

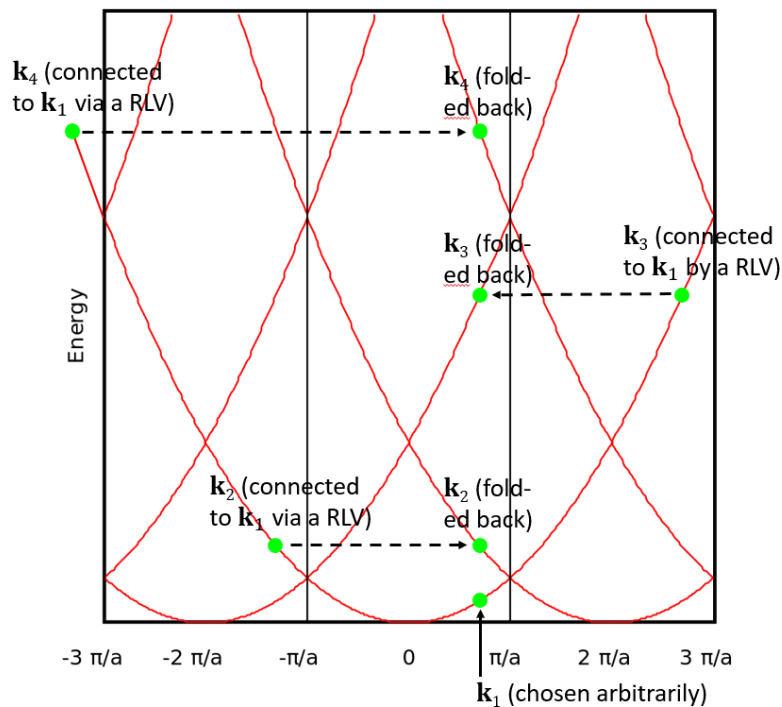
The Central Equation

by Dr. Colton, Physics 581 (last updated: Fall 2020)

This is the Central Equation; it essentially represents a Fourier transform of the Schrodinger equation:

$$(\lambda_k - E)C_k + \sum_{\mathbf{G}} U_{\mathbf{G}}C_{\mathbf{k}-\mathbf{G}} = 0$$

This actually represents an *infinite* set of equations for a given \mathbf{k} within the first Brillouin zone (BZ), let's call that \mathbf{k}_1 . That is, the first equation of the infinite set will have $\mathbf{k} = \mathbf{k}_1$. There is one equation for each \mathbf{k} which is "connected" to \mathbf{k}_1 by a reciprocal lattice vector (RLV), let's call those $\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4$, etc. Recall that in the empty lattice approximation, the energy for $\mathbf{k} + \text{a RLV}$ gets folded back into the first Brillouin zone (BZ) to the same \mathbf{k} value.



The energies that can be obtained from the Central Equation represent the infinite set of vertically stacked energies at \mathbf{k}_1 , which result from the folding back of the free electron parabola, combined with some knowledge of the actual potential energy function $U(\mathbf{r})$ which describes how the energy landscape departs from the free electron case.

More details:

- The \mathbf{G} vectors are the RLVs.
- The $U_{\mathbf{G}}$ terms are the Fourier components of $U(\mathbf{r})$. Remember from Chapter 2 that the 3D Fourier transform of a periodic function results in a summation over the reciprocal lattice vectors, $U(\mathbf{r}) = \sum_{\mathbf{G}} U_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}$.
- The $C_{\mathbf{k}}$ terms are the expansion coefficients of the wave function ψ , when written as a Fourier series of plane waves expanded over your infinite set of \mathbf{k} values, $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$, etc.: $\psi(\mathbf{r}) = \sum_i C_{\mathbf{k}_i}e^{i\mathbf{k}_i\cdot\mathbf{r}}$.

- λ_k is the energy of the free electron parabola corresponding to each k value in your infinite set, namely $\lambda_k = \frac{\hbar^2 k^2}{2m}$.

The equation can most easily be understood written in matrix form. Each row of the matrix equation is the Central Equation for one of the \mathbf{k} values in your infinite set.

$$\begin{pmatrix} \lambda_1 & U_{12} & U_{13} & \cdot & \cdot & \cdot \\ U_{21} & \lambda_2 & U_{23} & \cdot & \cdot & \cdot \\ U_{31} & U_{32} & \lambda_3 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = E \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

This is an infinite matrix equation! It's also an eigenvalue equation, where the allowed energies E are the eigenvalues, and the sets of plane wave expansion coefficients (C_1, C_2, C_3, \dots) are the eigenvectors. The U_{ij} terms are the Fourier components of the potential energy, where e.g. U_{23} is the Fourier coefficient for the specific RLV which connects \mathbf{k}_2 to \mathbf{k}_3 , i.e. $\mathbf{G} = \mathbf{k}_2 - \mathbf{k}_3$.

Multiplying out the first row or two of the matrix equation may convince you that it is equivalent to the Central Equation as given above.¹

Obviously one cannot find the eigenvalues of an infinite matrix, so the first thing one must do to solve this equation is decide where to cut off the matrix. That's exactly analogous to deciding how many terms of a Fourier series must be included to accurately represent a function, since the C_i coefficients are exactly the Fourier coefficients of the representation of $U(\mathbf{r})$.

The recipe for how to use the Central Equation to solve for the allowed energies, given a periodic potential energy function $U(\mathbf{r})$, is therefore as follows.

- 1) Pick a particular \mathbf{k} value you're interested in, within the first BZ. This is \mathbf{k}_1 , although it doesn't really have to be listed first in your set of \mathbf{k} values.
- 2) Decide where you want to truncate the matrix. That is to say, how many connected \mathbf{k} values do you want to consider? Connected means they are equal to \mathbf{k}_1 minus a reciprocal lattice vector. Form your finite set of \mathbf{k} values.
- 3) Calculate the λ_k values for your set of \mathbf{k} 's.
- 4) Calculate the Fourier expansion coefficients U_{ij} for the \mathbf{G} vectors which connect all of the \mathbf{k} 's in your set, or at least as many as reasonably possible. (In some cases the \mathbf{G} vector needed to connect \mathbf{k}_i to \mathbf{k}_j might be beyond where you'd like to take the expansion of $U(\mathbf{r})$.)
- 5) Write down the matrix and solve for the eigenvalues using your favorite method.

Let's do an example. This particular example is an actual final exam question from when I took this class as a graduate student at UC Berkeley.

¹ Disclaimer: I haven't included the U_0 terms in the matrix equation, namely the constant term of the Fourier series. If $U(\mathbf{r})$ has a non-zero average value, then U_0 will be non-zero and all diagonal terms will have U_0 added to them. This will simply have the effect of shifting all eigenvalues by U_0 so one can actually more simply solve for the eigenvalues without the U_0 terms present, then shift all of the eigenvalues (the energies) by U_0 at the end.

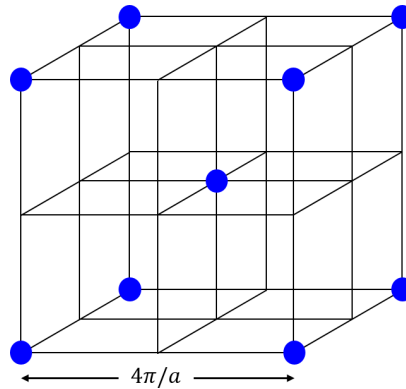
Worked Problem: Apply the Central Equation to GaAs to solve for the energies at $\mathbf{k} = (0,0,0)$. Only use RLVs with magnitude $G \leq \frac{4\pi}{a}$. Work out the equations to the level that you could solve for the energies were you to be given the $U(\mathbf{r})$ function.

Step 1: Pick a particular \mathbf{k} value you're interested in

The \mathbf{k} value of interest within the first BZ is given: $\mathbf{k}_1 = (0,0,0)$.

Step 2: Decide where you want to truncate the matrix

The problem says to consider all of the \mathbf{G} 's with $|\mathbf{G}| \leq \frac{4\pi}{a}$. To figure those out, we need to consider the lattice type. GaAs has an fcc lattice; the reciprocal lattice is bcc with lattice constant $4\pi/a$. Here's the unit cell of the reciprocal lattice:



By visualizing the expanded bcc lattice we can identify all of the specified \mathbf{G} vectors, which turn out to be the 14 shortest ones.

$\frac{4\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$	$\frac{4\pi}{a} \left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right)$	$\frac{4\pi}{a} (1,0,0)$	$\frac{4\pi}{a} (-1,0,0)$
$\frac{4\pi}{a} \left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$	$\frac{4\pi}{a} \left(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right)$	$\frac{4\pi}{a} (0,1,0)$	$\frac{4\pi}{a} (0,-1,0)$
$\frac{4\pi}{a} \left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right)$	$\frac{4\pi}{a} \left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right)$	$\frac{4\pi}{a} (0,0,1)$	$\frac{4\pi}{a} (0,0,-1)$
$\frac{4\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right)$	$\frac{4\pi}{a} \left(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right)$		

These are the 14 points on the bcc lattice which are closest to the origin: the eight body centered atoms of the eight cubes surrounding the origin, plus the six closest points along the $\pm x$, $\pm y$, $\pm z$ directions. All other RLVs have magnitudes larger than the specified cutoff. The first eight vectors have magnitudes of $\frac{2\pi}{a}\sqrt{3}$; the others have magnitudes of $\frac{4\pi}{a}$.

Because in this particular problem the \mathbf{k} point of interest is in fact the origin, those \mathbf{G} vectors, along with $(0,0,0)$, comprise our set of \mathbf{k} 's. Let's label them as follows:

$$\begin{aligned}
\mathbf{k}_1 &= (0,0,0) & \mathbf{k}_6 &= \frac{4\pi}{a} \left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right) & \mathbf{k}_{10} &= \frac{4\pi}{a} (1,0,0) & \mathbf{k}_{13} &= \frac{4\pi}{a} (-1,0,0) \\
\mathbf{k}_2 &= \frac{4\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) & \mathbf{k}_7 &= \frac{4\pi}{a} \left(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right) & \mathbf{k}_{11} &= \frac{4\pi}{a} (0,1,0) & \mathbf{k}_{14} &= \frac{4\pi}{a} (0, -1,0) \\
\mathbf{k}_3 &= \frac{4\pi}{a} \left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) & \mathbf{k}_8 &= \frac{4\pi}{a} \left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right) & \mathbf{k}_{12} &= \frac{4\pi}{a} (0,0,1) & \mathbf{k}_{15} &= \frac{4\pi}{a} (0,0, -1) \\
\mathbf{k}_4 &= \frac{4\pi}{a} \left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right) & \mathbf{k}_9 &= \frac{4\pi}{a} \left(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right) & & & & \\
\mathbf{k}_5 &= \frac{4\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right) & & & & & &
\end{aligned}$$

Step 3: Calculate the λ_k values for your set of \mathbf{k} 's.

There are actually only three different values of λ_k for our situation because there are only three magnitudes of k : \mathbf{k}_1 has $\lambda_k = 0$, then the next eight all have $\lambda_k = \frac{\hbar^2}{2m} \frac{12\pi^2}{a^2}$, which I will call λ_1 , and the final six all have $\lambda_k = \frac{\hbar^2}{2m} \frac{16\pi^2}{a^2}$, which I will call λ_2 .

Step 4: Calculate the Fourier expansion coefficients U_{ij}

We aren't given the details of $U(\mathbf{r})$ so we can't calculate the Fourier coefficients. We'll just assume that we could do that if we had the details. Note, however, that some of the U_{ij} terms will involve \mathbf{G} vectors longer than we were told to use. As an example, $\mathbf{k}_{10} - \mathbf{k}_{13} = \frac{8\pi}{a} (1,0,0)$. Terms like that don't need to show up in our matrix.

Step 5: Write down the matrix and solve for the eigenvalues

The allowed energies are the eigenvalues of this matrix:

$$\begin{pmatrix}
0 & U_{12} & U_{13} & \cdot & U_{1,15} \\
U_{21} & \lambda_1 & U_{23} & \cdot & \cdot \\
U_{31} & U_{32} & \lambda_1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot \\
U_{15,1} & \cdot & \cdot & \cdot & \lambda_2
\end{pmatrix}$$

The diagonal elements are the free electron parabola values. The off diagonal elements are the Fourier components of $U(\mathbf{r})$ —specifically, U_{ij} is the Fourier coefficient $U_{\mathbf{G}}$ for $\mathbf{G} = \mathbf{k}_i - \mathbf{k}_j \dots$ with some of the U_{ij} terms being set to zero if $|\mathbf{k}_i - \mathbf{k}_j|$ is too long. (I'm assuming the constant term in the Fourier expansion $U_0 = 0$, if not see footnote 1.)

The eigenvalues will give you an approximation to the 15 lowest energies at $\mathbf{k} = 0$. The eigenvectors tell you how the wave functions at each of those particular energy states are constructed from plane waves. A large coefficient for C_5 in your eigenvector, for example, would mean that the wave function for that particular energy state has a lot of $e^{i\frac{4\pi}{a}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \cdot \mathbf{r}}$ character to it, since $k_5 = \frac{4\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$.

And we're done! Without knowing the potential energy function that's as far as we can go.