

ASSIGNMENT 3: HARD WALL POTENTIALS

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HARD WALL POTENTIALS

PREREQUISITES

The chapter *Surface Scattering* from the *Theory Handbook*

INTRODUCTION

The scattering of helium atoms from a surface is one of the key processes used to probe surface structures. For this reason, it is important to understand how this scattering occurs, and the consequence of atom scattering. To achieve this, one of the tasks we must achieve is to construct a “hard wall potential” for a surface. In this tutorial, we will develop a model for the “hard wall potential” on a close packed plane.

HARD WALL POTENTIALS

In order to analyse the results from scattering experiments, it is useful to have a theoretical model that supports the experiment. This model must predict the scattering dynamics for a given surface. How do we make this model? The first step in constructing this is to generate a potential energy function that describes the potential on the same surface.

The simplest model for this potential energy function that we can use is known as a “hard-wall potential”. Covered comprehensively in the *Theory Handbook*, this takes the form:

$$V(\mathbf{R}, z) = \begin{cases} 0 & z > \zeta(\mathbf{R}); \\ \infty & z \leq \zeta(\mathbf{R}), \end{cases}$$

where V is the potential energy function, \mathbf{R} is the position vector of a point on the surface, z is the perpendicular distance of a point from the surface (see Figure 1), and $\zeta(\mathbf{R})$ is the “corrugation function”.

Within our model, it can be seen that the points given by $(\mathbf{R}, \zeta(\mathbf{R}))$ define a locus. What does this represent? This locus represents the points at which the incident atom will scatter, and begin to move away from the surface. This is reassuring - it is essentially the definition of

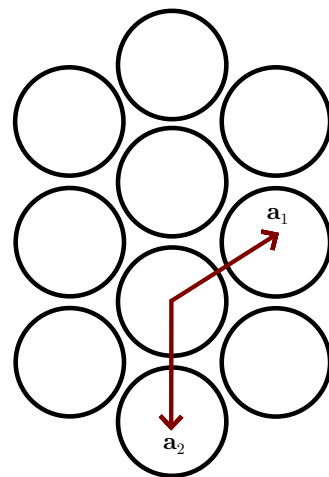


Figure 1 | The coordinate system used to define the potential function. The (001) family is set as the xy plane, and the [001] axis (not labelled) is denoted as the z axis, perpendicular to the surface. The circles are illustrative only - the true lattice has a dirac delta function located at the centre of each circle present.

the corrugation function. What can we say about the corrugation function's behaviour? As a starting point, we would expect the corrugation function to have two key features:

- Local maxima at the position of the surface atoms.
- Periodicity - respecting the symmetry of the lattice.

This information is sufficient to generate a corrugation function for a surface. In this tutorial, we will use Fourier series to construct a corrugation function for a close packed plane, satisfying the properties above. We will make use of the result that a function whose periodicity matches that of a Bravais lattice must take the form:

$$f(\mathbf{r}) = \sum_{\mathbf{G}} A_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}$$

where \mathbf{G} is a reciprocal lattice vector, and $A_{\mathbf{G}}$ is a constant. Where does this equation come from? Although it initially appears to be plucked out of thin air, it does make sense: whenever the argument \mathbf{r} is a multiple of a real space lattice vector, the argument of the exponential is a multiple of $2\pi i$. Evidently, this results in the function being periodic.

How do we approach the problem of constructing a corrugation function? Our strategy to begin is:

1. Determine the lattice that represents the surface.
2. Find the set of basis lattice vectors for the lattice in question, denoted \mathbf{a}_1 and \mathbf{a}_2 .
3. Find the corresponding reciprocal lattice vectors, denoted \mathbf{b}_1 and \mathbf{b}_2 .
4. Use the reciprocal lattice basis vectors to find reciprocal lattice vectors of the form:

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2,$$

where h and k are integers.

5. Use these reciprocal lattice vectors to construct a Fourier series for the corrugation function. Ensure that the coefficients of the terms in the Fourier series are chosen such that the function has local maxima occurring at the positions of the atoms.

In the case of a hexagonal lattice, much of this work has already been done for us! In the Fourier transforms tutorial, you found the reciprocal lattice basis vectors, denoted \mathbf{b}_1 and \mathbf{b}_2 , and you used these to plot the reciprocal lattice. We also need to choose the arguments of the terms in the Fourier series. Any reciprocal lattice vector \mathbf{G} is a suitable choice for the basis of the Fourier series. Figure 2 highlights the basis vectors of a close packed plane, naturally suggesting an elegant basis for the Fourier series.

The simplest possible corrugation function would be one that just uses the two basis reciprocal lattice vectors, \mathbf{b}_1 and \mathbf{b}_2 , to give a

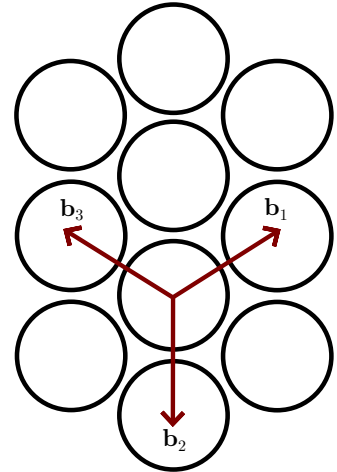


Figure 2 | The reciprocal lattice of a close packed plane. This is also a close packed plane! However, the spacing between the lattice points changes.

Fourier series with just two components. However, we will demonstrate that while this corrugation function would respect the periodicity of the lattice, it would not fully respect the hexagonal symmetry present. To represent this symmetry fully, we would need to use at least three reciprocal lattice vectors, such as \mathbf{b}_1 , \mathbf{b}_2 and \mathbf{b}_3 , in order to produce a suitable corrugation function.

TASK 1: TWO FOURIER COMPONENTS

Our first task is to construct a corrugation function for a close-packed plane, using just two Fourier components.

1. Find the reciprocal lattice basis vectors for the hexagonal surface.
2. Construct a Fourier series for the corrugation function using just two Fourier components: using one series for each reciprocal lattice basis vector. Ensure that the function has its maxima at the positions of the atoms (*i.e.* the lattice points). Use a lattice constant of $a = 4.52\text{\AA}$ and a corrugation height (*i.e.* the maximum value of the corrugation function) of $h = 1\text{\AA}$.
3. Produce a suitable plot. Convince yourself that the function does not fully respect the hexagonal symmetry of the system.

Tip 1

The lattice of a hexagonal surface was explored in the tutorial on graph plotting; the lattice vectors used here are the same as from that tutorial. The key result is that the two basis vectors are the same length a , and have an angle of 120° between them.

There is a formula for finding reciprocal lattice basis vectors from real space lattice basis vectors. This can be found in numerous sources. In addition, both the lattice vectors and the reciprocal lattice vectors can be calculated for you by the “auxCls” function, given in the solution.

Once you have calculated the reciprocal lattice vectors, \mathbf{d}_1 and \mathbf{d}_2 , the corrugation function is given by:

$$\zeta(\mathbf{R}) = A(\cos(\mathbf{R} \cdot \mathbf{d}_1) + \cos(\mathbf{R} \cdot \mathbf{d}_2))$$

where A must be chosen such that you get the correct corrugation height.

Note that we have used only cosine functions in the Fourier series so that the corrugation function peaks at the position of the top sites, as required.

Tip 2

When plotting a function on MATLAB, you need to sample the value of the function a set of points in space, and then plot your sampled values as a function of position. The points in space where you sample your function should take the form of a grid that respects the periodicity of the system.

In this case, the corrugation function that you need to plot is a function of two spatial dimensions, and so the function defines a surface in three-dimensional space (rather than a line in two-dimensional space that you would plot for functions of only one spatial dimension). To plot such a function, try the “surface” and/or “pcolor” functions in Matlab.

TASK 2: THREE FOURIER COMPONENTS

You may have noticed that the function plotted in the previous task did not respect the mirror symmetry of the close-packed surface. We are now going to construct a corrugation function that does fully respect the hexagonal symmetry of the system.

To do this, you will need to find three reciprocal lattice vectors. The three vectors labelled in Figure 2 are a suitable choice. Then you will have to construct a Fourier series as before, but this time with three Fourier components, one for each reciprocal lattice vector. You still need to ensure that the function has its maxima at the positions of the atoms. Use the same lattice constant and corrugation height as before, and produce a suitable plot. This time, you should see that your function does respect the hexagonal symmetry of the system.

Tip

We have already calculated \mathbf{b}_1 and \mathbf{b}_2 using the “auxCls” function. You should be able to see from Figure 2 that the third reciprocal lattice vector is given by:

$$\mathbf{b}_3 = \mathbf{b}_2 - \mathbf{b}_1.$$

SUMMARY

In this document, we have learned how to create a hard wall potential for a simple system. This skill will remain useful throughout your study of surface physics.