Lecture 11

Waves in Periodic Potentials

Today:

1. Inverse lattice definition in 1D.
2. Graphical representation of periodic and a-periodic functions using the ***k***-axis and inverse lattice vectors.
3. Series solutions to the periodic potential Hamiltonian – general form.

Questions you should be able to address after today's lecture:

1. What is the definition of an "inverse lattice"?
2. What is the form of a Fourier series in terms of the inverse lattice vector G.
3. How is a periodic function represented graphically on the *k*-axis?
4. How is an arbitrary function expressed as a linear combination of plane waves and how is this description different from a Fourier series?
5. Know how to expand a complex function in a complex Fourier series.
6. Know how to generate the series of equations that link the coefficients separated by inverse lattice vectors.
7. What is the resulting eigenvalues problem and how are its solutions related to the eigenfunction of the periodic Hamiltonian?

Direct and "Reciprocal lattice" in 1D and 3D

A 1D Bravais lattice is defined by the collection of vectors that have the form: $R = na$

a is called a primitive vector and the set of {R} form the Bravais lattice.

Clearly any point on the ***x***-axis can be written as: $x' = x + na,\ x \in [0, a]$

Suppose we found a set of vectors G that satisfy the following relation: $e^{i\vec{G}\cdot\vec{R}} = 1$

$e^{iGna} = 1 \rightarrow G = m\frac{2\pi}{a}$ $(m = ...-1,0,1,2...)$: This set of G's also comprise a Bravais lattice.

The ***reciprocal vectors*** form a lattice with reciprocal length dimensions (large separations between lattice points in direct lattice leads to small separation in reciprocal lattice and vice versa.)

Any point ***k*** in the reciprocal space (not necessarily a lattice point) can be expressed as:

$$k' = k + m\frac{2\pi}{a} = k + G,\ \textit{where}\ (1D):\ -\frac{\pi}{a} \le k \le \frac{\pi}{a}$$

This range is called the first Brilllouin Zone (BZ), it is the Wigner-Seitz cell of the reciprocal lattice.

A similar approach is used to define a 2D and 3D lattice: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Suppose we found a set of vectors G that satisfy the following relation: $e^{i\vec{G}\cdot\vec{R}} = 1$

These G's are called the reciprocal lattice vectors, and can be found in the following way:

$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$

Here ***a***'s are the set of primitive vectors for the direct lattice and the ***b***'s are the primitive vectors for the reciprocal lattice given by:

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)},\ \vec{b}_2 = 2\pi\frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)},\ \vec{b}_3 = 2\pi\frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Example simple cubic lattice: $\vec{a}_1 = a\hat{x},\ \vec{a}_2 = a\hat{y},\ \vec{a}_3 = a\hat{z}$

$$\vec{b}_1 = \frac{2\pi}{a}\hat{x},\ \vec{b}_2 = \frac{2\pi}{a}\hat{y},\ \vec{b}_3 = \frac{2\pi}{a}\hat{z}$$

<u>Properties of Crystal momentum *k*</u>.

Clearly ***k*** is a number (or vector) related to the eigenvalues of the discrete translational operator and has units of inverse length. We mentioned above that any vector of inverse length units can be written as a sum of a reciprocal lattice vector and a vector restricted to the first BZ.

$k' = k + \underbrace{m\frac{2\pi}{a}}_{G}$, where the first Brillouin zone defined by: $-\frac{\pi}{a} \le k \le \frac{\pi}{a}$

Going back to the eigenfunctions of the discrete translational operator.

Suppose we kept our ***k*** in the range specified above (BZ) and added to it a reciprocal lattice vector ***G***: $u_{k+G}(x) = e^{ikx}e^{iGx}f(x)$

This eigenfunction still corresponds to an eigenvalue of e^{ika} since by construction $e^{iGa} = 1$ and thus adding ***G*** to ***k*** may modify the functional form of the periodic term but will not obviously change the fact that it is periodic in ***a*** as e^{iGx} is itself a periodic function in ***a*** (therefore it can be taken to be part of $f(x)$).

In other words in terms of labeling the states it is sufficient to consider only *k*'s that are restricted to the first BZ as only they correspond to distinct eigenvalues of the discrete translational operator.

Numerical solution of the periodic potential: The eigenvalue problem

We are considering a periodic potential: $V\left(x+na\right)=V\left(x\right)$

Since the function is periodic with period "***a***" it can be expanded in a Fourier series where ***G***'s are the set of reciprocal lattice vectors, i.e. a periodic function can be expanded in terms of sine a cosine functions such that:

$$V\left(x\right)=\frac{V_0}{2}+\sum_{n=1}^{\infty}A_n\cos\underbrace{\frac{2\pi n}{a}}_{G_n}x+B_n\sin\underbrace{\frac{2\pi n}{a}}_{G_n}x$$

$$A_n=\frac{2}{a}\int_0^a V\left(x\right)\cos\frac{2\pi n}{a}xdx$$

$$B_n=\frac{2}{a}\int_0^a V\left(x\right)\sin\frac{2\pi n}{a}xdx$$

The reciprocal lattice as the collection of points $\left\{G\right\}$ defined by the relation: $e^{iGR}=1$

$$G=\frac{2\pi}{a}n=gn$$

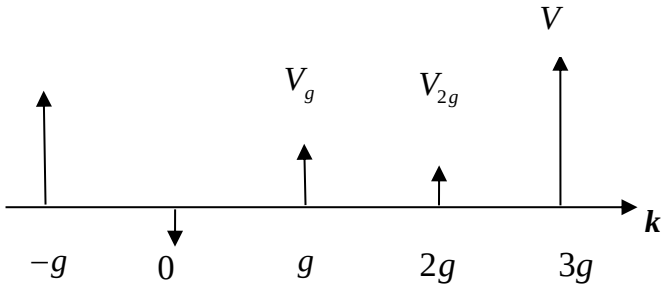
Then we can rewrite the Fourier series as:

$$V\left(x\right)=\frac{A_0}{2}+\sum_{G=g}^{\infty}V_G^{\cos}\cos Gx+V_G^{\sin}\sin Gx$$

$$V_G^{\cos}=\frac{2}{a}\int_0^a V\left(x\right)\cos Gxdx$$

$$V_G^{\sin}=\frac{2}{a}\int_0^a V\left(x\right)\sin Gxdx$$

The coefficients of the series can be represented graphically on the k axis.



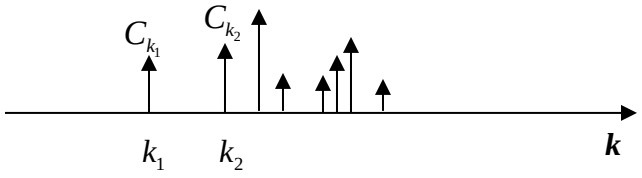
Since our functions are complex valued we will use the complex Fourier series:

$$V\left(x\right)=\sum_G V_G e^{iGx}$$

Now the Hamiltonian for the periodic potential has the following form:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\sum_G V_G e^{iGx}\right)\varphi(x)=Eu(x)$$

The eigenfunctions can be written as a series. Since there is no reason to assume that the eigenfunctions are periodic in lattice period we expand them in ***k***: $\varphi(x)=\sum_k C_k e^{ikx}$



Any particular solution *φ(x)* is completely defined by specifying the set of coefficients C_k. All ***k***'s are allowed so the ***k*** separation between two terms can be infinitesimal.

Substituting *φ(x)* into the periodic potential Hamiltonian:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\sum_G V_G e^{iGx}\right)\sum_k C_k e^{ikx}=E\sum_k C_k e^{ikx}$$

$$\frac{\hbar^2}{2m}\sum_k C_k k^2 e^{ikx}+\sum_G\sum_k V_G C_k e^{i(G+k)x}=E\sum_k C_k e^{ikx}$$

Since the sum over ***k*** is infinite and ***k*** is just a running index we can change our variable in the second sum from $k\to k-G$:

$$\frac{\hbar^2}{2m}\sum_k C_k k^2 e^{ikx}+\sum_G\sum_k V_G C_{k-G} e^{ikx}=E\sum_k C_k e^{ikx}$$

$$\sum_k\left(\frac{\hbar^2}{2m}k^2 C_k+\sum_G V_G C_{k-G}\right)e^{ikx}=\sum_k EC_k e^{ikx}$$

$$\sum_k\left(\left(\frac{\hbar^2}{2m}k^2-E\right)C_k+\sum_G V_G C_{k-G}\right)e^{ikx}=0$$

In order for this sum to be equal to zero every component has to be zero:

$$\left(\frac{\hbar^2}{2m}k^2-E\right)C_k+\sum_G V_G C_{k-G}=0\Rightarrow\frac{\hbar^2}{2m}k^2 C_k+\sum_G V_G C_{k-G}=EC_k$$

Unlike the situation we started with where the separation between two terms in the expansion could be infinitesimal this equation relates all the coefficients C_k that are

separated by an inverse lattice vector to each other forming a set of coupled algebraic equations (which in essence is a recursion formula).

Now all you need to do is to solve this infinite system of equations – i.e. find the energy eigenvalues E and the eigenvectors $\vec{C}$ composed of components C_k, which define our trial wavefunctions: $\varphi(x) = \sum_k C_k e^{ikx}$

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