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The Green's Function for the Hückel (Tight Binding) Model

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Applications of the Hückel (tight binding) model are ubiquitous in quantum chemistry and solid state physics. The matrix representation of this model is isomorphic to an unoriented vertex adjacency matrix of a bipartite graph, which is also the Laplacian matrix plus twice the identity. In this paper, we analytically calculate the determinant and, when it exists, the inverse of this matrix in connection with the Green's function, **G**, of the $N \times N$ Hückel matrix. A corollary is a closed form expression for a Harmonic sum (Eq. (12)). We then extend the results to $d-$dimensional lattices, whose linear size is N. The existence of the inverse becomes a question of number theory. We prove a new theorem in number theory pertaining to vanishing sums of cosines and use it to prove that the inverse exists if and only if $N + 1$ and d are odd and d is smaller than the smallest divisor of $N + 1$. We corroborate our results by demonstrating the entry patterns of the Green's function and discuss applications related to transport and conductivity.

Keywords: Matrix inverses, invertibility, Green's function, vanishing sums of cosines, quantum chemistry.

I. PROBLEM STATEMENT: THE HÜCKEL MODEL AND ITS GREEN'S FUNCTION

The Hückel or Tight Binding model was originally introduced to describe electron hopping on a one-dimensional chain or ring [13]. It has come to serve as a ubiquitous model in solid state chemistry and physics [3, 13]. Two typical forms of the Hückel matrix, for a linear chain of N atoms, and for a cycle of N atoms, are given in Eq. (3). The resulting banded matrix is isomorphic to the vertex adjacency matrix of a graph [12].

The diagonal entries of the Hückel Hamiltonian matrix are defined by the Coulomb integral, $\alpha = \langle \chi_i | \hat{H} | \chi_i \rangle$, where χ_i is the basis function of $2p_z AO$ of the ith carbon atom. The magnitude of α can be approximated by the ionization potential of a carbon atom. It is reasonable to assume that all carbon atoms have the same ionization potential, resulting in an approximation that all diagonal elements have the same value, which is denoted by just α.

An off-diagonal elements of the Hückel Hamiltonian matrix is typically called a resonance integral, $\beta_{i,j}$, defined as $\beta_{i,j} = \langle \chi_i | \hat{H} | \chi_j \rangle$. This is a measure of the interaction between the ith and j^{th} carbon atoms. Usually $\beta_{i,j}$ is neglected if there is no bond between the ith and j^{th} carbon atoms. It is reasonably assumed that all the carbon-carbon bonds have the same strength, resulting in an approximation that all non-zero off-diagonal elements have the same value, which is denoted by just β.

If there are no heteroatoms in the system, all Coulomb integrals can be considered identical. However, if there is a heteroatom, we need to modify the Coulomb integral properly. When one calculates a linear $\pi-$conjugated chain, namely a polyene, all resonance integrals cannot be considered identical, if there is bond alternation, as obtains normally. We address this problem later on. In a small $\pi-$conjugated cycle, termed annulene, there is no bond alternation, so all resonance integrals can be considered identical. However, as the cycle gets large, bond alternation sets in (see refs. [15, 29]).

Mathematical Statement of the Problem

Therefore, in the simplest version of both physical and chemical models, the matrix representation of the electronic Hamiltonian for a network of orbitals (one per atom, say carbon $2p_z$), is characterized by diagonal matrix elements α, which we may without loss of generality set equal to zero, and off-diagonal elements β (or t), where two atoms are neighbors. If we use units of β (β is negative), we may replace these nearest neighbor interactions by unity, 1. All other (non-nearest neighbor) interactions are set equal to 0.

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The eigenvalues and eigenvectors of these matrices are well known for the linear chain and cycles [13]. For the finite linear chain (the banded matrix at left in Eq. (3)), they can be written respectively as cosines and sines, as follows. Let λ_r and $|\psi_r\rangle$ be the rth eigenvalue and the corresponding r^{th} eigenvector, then

$$\lambda_r = 2\cos r\omega \qquad \text{in units of } \beta \tag{1}$$

$$|\psi_r\rangle = \sqrt{\frac{2}{(N+1)}} \left[\sin\left(r\omega\right), \sin\left(2r\omega\right), \ldots, \sin\left(Nr\omega\right)\right]^T, \tag{2}$$

where $\omega \equiv \frac{\pi}{N+1}$ and $1 \leq r \leq N$ is an integer. The Hückel matrix for a linear chain, whose matrix representation is a symmetric tridiagonal matrix [18, for a review], and a $N-$membered ring, which is a circulant matrix [6, 11], respectively are

$$H_1 = \begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & 1 & 0 & \ddots & \\ & & & \ddots & \ddots & 1 \\ & & & & 1 & 0 \end{bmatrix} \qquad H_1^c = \begin{bmatrix} 0 & 1 & & & & 1 \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & 1 & 0 & \ddots & \\ & & & \ddots & \ddots & 1 \\ 1 & & & & 1 & 0 \end{bmatrix}, \tag{3}$$

where to emphasize the one-dimensional structure of the molecular system we put a subscript 1 on H and denote the Hamiltonian by H_1. From now omitted entries are zeros; we will explicitly write down the zeros when it helps the presentation.

The Hückel model has found renewed significance in recent experimental and theoretical studies of molecular conductance, that is transmission of a current through a molecule [21, and references therein].

The Green's function matrix, **G**, is defined via the resolvent as

$$G\left(r,s\,;\,E\right) = \langle r|\frac{1}{E-H}|s\rangle, \tag{4}$$

where $G\left(r,s\,;\,E\right)$ is the r,s entry of the Green's function matrix, H is the Hamiltonian and E is an energy.

The Green's function plays an important role in the calculation of transport phenomena such as conductivity [5]. In the simplest form of the theory, the conductance between electrodes connected to sites r and s of a molecule is proportional to the square of the absolute value of the matrix element of the unperturbed Green's function,

$$G^{(0)}\left(r,s\,;\,E\right) = \sum_k \frac{C_{rk}C_{sk}^*}{E - \epsilon_k + i\eta}, \tag{5}$$

where C_{rk} is the coefficient of the rth atomic orbital in the kth molecular orbital (MO) in an orthogonal basis, ϵ_k is the kth MO energy, and η is an infinitesimal positive number to assure analyticity. The Fermi energy is equal to the Coulomb integral of the Hückel model and for convenience we set this energy to zero (see subsection "Level set of the Fermi Energy" below).

For the DC conductivity we want to evaluate the Green's function at the Fermi energy; therefore $E = 0$ in Eq. (4). By Sokhotski–Plemelj theorem, $\lim_{\eta \to 0^+} \frac{1}{x \pm i\eta} = P(\frac{1}{x}) \mp i\pi\delta(x)$, the real part of the Green's function (Eq. (5)) is

$$G^{(0)}\left(r,s\,;\,E=0\right) = -\sum_k \frac{C_{rk}C_{sk}^*}{\epsilon_k} \quad . \tag{6}$$

Therefore, the Green's function in the basis described above (Eqs. 1 and 2), for a finite open linear chain has entries that are:

$$G^{(0)}\left(r,s\,;\,E=0\right) = -\frac{1}{N+1}\sum_{k=1}^{N} \frac{\sin\left(rk\omega\right)\sin\left(sk\omega\right)}{\cos\left(k\omega\right)} \qquad \text{in units of } \beta^{-1} \tag{7}$$

$$\omega \equiv \frac{\pi}{N+1} \quad .$$

Below, for simplicity, we denote $G\left(r,s\right) \equiv G^{(0)}\left(r,s\,;\,E=0\right)$.

Remark 1. $\mathbf{G}^{(0)}$ is simply $-H_1^{-1}$ in the basis given by Eqs. (1) and (2). Generally, with energy set-point $E = 0$, the Green's function is minus the inverse of the Hamiltonian. We compute the inverses of H_1 and H_1^c in several ways– from general formulas for tridiagonal matrices, directly from simple equations for the first column of the inverses, and from factoring the matrix symbol $e^{i\theta} + e^{-i\theta}$.

Our goal is to prove the conditions under which the inverse of various forms of the Hückel model exists for different N and in $d-$spatial dimensions. When it exists, we analytically derive closed-form formulas for the Green's function $\mathbf{G}^{(0)}$.

Level set of the Fermi Energy

The position of the actual Fermi levels in a calculation of molecular transmission may vary. It has proven to be a good approximation to set it equal to the Coulomb integral of the Hückel method for most rings and chains (the limitations of this assumption will be mentioned later).

There is a good reason why we assume $E_F = \alpha$. The energy level of the $2p$ atomic orbital (AO) of carbon ($-11.4eV$, the same energy level as the Coulomb integral), is almost the same as that of the $6s$ AO of the widely used Au electrode ($-10.9eV$) [2]. Note that the electronic configuration of Au is $5d^{10}6s^1$. This approximation works well as long as significant charge transfer between the molecule and the electrode surface does not occur [30].

The assumption that the Fermi level is equal to the Coulomb integral of the Hückel method is probably valid for even-membered chains and rings with $4n + 2$ atoms.

II. DETERMINANTS AND ANALYTICAL EXPRESSIONS FOR H_1^{-1} AND $\left(H_1^c\right)^{-1}$

Open Chain, H_1

Lemma 1. H_1 *is only invertible when N is even, in which case* $\det\left(H_1\right) = (-1)^{N/2}$

Proof. Generally for any N

$$\det\left(H_N\right) = -\det\left(H_{N-2}\right) = \cdots = (-1)^{\frac{N-2}{2}}\det\left(H_2\right) = (-1)^{\frac{N-2}{2}}\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} = (-1)^{N/2} \quad N \text{ even,}$$

$$\det\left(H_N\right) = -\det\left(H_{N-2}\right) = \cdots = \det\left(H_1\right) = |0| = 0 \quad N \text{ odd,}$$

where we denoted H_1 of size $N \times N$, simply by H_N and the determinant of a matrix by $|\cdot|$. In Eq. (7), $\cos\left(k\omega\right)$ can take on a zero value if N is odd, whereby $G\left(r,s\right)$ is not defined. $\qquad\square$

Proposition 1. *When N is even, the entries of the Green's function* $G\left(r,s\right) \equiv -H_1^{-1}\left(r,s\right)$ *are*

$$G\left(r,s\right) = \begin{cases} (-1)^{\frac{r+s-1}{2}} & r < s \ : \ r \text{ odd and } s \text{ even} \\ (-1)^{\frac{r+s-1}{2}} & r > s \ : \ r \text{ even and } s \text{ odd} \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

$$G = -H_1^{-1} = \begin{bmatrix} 0 & -1 & 0 & +1 & 0 & -1 & \cdots \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & -1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & +1 & 0 & -1 & 0 & \cdots \\ \vdots & & & \vdots & & & \ddots \end{bmatrix} \tag{9}$$

Proof. Suppose we have a general tridiagonal matrix

$$A = \begin{bmatrix} b_1 & c_1 & & & \\ a_1 & b_2 & c_2 & & \\ & a_2 & b_3 & \ddots & \\ & & \ddots & \ddots & c_{N-1} \\ & & & a_{N-1} & b_N \end{bmatrix}$$

Then Usmani's formula [27] for the r,s entry of A^{-1} is

$$\alpha(r,s) = \begin{cases} (-1)^{r+s}\, c_r c_{r+1} \cdots c_{s-1}\ \theta_{r-1}\phi_{s+1}/\theta_N & r < s \\ \theta_{r-1}\phi_{r+1}/\theta_N & r = s \\ (-1)^{r+s}\, a_{s+1}a_{s+2}\cdots a_r\ \theta_{s-1}\phi_{r+1}/\theta_N & r > s \end{cases} \tag{10}$$

where θ_r and ϕ_s satisfy second order recursion relations

$$\begin{aligned} \theta_r &= b_r\theta_{r-1} - a_r c_{r-1}\theta_{r-2} & r = 1,2,\ldots,N-1,N \\ \phi_s &= b_s\phi_{s+1} - c_s a_{s+1}\phi_{s+2} & s = N,N-1,\cdots 2,1 \end{aligned}$$

with the initial conditions $\theta_{-1} = 0$, $\theta_0 = 1$, $\phi_{N+1} = 1$ and $\phi_{N+2} = 0$.

We are interested in the special case where $b_i = 0$, $c_i = a_i = 1$ for all i. The recursion relations are now given by

$$\begin{aligned} \theta_r &= -\theta_{r-2} & r = 2,3,\ldots,N \\ \phi_s &= -\phi_{s+2} & s = N,N-1,\ldots,2,1 \end{aligned}$$

The solutions, after imposing the initial conditions, are

$$\theta_r = \frac{i^r}{2}\left[1 + (-1)^r\right]; \qquad \phi_s = \frac{i^{-(N+1)+s}}{2}\left[1 - (-1)^s\right].$$

Substituting these in Eq. (10) and multiplying by -1, we obtain $\mathbf{G} = -H_1^{-1}$:

$$G(r,s) = \begin{cases} \frac{i^{3(r+s-1)}}{4}\left[1 + (-1)^{r-1}\right]\left[1 - (-1)^{s+1}\right] & r < s \\ \frac{i^{2(r-1)}}{4}\left[1 + (-1)^{r-1}\right]\left[1 - (-1)^{r+1}\right] & r = s \\ \frac{i^{3(r+s-1)}}{4}\left[1 + (-1)^{s-1}\right]\left[1 - (-1)^{r+1}\right] & r > s \end{cases} \tag{11}$$

$\square$

By symmetry we may focus on $r \geq s$. In Eq. (11) the only nonzero elements, for $r \geq s$, correspond to r even and s odd, in which case $G(r,s) = i^{3(r+s-1)} = (-1)^{\frac{r+s-1}{2}}$.

Corollary 1. *The closed form expression for the following sum gives the identity*

$$-\frac{1}{N+1}\sum_{k=1}^{N} \frac{\sin(rk\omega)\sin(sk\omega)}{\cos(k\omega)} = (-1)^{\frac{r+s-1}{2}} \tag{12}$$

when r is even and $s < r$ is odd. Otherwise, $G(r,s) = 0$ when $s \leq r$ and $G(r,s) = G(s,r)$ when $r \leq s$.

This is the Green's function in an orthonormal basis. A purely trigonometric derivation, that does not use the Hückel matrix and serves as an alternative proof of Eqs. (8) and (12), is presented in the appendix.

Remark 2. Formulas for the inverse of a tridiagonal Toeplitz matrix have been given by Schlegel [20] and Mallik [16] in terms of Chebyshev polynomials.

In quantum chemistry, it was known that $G(r,s) = 0$ when r and s have the same parity. These zeros can be derived from a property called "alternancy" (the original proof is due to C. A. Coulson and G. S. Rushbrooke [4]). If the interacting orbitals of a molecule can be divided into two disjoint sets, where the atoms of one set are adjacent only to atoms of the other set, the molecule is said to be alternant. For alternants, for instance the linear chain studied here, a number of results can be proved; for instance the energy levels are paired positive and negative, and in paired levels the coefficients of one set of atoms are just minus the coefficients of that set in the paired level. It follows that $G(r,s) = 0$ when r and s have the same parity. The other zeros and ± 1 entries, as far as we know, were not noticed.

In chemical applications one often has to deal with the special case of alternating bond strengths along a chain. The proposition below gives the form of the Hamiltonian and its corresponding Green's function.

Definition 1. The bond alternating Hamiltonian is defined by H_{alt} for N even, where

$$H_{alt} = \begin{bmatrix} 0 & \beta & & & & & \\ \beta & 0 & \alpha & & & & \\ & \alpha & 0 & \beta & & & \\ & & \beta & 0 & \ddots & & \\ & & & \ddots & \ddots & \alpha & \\ & & & & \alpha & 0 & \beta \\ & & & & & \beta & 0 \end{bmatrix}$$

Comment: In this special limit, the Toeplitz structure is lost. α in this definition is not related to the one discussed above, which stood for the diagonal elements and was taken to be zero.

Proposition 2. *The entries of the Green's function* $\mathbf{G} \equiv -(H_{alt})^{-1}$, *are given by*

$$G(r,s) = \begin{cases} \frac{(-1)^{\frac{r+s-1}{2}}}{4} \frac{1}{\beta} \left(\frac{\alpha}{\beta}\right)^{\frac{r-s-1}{2}} \left\{1 - (-1)^s\right\} \left\{1 + (-1)^r\right\}, & r \geq s \\[2ex] \frac{(-1)^{\frac{r+s-1}{2}}}{4} \frac{1}{\beta} \left(\frac{\alpha}{\beta}\right)^{\frac{s-r-1}{2}} \left\{1 - (-1)^r\right\} \left\{1 + (-1)^s\right\}, & r \leq s . \end{cases} \tag{13}$$

Proof. The form can be derived using the same techniques as above. □

Cyclic chain, H_1^c

The cyclic Hamiltonian is a circulant matrix and therefore diagonalizable in Fourier basis [6, 11, 22]. Let $\omega_j = \exp(2\pi i j/n)$, the eigenpairs are

$$\lambda_j = 2\cos(2\pi j/n), \qquad j = 0, 1, \ldots, n-1$$
$$v_j^T = \frac{1}{\sqrt{n}}\left(1, \omega_j, \omega_j^2, \ldots, \omega_j^{(n-1)}\right).$$

In particular when $n = 4j$, the matrix has zero eigenvalues and hence non-invertible. The following lemma sharpens this notion.

Lemma 2. *The determinant of H_1^c is given by*

$$\det(H_1^c) = \begin{cases} -1 & N = 2 \\ 2 & N = 2k+1 \\ 0 & N = 4k \\ -4 & N = 4k+2 \end{cases}, \qquad for \quad k \in \mathbb{N}.$$

Proof. When $N = 2$, trivially $\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} = -1$. When N is odd, we express

$$H_1^c = \begin{bmatrix} H_{N-1} & B \\ C & D \end{bmatrix}$$

where $C = [\,1\ 0\ \cdots\ 0\ 1\,]$, $B = C^T$, $D = 0$ and H_{N-1} is an $N-1 \times N-1$ version of H_1 (open chain) as defined above, which is invertible. With this decomposition, the structure of H_1^{-1} derived above, and the well-known fact about the determinant of block matrices we arrive at

$$\det(H_1^c) = -\det(H_{N-1})\det\left(CH_{N-1}^{-1}B\right) = \det\left(CH_{N-1}^{-1}B\right) = 2 \quad .$$

When N is a multiple of 4, one can easily check that the vectors $\mathbf{v}_1 \equiv [0, -1, 0, 1]^T$ and $\mathbf{v}_2 \equiv [1, 0, -1, 0]^T$ generate the kernel of H_1^c. Namely, if H_1^c is a $4k \times 4k$ matrix, then the $k-$fold concatenations $[\mathbf{v}_1\mathbf{v}_1\cdots\mathbf{v}_1]^T$ and $[\mathbf{v}_2\mathbf{v}_2\cdots\mathbf{v}_2]^T$ are

in the ker $\left(H_1^c\right)$. Moreover, since excluding the last two rows and columns of H_1^c gives H_{4k-2}, which is invertible, we conclude that the two vectors are a basis for the kernel of H_1^c.

Lastly, if N is even yet not a multiple of 4, we write $H_1^c = \begin{bmatrix} H_{N-2} & B \\ B^T & D \end{bmatrix}$, where $B^T = \begin{bmatrix} 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 \end{bmatrix}$ and $D = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Here H_{N-2} has a size that is a multiple of 4. Using the techniques above we obtain

$$
\begin{aligned}
\det\left(H_1^c\right) &= \det\left(H_{N-2}\right)\det\left(D - B^T H_{N-2}^{-1} B\right) = \det\left(D - B^T H_{N-2}^{-1} B\right) \\
&= \det\left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}\right) = -4 \quad .
\end{aligned}
$$

$\square$

Definition 2. A Toeplitz matrix is a matrix that is constant along diagonals. A circulant matrix is Toeplitz, and each column is a cyclic shift of the previous column [11, 23]. Thus the lower triangular part of a circulant determines the upper triangular part:

$$
\text{Toeplitz } A = \begin{bmatrix} x_0 & x_{-1} & x_{-2} \\ x_1 & x_0 & x_{-1} \\ x_2 & x_1 & x_0 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} x_0 & x_{-1} & \cdots & x_{-(N-1)} \\ x_1 & x_0 & & \vdots \\ \vdots & & \ddots & x_{-1} \\ x_{N-1} & \cdots & x_1 & x_0 \end{bmatrix}
$$

$$
\text{Circulant } A = \begin{bmatrix} x_0 & x_2 & x_1 \\ x_1 & x_0 & x_2 \\ x_2 & x_1 & x_0 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} x_0 & x_{N-1} & \cdots & x_1 \\ x_1 & x_0 & & x_2 \\ \vdots & & \ddots & \vdots \\ x_{N-1} & x_{N-2} & \cdots & x_0 \end{bmatrix}.
$$

The inverse of a circulant matrix is circulant. The inverse of a Toeplitz matrix is not in general Toeplitz.

A Toeplitz matrix T has (r,s) entries that depend on $r - s$. Therefore specifying the first row and the first column fully specifies the matrix. Specifying the first column(or row) is sufficient to specify a circulant matrix.

Proposition 3. *The $N \times N$ Hückel circulant matrix H_1^c is invertible for $N \neq 4k$. The first column of the inverse is*

$$
\begin{array}{lll}
N = 4k+1 & (x_0, x_1, x_2, x_3, \dots) & = \tfrac{1}{2}(1, 1, -1, -1, \text{ repeat}) \\
N = 4k+2 & (x_0, x_1, x_2, x_3, \dots) & = \tfrac{1}{2}(0, 1, 0, -1, \text{ repeat}) \\
N = 4k+3 & (x_0, x_1, x_2, x_3, \dots) & = \tfrac{1}{2}(-1, 1, 1, -1, \text{ repeat})
\end{array}
$$

The matrix representation is shown in Fig. 1.

Figure 1: The Toeplitz structure of $\mathbf{G}_1^c = -\left(H_1^c\right)^{-1}$.

Proof. H_1^c (see Eq. (3)), is a symmetric circulant matrix, so its inverse is also a symmetric circulant. Thus $x_k = x_{N-k}$ for $0 < k < N/2$. The matrix H_1^c (with two cyclic diagonals of 1's) multiplies the first column $(x_0, \ldots, x_{N-1})$ of its inverse to give the first column of the identity matrix:

$$\begin{bmatrix} 0 & 1 & & & 1 \\ 1 & 0 & 1 & & \\ & 1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ 1 & & & 1 & 0 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{N-1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

In the first row, symmetry changes $x_1 + x_{N-1} = 1$ to $2x_1 = 1$ and $x_1 = \frac{1}{2}$. Then the odd-numbered rows produce $x_3, x_5, x_7, \ldots$ with alternating signs:

$$x_1 + x_3 = 0 \quad \text{so that } x_3 = -\frac{1}{2}$$

$$x_3 + x_5 = 0 \quad \text{so that } x_5 = +\frac{1}{2} \tag{14}$$

$$\text{etc.}$$

The even numbered rows also produce alternating signs:

$$x_0 + x_2 = 0 \quad \text{so that } x_2 = -x_0 \tag{15}$$
$$x_2 + x_4 = 0 \quad \text{so that } x_4 = +x_0$$

$$\text{etc.}$$

Finally the last row gives $x_0 = -x_{N-2}$. This produces the three separate possibilities for the inverse matrix in Proposition 2:

$$\begin{array}{ll} N = 4k+1 & x_{N-2} = x_{4k-1} = -\frac{1}{2} \text{ by Eq. (14) and then } x_0 = \frac{1}{2} \\ N = 4K+2 & x_{N-2} = x_{4k} = x_0 \text{ by Eq. (15) and then } x_0 = -x_0 = 0 \\ N = 4k+3 & x_{N-2} = x_{4k+1} = +\frac{1}{2} \text{ by Eq. (14) and then } x_0 = -\frac{1}{2}. \end{array}$$

The alternating signs for $x_0, x_2, x_4, \ldots$ complete the inverse circulant matrix $\left(H_1^c\right)^{-1}$. The Green's matrix is defined as $\mathbf{G}_1^c \equiv -\left(H_1^c\right)^{-1}$ and is shown in Fig. 1. □

Remark 3. The same direct approach produces H_1^{-1} in the non-circulant case. The $(1, n)$ and $(n, 1)$ entries of H_1^c are now set to zero. Then the first equation in Eq. (14) is simply $x_1 = 1$. The other equations in Eq. (14) give alternating signs for $x_3, x_5, \ldots$.

Similarly, the last equation in Eq. (15) is now $x_{N-2} = 0$. The first column $(x_0, x_1, \ldots)$ of H_1^{-1} is seen to be $(0, 1, 0, -1, repeat)$. The last column of H_1^{-1} has these components in reverse order. Then by symmetry we also know the first and last rows of H_1^{-1}.

Because H_1 is tridiagonal, these two columns and two rows completely determine the rest of H_1^{-1}. On and above the main diagonal, all sub-matrices of H_1^{-1} have rank 1. (If H_1 is tridiagonal and invertible then H_1^{-1} is a "semiseparable" matrix [28].) It is easy to see that starting from the first and last rows and columns of $\mathbf{G}$ in Proposition 2, all other entries of $\mathbf{G}$ follow directly from the rank 1 requirement.

Proof. (alternative to Prop. 3) We now establish the inverse of H_1^c using a technique that is general to circulant matrices based on the factorization of the symbol. $H_1^c = S + S^{-1} = S + S^T$, where S is the $N \times N$ cyclic shift matrix: $S^N = I$. Since $S + S^{-1} = (\mathbb{I} - iS)(\mathbb{I} + iS) S^{-1}$, we have

$$\begin{aligned} \left(S + S^{-1}\right)^{-1} &= S(\mathbb{I} + iS)^{-1}(\mathbb{I} - iS)^{-1} \\ &= S \frac{\left(\mathbb{I} + (-i)S + \cdots + (-i)^{N-1}S^{N-1}\right)}{1 - (-i)^N} \frac{\left(\mathbb{I} + iS + \cdots + i^{N-1}S^{N-1}\right)}{1 - i^N}. \end{aligned} \tag{16}$$

The denominator is $\left(1 - i^N\right)\left(1 - (-i)^N\right) = \begin{cases} 0 & N \equiv 4k \\ 2 & N \equiv 4k+1 \\ 4 & N \equiv 4k+2 \\ 2 & N \equiv 4k+3 \end{cases}$. This confirms that H_1^c is singular for $N = 4k$.

The coefficient of S^N in the product given by Eq. (16) is the numerator:

$$i^{N-1} + (-i)\,i^{N-2} + (-i)^2\,i^{N-3} + \cdots + (-i)^{N-2}\,i + (-i)^{N-1} = \frac{i^N - (-i)^N}{i - (-i)} = \begin{cases} +1 & N \equiv 1 \ (\mathrm{mod}\ 4) \\ 0 & N \equiv 2 \ (\mathrm{mod}\ 4) \\ -1 & N \equiv 3 \ (\mathrm{mod}\ 4) \end{cases}.$$

When we divide by the denominators $2, 4, 2$ we find the main diagonal of $\left(H_1^c\right)^{-1}$ as the coefficients of $S^N = \mathbb{I}$ in $\left(S + S^{-1}\right)^{-1}$: $\frac{1}{2}, 0, -\frac{1}{2}$ for N: $4k+1, 4k+2, 4k+3$ respectively.

Now we find the coefficient of $S = S^{N+1}$ in Eq. (16). The numerator is: $1 + i^{N-1}\,(-i) + i^{N-2}\,(-i)^2 + \cdots + i\,(-i)^{N-1} = 1 + (i)\,(-i)\left[i^{N-2} + i^{N-1}\,(-i) + \cdots + (-i)^{N-2}\right]$. Simplifying the numerator we find $1 + \frac{i^{N-1} - (-i)^{N-1}}{i - (-i)} = 1, 2, -1$ for N: $4k+1, 4k+2, 4k+3$ respectively.

Dividing by $2, 4, 2$ in the denominator, we find $\frac{1}{2}$ on the diagonals ± 1 of $\left(S + S^{-1}\right)^{-1}$.

Finally, notice that diagonals $2, 3, 4, 5, \ldots$ of $\left(S + S^{-1}\right)^{-1}$ will have *opposite sign* to diagonals $0, 1, 2, 3, \ldots$. The multiplication in the numerator of Eq. (16) gives a cyclic convolution

$$\left(1, i, i^2, \ldots, i^{N-1}\right) \star \left(1, -i, (-i)^2, \ldots, (-i)^{N-1}\right)$$

for the coefficients of $S, S^2, \ldots$. Because $i^2 = -1$, the coefficient of S^{k+2} in the numerator of Eq. (16) is the negative of the coefficient of S^k. The denominators are still $2, 4, 2$ for $N \equiv 1, 2, 3$. So the pattern in $\left(S + S^{-1}\right)^{-1} = -\mathbf{G}_1^c$ (starting with the main diagonal) is:

$$
\begin{array}{ll}
N \equiv 4k+1 & \text{diagonals } \tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{1}{2} \text{ repeated} \\
N \equiv 4k+2 & \text{diagonals } 0, \tfrac{1}{2}, 0, -\tfrac{1}{2} \text{ repeated} \\
N \equiv 4k+3 & \text{diagonals } -\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \text{ repeated}.
\end{array}
$$

This completes the alternative proof. $\qquad\square$

Analogous to Prop. 2, the proposition below gives the form of the cyclic Hamiltonian with the special case of alternating bond strengths and its corresponding Green's function.

Definition 3. The cyclic bond alternating Hamiltonian is defined by (N even)

$$H_{alt}^c = \begin{bmatrix} 0 & \beta & & & & & & \alpha \\ \beta & 0 & \alpha & & & & & \\ & \alpha & 0 & \beta & & & & \\ & & \beta & 0 & \ddots & & & \\ & & & \ddots & \ddots & \ddots & & \alpha \\ & & & & & \alpha & 0 & \beta \\ \alpha & & & & & & \beta & 0 \end{bmatrix}$$

Comment: As before, this model is not circulant nor has it the Toeplitz structure.

Proposition 4. *The entries of the Green's function* $-\left(H_{alt}^c\right)^{-1}$, *are given by*

$$G\,(r,s) = -\frac{1}{4} \begin{cases} \dfrac{(-\alpha/\beta)^{\frac{r-s-1}{2}}}{\beta\left[1 - \left(-\frac{\alpha}{\beta}\right)^{N/2}\right]}\left[1 + (-1)^r\right]\left[1 - (-1)^s\right] + \dfrac{(-\beta/\alpha)^{\frac{r-s-1}{2}}}{\alpha\left[1 - \left(-\frac{\beta}{\alpha}\right)^{N/2}\right]}\left[1 - (-1)^r\right]\left[1 + (-1)^s\right] & r > s \\[2em] \dfrac{(-\alpha/\beta)^{\frac{N+r-s-1}{2}}}{\beta\left[1 - \left(-\frac{\alpha}{\beta}\right)^{N/2}\right]}\left[1 + (-1)^r\right]\left[1 - (-1)^s\right] + \dfrac{(-\beta/\alpha)^{\frac{N+r-s-1}{2}}}{\alpha\left[1 - \left(-\frac{\beta}{\alpha}\right)^{N/2}\right]}\left[1 - (-1)^r\right]\left[1 + (-1)^s\right] & r \leq s \end{cases} \qquad (17)$$

Proof. We obtain the inverse by solving for $\mathbf{y}$ in $H_{alt}^c \mathbf{x} = \mathbf{y}$; that is, we think of $\mathbf{y}$ as given and we solve for $\mathbf{x}$. This will give us $\mathbf{x} = \left(H_{alt}^c\right)^{-1} \mathbf{y}$. First we solve the even rows in terms of the last row x_N, which itself can be solved from $x_N = \sum_{i=1}^{N} \left[\left(H_{alt}^c\right)^{-1}\right]_{N,i} y_i$ to give

$$x_{2k} = \frac{1}{\beta}\{\sum_{m=0}^{k-1} \left(-\frac{\alpha}{\beta}\right)^m y_{2k-2m-1}\} + \left(-\frac{\alpha}{\beta}\right)^k x_N$$

$$x_N = \beta^{-1}\left[1 - (-\alpha/\beta)^{N/2}\right]^{-1} \sum_{m=0}^{\frac{N}{2}-1} \left(-\frac{\alpha}{\beta}\right)^m y_{N-2m-1}$$

Similarly the odd rows are obtained in terms of x_1, which itself can be solved $x_1 = \sum_{i=1}^{N} \left[\left(H_{alt}^c\right)^{-1}\right]_{1,i} y_i$ to give

$$x_{2k+1} = \frac{1}{\alpha}\{\sum_{m=0}^{k-1} \left(-\frac{\beta}{\alpha}\right)^m y_{2k-2m}\} + \left(-\frac{\beta}{\alpha}\right)^k x_1$$

$$x_1 = \alpha^{-1}\left[1 - (-\beta/\alpha)^{N/2}\right]^{-1} \{y_N - \frac{\beta}{\alpha} \sum_{m=0}^{\frac{N}{2}-1} \left(-\frac{\beta}{\alpha}\right)^m y_{N-2m-2}\}$$

Combining these equations to solve for the even and odd rows separately and multiplying by an overall minus sign we arrive at $\mathbf{G} = -\left(H_{alt}^c\right)^{-1}$ given by Eq. (17). $\square$

Comment: In the special case that $N = 2k\,(2k-1)$, G_1^c in Proposition 3 can be obtained from Eq. (17) by substituting $\alpha = \beta = 1$. Note that in this limit, it is necessary that $N \neq 4k$ for the denominator not to vanish in agreement with Lemma 2.

We now pose a more general (and difficult) question. When does the inverse exist in spatial dimension d and if it does, how can it be computed? In the next section we use mathematical techniques borrowed from quantum information theory and number theory to address some of these problems.

III. HIGHER DIMENSIONAL GREEN'S FUNCTION

The Green's function we derived is the negative of the inverse of the Hückel (tight binding) Hamiltonian, whose $N \times N$ matrix representation in Dirac notation [7] is

$$H_1 = \sum_{k=1}^{N} \{ |k\rangle\langle k+1| + |k+1\rangle\langle k| \} \quad , \tag{18}$$

where in units of β the coupling can be taken to be one.

To explore the $d-$dimensional analog H_d, we use tensor products of matrices. Recall that the tensor product of an $m \times n$ matrix A and an $p \times q$ matrix B is the $mp \times nq$ matrix defined by

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{bmatrix}.$$

The Hamiltonian, H_d, on a square lattice in $d-$spatial dimensions (square lattice in $d = 2$, cubic in $d = 3$, etc.), with the linear size N can succinctly be expressed as

$$H_d = \sum_{i=1}^{d} \mathbb{I}_{N^{i-1}} \otimes H_1 \otimes \mathbb{I}_{N^{d-i}} \tag{19}$$

where H_1 is given by Eq. (18), and the size of every identity matrix is indicated by its subscript. In dimensions 2 and 3, the Hamiltonians come from H_1 and $\mathbb{I} = \mathbb{I}_N$:

$$H_2 = (H_1 \otimes \mathbb{I}) + (\mathbb{I} \otimes H_1) \tag{20}$$

$$H_3 = (H_1 \otimes \mathbb{I} \otimes \mathbb{I}) + (\mathbb{I} \otimes H_1 \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{I} \otimes H_1) \quad . \tag{21}$$

Comment: The techniques apply more generally where the lattice can be constructed from d independent linear subsets.

Comment: When H_1 is a Toeplitz or a circulant matrix, the corresponding H_d is generally not a Toeplitz or a circulant matrix [18], but they will be block Toeplitz or block circulant respectively.

The eigenvalue decomposition of $H_1 = Q\Lambda Q^T$, where Λ is the $N \times N$ diagonal matrix of eigenvalues whose k^{th} entry is $2\cos k\omega$ and Q is the matrix of eigenvectors with r^{th} column given by Eq. (2). Since $\cos k\omega \neq 0$ for all $1 \leq k \leq N$, Λ is a diagonal matrix with no zero entries on the diagonal and H_1 is invertible, i.e., has a Green's function, as expected from our calculations.

The associated Green's function matrix in d dimensions is defined by $\mathbf{G}_d = -H_d^{-1}$. Obtaining an analytical expression for the inverse in higher dimensions, at first, might seem difficult because it involves sums of matrices. In $d = 2$ the size of the lattice is $N \times N$ and in $d = 3$ the size is $N \times N \times N$.

After the eigenvalue decomposition, the Hamiltonians in higher dimensions (e.g., Eqs. (20),(21)) reads

$$H_d \;=\; Q^{\otimes d} \left\{ \sum_{i=1}^{d} \mathbb{I}_{N^{i-1}} \otimes \Lambda \otimes \mathbb{I}_{N^{d-i}} \right\} \left(Q^T \right)^{\otimes d} \tag{22}$$

$$\equiv\; Q^{\otimes d} \left\{ \quad \Lambda_d \quad \right\} \left(Q^T \right)^{\otimes d} \tag{23}$$

where the matrix of eigenvectors denoted by $Q^{\otimes d} \equiv Q \otimes \cdots \otimes Q$ is a d-fold tensor product and the diagonal matrix of eigenvalues is $\Lambda_d = \sum_{i=1}^{d} \mathbb{I}_{N^{i-1}} \otimes \Lambda \otimes \mathbb{I}_{N^{d-i}}$. For example,

$$H_2 \;=\; \left(Q\Lambda Q^T \otimes \mathbb{I} \right) + \left(\mathbb{I} \otimes Q\Lambda Q^T \right) \tag{24}$$

$$=\; (Q \otimes Q)\; [(\Lambda \otimes \mathbb{I}) + (\mathbb{I} \otimes \Lambda)]\; \left(Q^T \otimes Q^T \right)$$

$$H_3 \;=\; \left(Q\Lambda Q^T \otimes \mathbb{I} \otimes \mathbb{I} \right) + \left(\mathbb{I} \otimes Q\Lambda Q^T \otimes \mathbb{I} \right) + \left(\mathbb{I} \otimes \mathbb{I} \otimes Q\Lambda Q^T \right) \tag{25}$$

$$=\; (Q \otimes Q \otimes Q)\; [(\Lambda \otimes \mathbb{I} \otimes \mathbb{I}) + (\mathbb{I} \otimes \Lambda \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{I} \otimes \Lambda)]\; \left(Q^T \otimes Q^T \otimes Q^T \right).$$

This change of basis allows us to diagonalize the Hamiltonians in any dimension, for example

$$\Lambda_2 \;=\; (\Lambda \otimes \mathbb{I}) + (\mathbb{I} \otimes \Lambda) \tag{26}$$

$$\Lambda_3 \;=\; (\Lambda \otimes \mathbb{I} \otimes \mathbb{I}) + (\mathbb{I} \otimes \Lambda \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{I} \otimes \Lambda). \tag{27}$$

Below we investigate the conditions under which the Green's function exists. For now suppose that it does. Its algebraic representation in d dimensions (compare with Eqs. (22) and (23)) is

$$\mathbf{G}_d = -Q^{\otimes d} \left\{ \sum_{i=1}^{d} \mathbb{I}_{N^{i-1}} \otimes \Lambda \otimes \mathbb{I}_{N^{d-i}} \right\}^{-1} \left(Q^T \right)^{\otimes d}. \tag{28}$$

It is clear that if $\mathbf{G}_d$ were to exist no eigenvalue can be zero. Namely, diagonal entries being all the possible sums should satisfy $2\sum_{i=1}^{d} \cos \left(\frac{k_i \pi}{N+1} \right) \neq 0$ for any choice of $1 \leq k_i \leq N$. Then, the corresponding eigenvalues of $\mathbf{G}_d$ are $-1 / \left\{ 2\sum_{i=1}^{d} \cos \left(\frac{k_i \pi}{N+1} \right) \right\}$.

As an illustration let us take $d = 2$. Then the energies are the diagonal entries of Λ_2 given by the sum

$$\Lambda_2 = 2 \begin{bmatrix} (\cos \omega)\,\mathbb{I} & & & \\ & (\cos 2\omega)\,\mathbb{I} & & \\ & & \ddots & \\ & & & (\cos N\omega)\,\mathbb{I} \end{bmatrix} + \begin{bmatrix} \Lambda & & & \\ & \Lambda & & \\ & & \ddots & \\ & & & \Lambda \end{bmatrix},$$

which is a matrix of size $N^2 \times N^2$; Λ and $(\cos k\omega)\,\mathbb{I}$ are $(N \times N)$. Since $\cos k\omega = -\cos\left[(N+1-k)\,\omega\right]$, each block of the sum is $2\left(\cos k\omega\right)\mathbb{I} + \Lambda$ for some $1 \leq k \leq N$ whose $(N+1-k)^{\text{th}}$ entry is zero. Therefore, the diagonal $N^2 \times N^2$ matrix Λ_2 has exactly N zeros on its diagonal, one in each of the N blocks, and hence noninvertible.

IV.   GREEN'S FUNCTION AND NUMBER THEORY

The existence of the Green's function, $\mathbf{G}_d$, in higher dimensions requires that H_d has non-zero eigenvalues, i.e., $\sum_{i=1}^d \cos\left(\frac{k_i\pi}{N+1}\right) \neq 0$ for any choice of $1 \leq k_i \leq N$.

Lemma 3. H_d^{-1} *does not exist in even spatial dimensions.*

Proof. Since $\cos k\omega = -\cos\left[(N+1-k)\,\omega\right]$ for any $1 \leq k \leq N$, we can always pair up the cosines such that each pair sums to zero implying that there is a zero eigenvalue. $\qquad\square$

Therefore, below we take d and $N+1$ to be odd (as N odd is already non-invertible in one dimension).

We need to prove the general conditions under which H_d is invertible, which is a problem in number theory. Recently there has been quite a bit of interest in a closely related question, which is under what conditions do sums of roots of unity vanish? Besides sheer theoretical interest, this problem is related to many mathematical structures. For example, Poonen and Rubinstein relate this problem to the number of interior intersection points made by the diagonals of a regular $n-$gon [19].

Let us denote $n \equiv N+1$. Suppose one asks for what natural numbers d do there exist n^{th} roots of unity $\alpha_1, \ldots, \alpha_d \in \mathbb{C}$ such that $\alpha_1 + \cdots + \alpha_d = 0$? Such an equation is said to be a vanishing sum of nth roots of unity of *weight d*. Let n have the prime factorization $p_1^{a_1} \cdots p_r^{a_r}$ $(a_i > 0)$, then we can define $W(n)$ to be the set of weights d for which there exists a vanishing sum $\alpha_1 + \cdots + \alpha_d = 0$; if the sum does not vanish then $W(n)$ is simply the empty set.

Before delving into the proof we introduce some notation and terminology presented in [14]. Let $\langle G \rangle$ be a cyclic group of order n and let ζ be a (fixed) primitive n^{th} root of unity. There exists a natural ring homomorphism φ from the integral group $\mathbb{Z}G$ to the ring of cyclotomic integers $\mathbb{Z}[\zeta]$, given by the equation $\varphi(z) = \zeta$, i.e., the map $\varphi : \mathbb{Z}G \to \mathbb{Z}[\zeta]$. An element of $\mathbb{Z}G$, say $x = \sum_{g\in G} x_g g$, lies in the kernel $\ker(\varphi)$ if and only if $\sum_{g\in G} x_g \varphi(g) = 0$ in $\mathbb{Z}[\zeta]$. Therefore, the elements of the ideal $\ker(\varphi)$ correspond precisely to all $\mathbb{Z}$-linear relations among the nth roots of unity. For vanishing sums of nth roots of unity, we have to look at elements $x = \sum_g x_g g \in \ker(\varphi)$ with $x_g \geq 0$; the number of non-zero coefficients x_g is denoted by $\epsilon_0(x)$. In other words one looks at $\mathbb{N}G \cap \ker(\varphi)$, where $\mathbb{N}G$ denotes the group semi-ring of G over $\mathbb{N}$.

A vanishing sum $\alpha_1 + \cdots + \alpha_d = 0$ is called *minimal* if no proper sub-sum is zero. Clearly, one can always multiply a vanishing sum by a root of unity to get another vanishing sum; we say the latter is *similar* to the former; i.e., one can be obtained from the other by a rotation. For any natural number n, ζ_n denotes a primitive n^{th} root of unity in $\mathbb{C}$.

In terms of roots of unity, a vanishing sum from the basic relations of the form

$$1 + \zeta_{p_i} + \zeta_{p_i}^2 + \cdots + \zeta_{p_i}^{p_i-1} = 0 \qquad 1 \leq i \leq r \tag{29}$$

is called a *symmetric* minimal elements in $\mathbb{N}G \cap \ker(\varphi)$. In general, there are vanishing minimal sums which are not similar to those in Eq. (29). The latter are called *asymmetric* sums.

The following theorem due to Lam and Leung IV [14], will help us prove our theorem pertaining to vanishing sums of cosines (Theorem 1).

Theorem. *[Lam and Leung, Theorem 4.8] Let G be a cyclic group of order $n = p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}$, where $p_1 < p_2 < \cdots < p_r$ are primes and let $\varphi : \mathbb{Z}G \to \mathbb{Z}[\zeta]$ be as above, where $\zeta = \zeta_n$. For any minimal element $x \in \mathbb{N}G \cap \ker(\varphi)$, we have either (A) x is symmetric, or (B) $r \geq 3$ and $\epsilon_0(x) \geq p_1(p_2-1) + p_3 - p_2 > p_3$.*

We shall utilize this theorem to prove the following (recall that $n = N+1$):

Theorem 1. *Let n be a positive odd integer and $k_1, k_2, \cdots, k_d$ be a set of integers such that $1 \leq k_i \leq n-1$. Then*

$$\sum_{i=1}^d \cos\left(\frac{k_i\pi}{n}\right) \neq 0 \tag{30}$$

for any choice of k_i's if and only if d is odd and is smaller than the smallest divisor of n.

Proof. By Lemma 3, we only need to consider d odd. Below we first work with roots of unity by writing the cosines in terms of the roots

$$\sum_{i=1}^d \cos\left(\frac{2k_i\pi}{2n}\right) = 2\left\{\sum_{i=1}^d \zeta_{2n}^{k_i} + \zeta_{2n}^{-k_i}\right\}. \tag{31}$$
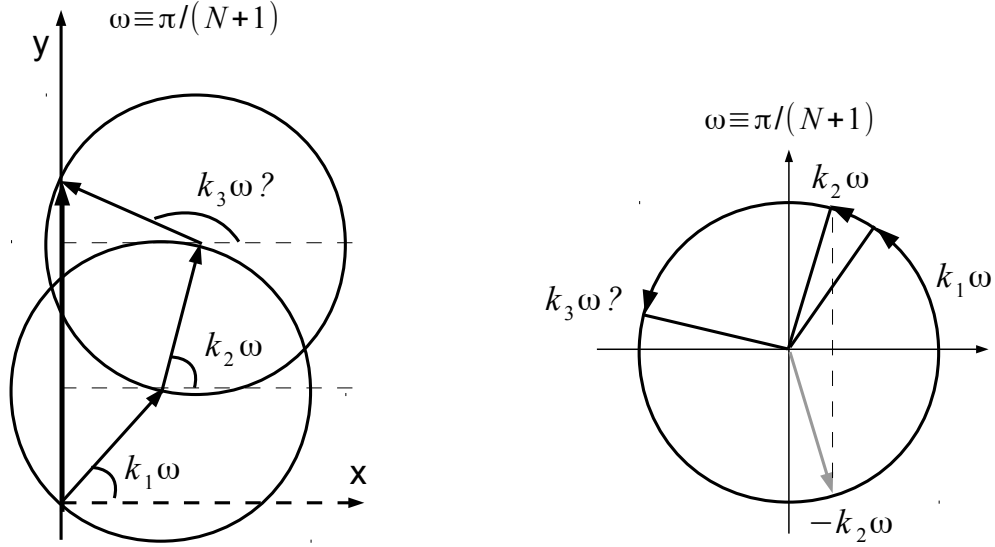
Figure 2: Left: $\cos\left(\frac{k_1\pi}{N+1}\right) + \cos\left(\frac{k_2\pi}{N+1}\right) + \cos\left(\frac{k_3\pi}{N+1}\right) = 0$ is equivalent to the phasors adding to a vertical vector. The circles shown are unit circles. Right: Vanishing sums of roots of unity imply vanishing sums of cosines on the upper half plane since one can reflect any phasor without changing the cosine.

So we have now a sum over $2d$ roots of unity. We first prove that this sum is never zero if $d < p_2$. Since $2n = 2p_2^{a_2}p_3^{a_3}\cdots p_r^{a_r}$ with all the p_i's being odd, we are guaranteed (from Theorem IV) that $p_1(p_2 - 1) + p_3 - p_2 = p_2 + p_3 - 2 < 2p_2$ therefore $2d \equiv \epsilon_0(x) < 2p_2$ and if there were vanishing sums they would be of type (A), which are symmetric, i.e., sums of minimal relations. When $d < p_2$, in Eq. (31) there would be fewer than $2p_2$ points on the unit circle all of which appear as complex conjugate pairs. For the sum to be of type (A) and vanish, there should be a symmetric sum with a prime p that vanishes. The corresponding roots are a subset of the original points that are a vanishing sum of roots of ζ_p with the prime $p \geq p_2 > d$, therefore it would involve a vanishing sum on more than half of the points of the original $2d$ terms in Eq. 31. Hence there must be at least one complex conjugate pair in the vanishing sum under consideration. But if there is one complex conjugate pair then all the roots should be complex conjugates as we can rotate any of the pth roots into one another. Since we have a vanishing sum of complex conjugate pairs but we allow only an odd number of terms there must be a real root. But we exclude the real roots (± 1). Therefore we reach a contradiction and the sum can never vanish.

Now we prove that the sum can be zero if $d \geq p_2$. It is sufficient to show that it vanishes for $d = p_2$ as for any odd $d > p_2$ we can always pair up the $2(p_2 - d)$ cosines to cancel as we did in the proof of Lemma 3. Suppose $d = p_2$. Then a symmetric sum over the roots of unity that vanishes implies that the sum over cosines vanishes as the cosines are the real part and geometrically one can reflect the roots to the upper half plane (see Fig. 2) . However, we need to exclude the possibility of ± 1 as roots and show that the sum still vanishes. The number of symmetric sums will be $\frac{2n}{p}$ but only 2 of them have ± 1 as roots. In the sum involving the symmetric sums we can exclude the ones that have ± 1 and still be left with vanishing symmetric sums. $\qquad\square$

Corollary 2. *The inverse of the Hückel matrix and hence its Green's function in d dimensions exists if and only if d is odd and is smaller than the smallest prime divisor of $N + 1$.*

For $d = 3$, this lemma and Eq. (30) have the geometrical interpretation shown in Fig. 2. Moreover, twice the left hand side of Eq. (30) is the expression for the energies of the Hückel matrix in d dimensions.

V. THE PHYSICAL CONSEQUENCES OF THE INVERSE OF THE HÜCKEL MATRIX AND THE ZEROES OF ITS GREEN'S FUNCTION

The Hückel formalism, in its physical and chemical context, is not, of course, restricted to a linear chain. Various two- and three-dimensional connectivities have been probed in the 80 years of its existence, to the immense benefit of practice and understanding in chemistry. But until recent time, there has been scant interest in the Green's function

of the Hückel matrix, and its inverse. Heilbronner used the inverse of the Hückel Matrix to form an undervalued bridge between the resonance structure of valence bond theory and molecular orbitals - thus bringing together two seemingly distinct, but in fact related, approaches to the electronic structure of molecules [13]. The graph theoretical context has led people to investigate the inverse of the vertex adjacency matrix [10]. In the work of Estrada, the relationship between the Green's function formalism and the inverse of the vertex adjacency matrix of a graph is consistently utilized [8, 9].

In a field that has attracted much attention both experimentally and theoretically in the last decade, the transmission of current across molecules, a striking phenomenon, quite nonclassical, is observed. This is quantum interference, zero or low conductance when electrodes are attached to specific sites across a molecule [5, 21]. Quantum interference occurs when the Green's function, whose absolute value squared is related to the current transmitted, vanishes. These are exactly the zeroes of Eq. (12). The inverse of the Hückel matrix has been directly related to this phenomenon in the work of Markussen and Stadler [17]. The chemical consequences of just these zeroes have been outlined in recent work by us [24].

The results we have obtained in this paper for the specific entries of the Green's function have been proven of great utility in describing the transmission of current through molecules. The Green's function expressions obtained in this paper also play an important role in designing a new molecular switches based on electrocyclic reactions, cycloadditions, and sigmatropic reactions in linear polyenes [21, 24]. In particular in a paper on linear polyenes, we have used the results to derive specifically the transmission across a chain, and its exponential falloff [26]. In the same paper, where it was important to have the Green's function elements for a cyclic polyene (annulene) with and without bond alternation, expressions from the current paper and some based on similar procedures, were used. Two kinds of zero values of the Green's function introduced in this paper, namely easy zero and hard zero, provide the bases for an important classification of quantum interference, and the connection between these zeroes and the non-disjoint or disjoint nature of diradical molecules has been clarified [25].

VI. ACKNOWLEDGEMENTS

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VII.   APPENDIX: FIRST PRINCIPLE DERIVATION FROM TRIGONOMETRICS

Proposition. *The following sum has a closed form solution*

$$-\frac{1}{N+1}\sum_{k=1}^{N}\frac{\sin\left(rk\omega\right)\sin\left(sk\omega\right)}{\cos\left(k\omega\right)}=e^{i\pi\left(\frac{r+s-1}{2}\right)} \tag{32}$$

when r is even and s < r is odd. Otherwise, when s ≤ r it is zero. Moreover s > r are symmetric, i.e., $G\left(r,s\right)=G\left(s,r\right)$.

Easy Zeros: Same parity of *s* and *r*

Using $\sin\left(rk\omega\right)\sin\left(sk\omega\right)=\frac{1}{2}\left\{\cos\left[\left(r-s\right)k\omega\right]-\cos\left[\left(r+s\right)k\omega\right]\right\}$, we can rewrite Eq. (7) as

$$G\left(r,s\right)=-\frac{1}{2\left(N+1\right)}\sum_{k=1}^{N}\frac{\left\{\cos\left[\left(r-s\right)k\omega\right]-\cos\left[\left(r+s\right)k\omega\right]\right\}}{\cos\left(k\omega\right)} \tag{33}$$

First let $r-s=2q$, this implies that r and s have the same parity (i.e., oddness or evenness). Therefore $r+s$ is also even, let it be $r+s=2q'$ for some $q'\in\mathbb{N}$. Eq. (33) becomes

$$G\left(r,s\right)=-\frac{1}{2\left(N+1\right)}\sum_{k=1}^{N}\left\{\frac{\cos\left[2qk\omega\right]}{\cos\left(k\omega\right)}-\frac{\cos\left[2q'k\omega\right]}{\cos\left(k\omega\right)}\right\}. \tag{34}$$

We now show that each sum is zero. Let us first show $\sum_{k=1}^{N}\frac{\cos[2qk\omega]}{\cos(k\omega)}=0$. Recall $\omega=\frac{\pi}{N+1}$ and expand the sum by adding the first to the last then the second to $N-1^{\text{st}}$ etc. to get

$$\sum_{k=1}^{N}\frac{\cos\left[2qk\omega\right]}{\cos\left(k\omega\right)}=\left(\frac{\cos\left[2q\omega\right]}{\cos\left(\omega\right)}+\frac{\cos\left[2qN\omega\right]}{\cos\left(N\omega\right)}\right)+\left(\frac{\cos\left[4q\omega\right]}{\cos\left(2\omega\right)}+\frac{\cos\left[2q\left(N-1\right)\omega\right]}{\cos\left(\left(N-1\right)\omega\right)}\right) \tag{35}$$

$$+\cdots+\left(\frac{\cos\left[2q\frac{N}{2}\omega\right]}{\cos\left(\omega N/2\right)}+\frac{\cos\left[2q\left(\frac{N}{2}+1\right)\omega\right]}{\cos\left(\left(\frac{N}{2}+1\right)\omega\right)}\right).$$

We now show that each of the parenthesis is identically zero. To do so we notice that each of the parenthesis is of the form

$$\frac{\cos\left[2qk\omega\right]}{\cos\left(k\omega\right)}+\frac{\cos\left[2q\left(N-k+1\right)\omega\right]}{\cos\left(\left(N-k+1\right)\omega\right)};\qquad k=1,2,\ldots,\frac{N}{2}.$$

But $\cos\left(\left(N-k+1\right)\frac{\pi}{N+1}\right)=\cos\left(-k\frac{\pi}{N+1}+\pi\right)=-\cos\left(k\frac{\pi}{N+1}\right)=-\cos\left(k\omega\right)$ by the double angle formula and evenness of the cosine. Moreover

$$\cos\left[2q\left(N-k+1\right)\omega\right]=\cos\left[2q\pi-2q\frac{k\pi}{N+1}\right]=\cos\left[-2q\frac{k\pi}{N+1}\right]$$

$$=\cos\left[2q\frac{k\pi}{N+1}\right]=\cos\left(2qk\omega\right)$$

Concluding that the numerators are equal but denominators differ in sign resulting in

$$\frac{\cos\left[2qk\omega\right]}{\cos\left(k\omega\right)}+\frac{\cos\left[2q\left(N-k+1\right)\omega\right]}{\cos\left(\left(N-k+1\right)\omega\right)}=\frac{\cos\left[2qk\omega\right]}{\cos\left(k\omega\right)}-\frac{\cos\left[2qk\omega\right]}{\cos\left(k\omega\right)}=0\quad.$$

The exact same argument with substitution q' for q in Eq. (35) proves that the second sum in Eq. (34) is zero. Together proving $G\left(r,s\right)=0$ if r and s have the same parity. There are other zeros that are harder to prove.

Harder Zeros

Let us make the sum in Eq. (7) centered by letting $m = k - \frac{N+1}{2}$, whereby

$$G(r,s) = -\frac{1}{N+1} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \frac{\sin\left[r\omega\left(m+\frac{N+1}{2}\right)\right] \sin\left[s\omega\left(m+\frac{N+1}{2}\right)\right]}{\cos\left[\omega\left(m+\frac{N+1}{2}\right)\right]}$$

where $\omega = \frac{\pi}{N+1}$ as before. Since, $\cos\left[\omega\left(m+\frac{N+1}{2}\right)\right] = -\sin(\omega m)$ and $\sin x = \frac{1}{2i}\left(e^{ix} - e^{-ix}\right)$

$$
\begin{aligned}
G(r,s) &= -\frac{ie^{i(r+s)\pi/2}}{2(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} e^{i\omega m(r+s-1)} \frac{\left(1 - e^{-2ir\omega\left(m+\frac{N+1}{2}\right)}\right)\left(1 - e^{-2is\omega\left(m+\frac{N+1}{2}\right)}\right)}{1 - e^{-2i\omega m}} \\
&= -\frac{ie^{i(r+s)\pi/2}}{2(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} e^{i\omega m(r+s-1)} \frac{\left[1 - (-1)^r e^{-2ir\omega m}\right]\left[1 - (-1)^s e^{-2is\omega m}\right]}{1 - e^{-2i\omega m}}
\end{aligned} \tag{36}
$$

This equation is general and will be used later for nonzero sums as well.

Since we proved that if r and s have the same parity the sum vanishes, we prove the harder zeros (see Eq. (9)) by letting r be odd and s even and enforcing $s < r$. We can let $r = 2q - 1$ and $s = 2p$ with integers p and q satisfying $0 < p < q \leq N/2$. Using these, Eq. (36) becomes

$$G(r,s) = -\frac{e^{i(p+q)\pi}}{2(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} e^{i2\omega m(p+q-1)} \frac{\left[1 + e^{-2i(2q-1)\omega m}\right]\left[1 - e^{-2i(2p)\omega m}\right]}{1 - e^{-2i\omega m}}$$

We now use the factorization $\frac{1-x^{2\ell}}{1-x} = 1 + x + x^2 + \cdots + x^{2\ell-1}$ with $x \equiv \exp(-i2m\omega)$ to get rid of the denominator

$$
\begin{aligned}
G(r,s) &= -\frac{(-1)^{p+q}}{2(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ e^{2i\omega m(p+q-1)}\left[1 + e^{-2i\omega m(2q-1)}\right] \right. \\
&\quad \times \left. \left[1 + e^{-2i\omega m} + e^{-4i\omega m} + \cdots + e^{-2i\omega m(2p-1)}\right] \right\}
\end{aligned}
$$

Multiplying the phase factor into the parenthesis inside the sum and substituting for ω we have

$$G(r,s) = -\frac{(-1)^{p+q}}{2(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left(e^{2i(p+q-1)\frac{\pi m}{N+1}} + e^{-2i(q-p)\frac{\pi m}{N+1}} \right) \left\{ 1 + e^{-2i\frac{\pi m}{N+1}} + e^{-4i\frac{\pi m}{N+1}} + \cdots + e^{-2i(2p-1)\frac{\pi m}{N+1}} \right\}. \tag{37}$$

Comment: The pre-factor multiplying the sum can only be $\frac{\pm 1}{2(N+1)}$, determined by the values of p and q : $G(r,s)$ vanishes iff the sum does.

We expand the summand in Eq. (37) to get

$$
\begin{aligned}
G(r,s) &= -\frac{(-1)^{p+q}}{2(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ \left[e^{2i(p+q-1)\frac{\pi m}{N+1}} + e^{2i(p+q-2)\frac{\pi m}{N+1}} + \cdots + e^{2i(q-p+1)\frac{\pi m}{N+1}} + e^{2i(q-p)\frac{\pi m}{N+1}} \right] \right. \\
&\quad + \left. \left[e^{-2i(q-p)\frac{\pi m}{N+1}} + e^{-2i(q-p+1)\frac{\pi m}{N+1}} + e^{-2i(q-p+2)\frac{\pi m}{N+1}} + \cdots + e^{-2i(p+q-2)\frac{\pi m}{N+1}} + e^{-2i(p+q-1)\frac{\pi m}{N+1}} \right] \right\} \\
&= -\frac{(-1)^{p+q}}{(N+1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ \cos\left[\frac{2\pi m(q-p)}{N+1}\right] + \cos\left[\frac{2\pi m(q-p+1)}{N+1}\right] + \cdots + \cos\left[\frac{2\pi m(p+q-1)}{N+1}\right] \right\}
\end{aligned} \tag{38}
$$

where in the last equation, to get the cosines, we paired the first term inside the first brackets with the last term inside the second brackets etc. and used the formula $e^{ix} + e^{-ix} = 2\cos x$. The factor of 2 cancelled the overall pre-factor $1/2$.

Comment: It is important to note that, since $q > p$, the exponents in the first bracket are all positive and in the second bracket the exponents are all negative.

We can write a more succinct expression

$$G(r,s) = -\frac{(-1)^{p+q}}{(N+1)} \sum_{t=0}^{2p-1} \left\{ 2 \sum_{m=\frac{1}{2}}^{\frac{N-1}{2}} \cos\left[\frac{2\pi m (q-p+t)}{N+1}\right] \right\}, \tag{39}$$

where we used evenness of cosines, to let m run from $1/2$, and switched the order of the sums. We now prove that the sum inside braces is $(-1)^t$. Let $\theta = \frac{2\pi(q-p+t)}{N+1}$, $n = m - 1/2$ and $N' = \frac{N}{2} - 1$ to rewrite the sum

$$2 \sum_{m=\frac{1}{2}}^{\frac{N-1}{2}} \cos\left[\frac{2\pi m (q-p+t)}{N+1}\right] \equiv 2 \sum_{n=0}^{N'} \cos\left[\left(n+\frac{1}{2}\right)\theta\right]$$

but $\cos\left[\left(n+\frac{1}{2}\right)\theta\right] = \cos(n\theta)\cos\left(\frac{\theta}{2}\right) - \sin(n\theta)\sin\left(\frac{\theta}{2}\right)$ and [1]

$$\sum_{n=0}^{N'} \cos(n\theta) = \frac{\cos\left(\frac{N'\theta}{2}\right)\sin\left[\frac{\theta}{2}(N'+1)\right]}{\sin(\theta/2)} \tag{40}$$

$$\sum_{n=0}^{N'} \sin(n\theta) = \frac{\sin\left(\frac{N'\theta}{2}\right)\sin\left[\frac{\theta}{2}(N'+1)\right]}{\sin(\theta/2)}. \tag{41}$$

Therefore $\sum_{n=1}^{N'} \cos\left(n+\frac{1}{2}\right)\theta = \sum_{n=1}^{N'} \left\{\cos(n\theta)\cos\left(\frac{\theta}{2}\right) - \sin(n\theta)\sin\left(\frac{\theta}{2}\right)\right\}$ gives

$$2 \sum_{n=0}^{N'} \cos\left(n+\frac{1}{2}\right)\theta = 2\left\{\cos\left(\frac{\theta}{2}\right)\frac{\cos\left(\frac{N'\theta}{2}\right)\sin\left[\frac{\theta}{2}(N'+1)\right]}{\sin(\theta/2)} - \sin\left(\frac{\theta}{2}\right)\frac{\sin\left(\frac{N'\theta}{2}\right)\sin\left[\frac{\theta}{2}(N'+1)\right]}{\sin(\theta/2)}\right\}$$

$$= 2\frac{\sin\left[\frac{\theta}{2}(N'+1)\right]}{\sin(\theta/2)}\left\{\cos\left(\frac{N'\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{N'\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\right\}$$

$$= 2\frac{\sin\left[\frac{\theta}{2}(N'+1)\right]}{\sin(\theta/2)}\left\{\cos\left(\frac{\theta}{2}(N'+1)\right)\right\} = \frac{\sin\left[(N'+1)\theta\right]}{\sin(\theta/2)} = \frac{\sin\left[N\theta/2\right]}{\sin(\theta/2)}.$$

However $\sin[N\theta/2] = \sin\left[\frac{(N+1)\theta}{2} - \frac{\theta}{2}\right] = \sin\left(\frac{(N+1)\theta}{2}\right)\cos\frac{\theta}{2} - \cos\left(\frac{(N+1)\theta}{2}\right)\sin\frac{\theta}{2}$. But $\sin\left(\frac{(N+1)\theta}{2}\right) = 0$, leaving us with

$$\frac{\sin[N\theta/2]}{\sin(\theta/2)} = \frac{\sin\left[\frac{\pi N(q-p+t)}{N+1}\right]}{\sin\left(\frac{\pi(q-p+t)}{N+1}\right)} = -\cos\left(\frac{(N+1)\theta}{2}\right) = -\cos(\pi(q-p+t)) = -(-1)^{q-p+t}. \tag{42}$$

Putting this back into the sum (Eq. (39))

$$G(r,s) = \frac{(-1)^{p+q}}{(N+1)} \sum_{t=0}^{2p-1} \left\{(-1)^{q-p+t}\right\}$$

$$= \frac{(-1)^{2q}}{(N+1)} \sum_{t=0}^{2p-1} (-1)^t = \frac{1}{(N+1)} \sum_{t=0}^{2p-1} (-1)^t \quad ;$$

zero comes out because we are summing alternating $+1$'s and -1's an even number of times. This completes the proof of the harder zeros. Note that we used $q > p$. For example if $q = p$, then $\cos \pi (q - p + t)$ would be 1 for $t = 0$ and the sum would give a $2p - 1$ on that term alone.

Recall $\frac{r+1}{2} = q$ and $\frac{s}{2} = p$ with integers p and q satisfying $0 < p < q \leq N/2$; for this choice

$$G (r, s) = 0 \quad .$$

Nonzero entries: ± 1's in the G

It remains to show that when r is even and s is odd, $G (r, s)$ is ± 1 as shown in Eq. (9). Let $r = 2q$ and $s = 2p - 1$ with $p \leq q$ (note that we allow for equality as well). Using Eq. (36) and previous techniques we have

$$G (r, s) = -\frac{i e^{i(2(p+q)-1)\pi/2}}{2 (N + 1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} e^{i2\omega m(p+q-1)} \frac{\left[1 - e^{-2i(2q)\omega m}\right] \left[1 + e^{-2i(2p-1)\omega m}\right]}{1 - e^{-2i\omega m}}$$

$$= -\frac{i e^{i(2(p+q)-1)\pi/2}}{2 (N + 1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left(e^{2i\omega m(p+q-1)} + e^{-2i\omega m(p-q)}\right)$$

$$\times \left\{1 + e^{-2i\omega m} + e^{-4i\omega m} + \cdots + e^{-2i(2q-1)\omega m}\right\} .$$

Once again we multiply the parenthesis into the braces to get (using $i e^{i(2(p+q)-1)\pi/2} = e^{i(p+q)\pi}$)

$$G (r, s) = -\frac{e^{i(p+q)\pi}}{2 (N + 1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ \left[e^{2i\omega m(p+q-1)} + e^{2i\omega m(p+q-2)} + \cdots + e^{2i\omega m(p-q)}\right] \right. \tag{43}$$

$$+ \left. \left[e^{-2i\omega m(p-q)} + e^{-2i\omega m(p-q+1)} + \cdots + e^{-2i\omega m(p+q-1)}\right] \right\}$$

Comment: Eq. (43) looks very similar to Eq. (38); however, it has a key difference. Since $q \geq p$, in either one of the brackets there will be a term with exponent zero. For example, if one looks at the first brackets the first term is $e^{2i\omega m(p+q-1)}$, which clearly has a positive exponent; however, the last term $e^{2i\omega m(p-q)}$ has either zero or negative exponent. If it is negative, then a term preceding it must have had zero exponent. Therefore, the sum for some choice of r and s can look like

$$G_{example} (r, s) = -\frac{e^{i(p+q)\pi}}{2 (N + 1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ \left[e^{2i\omega m(p+q-1)} + \cdots + e^{2i\omega m} + 1 + e^{-2i\omega m} + \cdots + e^{2i\omega m(p-q)}\right] \right. \tag{44}$$

$$+ \left. \left[e^{-2i\omega m(p-q)} + e^{2i\omega m} + 1 + e^{-2i\omega m} + \cdots + e^{-2i\omega m(p+q-1)}\right] \right\} \quad .$$

We can pair the terms to the left (right) of the 1 in the first bracket with those to the right (left) of the 1 in the right bracket to get the cosines as before. It is clear that the sum over 2 contributes a $2 (N - 1)$. We now show that the sum over the cosines contributes a 4, which together makes $2 (N + 1)$ and cancels the denominator in the pre-factor.

For any p and q, we can find a $t_0 = q - p \geq 0$ that makes the exponent zero. In the first bracket, there are $q - p$ terms to its left and there are $2q - (q - p + 1) = p + q - 1$ terms to its right (for a total of $2q$ terms). We can pair the terms to its left with the corresponding terms in the second bracket (now to the right of the 1) to get cosines and similarly pair terms to its right to get cosines. Then, we can break the sum in the foregoing equation to the sum over cosines obtained from terms to the left of t_0 in the first bracket, the sum over terms to its right and add a 2 for the term itself. Namely

$$G (r, s) = -\frac{e^{i(p+q)\pi}}{2 (N + 1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{2 \sum_{t=1}^{q-p} \cos [2\omega m t] + 2 + 2 \sum_{t=1}^{p+q-1} \cos [2\omega m t] \right\} \tag{45}$$

$$= -\frac{e^{i(p+q)\pi}}{(N + 1)} \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{\sum_{t=1}^{q-p} \cos [2\omega m t] + \sum_{t=1}^{p+q-1} \cos [2\omega m t] + 1 \right\} ,$$

where we cancelled the overall pre-factor of a 1/2. Let us evaluate each of the sums separately (switching order of summation, changing variables as before)

$$\sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \cos\left[2\omega mt\right] = 2\sum_{n=0}^{\frac{N}{2}-1} \cos\left[2\omega t\left(n+\frac{1}{2}\right)\right]$$

$$= 2\cos\left(\omega t\right)\sum_{n=0}^{\frac{N}{2}-1}\cos\left(2\omega tn\right) - 2\sin\left(\omega t\right)\sum_{n=0}^{\frac{N}{2}-1}\sin\left(2\omega tn\right)$$

The sum over cosines are evaluated using Eq. (40),41

$$\sum_{n=0}^{\frac{N}{2}-1}\cos\left(2\omega tn\right) = \frac{\cos\left(\left(\frac{N}{2}-1\right)\omega t\right)\sin\left[\omega t\left(N/2\right)\right]}{\sin\left(\omega t\right)}$$

$$\sum_{n=0}^{\frac{N}{2}-1}\sin\left(2\omega tn\right) = \frac{\sin\left(\left(\frac{N}{2}-1\right)\omega t\right)\sin\left[\omega t\left(N/2\right)\right]}{\sin\left(\omega t\right)}$$

which together give

$$\sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}} \cos\left[2\omega mt\right] = 2\frac{\sin\left[\left(\frac{N}{2}\right)\omega t\right]}{\sin\left(\omega t\right)}\left\{\cos\left(\left(\frac{N}{2}-1\right)\omega t\right)\cos\left(\omega t\right) - \sin\left(\left(\frac{N}{2}-1\right)\omega t\right)\sin\left(\omega t\right)\right\}$$

$$= 2\frac{\sin\left[\left(\frac{N}{2}\right)\omega t\right]}{\sin\left(\omega t\right)}\left\{\cos\left[\left(\frac{N}{2}\right)\omega t\right]\right\} = \frac{\sin\left(N\omega t\right)}{\sin\left(\omega t\right)} = \frac{\sin\left(\frac{\pi Nt}{N+1}\right)}{\sin\left(\frac{\pi t}{N+1}\right)}.$$

We calculated this ratio in Eq. (42) so we have

$$\frac{\sin\left(\frac{\pi Nt}{N+1}\right)}{\sin\left(\frac{\pi t}{N+1}\right)} = -\left(-1\right)^{t}\quad.$$

Using this we can evaluate Eq. (45)

$$G\left(r,s\right) = -\frac{e^{i(p+q)\pi}}{(N+1)}\left\{-\sum_{t=1}^{q-p}\left(-1\right)^{t} - \sum_{t=1}^{p+q-1}\left(-1\right)^{t} + \sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}}1\right\}.$$

If $q-p$ is even then $q-p=2k$ for some k and $p+q-1=2\left(k+p\right)-1$, which is odd. Also if $q-p=2k-1$, then $p+q-1=2\left(p+k-1\right)$, which is even. In either case one of the sums vanishes and the other evaluates to be -1. Therefore,

$$G\left(r,s\right) = -\frac{e^{i(p+q)\pi}}{(N+1)}\left\{1+\sum_{m=-\frac{N-1}{2}}^{\frac{N-1}{2}}1\right\} = -\frac{e^{i(p+q)\pi}}{(N+1)}\left(N+1\right) = -e^{i(p+q)\pi} \tag{46}$$

So we predict that if $p+q$ is odd then $G\left(r,s\right) = +1$ and if $p+q$ is even then $G\left(r,s\right) = -1$. What does this mean for r and s? Let us cover all of the cases one by one. Recall that r is even and s is odd and $q+p = \frac{r}{2}+\frac{s+1}{2}$

- $p+q$ is even, $G\left(r,s\right) = -1$, and q is even. This means, p is even. These implies that r and $s+1$ are multiples of 4. Looking at **G**, we see that these entries indeed are -1.

- $p+q$ is even, $G\left(r,s\right) = -1$, and q is odd. This means p is odd. These imply that r and $s+1$ are multiples of 2 but not 4. Looking at **G**, we see that the rest of the entries that are -1 have been covered.

- $p+q$ is odd, $G\left(r,s\right) = +1$, and q is even. This means p is odd. These imply that r is a multiple of 4 but $s+1$ is not (though of course even). This covers some of the $+1$'s in **G**.

- Lastly, $p + q$ is odd, $G(r,s) = +1$, and q is odd. This means p is even. These imply that r is not a multiple of 4 (though of course even), yet $s + 1$ is a multiple of 4. These cover the rest of $+1$'s seen $\mathbf{G}$,.

The final result Eq. (46) can be expressed in terms of r and s as

$$G(r,s) = -e^{i\pi\left(\frac{r+s+1}{2}\right)} = e^{i\pi\left(\frac{r+s-1}{2}\right)} \quad . \tag{47}$$

This completes our proof.

Remark 4. All the equations above for $G(r,s)$ were checked numerically.