1}\psi_{r-1} & \psi_{r+1}^2 & \cdots & \psi_{r+1}\psi_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \psi_n\psi_1 & \cdots & \psi_n\psi_{r-1} & \psi_n\psi_{r+1} & \cdots & \psi_n^2 \end{bmatrix} = \mathbf{0}.$$

Each set of values of $\{x_i\}$ thus extracts one factor $[\psi_r^2]$ from $\mathbf{A} - \lambda\mathbf{I}$. Since the matrix factor $[\psi_r^2]$ contains only one element, $\psi_r$ is the eigenfunction and $\psi_r^2 + \lambda$ is the corresponding eigenvalue.

## 5. Comparison with the cofactor method

The generality of the present algorithm is confirmed from (6). It has been found to be more efficient than the earlier cofactor method (numerically as in Streitwieser 1961) because (a) the latter can be derived from it, and (b) problems with multiple eigenvalue can be solved where the cofactor method fails. (a) can be deduced as follows.

Equation (8) is a consequence of (4). Now solving the characteristic equation, and using the eigenvalue $\lambda = \lambda_k$, $\{x_i\}$ can be obtained from (8). Then substitution of these $x_i$ values in (3), gives

$$\psi_r^{(k)} = \frac{1}{A_{sr}^{(k)}} \sum_{i=1}^{n} A_{si}^{(k)} \phi_i, \tag{20}$$

where $A_{sr}^{(k)}$ is the cofactor of the $(sr)$ element of $\det(\mathbf{A} - \lambda\mathbf{I})$ for $\lambda = \lambda_k$, and $\psi_r^{(k)}$ is the corresponding eigenfunction after normalisation. Ignoring $A_{sr}^{(k)}$, because this factor when non-zero is absorbed after normalisation, (20) reads the same as that given by the cofactor method when expanded along the $s$th row. When $A_{sr}^{(k)} = 0$, that is, the coefficient of $\phi_r$ in $\psi_r^{(k)}$ is zero, the difficulty of the present method compared to the cofactor method can be removed by choosing a second vertex ($\neq r$) for its application.

Sufficient examples in favour of (b) have been given. The following are some further merits of the present method over the cofactor method:

(i) It provides a means of obtaining complete description of the reduced graphs after factorisation.
(ii) For 'light' chemical graphs (where vertex weights are scarcely found and many of the edges are absent) separate evaluation of cofactors of all elements of a row is not necessary. In that case, if $r$ indicates a pendent vertex, solution sets $\{x_i\}$ can be obtained more easily from (5), (4) and (8).
(iii) It provides two ways for repeated application.

## 6. Concluding remarks

The method requires iteration in solving the final equation obtained from (4). This should not be regarded as a drawback 'since all eigenvalue techniques are essentially

iterative' (Wilkinson 1965). For heavily weighted graphs we have found that the labour necessary in the present method is nearly the same as in the cofactor method.

**Acknowledgement**

The author acknowledges his thanks to Dr Asok K Mukherjee of Burdwan Raj College for valuable discussions during the progress of this work.

**References**

D'Amato S S 1979a *Mol. Phys.* **37** 1363
D'Amato S S 1979b *Theor. Chim. Acta* **53** 319
Datta K K and Mukherjee A K 1988 *Proc. Indian Acad. Sci. (Chem. Sci.)* **101** 143
El Basil S 1984 *Theor. Chim. Acta* **65** 191
Givens J W 1958 *J. Soc. Ind. Appl. Math.* **6** 26
Gutman I and Polansky O E 1986 *Mathematical concepts in organic chemistry* (Berlin: Springer-Verlag)
Hall G G 1977 *Mol. Phys.* **33** 551
Householder A S 1958 *J. Assoc. Comput. Mach.* **5** 335
Householder A S 1964 *The theory of matrices in numerical analysis* (New York: Blaisdell)
Hosoya H 1972 *Theor. Chim. Acta* **25** 215
Jacobi C G J 1846 *Crelle's J.* **30** 51
Joshi A W 1980 *Matrices and tensors in physics* (Wiley Eastern) p. 9
Kassman A J 1985 *Theor. Chim. Acta* **67** 255
King R B 1977 *Theor. Chim. Acta* **44** 223
Mallion R B, Trinajstić N and Schwenk A J 1974 *Z. Naturforsch.* **A29** 1481
McClelland B J 1974 *J. Chem. Soc., Faraday Trans.* 2 **70** 1453
McClelland B J 1982a *Mol. Phys.* **45** 189
McClelland B J 1982b *J. Chem. Soc., Faraday Trans.* 2 **78** 911
Mukherjee A K and Datta K K 1989 *Proc. Indian Acad. Sci. (Chem. Sci.)* **101** 499
Sachs H 1962 *Publ. Math.* **9** 270
Sachs H 1963 *Publ. Math.* **11** 199
Streitwieser A (Jr) 1961 *Molecular orbital theory for organic chemists* (New York: John Wiley) p. 49
Wilkinson J H 1965 *The algebraic eigenvalue problem* (Oxford University Press) p. 570