

# Electrons in a Periodic Potential

## 1. Introduction

There are two basic ways we can attack this problem: we can choose to approximate the potential energy with a form for the potential for which we know how to solve Schrodinger's Equation exactly; or we can choose to use an exact form for the potential energy and then try to approximately solve Schrodinger's Equation. We will indicate one example of the first, but turn most of our attention to the second. But first we will introduce a very useful preliminary theorem.

## 2. Block Functions: a preliminary theorem

The theorem states that the solution of the Schrodinger's Equation for a periodic potential must be of the special form:

$$\psi(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \text{where } u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{T}),$$

where the  $\mathbf{T}$  vector is the translation vector (which is an integer number of lattice spacings in each of the lattice's three directions, i.e., an integer number of primitive lattice vectors).

The idea is that symmetry considerations demand that the probability of an electron being at any location,  $x$  [or  $\mathbf{r}$  vector in 3-D], should be the same as the probability of being at any other location separated by the translation vector,  $x+a$  [or  $\mathbf{r}+\mathbf{T}$  vector in 3-D]. Since the probability depends on  $\psi^* \psi$ , [the  $*$  indicates complex conjugate] the  $\psi(x)$  can differ from the  $\psi(x+a)$  only by a phase factor (denoted by  $e^{ikx}$ ). Note that the complex conjugate of the phase difference,  $e^{ikx}$ , is simply  $e^{-ikx}$ , and that  $e^{ikx} e^{-ikx} = 1$ .

The important consequence of this theorem is that we can now try to solve Schrodinger's Equation for  $u_{\mathbf{k}}(x)$  over only the limited range of  $0 < x < a$ . We then find the complete  $\psi(x)$  by multiplying the  $u_{\mathbf{k}}(x)$  by the phase factor  $e^{ikx}$  and then by matching boundary conditions.

## 3. The Kronig-Penney Model: a passing glance

One potential that we can solve for exactly is the constant potential. The Kronig-Penney Model assumes that the potential due to each ion core is some value,  $U_0$  from  $0 < x < b$ , and then the potential changes suddenly to 0 from  $b < x < a$  (where  $b$  is some distance less than that of the interatomic distance,  $a$ ).

The advantage of this model is that the Schrodinger's Equation can be **solved exactly**. The disadvantage is that the actual potential energy is most probably not of this form.

The result of working out the details of this model (which we will not do here) is that we **get energy gaps** predicted at the Brillouin zone boundaries. (Just as we did in the quasi-quantitative weakly interacting model.)