Vibrational dynamics in 2D crystal lattices of borophene

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Abstract. Vibration dynamics of crystalline borophene is considered in the framework of the Born–von Karman model. The vibrations perpendicular to the plane of 2D borophen lattice (flexural modes) are studied.

1. Introduction
One of the most interesting topics in the modern condensed matter physics is studying of crystalline graphene. As it is well known the crystalline graphene, due to the unusual geometry of the band structure, has exceptional mechanical [1,2], physical [3,4] and optical properties [5], which find applications [6] in various fields. Note here its record high thermal conductivity. For graphene, it was found, that it has unique properties of electrical conductivity and thermal conductivity, therefore, it is of great importance in microelectronics. The discovery of graphene sparked intense research activity. And later a whole class of new materials with no less unique properties appeared. One of these materials is borophene.

2. Borophene
The graphene lattice has a hexagonal honeycomb structure with 2 atoms in a unit cell. Unlike graphene, borophene has a triangular lattice with a single atom in the unit cell, but many elements of graphene symmetry are present in borophene.

Since borophene, unlike graphene, has only one atom in the unit cell, it has 3 acoustic modes like graphene, but no optical modes. Thus we have in borophene LA, TA and ZA modes. We have calculated the frequency spectrum $g(\omega)$ in borofen.

3. Calculations
3.1. Vibrations of a triangular lattice
Consider a triangular lattice, where each atom has 6 neighbors. Length of all links is $a$, the angle between the links is 60°. Let there be displacement vectors $e_1, e_2, e_3 = e_2 - e_1$ and three vectors opposite to them. Then $e_1, e_2$ is elementary lattice vectors, and there is only one atom in the unit cell. Let an atom be bound to its neighbors by springs that have rigidity $k$. In the Born–von Karman model, the equation of motion is

$$x''(r) = \frac{k}{m} \left( x(r+e_1) + x(r-e_1) - 2x(r) ight) + x(r+e_2) + x(r-e_2) - 2x(r) + x(r+e_3) + x(r-e_3) - 2x(r)$$
Figure 1. The triangular lattice. The first, second and third coordination sphere are marked in blue, orange, and green, respectively, and the connections to the third sphere are omitted.

Note that in fact it consists of three second-order finite differences. This circumstance will be useful to us. Indeed, we will look for solutions in the form of waves:

$$x(r) = e^{-i\omega t + ik \cdot r}$$

And note that then for any vector \( h \):

$$x(r + h) + x(r - h) - 2x(r) = x(r)(e^{i k \cdot h} + e^{-i k \cdot h} - 2) = -4x(r) \sin^2\left(\frac{k \cdot h}{2}\right)$$

And then we get the dispersion equation:

$$\omega^2 = 4\Omega_i^2 \left( \sin^2\left(\frac{k \cdot e_1}{2}\right) + \sin^2\left(\frac{k \cdot e_2}{2}\right) + \sin^2\left(\frac{k \cdot e_3}{2}\right) \right)$$

where \( \Omega_i^2 = \frac{\omega}{m} \).

Moreover, note that we did not use the angle between the bonds to derive this equation. We used only the fact that the atom is the center of the lattice inversion, and therefore 6 bonds are split into three pairs, each of which gives \( \sin^2 \). For a square lattice, for example, there will be a similar formula, but with two \( \sin^2 \) one for each pair of vectors. In addition, we will be able to apply this formula for subsequent coordination spheres.

3.2. General formula of dispersion for spheres with even \( N_i \)

Let us introduce the following notation: \( S_i \) is the set of position vectors drawn from some atom to the atoms of its \( i \)-th coordination sphere. For example, for triangular lattice \( S_1 = \{e_1, e_2, e_3, -e_1, -e_2, -e_3\} \).

\( D_i \) is the set of position vectors drawn to one from each pair of symmetric atoms of the \( i \)-th coordination sphere. Such a choice of vectors is ambiguous (one of the vectors can be arbitrarily chosen from each pair), but, as will be seen below, the dispersion equations do not depend on a particular choice. Of course, \( D_i \) is determined only when the number \( N_i \) of atoms in the \( i \)-th coordination sphere is even. For triangular lattice all of \( N_i \) are even (and equal to 6). \( D_i \) for it can be chosen, for example, as \( \{e_1, e_2, e_3\} \).

For small \( k \):

$$\sin^2\left(\frac{k \cdot h}{2}\right) = \frac{(k \cdot h)^2}{4} + O(|k|^4).$$
Let us write using the new notation

$$\omega^2 \approx \Omega_i^2 \sum_{l=1,2,3} (\mathbf{k} \cdot \mathbf{e}_l)^2 = \frac{\Omega_i^2}{2} \sum_{e \in \delta_i} (\mathbf{k} \cdot \mathbf{e})^2 = \frac{3}{2} \Omega_i^2 a^2 |\mathbf{k}|^2$$

where we went from the sum over three vectors to the sum over all six, the value of which is given to us by the previously obtained formula.

Moreover, it can be noted that all the considerations given here are also true for the following coordination spheres, if they have an even number of atoms. Then the exact formula of the dispersion of $N$ spheres is

$$\omega^2 = 2 \sum_i N_i \Omega_i^2 \sin^2 \left( \frac{\mathbf{k} \cdot \mathbf{e}}{2} \right)$$

where $\kappa_i$ is the stiffness of the bond with the atoms of the $i$th sphere, and the second summation is carried out over all vectors of the sphere.

Therefore, the condition for the dispersion to be non-linear at zero:

$$\sum_i N_i \Omega_i^2 \kappa_i^2 = 0$$

In particular, for a triangular lattice:

$$\Omega_1^2 + 3\Omega_2^2 + 4\Omega_3^2 = 0$$

### 3.3 Numerical results

Figure 2 shows the dependence of the $\omega$ dispersion law on $k$ in the Brillouin zone, taking into account one coordination sphere.

![Figure 2](image)

The linear dependence at the $\Gamma$ points indicates that these are phonons. To obtain the quadratic dispersion, it is necessary to take into account the neighbors from the second and third coordination spheres.

Figure 3 shows the dependence of the density of states $g(\omega)$. Linearity means that for small $\omega$, there are phonons with a linear law of dispersion, and the peak is the Van Hove singularity.
Figure 3. The dependence of the density of states \( g(\omega) \).

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Appendix
Let us prove the following lemma.

Let us find the next sum that will be needed further

\[
\sum (k \cdot e_i)^2
\]

where the summation is over vectors extended from the center to the vertices of a regular \( n \)-gon inscribed in a circle of radius \( r \) (that is, in fact, over a coordination sphere with \( n \) atoms).

Let us denote by \( \varphi \) the angle between \( k \) and the first of the vectors. Then the sum is

\[
|k|^2 r^2 \sum_{i=0}^{n-1} \cos^2 \left( \frac{2\pi i}{n} + \varphi \right) = \frac{n}{2} |k|^2 r^2
\]

so the direction of the vector \( k \) does not matter.

Moreover:

\[
\sum (k \cdot e)^4 = \frac{3n}{8} |k|^4 r^4
\]

\[
\sum k \cdot e = 0
\]

References
[1] Wirtz L and Rubio A 2004 Sol. State Comm. 131 141
[2] Hobson J P and Nierenberg W A 1953 Phys. Rev. 89 662
[3] Maradudin A A, Montroll E W, Weiss G H and Ipatova I P 1971 Theory of Lattice Dynamics in the Harmonic Approximation (New York: Academic Press)
[4] Weige A, Wellem G, Alvermann A and Feikse H 2006 Rev. Mod. Phys. 78 275
[5] Belukov Y M, Kozhuh V I and Parshin D A 2013 Phys. Rev. B 87 134203
[6] Belukov Y M and Parshin D A 2016 JETP Letters 104 552
[7] Falkovsky L A 2012 JETP 142 560
[8] Raikov I O et al 2020 J. Phys.: Conf. Ser. 1695 012179