We remark that π can be viewed as a matrix with rows indexed by $V(P)$ and columns indexed by $V(\Gamma)$ such that $\pi(v,x) = 1$ if $x \in V_v$ and 0 otherwise. Clearly, we have

$$\langle \phi_0 \pi A_j, f \rangle = |V_j| f(v_j).$$

Therefore, $\lambda' = |V_j| f(v_j)/f(v_0)$. □

Using Theorems 7.9, 7.10 and 7.12, we will show that the multiplicities of each eigenvalue can be determined from the contracted path P.

THEOREM 7.13. *For a distance-transitive graph Γ on n vertices, the multiplicity $m(\lambda)$ of an eigenvalue λ is*

$$m(\lambda) = \frac{n}{\| g \|^2} g^2(v_0)$$

where g is the corresponding eigenfunction of the weighted path P contracted from Γ from a fixed vertex v_0.

PROOF. Let g_i's denote eigenfunctions of P and f_i's denote the corresponding harmonic eigenfunctions. Note that $g(v_i) = \sqrt{k|V_i|} f(v_i)$ where k is the degree of Γ. We consider the following $n \times n$ matrix:

$$M_i = \sum_{j=0}^{D} f_i(v_j) A_j.$$

For a fixed i, the trace of M_i is just the trace of $f_i(v_0)A_0$. Hence

$$tr(M_i) = n f_i(v_0). \tag{7.3}$$

On the other hand, the eigenvalues of A_j are $|V_j| f_0(v_j)/f_0(v_0), |V_j| f_1(v_j)/f_1(v_0), \dots, |V_j| f_D(v_j)/f_D(v_0)$ of respective multiplicities $m(\lambda_0), \dots, m(\lambda_D)$. Therefore,

$$\begin{aligned} tr\ M &= \sum_{j=0}^{D} f_i(v_j)\ tr\ A_j \\ &= \sum_{j=0}^{D} f_i(v_j) \sum_{l=0}^{D} m(\lambda_l) f_l(v_j) \frac{|V_j|}{f_l(v_0)} \\ &= \sum_{j=0}^{D} f_i(v_j) m(\lambda_i) f_i(v_j) \frac{|V_j|}{f_i(v_0)} \\ &= \| g_i \|^2 \frac{m(\lambda_i)}{f_i(v_0)k}. \end{aligned}$$

Here, we use the fact that distinct eigenfunctions are orthogonal so that

$$\sum_i f_p(v_i) f_q(v_i) |V_i| k = \begin{cases} 0 & \text{if } p \neq q \\ \| g_p \|^2 & \text{if } p = q. \end{cases}$$

EXAMPLE 7.14. *The Petersen graph and intersection graphs*

The Petersen graph is a distance transitive graph on 10 vertices. The vertex set is labelled by all 2-subsets of $\{1,2,3,4,5\}$. Two vertices A and B are adjacent if and only if $A \cap B = \emptyset$. The eigenvalues are 0, $\frac{2}{3}$ (with multiplicity 5), and $\frac{5}{3}$ (with multiplicity 4). The Petersen graph is a special case of the intersection graph $G(n,r,k)$ with vertex set consisting of all r-subsets of $\{1,\dots,n\}$. The vertices A and B are adjacent if $|A \cap B| = k$. The symmetric group S_n acts on the graph with isotropy group $S_r \times S_{n-r}$. Since $(S_n, S_r \times S_{n-r})$ is a Gelfand pair [**97**], the spectral decompositions of the space $\mathcal{F}(v) = \{f : V \to R\}$ are quite special:

$$\mathcal{F}(v) = E_0 \oplus E_1 \oplus \ldots \oplus E_r$$

where the dimension of E_i satisfies $dim\ E_i = \binom{n}{i} - \binom{n}{i-1}$ for $i \geq 1$, and $dim\ E_0 = 1$.

7.5. Eigenvalues and group representation theory

A brute force method for computing eigenvalues of a connected graph on n vertices is to solve for x in the determinant, $det(xI - \mathcal{L})$, of an $n \times n$ matrix. Before starting such an arduous task, it makes sense to see if the matrix can be diagonalized into smaller blocks. Group representation theory is exactly the answer to such prayers when the graph is homogeneous.

Suppose Γ is a Cayley graph [**25**]with vertices labelled by a group $\mathcal{H}$ and with edge generating set $\mathcal{K}$. Let ρ denote an irreducible representation of $\mathcal{H}$ of dimension l. This means that ρ maps the elements of $\mathcal{H}$ into $l \times l$ matrices in such a way that matrix multiplication is consistent with the group multiplication, i.e., $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$. The eigenvalues of Γ are exactly the eigenvalues of the smaller matrix

$$I - \frac{1}{|k|} \sum_{g \in \mathcal{K}} \rho(g)$$

for ρ ranging over all irreducible representations of $\mathcal{H}$. Each eigenvalue of the $dim\ \rho \times dim\ \rho$ matrix has multiplicity $dim\ \rho$ in the graph Γ.

Suppose Γ is a homogeneous graph with associated group $\mathcal{H}$. The vertex set can be identified by $\mathcal{H}/\mathcal{I}$ where $\mathcal{I}$ is the isotropy group. The edge generating set $\mathcal{K} = \{g\mathcal{I} : v \sim gv\}$ for a fixed v is a union of double cosets

$$\mathcal{K} = \mathcal{I}\mathcal{K}\mathcal{I}$$

The eigenvalues of Γ are the eigenvalues of $I - \frac{1}{k} \sum_{g\mathcal{I} \in \mathcal{K}} \frac{1}{|\mathcal{I}|} \sum_{x \in g\mathcal{I}} \rho(x)$ where k is the degree of Γ.

The best way to illustrate the connection between homogeneous graph Γ and the irreducible representations of the associated group $\mathcal{H}$ is by examining concrete

We remark that for the Gelfand pairs in Example 7.15, all irreducible representations are 1-dimensional. This simplifies the computation of the eigenvalues of the corresponding homogeneous graphs.

In our final example we use terminology that may be unfamiliar to some readers. A quick summary of this can be found in [**85**] or [**84, 86**].

EXAMPLE 7.16. The Buckyball, a soccer ball-like molecule, consists of 60 carbon atoms. It corresponds to a Cayley graph on A_5 with edge generating set $\{(12345),(54321),(12)(23)\}$. The edges generated by $(12)(34)$ correspond to "double bonds" and the edges generated by $(12345),(54321)$ to "single bonds". The irreducible representations for the alternating group were determined by Frobenius [**134**] and they are of dimensions $1, 3, 3, 4$, and 5. This means the Laplacian can be diagonalized into blocks of sizes 1×1, 3×3 (with multiplicity 3), $3' \times 3'$ (a second type with multiplicity 3), 4×4 (with multiplicity 4), and 5×5 (with multiplicity 5). Note that $1^2 + 3^2 + 3^2 + 4^2 + 5^2 = 60$.

Suppose we consider the weighted graph with single bonds of weight 1 and double bonds of weight t. The eigenvalues of the adjacency matrix are exactly the eigenvalues of

$$\rho a + \rho a^{-1} + t\rho b$$

for any irreducible representation ρ and $a = (12345), b = (12)(34)$. For example, for the dimension 5 representation ρ_5 we have

$$\rho_5(a) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\rho_5(a^{-1}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\rho_5(b) = \begin{pmatrix} -1 & -1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Thus, the eigenvalues of the adjacency matrix are the roots of the characteristic polynomial

$$(x^2 + x - t^2 + t - 1)(x^3 - tx^2 - x^2 - t^2x + 2tx - 3x + t^3 - t^2 + t + 2).$$

In summary, the eigenvalues of the Buckyball can be written in closed form as roots of the following equations where the single bonds are weighted by 1 and the double bonds are weighted by t:

(a): $(x^2 + x - t^2 + t - 1)(x^3 - tx^2 - x^2 - t^2x + 2tx - 3x + t^3 - t^2 + t + 2) = 0$ with multiplicity 5;

(b): $(x^2 + x - t^2 - 1)(x^2 + x - (t+1)^2) = 0$ with multiplicity 4;

(c): $(x^2 + (2t+1)x + t^2 + t - 1)(x^4 - 3x^3 + (-2t^2 + t - 1)x^2 + (3t^2 - 4t + 8)x + t^4 - t^3 + t^2 + 4t - 4 = 0$ with multiplicity 3;

(d): $x - t - 2 = 0$ with multiplicity 1.

7.6. The vibrational spectrum of a graph

The Laplacian $\mathcal{L}$ of a graph Γ is an operator acting on the space of functions $\{f : V(\Gamma) \to \mathbb{R}\}$. A natural generalization is the *vibrational Laplacian* $\mathcal{L}_X$ which acts on the space $\mathcal{F}(V, X) = \{f : V(\Gamma) \to X\}$ for some vector space X. We use the word "vibrational" since the spectrum of the vibrational Laplacian $\mathcal{L}_X$ of a graph Γ for the special case of $X = \mathbb{R}^3$ is exactly the vibrational spectrum of the molecule whose atoms correspond to the vertices of Γ and whose bonds between atoms are just edges of Γ [**84**].

We start with a homogeneous graph Γ with the associated group $\mathcal{H}$ and isotropy group $\mathcal{I}$. We can generalize the Dirichlet sum (see Section 1.2) as follows: Suppose that to each edge, $e = \{u, v\}$, of the graph we associate a self-adjoint operator, A_e, on X; we then define the quadratic form Q on $\mathcal{F}(V, X)$ by

$$\langle g, \mathcal{L}_X g\rangle = \frac{1}{2}\sum [g(u) - g(v)] \cdot A_e \cdot [g(u) - g(v)] \tag{7.4}$$

where the sum ranges over all edges of Γ. Suppose ρ denotes a representation of $\mathcal{H}$ on X. Furthermore, suppose A_e in (7.4) satisfies

$$A_{ae} = \rho(a) A_e \rho(a)^{-1}$$

where ae denotes the edge $\{ab, ac\}$ and the edge e is denoted by $\{b, c\}$. Then it can be shown (see [**84**]) that the spectrum of $\mathcal{L}_X$ can be decomposed into the union of the spectra of the following operators over all irreducible representations γ of Γ:

$$\left(\sum_{g \in \mathcal{K}} A_g\right) \otimes I - \sum_{g \in \mathcal{K}} A_g \rho(g) \otimes \gamma(g) \tag{7.5}$$

describe a deviation from equilibrium, so that $\mathbf{u} + h(u)$ is the new position of the vertex u. Then the potential energy associated to h can be expressed as:

$$W(h) = \frac{1}{2}\sum k_{u,w}(\|\mathbf{u} + h(u) - (\mathbf{w} + h(w))\| - \|\mathbf{u} - \mathbf{w}\|)^2.$$

In the above expression, the sum is over all pairs $\{u, w\}$ of vertices connected by an edge, and $k_{u,w}$ is the spring constant of that edge. If h is sufficiently small so as to enable us to ignore terms quadratic in h, we then have

$$\begin{aligned} \|\mathbf{u} + h(u) - (\mathbf{w} + h(w))\| &\approx [\|\mathbf{u} - \mathbf{w}\|^2 + 2(\mathbf{u} - \mathbf{w}) \cdot (h(u) - h(w))]^{\frac{1}{2}} \\ &\approx \|\mathbf{u} - \mathbf{w}\| + \omega_{u,w} \cdot (h(u) - h(w)) \end{aligned}$$

where

$$\omega_{u,w} = \frac{\mathbf{u} - \mathbf{w}}{\|\mathbf{u} - \mathbf{w}\|}$$

is the unit vector from $\mathbf{u}$ to $\mathbf{w}$ and $\cdot$ denotes the scalar product on $\mathbb{R}^3$. Then the quadratic approximation to W is given by

$$W(h) = \frac{1}{2}\sum k_{u,w}[\omega_{u,w} \cdot (h(u) - h(w))]^2.$$

Hence, we may take A_e to be a 3×3 matrix:

$$A_e = \omega_{u,w} \otimes \omega^t_{u,w}$$

where e is the edge joining u to w.

We can now use the above methods and (7.5) to compute explicitly the vibrational spectra of a molecule in terms of the irreducible representations of A_5. The space of displacements is $\mathcal{F}(V, \mathbb{R}^3) = \{f : V \to \mathbb{R}^3\}$. We choose ρ to be the ordinary three-dimensional representation (which is just rotation in $\mathbb{R}^3$). Using irreducible representations of A_5, we can then evaluate explicitly all vibrational eigenvalues by treating $3 \times 3, 9 \times 9, 9 \times 9, 12 \times 12$, and 15×15 matrices.

We point out that the above methods not only determine the vibrational spectrum, but also the specific representation associated to each eigenvalue. This additional information is important in chemical applications. For the case of homogeneous molecules, we can, in advance of all computations and independent of specific models for the potential energy, determine the number of representations of each type by a simple application of the Frobenius reciprocity formula.

Now the space of displacements of the Buckyball has dimension $180 = 60 \times 3$. But the space of entire (infinitesimal) rigid displacements of the molecule as a whole is six-dimensional (the Lie algebra of the Euclidean group). By subtracting these six dimensions, we get

1. *The space of vibrational states is 174-dimensional.*

The 180-dimensional space is the tensor product of the regular representation with a three-dimensional representation. So we must decompose the regular repre-

the 180-dimensional displacement space decomposes into $48 = 3 \times 16$ irreducibles. Subtracting off two three-dimensional representations, we obtain:

2. *The number of distinct vibrational modes is at most 46.*

For a vibrational line to be visible as an absorption or emission line in the infrared (as a transition between the ground state and a one-photon state) it is necessary that the associated irreducible representation be equivalent to (the complexification of) the representation of $\mathcal{H}$ on the ordinary three-dimensional space $\mathbb{R}^3$ in which the molecule lies.

In the Raman experiment, light of a definite frequency is scattered with a change of frequency. This change, known as the Raman spectrum, is associated to those representations which intertwine with the space $S^2(\mathbb{R}^3)$ of symmetric two tensors. Therefore, both the infrared spectrum and Raman spectrum can be directly determined by using the Frobenius reciprocity formula. For details on this, the reader is referred to [**84, 230**].

3. *The space of classical vibrational states has dimension 174. Any force matrix, F, invariant under the group A_5 has (at most) 46 distinct eigenvalues yielding four lines visible in the infrared and ten in the Raman spectrum.*

Notes:

The proofs in Section 2 are mainly adapted from [**14**]. There are several chapters on distance transitive graphs in Biggs [**25**]. Here we have given slightly different proofs. The computation for the spectrum of the Buckyball graph is based on [**87**]. More reference on the vibrational spectrum of graphs can be found in [**84, 85, 86**].

[25] N.L. Biggs, *Algebraic Graph Theory*, (2nd ed.), Cambridge University Press, Cambridge, 1993.

[26] N.L. Biggs and M.H. Hoare, The sextet construction for cubic graphs, *Combinatorica* **3** (1983), 153-165.

[27] N.L. Biggs, E.K. Lloyd and R.J. Wilson, *Graph Theory 1736-1936*, Clarendon Press, Oxford, 1976.

[28] Y. Bishop, S. Fienberg, P. Holland, *Discrete Multivariate Analysis*, MIT Press, Cambridge, 1975.

[29] M. Blum, R.M. Karp, O.Vornberger, C. H. Papadimitriou, and M. Yannakakis, The complexity of testing whether a graph is a superconcentrator, *Inf. Proc. Letters* **13** (1981), 164-167.

[30] B. Bollobás, *Random Graphs*, Academic Press, New York (1987).

[31] B. Bollobás, *Extremal Graph Theory*, Academic Press, London (1978).

[32] B. Bollobás and F.R.K. Chung, The diameter of a cycle plus a random matching,*SIAM J. on Discrete Mathematics* **1** (1988), 328-333.

[33] B. Bollobás and I. Leader, Edge-isoperimetric inequalities in the grid, *Combinatorica* **11**(1991), 299-314.

[34] B. Bollobás and I. Leader, An isoperimetric inequality on the discrete torus, *SIAM J. Disc. Math.* **3** (1990), 32-37.

[35] B. Bollobás, and A. Thomason, Graphs which contain all small graphs, *European J. of Combinatorics* **2** (1981), 13-15.

[36] B. Bollobás and W.F. de la Vega, The diameter of random graphs, *Combinatorica* **2** (1982), 125-134.

[37] J.A. Bondy and M. Simonovits, Cycles of even length in graphs, *J. Combin. Theory Ser. B* **16** (1974), 97-105.

[38] R.B. Boppana, Eigenvalues and graph bisection: An average-case analysis, *28nd Symposium on Foundations of Computer Science*, IEEE Computer Society Press, (1987), 280-285.

[39] R. Bott and J.P. Mayberry, Matrices and trees, In *Economic Activity Analysis*, (O. Morgenstern, ed.), John Wiley and Sons, New York (1954), 391-340.

[40] A. Broder, A. Frieze and E. Upfal, Existence and construction of edge disjoint paths on expander graphs, *Proc. Sym. Theo. on Computing*, ACM (1992), 140-149.

[41] R. Brooks, The spectral geometry of k-regular graphs, Journal d'Analyse Mathématique, **57** (1991), 120-151.

[42] N.G. de Bruijn, A combinatorial problem, *Nederl. Akad. Wetensch. Proc.* **49** (1946), 758-764.

[43] D.A. Burgess, On character sums and primitive roots, *Proc. London Math. Soc.* **12** (1962) 179-192.

[44] P. Buser, Cayley graphs and planar isospectral domains, in *Geometry and Analysis on Manifolds* (T. Sunada, ed.), Springer Lecture Notes 1339 (1988), 64-77.

[45] P. Buser, Cubic graphs and the first eigenvalue of a Riemann surface, *Math. Z.* **162** (1978), 87-99.

[46] L. Caccetta, On extremal graphs with given diameter and connectivity, *Ann. New York Acad. Sci.* **328** (1979), 76-94.

[47] A. Cayley, A theorem on trees, *Quart. J. Math.* 23 (1889), 376-378.

[48] J. Cheeger, A lower bound for the smallest eigenvalue of the Laplacian, Problems in Analysis (R. C. Gunning, ed.), Princeton Univ. Press (1970), 195-199.

[49] Siu Yuen Cheng, Peter Li and Shing-Tung Yau, On the upper estimate of the heat kernel of a complete Riemannian manifold, *American Journal of Mathematics* **103** (1981), 1021-1063.

[50] R. Christensen, *Log-Linear Models*, Springer-Verlag, New York, 1990.

[51] F.R.K. Chung, Diameters and eigenvalues, *J. of Amer. Math. Soc.* **2** (1989), 187-196.

[52] F.R.K. Chung, Eigenvalues of graphs and Cheeger inequalities, in *Combinatorics, Paul Erdős is Eighty*, Volume 2, edited by D. Miklós, V. T. Sós, and T. Szőnyi, János Bolyai Mathematical Society, Budapest (1996), 157-172.

[53] F.R.K. Chung, V. Faber and T. A. Manteuffel, On the diameter of a graph from eigenvalues associated with its Laplacian, *SIAM. J. Discrete Math.* **7**(1994), 443-457.

[54] F.R.K. Chung, A. Grigor'yan, and S.-T. Yau, Upper bounds for eigenvalues of the discrete

[57] F.R.K. Chung and Prasad Tetali, Isoperimetric inequalities for cartesian products of graphs, preprint.

[58] F.R.K. Chung and S.-T. Yau, A Harnack inequality for homogeneous graphs and subgraphs, *Communications in Analysis and Geometry*, **2** (1994), 628-639.

[59] F.R.K. Chung and S.-T. Yau, Eigenvalues of graphs and Sobolev inequalities, *Combinatorics, Probability and Computing*, **4** (1995), 11-26.

[60] F.R.K. Chung and S.-T. Yau, Eigenvalue inequalities of graphs and convex subgraphs, *Communications in Analysis and Geometry*, to appear.

[61] F.R.K. Chung and S.-T. Yau, Eigenvalues, flows and separators of graphs, preprint.

[62] F.R.K. Chung and S.-T. Yau, Logarithmic Harnack inequalities, preprint.

[63] F.R.K. Chung, On concentrators, superconcentrators, generalizers and nonblocking networks, *Bell Systems Tech. J.* **58** (1978), 1765-1777.

[64] F.R.K. Chung, A note on constructive methods for Ramsey numbers, *J. Graph Th.* **5** (1981), 109-113.

[65] F.R.K. Chung, Diameters of communications networks, *Mathematics of Information Processing*, AMS Short Course Lecture Notes (1984), 1-18.

[66] F.R.K. Chung, Diameters of graphs: Old problems and new results, *Congressus Numerantium* **60** (1987), 295-317.

[67] F.R.K. Chung, Quasi-random classes of hypergraphs, *Random Structures and Algorithms* **1** (1990), 363-382.

[68] F.R.K. Chung and M.R. Garey, Diameter bounds for altered graphs, *J. of Graph Theory* **8** (1984), 511-534.

[69] F.R.K. Chung, Constructing random-like graphs, in *Probabilistic Combinatorics and Its Applications*, (B. Bollobas ed.), Amer. Math. Soc., Providence, (1991) 21-56

[70] F.R.K. Chung and R.L. Graham, Quasi-random hypergraphs, *Random Structures and Algorithms* **1** (1990), 105-124.

[71] F.R.K. Chung and R.L. Graham, Quasi-random tournaments, *J. of Graph Theory* **15** (1991), 173-198.

[72] F.R.K. Chung and R.L. Graham, Maximum cuts and quasi-random graphs, *Random Graphs* (Alan Frieze and Tomasz Luczak, eds.), John Wiley and Sons, New York (1992), 23-34.

[73] F.R.K. Chung and R.L. Graham, On graphs not containing prescribed induced subgraphs, in *A Tribute to Paul Erdős*, (A. Baker et al. eds.) Cambridge University Press (1990), 111-120.

[74] F.R.K. Chung and R.L. Graham, Quasi-random set systems, *J. Amer. Math. Soc.* **4** (1991), 151-196.

[75] F.R.K. Chung and R.L. Graham, Quasi-random subsets of Z_n, *J. Combin. Th. (A)* **61** (1992), 64-86.

[76] F.R.K. Chung, R.L. Graham and R.M. Wilson, Quasi-random graphs, *Combinatorica* **9** (1989), 345-362.

[77] F.R.K. Chung, The regularity lemma for hypergraphs and quasi-randomness, *Random Structures and Algorithms* 2 (1991), 241-252.

[78] F.R.K. Chung and R.L. Graham, Cohomological aspects of hypergraphs, *Trans. Amer. Math. Soc.* 334 (1992), 365-388

[79] F.R.K. Chung, R.L. Graham and S.-T. Yau, On sampling with Markov chains, *Random Structures and Algorithms* **9** (1996) 55-78.

[80] F.R.K. Chung and R.L. Graham, Random walks on generating sets of groups, preprint.

[81] F.R.K. Chung and R.L. Graham, Stratified random walks on an n-cube, preprint.

[82] F.R.K. Chung and C.M. Grinstead, A survey of bounds for classical Ramsey numbers, *J. Graph Theory* **7** (1983), 25-38.

[83] F.R.K. Chung and K. Oden, Weighted graph Laplacians and isoperimetric inequalities, preprint.

[84] F.R.K. Chung and S. Sternberg, Laplacian and vibrational spectra for homogenous graphs, *J. Graph Theory* **16** (1992), 605-627.

[85] F.R.K. Chung and S. Sternberg, Mathematics and the Buckyball, *American Scientist*, **81** (1993), 56-71.