Extracting the Dispersion of Periodic Lossless LC Circuits Using the White Noise

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Abstract: The spectral energy density (SED) method is used to obtain the phonon dispersion of solids in molecular dynamics tools, e.g., LAMMPS®. We show how the electric analog of the SED method is used to find the dispersion of periodic lossless LC circuits. The application of this idea is three-fold: (1) demonstrating how SED proves useful, should the analytic methods of calculating dispersion of a circuit render difficult (due to nonlinearity or having many elements), (2) teaching the concepts like Brillouin Zone, dispersion (or band structure), zone folding, gap formation and avoided crossing to students of physics and electrical engineering by highlighting the similarities of phonon and periodic circuits, and (3) studying the thermal devices, e.g., heat rectifiers using commercial circuit simulators.

Keywords: Dispersion, phonon, Molecular Dynamics, avoided crossing, Spectral Energy Density (SED), Spice, heat diode, topological circuits, parametric amplifiers, LAMMPS

1- Introduction:

Analogies between dispersion bands of vibrating atoms in a solid, energy band diagrams of electrons, and dispersion of voltage or current waves in a periodic discrete or distributed circuit were presented first by L. Brillouin [1]. In the 1950s, Gabriel Kron, an engineer from General Electrics, also proposed how the finite-difference form of partial differential equations can be simulated on periodic lattices of RLC circuits in one, two, or three dimensions [2]. The solution of the time-independent Schrödinger equation with potential wells was also represented by an array of periodic LC or CL circuits in [3]. Other examples of using circuit analogy are emulating Korteweg - De Vries (kdV) equation and soliton formation in Toda lattices in which nonlinear circuit elements like varactors are used [4][5].

Moreover, the physics of topologically protected states in condensed matters also sparked a new spate of research where people simulate different Hamiltonians and many-body interactions by periodic circuits with different dimensionalities and interconnections [6-8].

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Despite the insight and pedagogical value of the circuit analogy method, strong circuit simulators were not available at the time when Kron and others were trying to build the physics on circuits. Today, the availability of strong commercial circuit simulators which can treat circuits of all complexities in both time and frequency domains and in both linear and nonlinear regimes is an incentive to seek simpler ways of teaching concepts related to band structure in the condensed matter as well as investigating new physics and understandings using electric circuits. This approach will help both physics and engineering students because students are introduced to circuit analysis in their freshman college course, but band structure is a more advanced topic covered in solid state or device physics in later years.

This article shows how the concept of spectral energy density (SED) is implemented for periodic circuits. The SED method is widely used in the calculation of phonon dispersion of solids, e.g., graphene, and CNT [9][10]. The molecular dynamics codes like LAMMPS® solve equations of motion of atoms under different thermodynamical conditions called thermostats [11]. The equilibrated velocity of atoms as a function of time is then used to find quantities of interest, e.g., the density of state of phonons and thermal conductivity of the solid using the autocorrelation function of all atomic velocities. Furthermore, in the SED method, these time-recorded velocities are used to obtain the dispersion plots of phonons, i.e., the energy of phonons (ℏΩ) versus their wave vectors (q). This is useful in investigating which phonon branches are significant players in the heat-conducting mechanism. The broadening of each branch is a measure of how fast phonons lose their energy as a result of scattering. From this, the lifetime of phonons can be extracted. The slope of the dispersion plots is the group velocity of phonons. And from these two quantities (lifetime and group velocity), the mean free path of phonons is obtained. The mean free path is vital to deciding which nanostructure geometrical features affect heat transport [12-14].

Here we demonstrate how applying the SED method to a periodic circuit helps find the dispersion plots, i.e., frequency of propagating voltage/current wave (ω) versus the wave vector (k). Dispersion of a circuit, like that of phonons, has a wealth of information about the group velocity of propagating waves and stopbands within the circuit. This is useful in designing periodic nonlinear circuits for parametric amplification of microwave signals in quantum computing, sensing, and astronomy [15]. It also helps to find topologically protected bands in the circuit that emulates a given many-body Hamiltonian [6-8].

Teaching these analogies to electrical engineering, material science, and physics students is useful in increasing the student's grasp of concepts like BZ, dispersion, zone-folding, and
dynamical matrix. Also, in the case of periodic circuits of complex topology e.g., those with nonlinear inductors (using Josephson junctions) or nonlinear capacitors (using varactor diodes), the SED approach proves helpful in obtaining the dispersion without resorting to lengthy derivations first.

This article is organized in the following order. The SED formula is derived for a simple 1D solid, and its circuit analogy is presented using voltages/currents instead of the velocity of atoms. Then, the method of simulating the circuit in WRSpice®[16] to collect the voltages/currents is explained. Afterward, four circuits are presented as examples. Their dispersions are calculated based on the standard electrical engineering KVL/KCL methods and compared with those obtained from SED. The circuits are periodic LC, and periodic CL (which shows negative dispersion or left-handedness). The third one has a unit cell with two C’s and L’s to teach the concept of zone folding and bandgap (or stopband). The last one is the periodic LC coupled to a ring resonator in each unit cell to show the concept of avoided-crossing or degeneracy lifting (relevant to the degenerate time-independent perturbation theory). Avoided crossing and the creation of gaps are important concepts in designing RF/microwave filters [17] and improving the performance of superconducting parametric amplifiers [15, 18]. These concepts also have parallel analogs in optics, e.g., Bragg grating filters in fiber optics, optical amplifiers, and metamaterial design [19-21]. The SED method presented here is also applicable to periodic circuits of higher dimensions in 2 and 3D spatial dimensions.

2- Methods:
The working principle of SED is based on Parseval’s theorem which both physics and engineering learn about early in their college education when learning about Fourier transforms. The theorem simply states that the energy content of a signal is distributed in its harmonic content and can be found by adding the squared amplitudes of its harmonics, i.e., Fourier components. Derivation of the energy density formula is based on Parseval’s theorem [22][9][10], and here we only state the formula without the proof:

\[ \rho_E(k, \omega) = \frac{1}{4\pi\tau_0 N_T} \sum_\alpha \sum_\beta m_b \left| \int_0^{\tau_0} \sum_{n_{x,y,z}} \hat{u}_\alpha(n_{x,y,z}, b, t) e^{i(kr(n_{x,y,z})-i\omega t)} dt \right|^2 \]  

(2-1)

For the phonon case, the parameters in the above equation are as follows. \( N_T \) is the total number of unit cells, \( \tau_0 \) is the total integration time. Summation over \( \alpha \) runs over three different directions in the solid. The index \( b \) is the index of each atom, and \( B \) is the total number of
atoms in each unit cell. The inner summation runs over the number of unit cells and \( n_{x,y,z} \) is the index of each unit cell. The wave vector is shown by \( \mathbf{k} \) (sometimes shown by \( \mathbf{q} \)), and \( \mathbf{r} \) is the position in the 3D space wherein the phonon propagates. \( \dot{u} \) (The first derivative of oscillation amplitude \( u \)) is the velocity of atom number \( b \) along direction \( \alpha \) in the unit cell \( n_{x,y,z} \) as a function of time (\( t \)).

For a one-dimensional solid or circuit, the first summation does not exist. Also, the summation over the number of atoms is removed as in our 1D circuits; each LC section simulates one atom in every unit cell. The number of unit cells is the number of LC sections, and the index \( n_{x,y,z} \) is a number spanning 1 to \( N_T \) in one direction. The wave vector \( \mathbf{k} \) and position \( \mathbf{r} \) reduce to \( k_x \) and \( x \) in case of a one-dimensional solid or circuit along \( x \) direction. Therefore, the equation (2-1) is simplified as follows:

\[
\rho_E(k_x, \omega) = \frac{m_b}{4\pi \nu_0 N_T} \left| \int_0^{T_0} \sum_{n_x=1}^{N_T} \dot{u}_{n_x}(t) e^{-i\omega t} e^{ik_x x} dt \right|^2 = \beta \left| \sum_{n_x=1}^{N_T} e^{ik_x x} \int_0^{T_0} \dot{u}_{n_x}(t) e^{-i\omega t} dt \right|^2
\]

(2-2)

The summation and integral are interchanged by virtue of linearity, and perfectors are absorbed in \( \beta \). Note that the SED in this simplified form is two consecutive Fourier transforms. The inner-most transform is applied to the velocity to return the \( U(n_x, \omega) \) and the second transform is in the domain of \( n_x \), i.e., a discrete Fourier transform in space that returns \( \rho_E(k, \omega) \). The wave vector \( k_x \) is given by:

\[
k_x = \frac{2\pi n_x}{a_x N_T}
\]

(2-3)

where \( n_x = 0,1,2, \ldots, N_T \), which means the \( \rho_E(k, \omega) \) is a two-dimensional data matrix. In one direction, it stores the wave frequency, and in the other, it stores the wave vector values which span 0 to \( 2\pi \). For the periodic circuit, we assume the unit cell length to be one, \( a_x = 1 \), but note that the answers are not dependent nontrivially on the value of \( a_x \). The remaining steps are (1) injecting the white noise into the circuit and (2) running transient analysis for a long time and collecting the currents of each branch. The current and voltage are electrical analogs of velocity and force, respectively [23].

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The periodic circuits under study are simulated in the WRSpice® simulator from Whitley Research [16], but in principle, it can be done in any circuit simulator with time-domain (transient) analysis. The unit cell of each circuit is written in the netlist as a subcircuit. In the main netlist, 100 copies of the subcircuit are connected in series, and the input node is connected to a time-domain white noise voltage. The source parameters are standard deviation and mean voltage, and lattice, and interpolation. The mean value is chosen to be 0 as the definition of white noise mandates.

The simulation is performed for a sufficiently long time such that the possible back and forth reflections in the long discrete circuit due to impedance mismatch at the boundaries are settled. Total simulation time and the time step are typically $t_{tot} = 2000 \, ns$ and $dt = 5 \, ps$, respectively. Thereafter, the node voltages (or the branch currents) are saved in a $N_r \times N_c$ matrix in which the $N_r = 100$ is the number of rows (circuit nodes), and $N_c = t_{tot}/dt = 2000 \, ns / 5 \, ps = 4 \times 10^5$, is the number of columns.

The first Fourier transform is performed using the FFT function in MATLAB or python. This FFT corresponds to the inner-most Fourier transform in the SED formula in equation (2-2). The result of this part is a new matrix where the number of rows is still 100 (the number of nodes), but the number of columns is now the number of frequency points. This is determined in the first FFT step, and it should be large enough to include the highest frequency component of the voltage.

After the first transform, a new FFT is performed in the vertical direction, i.e., in the spatial (node) domain. This FFT corresponds to the outer-most Fourier transform, i.e., the one over space (atom indices or node indices) in the SED formula [equation (2-2)]. The matrix obtained in this step is visualized by surf or image functions in MATLAB or python, and the top view or the 2D rendering shows the trace of dispersion branches of the circuit. Each bright point on the branch corresponds to a peak. The sharpness of the peak depends on the number of points (pixels) along $k$ axis, meaning that increasing the number of unit cells to 500 and 1000 can make the branches very fine and sharp at the expense of time and memory.

In the next section, we show four different periodic circuits for which the above method is used to obtain their dispersion. The results are compared with the dispersions obtained using an analytic method based on Kirchhoff’s current and voltage laws and the eigenvalue problem, which is analogous to the dynamical matrix method for phonons [22].
3- Examples

3-1 One-dimensional periodic LC circuit:

The one-dimensional infinite and periodic array of the equal inductors \( (L) \) and capacitors \( (C) \) is shown in Figure 1(a). This circuit also serves as a discretized model of a continuous transmission line working at RF or microwave frequencies if we know the inductance per unit length \( (l') \) and capacitance per unit length \( (c') \) of the transmission line. We are interested in knowing which modes (waves of voltage or current) can propagate from –infinity to +infinity in this circuit with given inductance and capacitance determined by the geometry of the line.

![Figure 1](image)

Figure 1. The one-dimensional periodic circuits and their unit cells which is composed of (a) LC and (b) CL section. The circuit in (a) is a low-pass filter, and the one in (b) is a high-pass filter.

Like the method of treating periodic solids in solid-state physics [24], we define a unit cell, a cell of the minimum size that can be repeated by many periodic shifts to build the whole circuit. In this case, the unit cell is composed of parallel capacitor \( C \) and series inductor \( L \), as shown in Figure 1(a). The voltage of each node is \( V_n \) and the current entering the \( n \)’th unit cell \( I_n \). Kirchoff’s current law (KCL) relates the currents in unit cell \( n \) and its neighboring unit cell, i.e., \( n - 1 \) as follows:

\[
I_C = I_{n-1} - I_n \quad \rightarrow \quad C \frac{dV_n}{dt} = I_{n-1} - I_n
\]  

(3-1)
By taking time derivatives from both sides of equation (3-1) and noting that the relation between the magnetic flux inside the inductor and its current is \( \Phi = L.I \) and recalling Lens’ law which says \( V = -\frac{d\Phi}{dt} = \Phi \), equation (3-1) is then converted to a second-order differential equation relating the voltages of node \( n \) and its next neighbors.

\[
C \frac{d^2V_n}{dt^2} = \frac{1}{L} (V_{n-1} + V_{n+1} - 2V_n)
\]

(3-2)

To solve equation (3-2) a periodic trial solution is used by assuming that the solution, voltage at node \( n \), is of the form of a propagating wave with frequency, \( \omega \), and wave vector \( k.n.a \) (where \( a \) is the length of the unit cell) and complex amplitude of \( V_o \). After replacing \( V_n = V_0 e^{i(\omega t - k.n.a)} \) in equation (3-2), we get:

\[
-C \omega^2 V_0 e^{i(\omega t - k.n.a)} = \frac{1}{L} V_0 e^{i(\omega t - k.n.a)} (e^{-ika} + e^{ika} - 2) = \frac{1}{L} (2\cos(k.a) - 2)
\]

(3-3)

After solving for the frequency, we get:

\[
\omega^2 = \frac{4}{Lc} \sin^2 \frac{ka}{2}
\]

(3-4)

Equation (3-4) has two solutions: only the positive one is meaningful. Plotting the frequency \( (\omega/2\pi) \) versus the wave vector \( k \) or the normalized value \( (k.a) \) yields the dispersion as shown in Figure 2. As it is evident due to the periodicity of the dispersion, all information that we require to understand the dynamics of the circuit is contained in the interval of \( k.a = 2\pi \), i.e., \(-\pi \leq k.a \leq \pi \). This interval is the 1st Brillouin Zone (BZ). Everything outside the BZ is just a periodic replica of this information.

The group velocity of the propagating mode in the circuit is defined by \( v_g = \frac{\partial \omega}{\partial k} \). This quantity shows the velocity by which each mode (with wave vector \( k \)) propagates in the circuit or the discrete model of the transmission line. For example, suppose a pulse (superposition of different frequencies or wavelengths) enters the line. In that case, each mode propagates with a different velocity, and at the other end of the line, the pulse spreads or disperses (this is the reason behind the name, dispersion).
Figure 2. Dispersion of the 1D LC circuit shown in the first BZ ($-\pi < k.a < \pi$) for $L = 1 \, nH$ and $C = 1 \, pF$.

Note that at $k.a = \pm \pi$, the dispersion is slope less, i.e., the group velocity is zero. This suggests that the waves of this specific wavelength are stationary and do not move along the line. This resembles the Fermi level or Fermi surfaces in the solid’s electronic band structure, which should always be perpendicular to the 1st BZ boundaries [24]. Also, the maximum frequency in the dispersion is about 10 GHz, meaning that no mode can propagate with a higher frequency than this. This frequency (10 GHz) is called the cut-off or bandwidth of the circuit, and it is obtained from equation (3-4) by putting $k.a = \pm \pi$. For this example, with the values of capacitor and inductor as 1 $pF$ and 1 $nH$, respectively, we obtain,

$$\omega_{\text{cutoff}} = \frac{2}{\sqrt{LC}} \Rightarrow f_{\text{cutoff}} = \frac{1}{\pi \sqrt{LC}} \approx 10 \, GHz$$

Figure 3 shows the dispersion obtained by the SED method for the 1D LC circuit. The circuit simulated in this method is composed of 100 $LC$ unit cells. Fourier analysis of noise currents according to equation (2-2) resulted in Figure 3(a). As the cut-off frequency was designed to be 10 GHz, it is evident that there is no band (propagating mode) above 10 GHz, and the results are noisy. Half of the 1D BZ (50 $k_x$ points) in Figure 3(b) has all information in one branch, which is the same as Figure 3, which was obtained from equation (3-4) for $0 \leq k.a \leq \pi$. 
Figure 3. Dispersion of the 1D LC circuit obtained by the SED method. (a) The 2D top view of SED according to equation (2-2). Note that the data above the cut-off frequency of 10 GHz is noise. Below 10 GHz, two replicas of branches are visible. (b) The half of the BZ is shown, with one branch. The number of points along $k_x$ is determined by the number of unit cells. Obtaining higher resolution requires a larger number of unit cells.

Note that the second branch in Figure 3(a) is the mirror image of the first one, and it can be easily shifted to the negative $k_x$ values to make it the exact replica of Figure 2. However, one branch has all the necessary information about the circuit.

3-2 One-dimensional periodic CL circuit (Left-handed circuit):

Now we replace the unit cell of the LC circuit with its dual, i.e., a series capacitor and a parallel inductor [see Figure 1(b)]. As we will see, this circuit shows negative group velocity from which the name, left-handed, originated. Meaning that the circuit allows the propagation of waves towards the $-x$ direction. Additionally, it has high pass filter characteristics.

Writing the KVL around the capacitor in unit cell $n$ yields:

$$V_{n-1} - V_n = V_c$$  \hspace{1cm} (3-5)

$$L \frac{dt_{n-1}}{dt} - L \frac{dt_{n}}{dt} = V_c$$  \hspace{1cm} (3-6)

The current going through $n$’th capacitor is as follows:
\[ C_L \frac{dV_c}{dt} = i_n + C \frac{d}{dt} (V_n - V_{n+1}) \]  \hspace{1cm} (3-7)

By replacing (3-7) in equation (3-6), we get the 2nd order differential form:

\[ C_L \frac{d^2i_{n-1}}{dt^2} - LC \frac{d^2i_n}{dt^2} = i_n + LC \frac{d^2i_n}{dt^2} - LC \frac{d^2i_{n+1}}{dt^2} \]  \hspace{1cm} (3-8)

\[ C_L \left( \frac{d^2}{dt^2} (i_{n+1} + i_{n-1} - 2i_n) \right) = i_n \]  \hspace{1cm} (3-9)

Using the periodic trial solution \( i_n = I_0 e^{i(\omega t - kna)} \) we have:

\[ LC \left( 2\omega^2 - \omega^2 (e^{ika} + e^{-ika}) \right) = 1 \]  \hspace{1cm} (3-10)

\[ LC \left( 2\omega^2 - 2\omega^2 \cos (ka) \right) = 1 \]  \hspace{1cm} (3-11)

\[ \omega^2 = \frac{1}{4LC \sin^2 (\frac{ka}{2})} \]  \hspace{1cm} (3-12)

Figure 4 shows the dispersion of the 1D CL circuit. The negative slope of the dispersion explains why the left-propagating waves are allowed because the group velocity is negative. Also, the circuit shows a high pass filter feature as it allows all low \( k \) values (small wavelength) frequencies to be propagated. Below a certain frequency, determined by \( L \) and \( C \) there is no frequency available for all \( k \) values. This low cut-off frequency is found in equation (3-12) by putting \( ka = \pm \pi \). For \( L = 1 \text{ nH} \) and \( C = 1 \text{ pF} \) we obtain (see Figure 4),

\[ f_{cutoff} = \frac{1}{4\pi \sqrt{LC}} \approx 2.517 \text{ GHz} \]
Figure 4. The dispersion of 1D periodic CL (lefthanded) circuit for $L = 1nH$ and $C = 1 pF$. The low cut-off frequency is $2.157 GHz$. Note that only the right half of BZ is shown.

The dispersion calculated by SED is shown in Figure 5, which closely matches the one found in Figure 4. The number of unit cells ($k_x$ points) is 100, with the same capacitance and inductance values as for LC circuit. Note that there are two replicas of branches in the $[0, \pi]$ interval. The noisy data at the bottom shows the stop band below the cut-off frequency ($2.157 GHz$). Figure 5(b) shows half of the BZ (50 $k_x$ points). At low $k_x$ values, the branch is steeply rising to infinity, occupying one- or two-pixel areas. By increasing the number of unit cells to 1000, the resolution of this part will be better.
Figure 5. (a) The 2D view of SED for the lefthanded circuit shows two dispersion branch replicas and a low cut-off frequency of about 2 GHz. (b) The 1st half of BZ. The poor resolution at low $k_x$ values are due to the steep part of the plot, which occupies only one or two $k_x$ pixels.

### 3.3 Unit cell with two capacitors and two inductors:

Now assume that each unit cell is composed of two inductors and two capacitors of different values, i.e., $L_1$, $l_1$, $C_1$ and $C_2$ as shown in Figure 6(a). For simplicity, let $L = L_1 = L_2$ but we keep $C_1$ and $C_2$ to be different for the generality of the discussion. The treatment is like the calculation of phonon dispersion for a 1D solid with two different atomic masses ($m_1$ and $m_2$) and connected by two springs of stiffness $K_1$ and $K_2$ in the same unit cell [24]. The only difference is that the second Newton law is used to set up two coupled second-order differential equations for phonon, but for circuits, KVL/KCL is used instead.

In each unit cell there are two nodes with voltages $U_n$ and $V_n$, respectively. For both nodes, we write KCL and, like the previous discussion, for a simple $LC$ line:

For $C_2$: \[
\frac{dI_{C_2}}{dt} = \frac{d}{dt}(I_{n-1} - I_n) = \frac{\Phi_{left}}{L} - \frac{\Phi_{right}}{L}, \tag{3-13}
\]

Where left means the left side of $C_2$ and right means the right side of $C_2$.

For $C_1$: \[
\frac{dI_{C_1}}{dt} = \frac{d}{dt}(I_n - I_{n+1}) = \frac{\Phi_{left of C_1}}{L} - \frac{\Phi_{right of C_1}}{L} \tag{3-14}
\]
Using Lens’ law and replacing each flux time-derivation with the voltage difference on each inductor, and noting that the current going through each capacitor \((C)\) is \(I = C \, dv/dt\), we obtain:

\[
C_1 \frac{d^2 V_n}{dt^2} = \frac{1}{L} (U_{n-1} - V_n) - \frac{1}{L} (V_n - U_n) = \frac{1}{L} (U_{n-1} + U_n - 2V_n) \quad (3-15)
\]

\[
C_2 \frac{d^2 U_N}{dt^2} = \frac{1}{L} (V_n - U_n) - \frac{1}{L} (U_N - V_{N+1}) = \frac{1}{L} (V_n + V_{n+1} - 2U_n) \quad (3-16)
\]

The equations (3-15) and (3-16) are coupled, i.e., the right-hand sides contain both \(U\) and \(V\), which are unknown. Using the Ansatz for both \(U\) and \(V\) and replacing them in equations (3-15) and (3-16), this set of second-order differential equations are converted to an algebraic equation relating frequency \((\omega)\) and weave vector \((k)\).

![Diagram](image)

**Figure 6.** (a) The periodic 1D circuit with two different \(LC\) sections in each unit cell. (b) A periodic 1D LC circuit with coupling to a resonator of fixed frequency \(\omega_0\) in each unit cell.

By replacing \(U_n = \sum_k \bar{U}_k e^{i(kn \alpha - \omega t)}\) and \(V_n = \sum_k \bar{V}_k e^{i(kn \alpha - \omega t)}\) (which are superpositions of planar waves of different wavevectors \(k\)) in the above equations, using \(\beta_1 = 1/LC_1\) and \(\beta_2 = 1/LC_2\) and factoring out common terms from both sides, we obtain,
\[-\omega^2 V_k = \beta_2 (1 + e^{-ika}) U_k - 2 V_k \]  
(3-17)

\[-\omega^2 \bar{U}_k = \beta_1 (1 + e^{+ika}) \bar{V}_k - 2 \bar{U}_k \]  
(3-18)

It is instructive to write these equations in matrix form as follows:

\[
\begin{bmatrix}
\beta_2 (1 + e^{-ika}) & \omega^2 - 2\beta_2 \\
\omega^2 - 2\beta_1 & \beta_1 (1 + e^{+ika})
\end{bmatrix}
\begin{bmatrix}
U_k \\
V_k
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix}
\]  
(3-19)

The above matrix equation is of the form \( A X = 0 \), hence, to have a non-zero solution, its determinant should be zero [i.e., \( det(A) = 0 \)]. As a result, the following equation is obtained:

\[\omega^4 - 2(\beta_1 + \beta_2)\omega^2 + 4\sin^2 \left(\frac{ka \pi}{2}\right) \beta_1 \beta_2 = 0 \]  
(3-20)

Solving the above equation and keeping the positive (physical) frequency solutions yields:

\[\omega^2 = \frac{1}{l} \frac{C_1 + C_2}{C_1 C_2} \pm \frac{1}{l C_1 C_2} \sqrt{(C_1 + C_2)^2 - 4 C_1 C_2 \sin^2 \frac{ka \pi}{2}} \]  
(3-21)

After plotting this, the dispersion shown in Figure 7 is obtained.

Figure 7. The 1st BZ of the periodic circuit with \( L = L_1 = L_2 = \frac{1}{2} nH \) and \( C_1 = 1 \mu \text{F} \) and \( C_2 = 2 \mu \text{F} \) in each unit cell.
Recall that this resembles the dispersion of vibrational energies of a two atomic unit cell solid composed of two different masses, e.g., $m_1$ and $m_2$. Even the factor $\frac{C_1 + C_2}{C_1 C_2}$ is formally like $\frac{m_1 + m_2}{m_1 m_2}$ in the case of phonons. In the latter case, the 1st branch is called the acoustic, and the top (second) one is called the optical branch. The modes on $k \alpha = \pm \pi$ have zero group velocity, which means they are standing waves in the circuit and do not propagate. The frequencies between 5 GHz and about 7 GHz cannot propagate in the circuit because there is no corresponding wave vector available for them. This frequency band is called the stop band or bandgap of the circuit. The bottom and top edges of the bandgap are found by putting $k \alpha = \pm \pi$ in equation (3-21),

$$f_{low} = \frac{\sqrt{2}}{\pi \sqrt{LC_2}} = 5.03 \text{ GHz} \quad \text{and} \quad f_{high} = \frac{2}{\pi \sqrt{LC_1}} = 7 \text{ GHz}$$

The maximum frequency of the second dispersion branch (cut off) is 8.7 GHz which is found using equation (3-21) by putting $k_x = 0$,

$$f_{cutoff} = \frac{\sqrt{2(C_2 + C_2)}}{\pi \sqrt{LC_1 C_2}} = 8.7 \text{ GHz}$$

For phonons, this is called the maximum frequency of optical phonons. It is instructive to rewrite the matrix equation $(A \cdot X = 0)$ in a slightly different form as follows:

$$\omega^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} U_k \\ V_k \end{bmatrix} = \begin{bmatrix} 2\beta_1 & -\beta_1(1 + e^{+ika}) \\ -\beta_2(1 + e^{-ika}) & 2\beta_2 \end{bmatrix} \begin{bmatrix} U_k \\ V_k \end{bmatrix}$$

(3-22)

This can be written in the form of an eigenvalue problem as:

$$D_k \cdot X = \omega^2 \cdot I \cdot X,$$

(3-23)

where $D_k$ is called Dynamical Matrix and $X$ is the eigenvector and is composed of complex wave amplitudes. The eigenvalue, $\omega^2$, is found by diagonalizing $D_k$. For example, $[\text{amp}, \text{omega2}] = \text{eig}(D_k)$ in MATLAB returns the eigen values and eigen waves. In case the Dynamical Matrix is available, it is enough to diagonalize it for each given discrete $k \alpha$ within [0, $\pi$] interval and plot the eigenvalues for each $k \alpha$ value to obtain the dispersion.
Executing the SED method for this circuit results in Figure 8. The highest cut-off frequency is about 8.7 GHz, as previously determined by equation (2-21) using $L = 1\, nH$ and $C_1 = 1\, pF$, $C_2 = 2\, pF$. Also there is a bandgap or stop band from 5.03 GHz to 7 GHz, like the dispersion found in equation (3-31). Note that since the number of unit cells is 50 this time, the 100-point range of $k_\chi$ includes two BZs [recall equation (3-4)]. Figure 8(b) shows the 25 $k_\chi$ points (half of BZ), which is the same as the left half of Figure 7.

### 3-4 Coupled Resonators (Avoided Crossing):

Now consider Figure 6(b), where each inductor of the discrete transmission line is mutually coupled to a series of lumped resonator rings (composed of $L_s$ and $C_s$). The mutual coupling inductance is $M$. This example helps in teaching the concept of avoided crossing and is relevant to the case of time-independent perturbation with degeneracy. In this case, we show how, at a certain $k_\chi$ point, there are two degenerate and equal eigen frequencies (5 GHz), and this is lifted by the amount, which is determined by the coupling constant $M$. It is also helpful to show the students what kind of structure leads to a flat line in the dispersion, i.e., a constant frequency (energy) line for all values of $k$. In our case, a lumped (localized) resonator led to the constant 5 GHz line.

To find the dispersion of a $LC$ line coupled with the resonator, we first write the KCL in the $n$’th node. The current and voltage in the $LC$ line are represented by $i_n$ and $v_n$. The
corresponding quantities for the \( n \)'th \( L_s C_s \) loop are shown by adding a tilde on top, e.g., \( i_n \) and \( \tilde{U}_n \).

\[
i_{n-1} = i_n + C \frac{d\psi_n}{dt} \tag{3-24}
\]

After differentiating both sides with respect to time, we have:

\[
\frac{d^2i_{n-1}}{dt^2} = \frac{d^2i_n}{dt^2} + C \frac{d^2\psi_n}{dt^2} \tag{3-25}
\]

For each unit cell, due to the mutual inductance, the following voltage relations for \( (n - 1) \) and \( n \) unit cells hold:

\[
\frac{d\psi_{n-1}}{dt} = v_{n-1} - v_n - M \frac{d\psi_{n-1}}{dt} \tag{3-26}
\]

\[
\frac{d\psi_n}{dt} = v_n - v_{n+1} - M \frac{d\psi_n}{dt} \tag{3-27}
\]

Plugging in the above in equation (3-25), we have:

\[
v_{n+1} + v_{n-1} - 2v_n - LC \frac{d^2\psi_n}{dt^2} = M \frac{d\psi_{n-1}}{dt} - M \frac{d\psi_n}{dt} \tag{3-28}
\]

To write \( \tilde{i}_n \) in terms of \( \tilde{U}_n \), note that the current inside each \( L_s C_s \) loop is found from the capacitor voltage:

\[
\tilde{i}_n = -C_s \frac{d\tilde{\psi}_n}{dt} \tag{3-29}
\]

Replacing (3-29) in (3-28), we have:

\[
v_{n+1} + v_{n-1} - 2v_n - LC \frac{d^2\psi_n}{dt^2} = -M C_s \frac{d^2\tilde{\psi}_{n-1}}{dt^2} + M C_s \frac{d^2\tilde{\psi}_n}{dt^2} \tag{3-30}
\]

Equation (3-30) is the first one required to find the dispersion modes, and it is written in terms of two voltages: \( \psi \) and \( U \). Now, a KVL is written inside the \( n \)'th \( L_s C_s \) loop using equation (3-29):
\[ L \frac{d^2 n}{dt^2} + M \frac{dn}{dt} = \bar{U}_n \quad (3-32) \]

Thereafter, \( \frac{dn}{dt} \), is replaced with its equivalent given in equation (3-27) and \( \frac{dn}{dt} \) is replaced with the help of equation (3-29). We get:

\[ -C_s L_s \frac{d^2 \bar{U}_n}{dt^2} + \frac{M}{L} (L \frac{dn}{dt}) = \bar{U}_n \quad (3-33) \]
\[ -C_s L_s \frac{d^2 \bar{U}_n}{dt^2} + \frac{M}{L} (v_n - v_{n+1} - M \frac{dn}{dt}) = \bar{U}_n \quad (3-34) \]

Using equation (3-29), equation (3-24) is also expressed in terms of \( v \) and \( U \) only. Also, for the sake of brevity, the dot notation is used for differentiation with respect to time, i.e., \( \frac{dv}{dt} = \dot{v} \).

\[ \frac{M}{L} (v_n - v_{n+1}) + \frac{M^2 C_s}{L} \bar{U}_n - C_s L_s \ddot{U}_n - U_n = 0 \quad (3-35) \]

Equations (3-35) and (3-30) are grouped in matrix form.

\[ \begin{bmatrix} v_{n+1} + v_{n-1} - 2v_n - LC \dot{v}_n + MC_s (\ddot{U}_{n-1} - \ddot{U}_n) \\ \frac{M}{L} (v_n - v_{n+1}) + \frac{M^2 C_s}{L} \bar{U}_n - C_s L_s \ddot{U}_n - U_n \end{bmatrix} = 0 \quad (3-36) \]

By replacing the trial solutions like \( U_n = \sum_k U_k e^{i(kn \alpha - \omega t)} \) and \( V_n = \sum_k V_k e^{i(kn \alpha - \omega t)} \), the following numerical matrix equation is found,

\[ \begin{pmatrix} e^{ika} + e^{-ika} - 2 + LC \omega^2 \\ \frac{M}{L} (1 - e^{-ika}) \end{pmatrix} \begin{pmatrix} M C_s \omega^2 (1 - e^{ika}) \\ - \frac{M^2 C_s \omega^2}{L} + L_s C_s \omega^2 - 1 \end{pmatrix} \begin{pmatrix} V_k \\ U_k \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (3-37) \]

Using the shorthand notations \( \omega_0 = 1/\sqrt{LC} \) and \( \Omega = 1/\sqrt{L_s C_s} \) we have:

\[ \begin{pmatrix} 2 \cos (ka) - 2 + \frac{\omega^2}{\omega_0^2} M C_s \omega^2 (1 - e^{ika}) \\ \frac{M}{L} (1 - e^{-ika}) - \frac{M^2 C_s \omega^2}{L} + \frac{\omega^2}{\Omega^2} - 1 \end{pmatrix} \begin{pmatrix} V_k \\ U_k \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (3-38) \]
To have a non-zero solution, the determinant of the above matrix is set equal to zero. From this, the dispersion relation is extracted,

\[ \cos(ka) = 1 - \frac{LC}{2} \omega^2 + \frac{\omega^4}{\omega^2 - \Omega^2} \left( \frac{M^2C}{2L_s} \right) \]  \hspace{1cm} (3-39)

Note that in contrast to equations (3-4), (3-12), and (3-21), where \( \omega \) was a function of \( k \), here \( k \) must be found numerically by sweeping the frequency, \( \omega \). With the example values of \( L_s = 1 \ nH, \ C_s = 1 \ pF, \ L = 1 \ nH, \) and \( C = 0.25 \ pF \); the resulting dispersion is plotted in Figure 9. It is shown that the bandgap (stopband) begins at 5.035 \( GHz \) and ends at 5.812 \( GHz \). Note that if coupling did not exist, i.e., \( M = 0 \), we would have the same dispersion as the one for \( LC \) circuit (section 3-1) plus a horizontal line at 5 \( GHz \) for all values of \( k \) as the resonance frequency of the ring resonator is always \( \frac{\Omega}{2\pi} = \frac{1}{2\pi\sqrt{L_sC_s}} = 5 \ GHz \), and the localized oscillation on this resonator needs all \( k \) (wavelength) values in order to get formed. This resembles the physics of a defect in a crystal on which an electron is localized or trapped, and as a result, in the nanostructure (dispersion), a flat constant-energy line is observed.

![Figure 9. Avoided crossing in the dispersion plot of a \( LC \) circuit interacting with a ring resonator of \( f_s = 5 \ GHz \) in each unit cell. The coupling (interaction) causes a gap formation from 5.035 \( GHz \) to 5.812 \( GHz \).](image-url)
By turning on the coupling (here $M = 0.5$), the dispersion plots on the overlapping point (same frequency of 5 GHz) split into two branches of different frequencies. This is what is called avoided crossing. Note that in solving the equation (3-41), in contrast to the previous cases, the frequency is swept from 0 to values higher than the cut-off, and the available $k$ values are recorded. The straight horizontal and vertical lines in Figure 9 are artifacts of plotting and have no physical meaning.

The SED method returns Figure 10(a), in which two replicas of branches in the BZ are shown. The 1st half of the BZ is shown in Figure 10(b), that is like the one obtained by the analytic method in Figure 9. Note the resemblance of avoided crossing (noisy part of the figure) and the highest cut-off frequency, which is 23.6 GHz in both methods.

Figure 10. (a) Top view of SED for $LC$ circuit coupled to ring resonator in each unit cell for the values of inductance and capacitance given in the text. (b) The 1st half of BZ with the avoided crossing and highest cut-off frequency.
4- Conclusions:
We showed how the band structure or dispersion concept, first Brillouine Zone (BZ), zone folding, gap formation, and avoided crossing can be discussed and taught based on periodic lossless LC circuits. We showed implementing the spectral energy density (SED) method using the circuit analog quantities for phonons. From that, we obtained dispersion of four different periodic 1D circuits based on discrete unit cells composed of L and C. While the examples presented in this work are trivial and circuit analysis seems to be the easier way to get the dispersion, firstly, the proposed approach is helpful in increasing the student's grasp of the concepts like BZ, dispersion, zone-folding, and dynamical matrix. Secondly, in the case of a periodic circuit of a complex or nonlinear topology for which the standard KVL/KCL-based method is not straightforward, the SED approach proves helpful. Thirdly, the presented approach can be used in emulating the thermal transport physics of nanomaterials, e.g., heat rectifiers [25 - 27], heat transistors, etc., by using commercial circuit simulators and translating the language of mass and spring to that of inductance and capacitance.

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