Lecture 06

Thursday, January 26, 2012

Born - von Karman boundary condition

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In solid state physics, we often use the **Born - von Karman boundary condition**, which is often called **periodic boundary condition**. Consider a crystal with lattice points, $\vec{R} = \sum_i n_i \vec{a}_i$, with $n_i = 0, \ldots, N_i - 1$. That is, this crystal has $\Pi_i N_i$ bases.

Born - von Karman boundary condition

$$n_i = n_i \,\%\, N_i$$

where $a \,\%\, b$ = remainder of a/b.

Under the Born - von Karman boundary condition, a one dimensional crystal can be viewed as a circle, a two dimensional crystal as a torus, and a three dimensional crystal as a hyper torus.

Born - von Karman (BvK) boundary condition will be used throughout this course [as in the next topics that we will discuss below].

- Why use BvK? The math becomes very nice.
- Is it absolutely necessary? No. Sometimes it may even be harmful (see below).
- When is it OK to use? For a large crystal size and for the bulk property. I.e. for the majority of topics in a course like this.
- When should you not use this or at least re-examine this boundary condition? For surface, interface, or nano-scale physics.

Waves in Crystal I

By wave in crystal, we will mean a wave (quantum or classical) with amplitude

$$A(\vec{r}) = P(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$

Only the spatial dependence is noted explicitly here, with the time dependence ($e^{-i\omega t}$) implicit. $P(\vec{r})$ is a function that is periodic as the lattice is, i.e. $P(\vec{r}+\vec{R}) = P(\vec{r})$ for any lattice vector $\vec{R}$. Notice that $P(\vec{r}+\vec{a}_i) = P(\vec{r})$ for each i would sufficient. In any case, we call function like $P(\vec{r})$ a **lattice-periodic function**. All waves that we consider in this course has the functional form of $A(\vec{r})$.

Such wave in crystals has distinct properties. Here are couple of important ones.

Under the BvK BC, waves in crystal must have

! →

$$\boxed{k_i = a_i^* \frac{n_i}{N_i}, \qquad n_i = \text{integer}, \qquad a_i^* = |\vec{a}_i^*|}$$

where we assume that the crystal consists of lattice points $\vec{R} = \sum_i l_i \vec{a}_i$, with N_i lattice points along each direction $\vec{a}_i$. So in total there are $N = \Pi_i N_i$ lattice points in the crystal.

It suffices to show this in 1D, since extension to higher D is straightforward. In 1D,

$$A(x) = P(x)e^{ikx}$$

To satisfy the BvK BC, $A(x+Na) = A(x)$. $A(x+Na) = P(x+Na)e^{ik(x+Na)} = P(x)e^{ikx}e^{ikNa} = A(x)e^{ikNa}$. And so, we need to have $kNa = 2\pi n$, where $n =$ integer. So, in 1D

$$k = \frac{2\pi}{a}\frac{n}{N} \qquad \text{QED.}$$

Now, how many allowed k points are there in a reciprocal cell? There are exactly N points since $k(n+N) = \frac{2\pi}{a} + k(n)$. This is true in any dimension: there are $N = \Pi_i N_i$ points of allowed wave vectors in a reciprocal cell.

There are exactly as many allowed wave vectors per reciprocal cell as there are lattice points in real space.

This is a very important point. What is happening is that the wave vector becomes quantized due to the finite size of the real space, i.e. the crystal. The volume per

! → wave vector is $J\Pi_i \frac{a_i^*}{N_i}$, and the total number of allowed wave vectors in a reciprocal cell is then the volume of the reciprocal cell, $J\Pi_i a_i^*$, divided by this volume per wave vector. [J: a number that is due to the possible non-orthogonal nature of $\vec{a}_i^*$'s.] The result is $\Pi_i N_i = N$. Notice that the reciprocal cell here can be any valid reciprocal cell, since what matters is its volume only.

Some important math

Now that we have quantized wave vectors, we have some nice identities, which will come useful throughout this course.

$\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} = N\delta_{\vec{k},\vec{G}}$	Sum over all lattice points. N is the total number of lattice points.
$\int_{V_t} d\vec{r}e^{i\vec{k}\cdot\vec{r}} = V_t\delta_{\vec{k},0}$	V_t is the total volume of the crystal
$\int_{V_c} d\vec{r}e^{i\vec{G}\cdot\vec{r}} = V_c\delta_{\vec{G},0}$	V_c is the volume of the unit cell. Integration is over *any* unit cell.

All δ symbols = Kronecker delta

Proof (essential, not full)

$$\textcircled{1}\ \sum_{R} e^{ikR} = \sum_{n=0}^{N-1} e^{ikna} \underset{\substack{\uparrow \\ k=\frac{2\pi l}{Na}}}{=} \frac{1-e^{i\frac{2\pi l}{Na}aN}}{1-e^{i\frac{2\pi l}{Na}a}} = \frac{1-e^{i2\pi l}}{1-e^{i\frac{2\pi l}{N}}} = N\delta_{l\%N,0}$$

(1D only)
extension to higher D is easy

$$\textcircled{2}\ \int_{V_t} d\vec{r}\, e^{i\vec{k}\cdot\vec{r}} = 0 \quad \text{unless} \quad \vec{k}=0$$

since with BvK BC the period of $e^{i\vec{k}\cdot\vec{r}}$ along any direction $\vec{a}_i$ is the full length $N_i a_i$ divided by an integer.

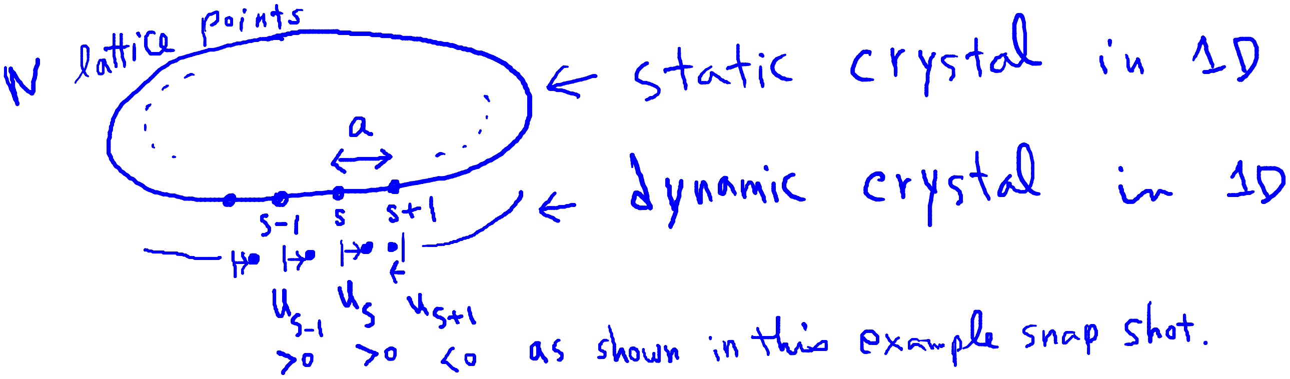
$$\textcircled{3}\ \int_{V_c} d\vec{r}\, e^{i\vec{G}\cdot\vec{r}} = 0 \quad \text{unless} \quad \vec{G}=0$$

since the length of the unit cell along any direction $\vec{a}_i$ is integer × the period of $e^{i\vec{G}\cdot\vec{r}}$.

Phonons

Phonons are the 1st example of waves/quantum particles in crystal. We will do good old Classical Mechanics to start this subject!

Lattice vibration modes in classical mechanics



Consider a one dimensional crystal with one atom per unit cell, as pictured above. Let us also assume that there are N lattice points, and thus N atoms.

The fact that a crystalline state is found to be a low temperature stable state for many substances means that it can be perturbed slightly and we expect that perturbation to give rise to a harmonic potential energy behavior in the first approximation. Specifically in this case, one simple, and widely used, model is that each bonding in the nearest neighbor be thought of as a spring with the equilibrium constant a, the lattice constant, and the spring constant C. Thus, with $u_s =$ the displacement of the lattice point s relative to the equilibrium position, the Hamiltonian of the system is:

$$H\ = T + V = \frac{1}{2}m\sum_s \dot{u}_s^2 + \frac{1}{2}C\sum_s (u_s - u_{s+1})^2$$

In this equation, the summation index s can be taken to run from any integer s_0 to $s_0 + N - 1$, since we are using the BvK boundary condition, which means that

$$u_s = u_{s+N}$$

By convention, let us take $s_0 = 0$. The equation of motion, given the above Hamiltonian, is

$$m\ddot{u}_s = -C(u_s - u_{s-1}) - C(u_s - u_{s+1})$$

Let us try the travelling wave solution:

$$u_s = ue^{i(kx_s - \omega_k t)} \quad \text{with } x_s = sa$$

While u_s is defined only on a discrete values of $x = sa$, it does have the wave form $P(x)e^{ikx}$ with $P(x) = u\delta_{x,sa}$ (Kronecker delta) and so the k quantization in the last section applies.

$$k = \frac{2\pi n}{Na}$$

Then,

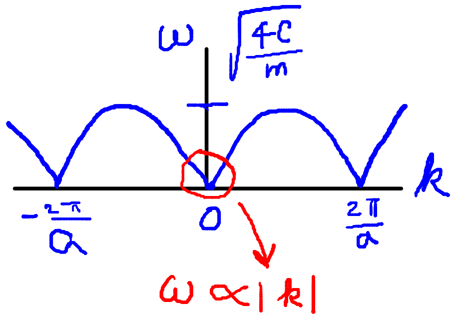
$$m\ddot{u}_s = -m\omega_k^2 u_s$$

$$u_{s\mp 1} = e^{\mp ika} u_s$$

$$-C(u_s - u_{s-1}) - C(u_s - u_{s+1}) = -C\left(2 - e^{-ika} - e^{ika}\right)u_s$$
$$= -2C(1 - \cos(ka))u_s = -4C\sin^2\left(\frac{ka}{2}\right)u_s$$

Equating $m\ddot{u}_s$ and $-k(u_s - u_{s-1}) - k(u_s - u_{s+1})$, and canceling out u_s (requiring $u \neq 0$), we get

$$-m\omega_k^2 = -4C\sin^2\left(\frac{ka}{2}\right)$$
$$\omega_k = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



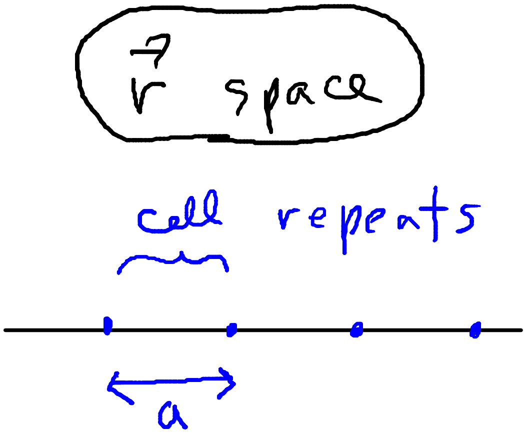
Note is that, for long wavelength ($k \to 0$), we have

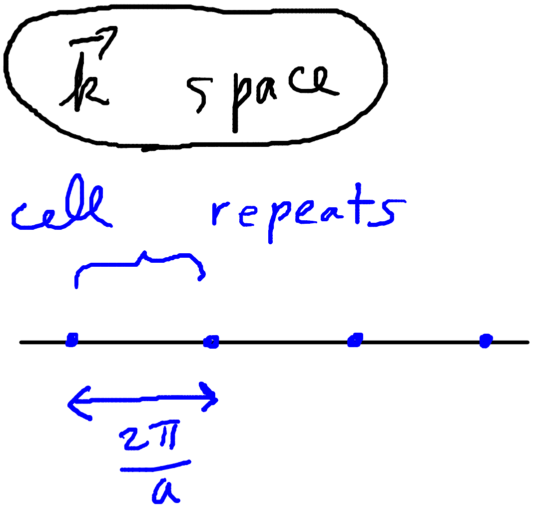
$$\omega_k = \sqrt{\frac{C}{m}}a|k|$$

This is the sound wave in a 1D crystal with the speed of sound $= \sqrt{\frac{C}{m}}a$.

Note that ω_k as a function of k has the period of $\frac{2\pi}{a}$, the length of the reciprocal cell. Also, with $u_s \propto e^{iksa} = e^{i\frac{2\pi n}{a N}sa} = e^{i\frac{2\pi ns}{N}}$, it follows that $u_s(n) = u_s(n+N)$, i.e. $u_s(k) = u_s\left(k + \frac{2\pi}{a}\right)$. In analogy with the lattice periodic function $P(x)$ defined above in the real space, we will call a $\vec{k}$-space function $\mathbb{P}(\vec{k})$ **lattice-periodic** also if it satisfies $\mathbb{P}(\vec{k}) = \mathbb{P}(\vec{k} + \vec{G})$. The fact that $\omega(k)$ and $u_s(k)$ are lattice periodic in the reciprocal space is not a coincidence at all, but reflects the general property of waves in crystal.

Waves in Crystal II





$\vec{x}$ and $\vec{x}+\vec{R}$ are equivalent.

$\boxed{\vec{k} \text{ and } \vec{k}+\vec{G} \text{ are equivalent.}}$

The fact that $\vec{k}$ and $\vec{k}+\vec{G}$ are equivalent was demonstrated for the solutions discussed above. This is the general property of *any* wave in crystal, as we will see later. The reason for this is the periodicity of the crystal, which is the background environment for the wave. We also have seen this once before. The Bragg diffraction condition $\vec{k}' = \vec{k}+\vec{G}$ can be thought of as coming from the fact that $\vec{k}$ and $\vec{k}+\vec{G}$ are equivalent in a crystal: if a wave in crystal has wave vector $\vec{k}$ then it also must have $\vec{k}+\vec{G}$; therefore if we prepare a beam of wave vector $\vec{k}$ and shine it on a crystal, it is no wonder that waves with wave vectors $\vec{k}+\vec{G}$ comes out!

Quantum mechanical derivation of phonons

The true lovers of QM: read thoroughly.
otherwise, take it easy.

In the above discussion, we showed that there are N travelling wave solutions $u_s = ue^{i(kas-\omega t)}$ corresponding to N k values in the unit cell. For a given k, one can identify $ue^{-i\omega t}$ as a generalized coordinate. Note that u, ω are implicitly k-dependent.

Of course, in general, u_s should be a linear superposition of normal mode coordinates. It is customary to express u_s in terms of the complex generalized coordinate q_k with the $1/\sqrt{N}$ factor, as follows.

$$u_s = \frac{1}{\sqrt{N}} \sum_k q_k e^{ikas}$$

The sum over k should be that over the unit cell, without any overlap. For instance sum over $n = 0,1,2,\dots,N-1$ will do, with $k = \frac{2\pi n}{Na}$. However, more frequently, we take the sum to be over the Wigner-Seitz cell: $n = -\frac{N}{2}+1,\dots,0,\dots,\frac{N}{2}$ (for even N) or $n = -\frac{N-1}{2},\dots,\frac{N-1}{2}$ (for odd N). Without loss of generality, we will assume that N is even and take the k sum to mean $n = -\frac{N}{2}+1,\dots,0,\dots,\frac{N}{2}$.

Consider $\frac{1}{\sqrt{N}}\sum_s u_s e^{-ikas}$. Using the above equation, this equals $\frac{1}{N}\sum_s \sum_{k'} q_{k'} e^{i(k'-k)as}$. Using $\sum_s e^{i(k'-k)as} = N\delta_{k'-k,G}$ and the fact that k and k' is from the same unit cell and so that they have to be equal to satisfy $k'-k=G$, we see that this evaluates to q_k. Thus, we get the inverse transformation of the above equation.

$$q_k = \frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} u_s e^{-ikas}$$

Note that $q_{-k} = q_k^*$.

It is straightforward to express the Hamiltonian in terms of q_k's, using the lattice sum identity (left as exercise):

$$H = \frac{1}{2} m \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \left(|\dot{q}_k|^2 + \omega_k^2 |q_k|^2\right)$$

Here $\omega_k = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$, the same as above, now derived in another way.

Recall from the the theory of coupled oscillators in Classical Mechanics, that the Hamiltonian should be written as that of N *independent* normal modes with *real* coordinates. Indeed, there are exactly N such normal modes. Their coordinates are $q_{k,r}$ and $q_{k,i}$(these coordinates are shared by $\pm k$, for $k \neq 0, \pm N/2$), and $q_{k,r}$ (for $k = 0, \pm N/2$; the "high symmetry points" for which $q_{-k} = q_k^* = q_k$ so q_k is real).
The above Hamiltonian is indeed a sum over the simple harmonic oscillator Hamiltonian for each of these normal modes, since $|\dot{q}_k|^2 + \omega_k^2|q_k|^2 = \dot{q}_{k,r}^2 + \omega_k^2 q_{k,r}^2 + \dot{q}_{k,i}^2 + \omega_k^2 q_{k,i}^2$. Each normal mode can be quantized. That quantized particle is called phonon.

While this is quite clear, it is customary to continue to work with the complex coordinate q_k and treat q_k and q_{-k} as independent. This is quite attractive, since each normal mode is assigned to each wave vector in a more straightforward manner.

How do we quantize q_k? The conjugate momentum is *not* $m\dot{q_k}$. Rather $p_k = \frac{\partial L}{\partial \dot{q}_k} = m\dot{q}_k^* = m\dot{q}_{-k}$. So, the Hamiltonian can be written as

$$H = \frac{1}{2m}\sum_k \left(p_k p_{-k} + m^2\omega_k^2 q_k q_{-k}\right)$$

The canonical quantization condition $[q_k, p_{k'}] = i\hbar\delta_{k,k'}$ can be used to quantize the problem. [Note that this quantization condition can also be *derived* from the canonical quantization condition that you would impose on u_s and $p_s = m\dot{u}_s$.]

These coordinates q_k, p_k are known as phonon coordinates.

We absolutely expect that q_k will satisfy the simple harmonic equation of motion. Using the Heisenberg picture of quantum mechanics and the above canonical quantization condition, this is easy to show.

$$\dot{q_k} = \frac{i}{\hbar}[H, q_k] = \frac{p_{-k}}{m}$$

Then, $\ddot{q_k} = \frac{i}{\hbar m}[H, p_{-k}] = \frac{i}{\hbar m} i\hbar m\omega_k^2 q_k = -\omega_k^2 q_k$, QED.

Thus, the energy spectrum for each k channel must be $\left(n + \frac{1}{2}\right)\hbar\omega_k$, with $n = 0,1,2,\ldots.$

To show this explicitly amounts to defining the annihilation operator a_k (and its complex conjugate, which is the creation operator $a_k^\dagger$). Normally, $a = \sqrt{\frac{m\omega_k}{2\hbar}}\left(x + \frac{ip}{m\omega_k}\right)$, but here so we need the following.

$$a_k = \sqrt{\frac{m\omega_k}{2\hbar}}\left(q_k + \frac{ip_{-k}}{m\omega_k}\right)$$

[This can be *derived* from $a_k = \frac{1}{\sqrt{N}}\sum_s e^{-ikas}\sqrt{\frac{m\omega_k}{2\hbar}}\left(u_s + i\frac{ip_s}{m\omega_k}\right)$ where p_s is the conjugate momentum for u_s.]

Then,

$$a_k^\dagger = \sqrt{\frac{m\omega_k}{2\hbar}}\left(q_{-k} - \frac{ip_k}{m\omega_k}\right)$$

as $q_k^\dagger = q_{-k}$ and $p_k^\dagger = p_{-k}$.

Using $[q_k, p_{k'}] = i\hbar\delta_{k,k'}$, the canonical quantization condition can be shown.

$$[a_k, a_{k'}^\dagger] = \delta_{k,k'}$$

The inverse transformation can be derived from the above.

$$q_k = \sqrt{\frac{\hbar}{2m\omega_k}}\left(a_k + a_{-k}^\dagger\right), \qquad p_k = i\sqrt{\frac{\hbar m\omega_k}{2}}\left(a_k^\dagger - a_{-k}\right)$$

Using this,

$$\begin{aligned}
H &= \sum_k \frac{1}{2m}\left(p_k p_{-k} + m^2\omega_k^2 q_k q_{-k}\right) \\
&= \sum_k \frac{1}{2m}\left(-\frac{\hbar m\omega_k}{2}\left(a_k^\dagger - a_{-k}\right)\left(a_{-k}^\dagger - a_k\right) + m^2\omega_k^2\frac{\hbar}{2m\omega_k}\left(a_k + a_{-k}^\dagger\right)\left(a_{-k} + a_k^\dagger\right)\right) \\
&= \sum_k \frac{1}{4}\hbar\omega_k\left(\left(a_k + a_{-k}^\dagger\right)\left(a_{-k} + a_k^\dagger\right) - \left(a_k^\dagger - a_{-k}\right)\left(a_{-k}^\dagger - a_k\right)\right) \\
&= \sum_k \frac{1}{4}\hbar\omega_k\left(a_k a_k^\dagger + a_k^\dagger a_k + a_{-k}^\dagger a_{-k} + a_{-k}a_{-k}^\dagger\right) \\
&= \sum_k \left(\frac{1}{2}\hbar\omega_k + \frac{1}{2}a_k^\dagger a_k + \frac{1}{2}a_{-k}^\dagger a_{-k}\right) = \sum_k \left(\frac{1}{2}\hbar\omega_k + \frac{1}{2}a_k^\dagger a_k + \frac{1}{2}a_k^\dagger a_k\right)
\end{aligned}$$

$\sum_k f(-k) = \sum_k f(k)$ for any lattice-periodic $f(k)$ and sum over any reciprocal cell.

$$\boxed{H = \sum_k \left(a_k^\dagger a_k + \frac{1}{2}\right)\hbar\omega_k}$$

This is of course the sum over the familiar quantum simple harmonic Hamiltonian. Note that a_k and $a_k^\dagger$, usually called the lowering operator and the raising operator, are to be understood as the annihilation operator and the destruction operator of the **phonon** with the wave vector k.

$$\boxed{n_k = a_k^\dagger a_k}$$

is the number operator for the phonon with the wave vector k.

- Classically, a_k should be read as amplitude, up to a multiplicative constant. In classical mechanics, the amplitude is continuous and can be set to zero. In quantum mechanics, it is discontinuous, since the eigenvalue of $n_k = 0, 1, 2, \ldots$. And, furthermore, the amplitude cannot be set to be zero. Instead the **zero point energy**, $\frac{1}{2}\hbar\omega_k$ represents the quantum fluctuation that one can never suppress!
- **Phonons are bosons**, since you can put many bosons in the same state ($n_k > 1$).
- In higher dimensions, the polarization of phonons need to be accounted for. So, in addition to the wave vector label, k, polarization label should be added for each creation/annihilation operator.
- The theory above shows how phonons emerge as a consequence of having a crystal. It turns out that for photons, the identical mathematical structure above, namely the amplitude quantized through a_k and $a_k^\dagger$ and $H = \sum_k \left(a_k^\dagger a_k + \frac{1}{2}\right)\hbar\omega_k$ work exactly the same way. In the case of photons, $\omega_k = ck$, which, while different from that of phonons, even have the same functional form as that of phonon ($\omega \propto k$) at long wave length! The big difference between the phonon and the photon is that we have basically no idea yet what is vibrating in the case of the photon.