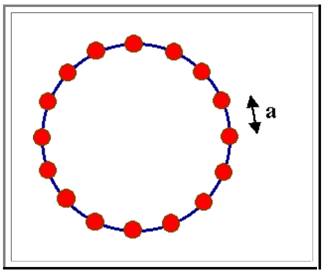
Simple Proofs of Bloch's Theorem

The Proof

- We first give a very short proof for a special case which is taken from the book of Kittel ("Quantum Theory of Solids"). It treats the one-dimensional case and is only valid if ψ is not degenerate, i.e. there exists no other wavefunction with the same $\boldsymbol{k}$ and energy $\boldsymbol{E}$.

  - We consider a one-dimensional ring of lattice points with the geometry as shown in the picture.



  - This is of course just a representation of a one-dimensional crystal consisting of $\boldsymbol{N}$ atoms with spacing $\boldsymbol{a}$ and periodic boundary conditions.
  - The potential $\boldsymbol{V}$ thus is periodic in $\boldsymbol{x}$ with period length $\boldsymbol{a}$, i.e. we have $V(x) = V(x + s \cdot a)$ with $s =$ integer.

- The decisive thought invokes *symmetry arguments*. Since no particular coordinate $\boldsymbol{x}$ along the ring is different in any way from the coordinate $(x + a)$, we expect that the value of any wave function $\psi(x)$ will differ at most by some factor $\boldsymbol{C}$ from the value at $(x + a)$, i.e.

$$\psi(x + a) = C \cdot \psi(x)$$

  - If we now proceed from $(x + a)$ to $(x + 2a)$, or to $x + Na$, we obtain

$$\psi(x + 2a) = C^{2} \cdot \psi(x)$$

$$\psi(x + Na) = C^{N} \cdot \psi(x) = \psi(x)$$

  - because after $\boldsymbol{N}$ steps we are back at the beginning.
  - We thus have $C^N = 1$ and $\boldsymbol{C}$ must be one of the $\boldsymbol{N}$ roots of **1**, i.e.

$$C = \exp\frac{i \cdot 2\pi s}{N}$$

  - With $s = 0, 1, 2, 3, \ldots, N - 1$

- We now have $\psi(x + a) = \psi(x) \cdot \exp(i2\pi s/N)$ and this equation is satisfied if

$$\psi(x) = u_k(x) \cdot \exp\frac{i \cdot 2\pi \cdot s \cdot x}{N \cdot a}$$

  - With $u_k(x) = u_k(x + a)$, i.e. for any function **u** that has the periodicity of the lattice.
  - Try it:

$$\psi(x+a) = u_k(x+a)\cdot\exp\frac{i\cdot 2\pi\cdot s\cdot(x+a)}{N\cdot a}$$

$$\psi(x+a) = u_k(x)\cdot\exp\frac{i\cdot 2\pi\cdot s\cdot x}{N\cdot a}\cdot\exp\frac{i\cdot 2\pi\cdot s}{N} = \psi(x)\cdot\exp\frac{i\,2\pi\cdot s}{N}$$

- If we introduce $\boldsymbol{k} = 2\pi s/Na$ we have Bloch's theorem for the one-dimensional case.
  q.e.d.

The Problem

- This "proof", however, is not quite satisfactory. It is not perfectly clear if solutions could exist that do not obey Bloch's theorem, and the meaning of the index **k** is left open. In fact, we could have dropped the index without losing anything at this stage.
  - It does, however, give an idea about the power of the symmetry considerations.
- A very similar proof is contained in the relevant Alonso–Finn book ("Quantum and Statistical Physics"). It uses a slightly different approach in arguing about symmetries.
  - Again, we consider the one-dimensional case, i.e. $V(x) = V(x+a)$ with a = lattice constant.
  - But now we argue that the *probability* of finding an electron at x, i.e. $|\psi(x)|^2$, must be the same at any indistinguishable position, i.e.

$$|\psi(x)|^2 = |\psi(x+a)|^2$$

  - This implies

$$\psi(x+a) = C\cdot\psi(x)$$

$$|C|^2 = 1$$

  - We thus can express C as

$$C = \exp(i\cdot k\cdot a)$$

  - for all a and k. At this point k is an arbitrary parameter (with dimension **1/m**). This ensures that $|C|^2 = \exp(ika)\cdot\exp(-ika) = 1$
  - We thus have

$$\psi(x+a) = \exp(ika)\cdot\psi(x)$$

  - And this is already a very general form of Blochs theorem as shown below.
- Writing it straight forward for the three-dimensional case we obtain the general version of Bloch's theorem:

$$\psi_k(\underline{r}+\underline{T}) = \exp(i\underline{k}\cdot\underline{T})\cdot\psi_k(\underline{r})$$

  - with $\underline{T}$ = translation vector of the lattice and $\underline{r}$ = arbitrary vector in space.
  - The index **k** now symbolizes that we are discussing that particular solution of the Schrödinger equation that goes with the wave vector $\underline{k}$.
- The generalization to three dimensions is not really justified, but a rigorous mathematical treatment yields the same result. The more common form of the Bloch theorem with the modulation function **u(*k*)** can be obtained from the (one-dimensional) form of the Bloch theorem given above as follows:

- Multiplying ψ $(x) = \exp(-ika) \cdot \psi(x + a)$ with $\exp(-ikx)$ yields

$$\exp(-ikx) \cdot \psi(x) \;=\; \exp(-ikx) \cdot \exp(-ika) \cdot \psi(x + a) \;=\; \exp(-ik \cdot [x + a]) \cdot \psi(x + a)$$

This shows unambiguously that $\exp(-ikx) \cdot \psi(x) = u(x)$ is periodic with the periodicity of the lattice.

- And this, again, gives Bloch's theorem:

$$\psi(x) \;=\; u(x) \cdot \exp(ikx)$$

Once more, no index **k** at ψ or **u** is required. We also did not require specific boundary conditions. The meaning of ***k***, however, is left unspecified. Of course, the plane wave part of the expression makes it clear that ***k*** has the role of a wave vector, but it has not been explicitly introduced as such.