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ORIGINAL PAPER

Phased graphs and graph energies

Douglas J. Klein · Vladimir R. Rosenfeld

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Abstract We define a *phased* graph G to yield an adjacency matrix $A(G)$ having general magnitude-1 values in the same locations as the usual unphased case, but subject to the restriction that A be Hermitian. Some characteristics of such phased graphs and their eigenspectra are contemplated and to some extent described. Different graph energies are defined as suitable sums over adjacency-matrix eigenvalues, with "occupation-number" coefficients $\in \{0, 1, 2\}$.

Keywords Phases · Phased graph · Eigenvalue · Eigenvector · Eigenspectrum · Total energy

1 Introduction

Modifications to a graph's adjacency matrix might entail different possible weightings. Here, we consider a particular type of weighting by *phases*, which is to say that each element $a_{jk} = 1$ appearing in the adjacency matrix A is replaced by $e^{i\theta_{jk}}$, where θ_{jk} is real and such that $\theta_{kj} = -\theta_{jk}$. Thus, A keeps each of its entries with the same modulus, 0 or 1, such that the result is a Hermitian matrix ($A^\dagger = A$). Being Hermitian, all the eigenvalues remain real.

Such *phased* matrices arise in several different contexts. First, they arise for cyclic "polymer" graphs G when their cyclic (or translational) symmetry is used to block-diagonalize the total parent graph—each block is a phased graph related

D. J. Klein (✉) · V. R. Rosenfeld
Mathematical Chemistry Group, Department of Marine Sciences, Texas A&M University at Galveston, Galveston, TX 77553–1675, USA
e-mail: kleind@tamug.edu

V. R. Rosenfeld
e-mail: rosenfev@tamug.edu; vladimir_rosenfeld@yahoo.com

to that of the basic repeat unit in G—see, e.g., [1] and a similar picture with more phases occurs as the result of multicyclic symmetries for two- or three-dimensional crystals, with the underlying idea going back to Bloch [2] in 1929. Second, phased graphs arise in the quantum-theoretic Hückel-model description in the presence of a magnetic field—see, e.g., London [3] or also [4]. Third, phased cycles sometimes arise as solutions to the cyclic (intrinsically graph-theoretical) Hubbard model near the atomic limit. Fourth, phased graphs may sometimes be interpreted as representing an acyclic reference system in Aihara's approach [5–8] to resonance energy. Fifth, yet further, there is a possibility that such a weight be relevant in the context of inorganic "aromaticity"—see, e.g., [9]. Yet further phased graphs extend the notion of "signed" graphs, such as have several times been defined and studied [10–16]. But there is another general circumstance of long interest involving "flow" graphs, as reviewed in [17]—for such cases, there is an orientation on the graph with a skew adjacency matrix whose nonzero entries $= \pm 1$ corresponding to edges $\{j, k\}$ with the "+" sign for a_{jk} in agreement with the orientation and the "–" sign when counter to the orientation—here if one multiplies A by i to give a new Hermitian adjacency matrix $A' = iA$, then A' is seen to be that for a phased graph, with every phase $\doteq \pm\pi/2$. A similar remark applies for the skew adjacency matrices of Kasteleyn [18].

Here, we pursue the general theory of phased graphs, utilizing standard graph-theoretic notation—with a graph $G = (V, E)$ specified in terms of vertex and edge sets, V and E. The adjacency matrix A is allowed in our current investigation to be phased. Further, following chemical tradition, reference is made to molecular energies as $\sum_k n_k \lambda_k(G)$, where $\lambda_k(G)$ are eigenvalues, and different choices may be contemplated for the occupation numbers $n_k \in \{0, 1, 2\}$. The *chemical energy* is

$$\varepsilon_0(G) = \max_n \sum_k n_k \lambda_k(G), \tag{1}$$

where the choices of n_k are taken to maximize the sum subject to the restriction that the n_k sum to n. This constraint gives neutral (uncharged) species, while other choices for the n_k correspond to ions and/or excited states. Another natural choice maximizes the sum in (1) without the constraint that the occupation numbers sum to n. In such cases, one maximizes the sum without restriction on the value $\sum_k n_k$ (but still $n_k \in \{0, 1, 2\}$) to obtain

$$\varepsilon_{\text{opt}} = \max_{\text{opt}} \sum_k n_k \lambda_k(G). \tag{2}$$

Thus, the $n_k = 2$ for $\lambda_k > 0$ and $n_k > 0$ for $\lambda_k < 0$, while we further understand that $n_k = 1$ for $\lambda_k = 1$. Then, one identifies

$$q_{\text{opt}} \equiv n - \sum_k n_k \tag{3}$$

as the associated *charge*. Note a contrast to Gutman's [19] *mathematical energy*

$$\varepsilon_{\text{math}}(G) = \sum_{k}^{\text{all}} |\lambda_k(G)|, \tag{4}$$

which seems to have been intended to be an approximation to $\varepsilon_0(G)$—see also McClelland [20] and Aihara [21]. A natural question is whether (and if so, when) any of these examples might agree.

2 First results

A *bipartite* (or alternant) graph is recalled to be one for which the sites may be bipartitioned into two sets of *starred* ($*$) and *unstarred* ($\circ$) sites such that the neighbors of a site of one type are of the other type. Now, in a separate paper [22], it is found for the phased cycle that, though the eigenvalues moved around with the choice of phases, the even cycles maintained a symmetric distribution about 0, as was noted for unphased bipartite graphs [23] by Coulson and Rushbrooke (in 1940). But in fact, their eigenspectral symmetry is retained for phased graphs:

Theorem 1 *Let G be a bipartite phased graph. Then, its (real) eigenvalue spectrum is symmetric about* 0. *Moreover, let Φ be a diagonal matrix which acts as the identity on the $*$-space and as minus the identity on the $\circ$-space, whence $\Phi A = -A\Phi$. Also, if $A\vec{c} = \lambda\vec{c}$, then $\Phi\tilde{c}$ (if $\neq 0$) is an eigenvector to A with eigenvalue $-\lambda$.*

Proof The proof follows quite closely the proof for the unphased graph. It is easily seen that A and Φ anticommute: $A\Phi = -\Phi A$. Then, for an eigenvector $\vec{c}$ with eigenvalue λ, we see that A acts on $\vec{c'} \equiv \Phi\tilde{c}$ thusly $A\vec{c'} = A\Phi\tilde{c} = -\Phi A\tilde{c} = -\lambda\vec{c'}$.

Indeed, the result persists for arbitrary magnitude entries as well—the single condition of Hermiticity being maintained. The formulation in terms of the anticommuting operator Φ need not be introduced, with one just looking at the eigenproblem expressed in terms of the block components A_{**}, $A_{*\circ}$, $A_{\circ *}$, $A_{\circ\circ}$ of A as well as $\vec{c}_*$ and $\vec{c}_\circ$ of $\vec{c}$, and seeing that the replacement of $\vec{c}_* + \vec{c}_\circ$ by $\vec{c}_* - \vec{c}_\circ$ yields an eigenvalue $-\lambda$. But the formulation in terms of an anticommuting operator like Φ is useful in extensions [24–27] to Hubbard and PPP models. Indeed, if the electron hopping parameter is phased in these extended models, the present Φ may be suitably modified for these models in the bipartite case.

A further straightforward result concerns (necessary and sufficient) conditions for the chemical and mathematical energies to agree:

Proposition 2 *Let G be a phased graph. The equality $\varepsilon_0(G) = \varepsilon_{math}(G)$ holds iff the numbers $\#_+(G) and \#_-(G)$ of positive and negative eigenvalues are both $\leq n/2$.*

Proof This easily follows a result of Gutman and Trinajstić [28,29] for unphased graphs.

Again, the result also persists for arbitrary magnitude entries, while maintaining the condition of Hermiticity. As an immediate consequence of Propositions 6 and 7, we

have an extension of a more widely-known (for unphased graphs) condition for agreement between $\varepsilon_{\text{math}}$ and the chemical energy ε_0—namely that $\varepsilon_{\text{math}}(G) = \varepsilon_0(G)$ for bipartite G. But what seems to us much more (chemically) interesting is that:

Theorem 3 *For a general phased graph* $\varepsilon_{math}(G) = \varepsilon_{opt}(G)$.

Proof Since $\text{tr}A = 0$; and since the trace operation is invariant under unitary transformation UAU^T, the negative eigenvalues sum to the negative of the sum of the positive eigenvalues: $\sum_{\lambda<0} \lambda = -\sum_{\lambda>0} \lambda$. Thus, $2\sum_{\lambda>0} \lambda = \sum_{\lambda>0} \lambda - \sum_{\lambda<0} \lambda = \sum |\lambda| = \varepsilon_{\text{math}}(G)$.

This is a straightforward result, giving a perfectly well-defined chemical meaning to $\varepsilon_{\text{math}}(G)$ in general, but still seems not to have been previously clearly enunciated.

Also, upon taking the complex conjugate of the eigenvalue equation, one obtains:

Proposition 4 *If all the phases of a phased graph are changed in sign, then the eigenvalue spectrum remains fixed, while the eigenvectors change to their complex conjugates.*

3 Transformation by di-uns

For the single cycle and beyond it proves of use to consider the effect of diagonal unitary transformations, or *di-uns*, on a phased adjacency matrix: $A \rightarrow UAU^{\dagger}$, where U is a diagonal unitary matrix—earlier considered by McWeeny [30] and by Mallion [31]. Being a similarity transformation, this di-un preserves eigenvalues, and moreover, the eigenvectors are simply related, with corresponding components of the same magnitude.

The *cyclomatic number* of a graph G is the minimum number of edges needed to be deleted in order to render the result acyclic. It is well-known (e.g., [32], Ch. 1) that for a connected G, $\gamma = |E| - |V| + 1$. For a connected graph, deletion of the maximum number γ of edges while retaining connectivity leaves a spanning tree T, and each edge of G not in T is termed a *chord* (of G with respect to T).

Proposition 5 *Let* T *be a tree with an unphased adjacency matrix* $A(T)$ *and a phased adjacency matrix* $W(T)$. *Then, there exists a diagonal unitary matrix* U *such that* $UWU^{\dagger} = UWU^{-1} = A$. *Phasing does not influence the eigenspectrum of a tree.*

Proof We show by an inductive argument that the required unitary matrix exists. It is clear that for $n = 1$ vertices such a matrix exists. Now, let j be a terminal vertex of T and T_1 be that tree with vertex j deleted (along with its incident edge), and let U_1 be a diagonal unitary matrix such that $U_1 A_1 U_1^{\dagger}$ is unphased (where A_1 is the $(n-1)\times(n-1)$ submatrix of A corresponding to T_1). Let $e^{i\varphi_k}$ be the diagonal value for the vertex k to which j is adjacent in T. Now, let U be the diagonal unitary matrix for which its j-th diagonal entry is $e^{i(\varphi_k - \theta_{jk})}$ and with remaining diagonal entries as in U_1. Then, clearly, in $UAU^{\dagger}$, the phase of each edge in T_1 is eliminated, and for the (j,k)-th entry of $UAU^{\dagger}$ one has $(UAU^{\dagger})_{jk} = U_{jj} A_{jk} U^*_{kk} = e^{i(\varphi_k - \theta_{jk})} e^{i\theta_{jk}} e^{-i\varphi_k} = 1$. Thus an unphasing di-un has been achieved.

Theorem 6 *All phased single cycles with the same value of θ_0 are equivalent under di-uns.*

Proof If we pick a di-un with the j-th diagonal entry $= e^{i\theta_{j,j+1}}$, $j \in [1, n-1]$, and n-th diagonal entry $= 1$, then UAU^{-1} is unphased except for the edge $\{1, n\}$, which ends up with phase θ_0 for the arc from n to 1. Conversely, the inverse transformation (by U^{-1}) carries this special phased cycle, with all the phase localized in edge $\{1, n\}$, to any other phased cycle with net phase θ_0, and thence they all occur in the same di-un equivalence case.

Corollary 6.1 *The nonzero phases of a phased cycle may be localized entirely in any one of the edges of the cycle, whence this exceptional edge has weights $e^{\pm i\theta_0}$. The nonzero phase θ_0 of a phased cycle may be uniformly distributed over all the edges, whence the directed edges $(j, j+1)$ have weights $e^{i\theta_0/n}$.*

This last uniformly-distributed case evidently "explains" the cyclic symmetry found in Theorem 2 of our accompanying paper [22]. That is, the di-uns manifestly reveal a cyclic symmetry directly in the adjacency matrix, which then appears in the eigenspectrum.

Corollary 6.2 *Let A be the adjacency matrix of the phased n-cycle, let C_0 be the (unphased) matrix with (j,k)-th entry $\delta_{j+1,k}$, and let $\sigma_p = C_0^p \sigma_0 C_0^{-p}$. Then, $\sigma_p A \sigma_p = A^*$, whence $\theta_0 = 0$ gives commutation $\sigma_p A = A\sigma_p$. If there is uniform distribution with $\theta_{j,j+1} = \pi/2$, then $\sigma_p A \sigma_p = -A$, which is anticommutation.*

Theorem 7 *Let G be a connected phased graph with cyclomatic number $\gamma(G)$. Then, there is a di-un which brings the phased adjacency matrix $W(G)$ to another $W'(G)$ with no more than $\gamma(G)$ nonzero phases for $\gamma(G)$ chords.*

Proof Let $\mathcal{E}(G)$ be a set of $\gamma(G)$ chords in G, whence removal of these from G leaves a tree T. By Proposition 5, there is a unitary transformation which will bring the phases on this subtree all to 0. Thence, any (possible) nonzero phases are left solely on the edges of $\mathcal{E}(G)$.

Along with this result, our consideration on the symmetries for the phased cycle shed some light on what symmetries might persist for more general phased graphs. Evidently, one should adjust the phasing through the judicious use of di-uns so as to obtain a (visual) weighting pattern (with directed, weighted edges) preserving as much of the unphased symmetry as possible—whence it is that symmetry which persists.

We say that two ordered sequences $(a_1, a_2, \ldots, a_n)$ and $(b_1, b_2, \ldots, b_n)$ are 1-*interlaced* if either $a_1 \le b_1 \le a_2 \le b_2 \le \cdots \le a_n \le b_n$ or $b_1 \le a_1 \le b_2 \le a_2 \le \cdots \le b_n \le a_n$. We say that ordered sequences $(a_1, a_2, \ldots, a_n)$ and $(c_1, c_2, \ldots, c_n)$ are *m-interlaced*, $m-1 \in \mathbb{Z}_+$, if there exists a sequence $(b_1, b_2, \ldots, b_n)$ which is $(m-1)$-interlaced with $(a_1, a_2, \ldots, a_n)$ and 1-interlaced with $(c_1, c_2, \ldots, c_n)$. Equivalently, when $p + q = m$ and $p, q \in \mathbb{Z}_+$, sequences $(a_1, a_2, \ldots, a_n)$ and $(b_1, b_2, \ldots, b_n)$ are interlaced iff there is a sequence $(b_1, b_2, \ldots, b_n)$ p-interlaced with $(a_1, a_2, \ldots, a_n)$ and q-interlaced with $(c_1, c_2, \ldots, c_n)$.

Theorem 8 *For $\gamma =$ cyclomatic number of G, the eigenvalue spectrum of the phased G is 2γ-interlaced with the eigenvalue spectrum of the unphased correspondent graph.*

Proof As preparation, recall the standard result [33] (p. 119) that on deletion of a given vertex (or better placing 0 in all the positions of a row and corresponding column) of $A = A(G)$, a new matrix A_0 is obtained which is 1-interlaced with A. We denote the 1-interlacing $A_0 \sim_1 A$. Thus, if first a vertex is so disconnected in A, then reconnected with phased weights to give A', one has $A \sim_1 A_0 \sim_1 A'$, so that A and A' are 2-interlaced. Now, via Theorem 7, the nonunity phases may be localized in no more than γ edges. Doing so and treating (disconnecting and reconnecting) a vertex in each one of these $\leq \gamma$ edges, then yields a sequence of ever higher interlacing relations up to 2γ-interlacing.

Note that this theorem applies even for trees, when we take 0-interlacing to mean that the 2 eigenspectra are equal.

Next, let $\gamma' \equiv \gamma'(G)$ denote the minimum number of vertices which need to be removed from G to make it acyclic. Then

Theorem 9 *The eigenvalue spectrum of a phased G is* $2\gamma'$*-interlaced with the eigenspectrum of the unphased correspondent graph.*

Proof The proof is quite parallel to that of Theorem 8. One needs to note that in the proof of Theorem 7, the edges on which the phases are localized may be chosen to be those that are coincident at the set of γ' vertices which when deleted make G acyclic.

In general $\gamma' \leq \gamma$, and in some cases $\gamma' < \gamma$, so that Theorem 9 then improves on Theorem 8.

4 Conclusion

Several first results for phased graphs and for graph energies have been noted.

Also, some chemical aspects of graph energies so widely considered in mathematical literature have been clarified.

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