Effects of Boundary Conditions on Phonon Dispersions, and Tamm- and Shockley-like Surface States in Solids, Shown in 1D Phonic Systems

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This essay aims to compare different boundary conditions and their effects on phonon dispersion spectra in 1D atomic chains as an example of solids. Firstly, a theoretical analysis is done to compare periodic and fixed boundary conditions' dispersion relations on 1D monoatomic chains, allowed wave vectors and density of states, and their behaviors at thermaldynamic limit. Second quantization of phonons under both boundary conditions are performed to illustrate the boson properties, Goldstone modes and the existence of zero-point energy of these phonons. Then, Tamm- and Shockley-like states are introduced to this system by changing the conditions on the edges or changing the topological bulk properties, and additional surface states are successfully observed. Floquet boundary conditions in pressure acoustic simulations are also compared to periodic boundary conditions to show their similarity and the fact that discrete translational symmetry introduces dispersion. Finally, some beneficial questions are discussed.

I. INTRODUCTION

In the study of solid state physics, periodic boundary conditions (PBCs) are a very convenient choice when handling macroscopic crystals, mimicking an infinite system by joining together cells on the boundaries, naturally inducing quantized travelling-wave-like solutions. However, it does not necessarily accurately describe the real situation, as the crystals themselves are clearly not infinite. Hereby, we want to compare different boundary conditions (BCs), including fixed boundary conditions (FBCs) and free boundary conditions (Free BCs), especially on their different effects on electronic band structures and phonon spectra of crystals.

Also, in a similar field of phononic crystals[1] (or sonic crystals), many thoretical[2] and practical[3–5] methods, along with actual computations on specific structures[6–8] have been done to simulate the dispersion spectra of phononic crystals, using Finite Element Method (FEM) and pressure acoustic method. More recently, it has been transplanted to the simulations of electronic band structures of actual crystals, such as graphenes[9,10]. In these researches, a boundary condition called Floquet boundary condition (Floquet BC) is commonly used as a type of PBC. Hereby, we also want to discuss its similarity and difference between ordinary PBC.

II. MODEL AND CALCULATIONS FOR 1D MONOATOMIC CRYSTALS

A. Model

For simplicity, we adopt an 1D monoatomic chain with total number of N primitive cells and a lattice vector of $\boldsymbol{a} = a\hat{x}$.

B. Phonon Dispersion

We assume that the only interactions between atoms are the linear resilience force between nearest neighbors (NNs) with a Hooke factor K. Also, we denote u_n as the deviation from balanced position of the nth atom. Therefore, Newton's second law yields

$$\begin{aligned} M\frac{\partial^2 u_n}{\partial t^2} &= -K(u_n - u_{n-1}) - K(u_n - u_{n+1}) \\ &= -K(-u_{n-1} + 2u_n - u_{n+1}) \end{aligned} \tag{1}$$

From translational symmetry of the model, we assume that the eigensolution of Eq. (1) is a wave-like solution, which is

$$u_n = A\exp i(qx_n - \omega t) + B\exp i(-qx_n - \omega t) \tag{2}$$

in which q serves as a wave vector living in reciprocal space (q-space) and ω serves as the frequency of time domain.

Substituting Eq. (2) into Eq. (1):

$$-\omega^2 u_n = \frac{K}{M}(u_{n-1} - 2u_n + u_{n+1}) \tag{3}$$

or

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$$\begin{aligned}\omega^2 &= -\frac{K}{M}(\exp(-iqa) - 2 + \exp(iqa)) \\ &= \frac{4K}{M}\sin^2\Big(\frac{qa}{2}\Big)\end{aligned} \tag{4}$$

Abandon negative branch of ω:

$$\omega(q) = \sqrt{\frac{4K}{M}}\left|\sin\Big(\frac{qa}{2}\Big)\right| \tag{5}$$

This is the general phonon dispersion for 1D monoatomic crystal we consider, as is shown in Fig. 1(c). However, to actually determine the forms of allowed solutions, which is different linear combinations of eigensolutions, and allowed values of q, we must take different BCs into account.

PBC

PBC infinitely joins the same N primitive cells on both boundaries, forming a (topologically) ring-like **supercell** containing N primitive cells, as is shown in Fig. 1(a). That is to say,

$$u_n = u_{n+N} \tag{6}$$

Substituting Eq. (6) into Eq. (2), we get:

$$\exp(iqNa) = 1 \tag{7}$$

which is to say,

$$q_j = j\frac{2\pi}{Na}, j = 0, \pm1, \pm2, ... \tag{8}$$

These are the allowed values of q; these collective vibrational modes are called (acoustic) **phonons**, since they exhibit a similar behavior of quantized bosons and energies like photons, as will be showned below in section III. There are N allowed q values in 1st Brillouin zone (BZ), possesing 2-fold degeneracy of energy except for $q = 0$.

Thus, we can write the eigensolutions under PBC as

$$u_n = A\exp i\Big(2\pi j\frac{n}{N} - \omega t\Big) \tag{9}$$

which is a *travelling* wave solution with a group velocity

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}q} = \mathrm{sgn}(q)\cdot a\sqrt{\frac{K}{M}}\cos\Big(\frac{qa}{2}\Big) \tag{10}$$

as is shown in Fig. 1(e). It represents how fast energy propagates with a wavevector q. For q near 0 (long wavelength limit), there is nearly no dispersion, because dispersion relation is nearly linear around $q = 0$, as is shown in Fig. 1(c); however, for q near the boundaries of 1st BZ (short wavelength limit), energy propagates relatively slowly through sound, hence the name "*dispersion*".

When q exceeds the boundaries of 1st BZ, the dispersion relations repeats periodically in q-space. In the prospective of digital signal processing, if we consider the vibrations of atoms as a *sample* of a non-existing continuous travelling wave at a given position and time, this periodicity naturally comes from **Nyquist-Shannon Sampling Theorem**[11], when a space frequency exceeding Nyquist frequency (in this case, the boundary of 1st BZ π/a), the actual effect is equivalent with a wave with $q' = q - \pi/a$, folding back to 1st BZ, as is shown in Fig. 1(f). Therefore, it's enough to only consider qs inside 1st BZ.

Specifically, for the state $q = 0$, we also have $\omega = 0$; it represents a monolithic translation without any vibrations, carrying a slow amount of kinetic energy, which is ignorable compared to $q \neq 0$ modes at low velocities. These gap-less low-energy modes are called **Goldstone modes** (or **Nambu-Goldstone bosons**) in statistical physics and quantum field theory, originating from a spontaneously-broken continuous symmetry (in our case, continuous translational symmetry) [12]. In our calculations, we can safely neglect them, as we usually only consider crystals at stationary states.

For density of states (DOS), each mode occupies $2\pi/(Na)$ in q-space, so DOS in q-space

$$D(q) = \frac{Na}{2\pi} \tag{11}$$

However, we also want to know DOS in frequency domain $g(\omega)$. Here we can construct a equivalence relation

$$g(\omega)\,\mathrm{d}\omega = D(q)\,\mathrm{d}q \times 2 - 1 \tag{12}$$

where 2 originates from 2-fold degeneracy. Then, substituting Eq. (1)(0), at $n \to \infty$ we get

$$g(\omega) = \frac{Na}{\pi}\left|\frac{\mathrm{d}q}{\mathrm{d}\omega}\right| = \frac{2N}{\pi\sqrt{\omega_{\max}^2 - \omega^2}} \tag{13}$$

where $\omega_{\max} = \sqrt{4K/M}$.

FBC

FBC requires the atoms on the boundaries of supercells to be stationary; that is to say, we can append 2 virtual atoms with number 0 and $N + 1$ denoting them, then

$$u_0 = u_{N+1} = 0 \tag{14}$$

preserving N total degrees of freedom.

Phonon dispersion relation of FBC is the same as PBC, both with Eq. (5), due to the unchanged interaction model we adopt. However, the eigensolutions are not the same due to changed BCs. Substituting Eq. (1)(4)'s left side into Eq. (2), we get:

$$A + B = 0 \tag{15}$$

which makes the eigensolution

$$u_n = 2iA\sin(qx_n)\exp(-i\omega t) \tag{16}$$

which is a *standing* wave.

Also, Substituting Eq. (1)(4)‘ s right side into Eq. (1)(6), we get:

$$0 = \sin(q(N+1)a) \tag{17}$$

giving out the allowed q values:

$$q_j = j\frac{\pi}{(N+1)a}, j \in \mathbb{Z}$$

However, with *standing* wave solutions, q and $-q$ actually denotes the same wave (with the same wavelength, which is a natural conclusion of linear combinations of mathematical eigensolutions in Eq. (1)(5) and Eq. (1)(6)); also, when $q = 0$, we get a trivial solution of $u_n = 0$, which we neglect. What's more, for the same reason of Nyquist frequency, we neglect all j values more than N, since they represent the same waves as in $[1, N]$. Thus, the actual allowed q values are:

$$q_j = j\frac{\pi}{(N+1)a}, j = 1, 2, ..., N \tag{18}$$

as is shown in Fig. 1(d).

For DOS, we follow a similar process of PBC:

$$D(q) = \frac{Na}{\pi} \tag{19}$$

$$g(\omega) = \frac{Na}{\pi}\left|\frac{\mathrm{d}q}{\mathrm{d}\omega}\right| = \frac{2N}{\pi\sqrt{\omega_{\max}^2 - \omega^2}} \tag{20}$$

Notice that the 2-fold degeneracy in PBC doesn't exist in FBC.

C. Thermaldynamic Limit

With thermaldynamic limit of $N \to \infty$, allowed q values approaches continuity, making phonon dispersion and DOS continuous; also from calculations above, DOS in ω domain is the same in PBC and FBC when $N \to \infty$.

D. Numerical Calculations

For $N \in [1, 50]$, we plot N vs. energy levels under both PBC and FBC, as is shown in Fig. 1(g). In the graph, we can clearly see that: i) PBC possesses a 2-fold degeneracy except for $q = 0$, while FBC doesn't possess any degeneracy; ii) as N goes higher, the level spacings gradually become equal; however, iii) the energy states at higher ωs are denser than those at lower ωs.

We can also draw N vs. standard deviations of level spacings graph as in Fig. 1(h) and the distribution of level spacings of both BCs at $N = 50$ as in Fig. 1(i), which further proves point ii) and iii).

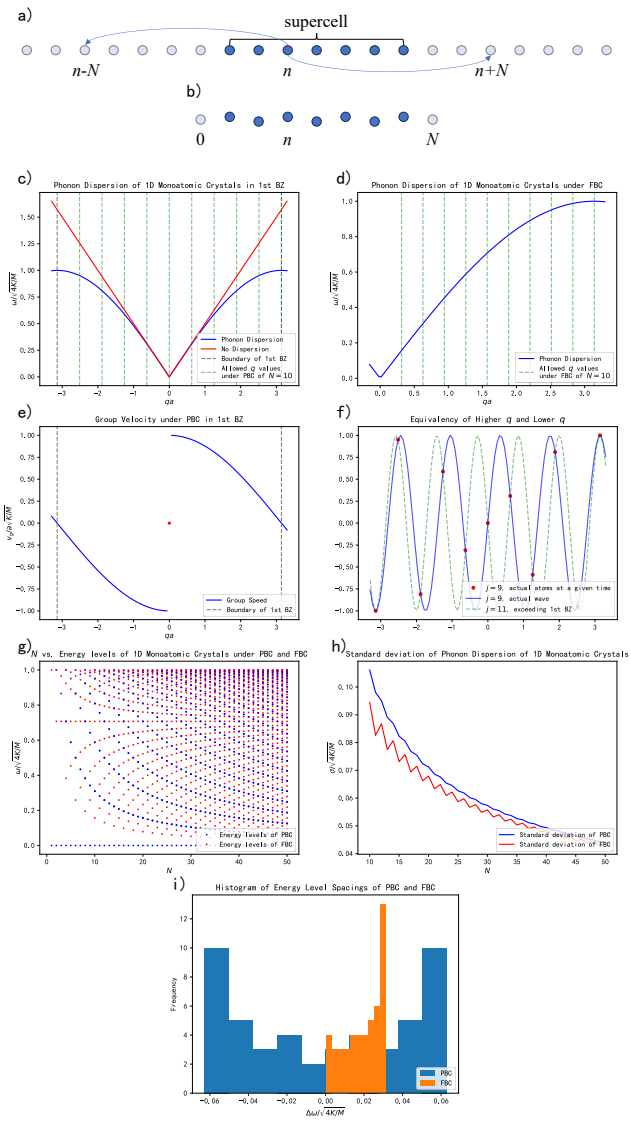

FIG. 1: Phonon dispersion relation and following calculations. a) Illustration of PBC supercell; b) illustration of FBC; c) phonon dispersion and allowed q values under PBC; d) phonon dispersion and allowed q values under FBC; e) group velocity $v_g(q)$ under PBC; f) illustration of equivalency of the spacial frequency higher than 1st BZ and that lower; g) N vs. energy levels of PBC(blue) and FBC(red), $N \in [10, 50]$; h) N vs. standard deviations of energy level spacing, $N \in [10, 50]$; i) distribution of level spacings at $N = 50$.

III. DIFFERENCE BETWEEN PBC AND FBC, AND SECOND QUANTIZATION OF PHONONS

The difference of allowed q values between PBC and FBC originates from the discrete translational symmetry of supercells. In PBC, periodicity of supercells allows us to do a Fourier transformation to transform real space vectors u_n into q-space;

however, in FBC, this periodicity is broken. Still, we can transform them using sine series. We will construct the creation/annihilation operators ($a^\dagger$ and a) for phonons under both BCs to further discuss this issue.

A. Hamiltonian

From our 1D elastic monoatomic chain model,

$$H = \sum_{n=1}^{N} \left(\frac{p_n^2}{2m} + \frac{K}{2}(u_n - u_{n-1})^2 \right) \tag{21}$$

B. PBC

From discrete periodicity of supercells, we can transform u_n and p_n into q-space by discrete Fourier Transformation (DFT):

$$\begin{aligned} u_n &= \frac{1}{\sqrt{N}} \sum_q u_q \exp(iqna) \\ p_n &= \frac{1}{\sqrt{N}} \sum_q p_q \exp(-iqna) \\ q &= j\frac{2\pi}{Na}, j = 0, \pm 1, \pm 2, ... \end{aligned} \tag{22}$$

in which $u_q^\dagger = u_{-q}$ and $p_q^\dagger = p_{-q}$ in order to maintain Hermitian u_ns and p_ns.

Also, from orthonormality relations of Fourier basis,

$$\frac{1}{N} \sum_q \exp(i(q - q')na) = \delta_{q,q'} \tag{23}$$

We can prove that u_q and p_q preserve a corresponding commutating relation:

$$\left[u_q, p_{q'}\right] = i\ \hbar\ \delta_{q,q'} \tag{24}$$

Substituting Eq. (2)(2) and Eq. (2)(3) into Eq. (2)(1), we get:

$$\begin{aligned} \sum_n p_n^2 &= \frac{1}{N} \sum_n \sum_{q,q'} p_q p_{q'} \exp(-i(q + q')na) \\ &= \sum_q p_q p_{-q} \\ \sum_n (u_n - u_{n-1})^2 &= \frac{1}{N} \sum_n \sum_q \left(u_q \exp(iqna)(1 - e^{-iqa})\right)^2 \\ &= \frac{1}{N} \sum_n \sum_{q,q'} \Big(u_q u_{q'} \exp(i(q + q')na) \\ &\quad (1 - e^{-iqa})\left(1 - e^{-iq'a}\right)\Big) \\ &= \sum_q 4\sin^2\left(\frac{qa}{2}\right) u_q u_{-q} \end{aligned}$$

which is to say,

$$H = \frac{1}{2m} \sum_q p_q p_{-q} + \frac{m}{2} \sum_q \omega_q^2 u_q u_{-q} \tag{25}$$

Using Eq. (2)(4), we can construct the the creation/annihilation operator of phonons:

$$\begin{aligned} a_q &= \sqrt{\frac{m\omega_q}{2\hbar}} \left(u_q + \frac{i}{m\omega_q} p_{-q} \right) \\ a_q^\dagger &= \sqrt{\frac{m\omega_q}{2\hbar}} \left(u_{-q} - \frac{i}{m\omega_q} p_q \right) \end{aligned} \tag{26}$$

the commutator of those

$$\left[a_q^\dagger, a_q\right] = 1 \tag{27}$$

indicating that phonons here are **bosons**; We can also construct Hamiltonian using these:

$$H = \sum_q \hbar\ \omega_q \left(a_q^\dagger a_q + \frac{1}{2} \right) \tag{28}$$

in which $E_0 = \sum_q 1/2\ \hbar\ \omega_q$ is the **zero-point energy** of this system; it is related to the crystal constants a and the mass of atoms M, thus can be, and has been experimentally observed via phenomena like Casimir effect, yet it's much weaker than that induced by vacuum zero-point energy[13]. However, unlike real Casimir effect, zero-point energy won't diverge like real Casimir effect, due to limited size of crystals.

Furthermore, we can define the **number operator**

$$N_q = a_q^\dagger a_q \tag{29}$$

It's provable that its eigenvalue n_q is a natural integer (including 0), and $\left[N_q, H\right] = 0$. Therefore, n_q is a "good quantum number", indicating the amplitude of activation of each vibration mode q; we can denote the whole system as $\left|\{n_q\}\right\rangle = |(n_1, n_2, ...)\rangle$ (called **Fock states**), and each n_k stays the same as its initial value unless there are external forces.

The process above is called **Second Quantization** of phonons; it's a quantization process of the "wave field" u in the crystals.

C. FBC

With FBC, we cannot do DFT properly due to broken discrete translational symmetry of supercells. However, with these eigensolutions, we can use discrete Sine Transformation (DST)

$$\begin{aligned} u_n &= \sqrt{\frac{2}{N+1}} \sum_q u_q \sin(nqa) \\ q &= \frac{j\pi}{(N+1)a}, j = 1, 2, ..., N \end{aligned} \tag{30}$$

to do a similar job. With a similar process, we can get:

$$\begin{aligned} a_q &= \sqrt{\frac{m\omega_q}{2\hbar}}\left(u_q + \frac{i}{m\omega_q}p_{-q}\right) \\ a_q^\dagger &= \sqrt{\frac{m\omega_q}{2\hbar}}\left(u_{-q} - \frac{i}{m\omega_q}p_q\right) \\ H &= \frac{1}{2m}\sum_q p_q^2 + \frac{m}{2}\omega_q^2 u_q^2 \\ &= \frac{1}{2}\,\hbar\,\omega_q\left(a^\dagger a + \frac{1}{2}\right) \end{aligned} \tag{31}$$

which are the same forms as in PBC. This reflects the unchanged **bulk** properties - hence the dispersion relation - of our model. However, if we make abrupt changes on the edges (surfaces) of the model, some new modes (or **surface states**) will exist.

IV. SURFACE STATES

A. Theory

When we add a sharp transition at the surface of solids, some states localized at the surfaces can be observed, thus being called "surface states"[14,15]. Usually, surface states are divided into 3 categories: Tamm states, usually derived from tight-binding model; Shockley states, usually derived from the Schrödinger equation in nearly-free electron approximation; and topological surface states, from non-trivial topological invariants of the system.

In this chapter, we try to realize Tamm-like and Shockley-like states in 1D phononic systems.

B. Tamm-like states in 1D Tight-binding-like Phonon Model

As is mentioned above, Tamm states are usually derived using electronic tight-binding model. For simplicity, we use a similar model, introducing surface states by changing the surface condition of the aforementioned 1D phonon model in section II A.

Construction of the Matrix

We use FBC to achieve surface states. Notice that under FBC, the atoms $n = 1$ and N satisfies

$$\begin{aligned} M\frac{\partial^2 u_1}{\partial t^2} &= -K(u_1 - 0) - K(u_1 - u_2) \\ M\frac{\partial^2 u_N}{\partial t^2} &= -K(u_N - u_{N-1}) - K(u_N - 0) \end{aligned} \tag{32}$$

Combining Eq. (3) and Eq. (3)(2), we can turn them into an eigenequation of a matrix:

$$\begin{aligned} &\begin{pmatrix} \frac{K_{0,1}}{M_0} & -\frac{K_{0,1}}{M_0} & \cdots & & \\ \vdots & \ddots & & & \\ & -\frac{K_{n-1,n}}{M_n} & \frac{K_{n-1,n}+K_{n,n+1}}{M_n} & -\frac{K_{n,n+1}}{M_n} & \\ & & & \ddots & \vdots \\ & & \cdots & -\frac{K_{N,N+1}}{M_{N+1}} & \frac{K_{N,N+1}}{M_{N+1}} \end{pmatrix}\boldsymbol{u} \\ &= \omega^2\boldsymbol{u} \end{aligned} \tag{33}$$

in which $\boldsymbol{u} = (u_1, ..., u_N)^{\mathrm{T}}$. Using this matrix, we can use numerical methods to diagonize and solve the eigenvalues of it, thus getting the actual dispersion relation.

In order to realize Tamm states, we set the parameters as the following:

$$\begin{gathered} K_{0,1} \neq K_{N,N+1} \neq K_{1,2} = K_{2,3} = ... \\ M_1 = M_2 = ... = M_N \end{gathered} \tag{34}$$

changing the kinetic condition of the 2 atoms on the surface. Thus, we can induce Tamm-like surface states localized on the surface with isolated energy levels in prohibited area.

Numerical Computations

We write a simple program in `Python` to solve the states of the model. Particularly, we use `numpy.linalg.eigh()` to solve the real symmetric matrix above and get the eigen values ω^2 s; to get the adjoint q values, we use the eigenvectors from it[1] and do a DST[2] on them, as is performed in Eq. (3)(0).

The whole program can be found in [19].

Parameters

We use a parameter set as the following:

$$\begin{gathered} M = 1 \\ K = 1 \\ k_{\text{left}} = 5, k_{\text{right}} = 10 \\ a = 1 \\ N = 100 \end{gathered}$$

Results

We get the result as is shown in Fig. 2. The dots fitting the original dispersion relation represents the *bulk* states of the model, originating from the supercell. We can also draw the eigenvector corresponding to the lowest energy, which is a standing wave solution with its wavelength $\lambda = Na/2$,

[1] It is worth mentioning that the output eigenvectors in the return value of `numpy.linalg.eigh()` lives in the *second* dimension of the output 2D array (like `vecs[:,i]` for the ith eigenvector, which is a vertical)[16], unlike that in other tools like `mathematica` which directly output them directly in a list of (horizontal) vectors (like `vecs[i]`); that is to say, the output matrix needs to be transposed first. *We defenitely was not confused by this issue and debugging for days...*[17]

[2] More specifically, DST-I[18].

same as the unchanged model, which further validates our computational method. As we approach the thermaldynamic limit $N \to \infty$, the bulk states become continuoous, forming a literal energy "band" below, as is seen in Fig. 2(d)

However, our changes to the surfaces of the chain give rise to 2 isolated points on the dispersion relation, living in the prohibited area higher than the maximum ω (Fig. 2(c)), and creating band gaps (Fig. 2(d)). These states are just the Tamm-like surface states we created.

Furthermore, we can illustrate 2 isolated Tamm-like states in its wave form by drawing the corresponding eigenvectors. As is shown in Fig. 2(b), 2 Tamm-like states separately occupies the 2 edges of the chain, strongly localized, exhibiting a heavily damping behavior as they "penetrate" into the bulk area. In q-space, the spacial spectral is a wide, smooth peak like a certain "impulse" (like in Fig. 2(b)), as is showned in Fig. 2(e), in contrast to a near-monochromatic peak corresponding to typical standing sine waves, as is showned in Fig. 2(f).

C. Shockley-like states in 1D Diatomic Phonon Model

In contrast with Tamm states, Shockley states arise from the internal (trivial) topological bulk properties of the crystal, along side with surfaces to localize them. From a similar process from above, we can induce a Shockley-like surface state in a diatomic chain.

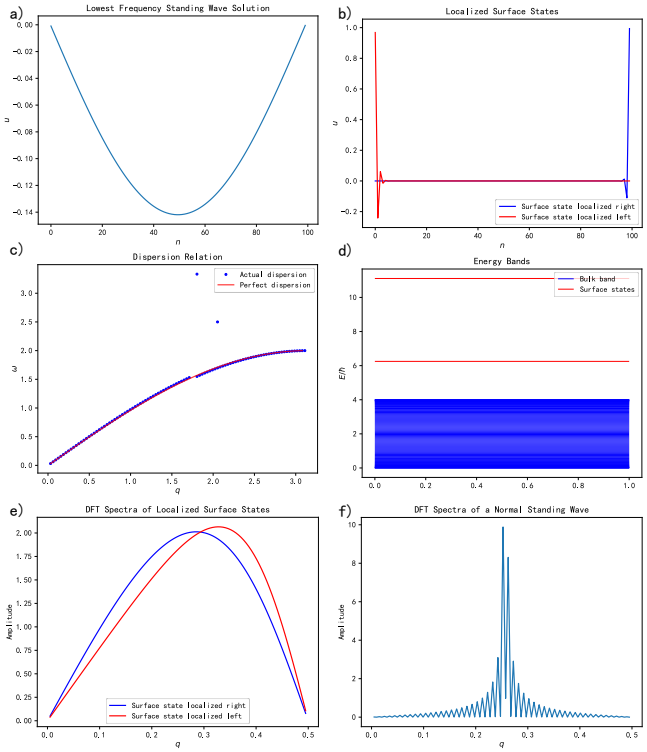

FIG. 2: Tamm-like states realized in 1D monoatomic chain with FBC. a) Lowest energy eigensolution of standing waves; b) localized surface states at both ends; c) dispersion relation, notice the isolated points representing Tamm-like states; d) energy bands with isolated Tamm-like states; e) q spectra of 2 Tamm-like states; f) q spectra of a standing wave eigensolution.

Construction of the Matrix

In essence, our construction of the so-called kinetic matrix is build as $M^{-1}K$. In order to make full use of real symmetric matrices, we make the following settings: all atoms are the same, yet the elastic coefficients alternate in each gap between atoms. Consider $2N+1$ atoms, our matrix is

$$\begin{pmatrix} \frac{K+k}{M} & -\frac{K}{M} & \cdots & & \\ -\frac{K}{m} & \frac{K+k}{m} & -\frac{k}{m} & \cdots & \\ \vdots & \ddots & & & \\ & & & \ddots & \vdots \\ & \cdots & -\frac{K}{m} & \frac{K+k}{m} & -\frac{k}{m} \\ & & \cdots & -\frac{k}{M} & \frac{K+k}{M} \end{pmatrix} \tag{35}$$

in which $M = m$.

Parameters

We set

$$\begin{gathered} M = m = 1 \\ K = 1 \\ k = 5 \\ a = 1 \\ N = 100 \end{gathered}$$

Results

Slightly modifing our program[19], the results are shown in Fig. 3. We still get an isolated surface state in the prohibited band; however, there is only 1 of them, strongly localized at the weaker ("more free") end, and energy of this state is in between the maximum and minimum energy, lowering the band gaps, unlike Tamm-like states above. The q-spectrum of this state shows multiple wide peaks.

More interestingly, Tamm-like states are induced directly by altering the conditions at the surface, yet the Shockley-like state seems to be induced by the bulk state itself with a terminating surface, which agrees with the thoretical contents mentioned above.

V. FLOQUET BC, AND DEGENERACY FROM CONTINUOUS TRANSLATIONAL SYMMETRY TO DISCRETE ONE

In some simulation softwares like COMSOL, a special type of PBC - Floquet BC - is used to simulate continuous systems such as phononic crystal under pressure acoustics methods. Typically, this BC is stated as:

$$p_{\text{dst}} = p_{\text{src}} \exp(-i\boldsymbol{k}_F \cdot (\boldsymbol{r}_{\text{dst}} - \boldsymbol{r}_{\text{src}})) \tag{36}$$

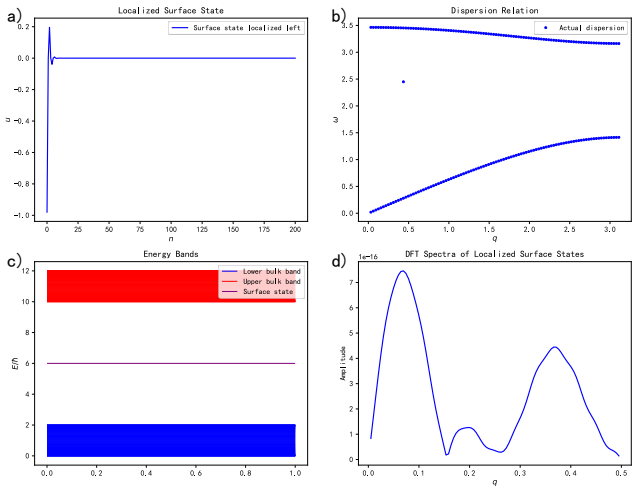

FIG. 3: Shockley-like state realized in 1D diatomic chain with FBC and alternating elastic coefficients. a) localized surface state at the "more-free" end; b) dispersion relation, notice the isolated point representing Shockley-like state; c) energy bands with isolated Shockley-like state lying in the prohibited band; d) q spectra of Shockley-like state.

It's a continuous version of Bloch theorem, also assuming that the pressure waves in the system satisfy travelling wave eigensolutions, thus also applies in discrete systems such as phononic crystals. In fact, we can achieve a similar "dispersion" relation with a simple pseudo-1D pressure acoustic model to show that degeneracy from continuous translational symmetry to discrete one introduce dispersion, similar as the result shown in section II.

A. Model

We use a rectangular acoustic cavity cell to simulate a system with 1D continuous translational symmetry along x axis, by applying Floquet BC to a pair of opposite edges on x axis, as is shown in Fig. 4(a). A large width-height ratio (10:1) is to ensure no extra high-frequency modes along y axis appears in our interested zone, decoupling 2 directions. To let its symmetry degenerate to discrrete translational symmetry, we introduce a square hole in the middle of each cell, as is shown in Fig. 4(c).

B. Result

The dispersion relation of the first system exhibits a perfect straight line folded in the 1st BZ, as is shown in Fig. 4(b), indicating that no dispersion exists. However, when we add the hole in the system, dispersion appears, opening band gaps, as is shown in Fig. 4(d).

This simple comparison shows that dispersion is introduced by breaking the continuous translational symmetry with discrete translational symmetry.

What's more, if we let our 1D monoatomic chain's $a \to \infty$, the dispersion relation shown in Fig. 1(b) degenerates into an infinitely-extending straight line from the origin, proving that

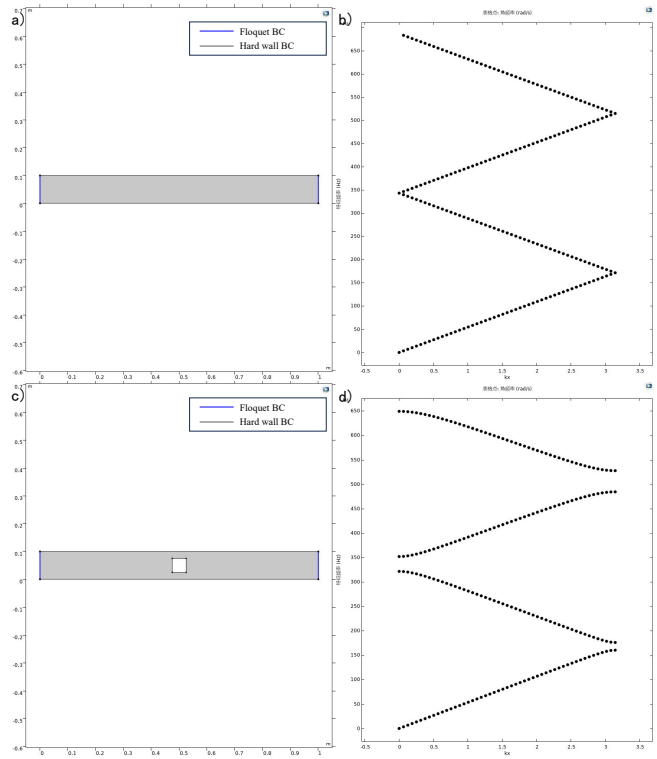

FIG. 4: COMSOL models and results. a) 1D simple rectangular cavity; b) dispersionless f-q relation of (a); c) adding a hole to break (a)'s continuous translational symmetry; d) f-q relation of (c).

our pressure acoustic model is similar with the phonon model in respect of physical essence, and combining Floquet BC and PBC together as representations of translational symmetry.

VI. DISCUSSION QUESTIONS

Q: *Why do most solid state physics textbooks adopt periodic boundary conditions? What are their advantages?*

A: For several reasons.

- PBC preserves discrete translational symmetry of the system, making it possible to use Bloch theorem and DFT to analyze the whole problem in q-space with travelling waves eigensolutions, making the whole problem a LOT simpler for mathematical analysis.
- FBC might be more realistic, but from the analysis above, we see that FBC and PBC share the same dispersion relation and DOSes as long as the bulk properties don't change; therefore, when approaching thermaldynamic limit, the energy band structures become the same continuous band for both BCs.
- Travelling waves are more convenient and physically clear when dealing with problems such as phononic scattering and heat transferring.

Thus, we can adopt a simpler method of PBC rather than FBC.

Q: *Can fixed boundary conditions be used to describe the bulk properties of a real crystal? If yes, under what condition?*

A: Yes, when we want to study the surface states of a limited-size system.

Q: *How do the electronic energy levels of a nanocrystal (quantum dot, nanowire) differ from bulk bands? Which boundary condition is more appropriate in such cases?*

A: These systems are highly localized and of limited-size, hence inducing many surface states in between prohibited areas. Thus, we need to use FBC.

Q: *What possible effects could surface states have on optical absorption, catalytic activity, or electrical conductivity?*

A: As we see in Shockley-like states, the band gaps are lowered by introducing surfaces, which may lower the activation energy of several related reactions or extend the range of response energies, like in the case of photonic catalysts and surface photonics. Pretty useful!

VII. CONCLUSIONS

This paper investigates the effects of different BCs on phonon dispersion spectra in 1D atomic chains, and further realizes Tamm-like and Shockley-like surface states in 1D phononic systems, while clarifying the physical essence of Floquet boundary conditions and the relation between dispersion and discrete translational symmetry.

Firstly, taking the 1D monoatomic chain with nearest-neighbor linear interactions as the basic model, this paper theoretically compares PBCs and FBCs. It is found that the two BCs share the identical phonon dispersion relation due to unchanged bulk interaction properties, but differ significantly in allowed wave vectors q, eigensolutions and degeneracy: PBCs produce travelling wave solutions and 2-fold degeneracy (except at $q = 0$), while FBCs generate standing wave solutions and no degeneracy. Numerical calculations for $N \in [10, 50]$ verify these differences, and both theoretical and numerical results confirm that DOSes of the two BCs converge to the same continuous form in the thermodynamic limit ($N \to \infty$).

The second quantization of phonons is further performed, showing that DFT applies to PBCs while DST is suitable for FBCs, and the Hamiltonian forms remain consistent, reflecting the invariance of bulk properties. Goldstone modes and zero-point energy are discovered during the analysis.

Secondly, the paper successfully realizes Tamm-like and Shockley-like surface states in 1D phononic systems by modifying boundary conditions and bulk topological properties respectively. Tamm-like states are induced by changing the elastic coefficients of the two end atoms in the monoatomic chain with FBCs, which appear as isolated energy levels above the maximum bulk frequency and are strongly localized at both ends of the chain with exponentially damped amplitudes into the bulk. In contrast, Shockley-like states are realized in a 1D diatomic chain with alternating elastic coefficients, presenting a single isolated state within the band gap that is localized only at the "more free" end of the chain. Their different physical origins are further confirmed: Tamm-like states arise from direct surface modification, while Shockley-like states originate from the bulk (trivial) topological properties combined with surface termination.

Thirdly, the paper explores Floquet BCs commonly used in pressure acoustic simulations, demonstrating that it is essentially a continuous version of Bloch's theorem. Through COMSOL simulations of rectangular acoustic cavity cells, it is verified that breaking continuous translational symmetry into discrete translational symmetry introduces phonon dispersion and opens band gaps, which is consistent with the physical mechanism of the 1D atomic chain model.

Finally, the paper discusses the practical significance of different BCs: PBCs are widely adopted in solid state physics textbooks because they preserve discrete translational symmetry, simplify mathematical analysis via Bloch theorem, and are equivalent to FBCs for bulk properties in the thermodynamic limit. FBCs are more appropriate for describing finite-size systems such as nanocrystals, where surface states play a significant role. Additionally, surface states can reduce band gaps, lower reaction activation energies and extend optical response ranges, showing important application prospects in photocatalysis, surface photonics and other fields.

This work provides a clear and intuitive theoretical framework for understanding boundary effects and surface states in solid state systems.

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