Lattice Vibration and Field Model for Phonons

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Abstract. In this letter, we first briefly review Hamiltonian and Newtonian method for solving lattice vibration. Second, the equivalence between phonons and Klein-Gordon particles is proven. Finally, we use the new method to analyse some simple models and compute their phonon spectrum as well as Berry curvature.

1. Mechanical Modes and Klein-Gordon Operators

1.1. Hamiltonian of Lattice Vibration and Three Equivalent Methods

Hamiltonian describing lattice vibration is generally written by:

\[ H = \sum_i \frac{\hat{p}_i^2}{2m} + V(\hat{x}_i) = V(\hat{x}_i - \hat{x}_j) = \sum_{i,j} \frac{\hat{p}_i^2}{2m} + V(\hat{x}_i - \hat{x}_j) \]  

where \( \hat{x}_i \) and \( \hat{p}_i \) are position and momentum vectors for \( i \)-th atom, \( \frac{\hat{p}_i^2}{2m} \) are kinetic energy terms, and total potential energy is just sum over potential between each two particles. We usually Taylor expand \( V(\hat{x}_i - \hat{x}_j) \):

\[ V = V_0 + \vec{V}_1 \cdot (\hat{x}_i - \hat{x}_j) + \vec{V}_2 : (\hat{x}_i - \hat{x}_j)^{\Theta^2} + \ldots \]  

Here, \( V_0 \) is a constant, which contribute nothing to lattice vibration; \( \vec{V}_1, \vec{V}_2 \) are first and second order derivatives of \( V \) and similar for subsequent terms. Since potential energy near equilibrium are small, \( \vec{V}_1 \approx 0 \) approximately. Second order derivatives can be written in indices form [2]:

\[ \frac{1}{2} \vec{V}_2^{(2)} : (\hat{x}_i - \hat{x}_j)^{\Theta^2} = \sum_{\mu \nu} \frac{1}{2} \kappa_{\mu \nu} (x_i^{\mu} - x_j^{\mu}) (x_i^{\nu} - x_j^{\nu}) \]  

\( \kappa_{ij}^{\mu\nu} \) represent elastic interaction among atoms, which can be measured experimentally. If we want to have a kindred form like one dimensional harmonic oscillator, we can set \( \omega_{\mu\nu}^2 = \frac{\kappa_{ij}^{\mu\nu}}{m} \).

We utilize Newtonian method and dynamical matrix equation method practically. Plugging (1) into canonical equation \( \frac{\partial H}{\partial \dot{x}_i} = -\ddot{p}_i \) and using non-relativistic momentum-velocity relation \( \dot{p}_i = m\ddot{x}_i \), we have:

\[
- \sum_\nu \kappa_{ij}^{\mu\nu} (\ddot{x}_i^\nu - \dot{x}_j^\nu) = m\ddot{x}_i^\mu
\]  

(4)

It has the same meaning with Newton’s second law,

\[
F_\mu = m\ddot{x}_\mu
\]  

(5)

Because of transition symmetry in lattice, we try solutions \( x_{\mu,i} = x_{\mu,k} e^{i(kr_i - \omega t)} \). After some simple manipulation, we attain:

\[
Dx = -\ddot{x}
\]  

(6)

where \( x \) is column vector made up with different degrees of freedom from inequivalent sites. Or we can set \( x = x_0 + u \), and only considering homogeneous part. Therefore,

\[
Du = -\ddot{u}
\]  

(7)

It is the commonly used dynamical equation and we acquire dispersion relation of lattice vibration (phonons) by solving eigenvalues of matrix \( D \).

1.2. Field Model for Phonon, and Klein-Gordon Operators

The abovementioned argument concern about lattice vibration, but generally we consider quantized lattice wave as quasiparticles-- phonons. It is well known that phonon has 0 spin, which only succeed in Klein-Gordon equation. K-G equation is a second order partial differential equation, and dynamical equation is also a second order equation confidently. We conclude that square of phonon’s Hamiltonian is:

\[
H^2 = \begin{pmatrix} D & 0 \\ 0 & D^T \end{pmatrix}
\]  

(8)

Here we combine dynamical matrix of phonon and its supersymmetric phonon to construct a bigger matrix.

Second quantization model for phonon is given [1]

\[
H^2 = \frac{1}{2} \hbar^2 A_2 + \frac{1}{6} \hbar^2 A_3 + \cdots
\]  

(9)

where,

\[
A_2 = \sum_{\mu,\nu,i,j} \kappa_{ij}^{\mu\nu} [(a_{\mu,i}^{\dagger} - a_{\mu,j}^{\dagger})(a_{\nu,i} - a_{\nu,j}) + (a_{\mu,i} - a_{\mu,j})(a_{\nu,i}^{\dagger} - a_{\nu,j}^{\dagger})],
\]

\[
A_3 = \sum_{\mu,\nu,\xi,i,j} V_{\mu,\nu,\xi} \left[(a_{\mu,i}^{\dagger} - a_{\mu,j}^{\dagger})(a_{\nu,i} - a_{\nu,j})(a_{\xi,i} - a_{\xi,j}) + (a_{\mu,i} - a_{\mu,j})(a_{\nu,i}^{\dagger} - a_{\nu,j}^{\dagger})(a_{\xi,i} - a_{\xi,j}) + (a_{\mu,i} - a_{\mu,j})(a_{\nu,i} - a_{\nu,j})(a_{\xi,i}^{\dagger} - a_{\xi,j}^{\dagger}) + \text{h.c.} \right]
\]

\( a_{\mu,i}^{\dagger} \) creates a \( \mu \)-type phonon on site \( i \), which means oscillating degrees of freedom on \( \mu \) direction.
This model (9) has already included inharmonic effects, and it can be solved by mean field theory, exact diagonalization etc. But in most of cases we only concentrate on harmonic part:

\[ H^2 = \frac{1}{2} \hbar^2 \sum_{\mu,\nu,i,j} \kappa_{\mu\nu} \left[ (a^{\dagger}_{\mu,i} - a^{\dagger}_{\mu,j})(a_{\nu,i} - a_{\nu,j}) + (a_{\mu,i} - a_{\mu,j})(a^{\dagger}_{\nu,i} - a^{\dagger}_{\nu,j}) \right] \] (10)

In standard basis \( \Psi^+ = (a^{\dagger}_{\mu,1}, ..., a^{\dagger}_{\mu,N}, a_{\nu,1}, ..., a_{\nu,N}) \), the matrix representation:

\[ H^2 = \frac{1}{2} \hbar^2 \begin{pmatrix} D & 0 \\ 0 & D^T \end{pmatrix} \] (11)

On the other hand, K-G equation is equivalent to scalar field,

\[ S_E = \frac{1}{2} \sum_{i,j} a^2 \phi_i \left( \partial^2_{\mu} \phi_j + m^2 \right) \]

Where \( a \) is lattice constant and \( \partial^2_{\mu} \phi(x_i) = \sum_{\mu} \frac{1}{a^2} (2\phi(x_i) - \phi(x_i + a\mu) - \phi(x_i - a\mu)) \) is square of difference operator defined in [5].

If comparing (12) with (10), we assert that phonon field is a massless scalar field involving higher order coupling in Euclidean space.

Euclidean action for phonon:

With the formula of interaction operators expanding by number, \( \delta = \sum_{j=1}^{n} \delta_j^{(1)} + \frac{1}{2} \sum_{j=1}^{n} \delta_j^{(2)} + \frac{1}{3} \sum_{j=1}^{n} \delta_j^{(3)} + \ldots \) we know \( \delta^2 = \sum_{j=1}^{n} \delta_j^{(1)} + \frac{1}{2} \sum_{j=1}^{n} \delta_j^{(2)} + \frac{1}{3} \sum_{j=1}^{n} \delta_j^{(3)} + \ldots + \) crossing terms. It is easy to check crossing term would not appear in terms which \( A_n(t \leq 3) \)

\[ S_E = \frac{1}{2} \sum_{i,j} a^2 g_2 \phi_i \left( \partial^2_{\mu} \phi_j + m^2 \right) \phi_j + \sum_{n>2} \sum_{i,j} \frac{g_{an}}{n!} (\phi_i - \phi_j)^n \] (13)

Finally, if taking the same procedure in equilibrium matrix choosing as [6], we have:

\[ H = \begin{pmatrix} 0 \\ Q^T \end{pmatrix} \]

where \( D = QQ^T, Q \) is so called equilibrium matrix.

2. Examples

2.1. One Dimensional Model

Let us calculate a simple 1D model.

\[ H = \sum_i c_1 a^{\dagger}_i a_i - c_2 a_i a_{i+1} + h.c. \] (15)

By Fourier transform,

\[ a_{\mu,i} = \frac{1}{\sqrt{N}} \sum_{k} e^{ikr_i} a_{\mu,k}, a^{\dagger}_{\mu,i} = \frac{1}{\sqrt{N}} \sum_{k} e^{-ikr_i} a^{\dagger}_{\mu,k} \] (16)

We obtain momentum space Hamiltonian in basis \( \Psi^+ = (a^{\dagger}_k, a_k) \):
\[ H = \begin{pmatrix} 0 & c_1 - c_2 e^{ika} \\ c_1 - c_2 e^{-ika} & 0 \end{pmatrix} \] (17)

At last the energy spectrum is computed:

\[ \omega(k) = \pm \sqrt{c_1^2 + c_2^2 - 2c_1c_2 \cos ka} \] (18)

This is SSH model for phonon, having similar matrix and dispersion relation with electronic case.

2.2. Two Dimensional Models

2.2.1. Hexagonal Lattice. Next, we will analyze two important 2D model in topological photonics, hexagonal and Kagome lattice.

Only focusing nearest neighbor interaction, phonon’s Hamiltonian in hexagonal lattice could be represented by block matrix in momentum space:

\[ H^2 = \begin{pmatrix} H^2_{aa} & H^2_{ab} \\ H^2_{ba} & H^2_{bb} \end{pmatrix} \] (19)

In the matrix,

\[ H^2_{aa} = \sum_{j=1}^{3} \begin{pmatrix} \omega^2 a_{11} & \omega^2 a_{12} \\ \omega^2 a_{21} & \omega^2 a_{22} \end{pmatrix} \]

\[ H^2_{bb} = \sum_{j=1}^{3} \begin{pmatrix} -\omega^2 a_{11} & -\omega^2 a_{12} \\ -\omega^2 a_{21} & -\omega^2 a_{22} \end{pmatrix} \]

\[ H^2_{ab} = \sum_{j=1}^{3} \begin{pmatrix} -\omega^2 a_{11} y_k & -\omega^2 a_{12} y_k \\ -\omega^2 a_{21} y_k & -\omega^2 a_{22} y_k \end{pmatrix} \]

\[ H^2_{ba} = \sum_{j=1}^{3} \begin{pmatrix} -\omega^2 a_{11} y_k & -\omega^2 a_{12} y_k \\ -\omega^2 a_{21} y_k & -\omega^2 a_{22} y_k \end{pmatrix} \]

form factor \( Y_{k1} = e^{i(x-k_k^2)} \), \( Y_{k2} = e^{i(x-k_k^2)} \), \( Y_{k3} = e^{-ika} \);

basis \( \Psi^+ = (a_{1,k}^+, a_{2,k}^+, b_{1,k}^+, b_{2,k}^+) \);

coefficient \( \omega_{ij}^2 \nu \) means vibrating frequency between atom with degrees of freedom \( \nu \) at site \( j \) and atom with d.o.f. \( \nu \) at site \( j \). If we assume lattice system is isotropic and homogeneous, mass \( m = 1 \), then \( \omega_{11}^2 = \frac{1}{4} \), \( \omega_{12}^2 = \frac{1}{4} \), \( \omega_{13}^2 = 1 \), \( \omega_{14}^2 = \frac{1}{4} \), \( \omega_{21}^2 = -\frac{\sqrt{3}}{4} \), \( \omega_{22}^2 = 0 \), \( \omega_{23}^2 = \frac{3}{4} \), \( \omega_{24}^2 = \frac{3}{4} \), \( \omega_{31}^2 = 0 \).

After substituting in, the Hamiltonian would become:

\[ H^2 = \begin{pmatrix} \frac{3}{4} & 0 & -\frac{1}{2} e^{-i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} - e^{i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} \\ 0 & \frac{3}{4} & \frac{1}{2} e^{-i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} - \frac{1}{2} e^{i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} \\ -\frac{1}{2} e^{i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} - e^{-i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} & \frac{1}{2} e^{-i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} - \frac{1}{2} e^{i\frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y} & 0 \end{pmatrix} \] (20)

Finally, we compute energy spectrum,

\[ E_{1,2,3,4} = \hbar \left( \frac{3}{4} \pm \sqrt{\frac{1}{4} + \cos \left( \frac{3k_x}{2} \right) + \cos^2 \left( \frac{\sqrt{3}}{2} k_y \right)} \right)^{1/2} \]

\[ , \hbar \sqrt{3}, 0, \text{and Berry curvature. Their 3D plot is showed in figure 1 and 2.} \]
2.2.2. Kagome Lattice. Similar as (19), Hamiltonian matrix in K space can be computed.

\[ H^2 = \begin{pmatrix} H_{aa}^2 & H_{ab}^2 & H_{ac}^2 \\ H_{ba}^2 & H_{bb}^2 & H_{bc}^2 \\ H_{ca}^2 & H_{cb}^2 & H_{cc}^2 \end{pmatrix} \]  

(21)

In the matrix,

\[ H_{aa}^2 = \begin{pmatrix} \omega_{11}^2 a_1 b_1 + \omega_{11}^2 a_2 b_2 & \omega_{12}^2 a_1 b_1 + \omega_{12}^2 a_2 b_2 \\ \omega_{12}^2 a_1 b_1 + \omega_{12}^2 a_2 b_2 & \omega_{11}^2 a_1 b_1 + \omega_{11}^2 a_2 b_2 \end{pmatrix} \]

\[ H_{ab}^2 = \begin{pmatrix} -\omega_{11}^2 a_1 b_1 \gamma_k a_1 b_1 - \omega_{11}^2 a_2 b_2 \gamma_k a_1 b_1 \\ -\omega_{12}^2 a_1 b_1 \gamma_k a_1 b_1 - \omega_{12}^2 a_2 b_2 \gamma_k a_1 b_1 \end{pmatrix} \]

\[ H_{ac}^2 = \begin{pmatrix} -\omega_{11}^2 a_1 c_1 \gamma_k a_1 c_1 - \omega_{11}^2 a_2 c_2 \gamma_k a_1 c_1 \\ -\omega_{12}^2 a_1 c_1 \gamma_k a_1 c_1 - \omega_{12}^2 a_2 c_2 \gamma_k a_1 c_1 \end{pmatrix} \]

\[ H_{bc}^2 = \begin{pmatrix} -\omega_{11}^2 b_1 c_1 \gamma_k b_1 c_1 - \omega_{11}^2 b_2 c_2 \gamma_k b_1 c_1 \\ -\omega_{12}^2 b_1 c_1 \gamma_k b_1 c_1 - \omega_{12}^2 b_2 c_2 \gamma_k b_1 c_1 \end{pmatrix} \]

\[ \omega^2 \text{ and } \gamma_k \text{ are symmetric for upper and lower indices; } \]

nearest neighbor form factors

\[ \gamma_k^{a_1 b_1(2)} = e^{\pm i k_x a}, \gamma_k^{a_1 c_1(2)} = e^{\pm i (\frac{1}{2} k_x + \frac{\sqrt{3}}{2} k_y)}, \gamma_k^{b_1 c_1(2)} = e^{\pm i (\frac{1}{2} k_x + \frac{\sqrt{3}}{2} k_y)} \]

We still take isotropic approximation and set \( m = 1 \) for all atoms, then Hamiltonian:

\[ H = \begin{pmatrix} \frac{\gamma}{2} & -\frac{\sqrt{3}}{2} & -2 \cos k_x & 0 & -\frac{\sqrt{3}}{2} \cos \left( \frac{k_x}{2} - \frac{\sqrt{3}}{2} k_y \right) \\ -\frac{\sqrt{3}}{2} & \frac{\gamma}{2} & 0 & 0 & -\frac{\sqrt{3}}{2} \cos \left( \frac{k_x}{2} + \frac{\sqrt{3}}{2} k_y \right) \\ -2 \cos k_x & 0 & \frac{\gamma}{2} & -\frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} \cos \left( \frac{k_x}{2} + \frac{\sqrt{3}}{2} k_y \right) \\ 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\gamma}{2} & -\frac{\sqrt{3}}{2} \cos \left( \frac{k_x}{2} - \frac{\sqrt{3}}{2} k_y \right) \\ -\frac{1}{2} \cos \left( \frac{k_x}{2} - \frac{\sqrt{3}}{2} k_y \right) & -\frac{\sqrt{3}}{2} \cos \left( \frac{k_x}{2} - \frac{\sqrt{3}}{2} k_y \right) & -\cos \left( \frac{k_x}{2} + \frac{\sqrt{3}}{2} k_y \right) & -\frac{\sqrt{3}}{2} \cos \left( \frac{k_x}{2} + \frac{\sqrt{3}}{2} k_y \right) & 1 \end{pmatrix} \]

Finally, its energy spectrum and Berry curvature are shown.

(a) (b)

**Figure 1.** Energy spectrum for phonon in hexagonal (a) and Kagome (b) lattice.
3. Summary
We have developed a simple field model for lattice vibration and show equivalence between scalar field and phonon field. By brief calculation, we find an identical result to classical dynamic matrix method. Finally, it would be interested to study anharmonic and topological effects for phonons further.

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