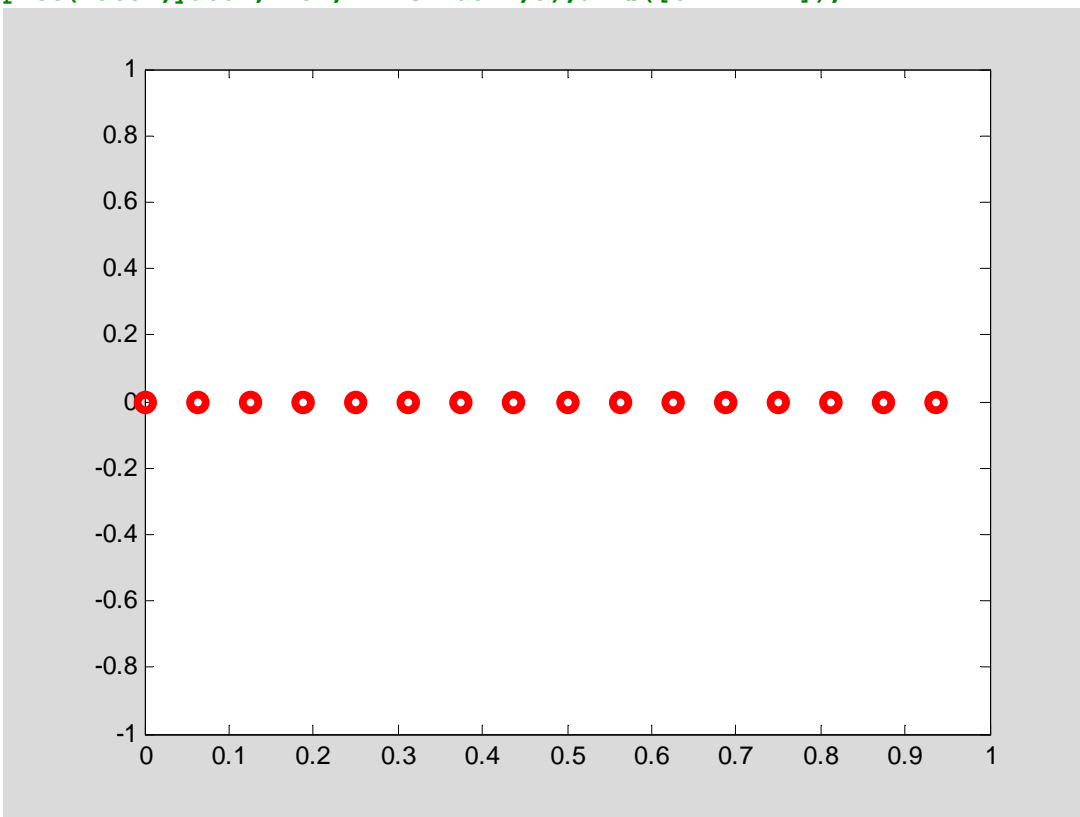


Visualisierung von Bloch Wellen

Im perfekten Festkörper (bei $T=0$) müssen die Lösungen der Schrödinger-Gleichung sowohl im Ortsraum als auch im k-Raum die Gittersymmetrie widerspiegeln.

Um sich ein "Bild" von diesen Symmetrien zu machen, betrachten wir zuerst einmal eindimensionale einfache Gitter. Im äquidistanten Abstand a sind die Gitterbausteine (z.B. Atome) angeordnet.

```
Natom=16;
a=1/Natom;
xatom=[0:a:(Natom-1)*a];
yatom=zeros(1,Natom);
plot(xatom,yatom,'ro','Linewidth',3);axis([0 1 -1 1]);
```

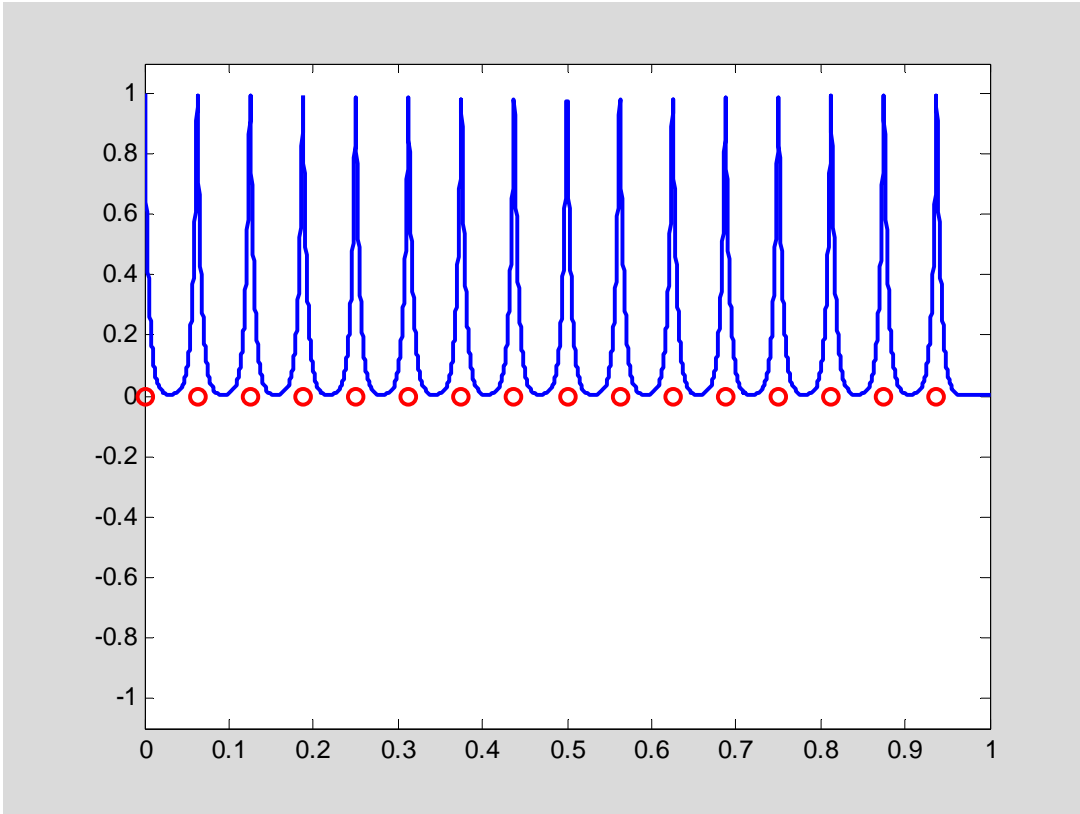


Jetzt ordnen wir an jedem Gitterpunkt eine lokalisierte Wellenfunktion an.

```
Nx=4000;
x=linspace(0,1,Nx);
alpha=0.005;

wellenfunktion=zeros(1,Nx);
for i1=1:Natom
wellenfunktion = wellenfunktion +exp(-(abs(x-xatom(i1))/alpha));
end
```

```
plot(x,wellenfunktion,xatom,yatom,'ro','Linewidth',2);axis([0 1 -1.1 1.1]);
```

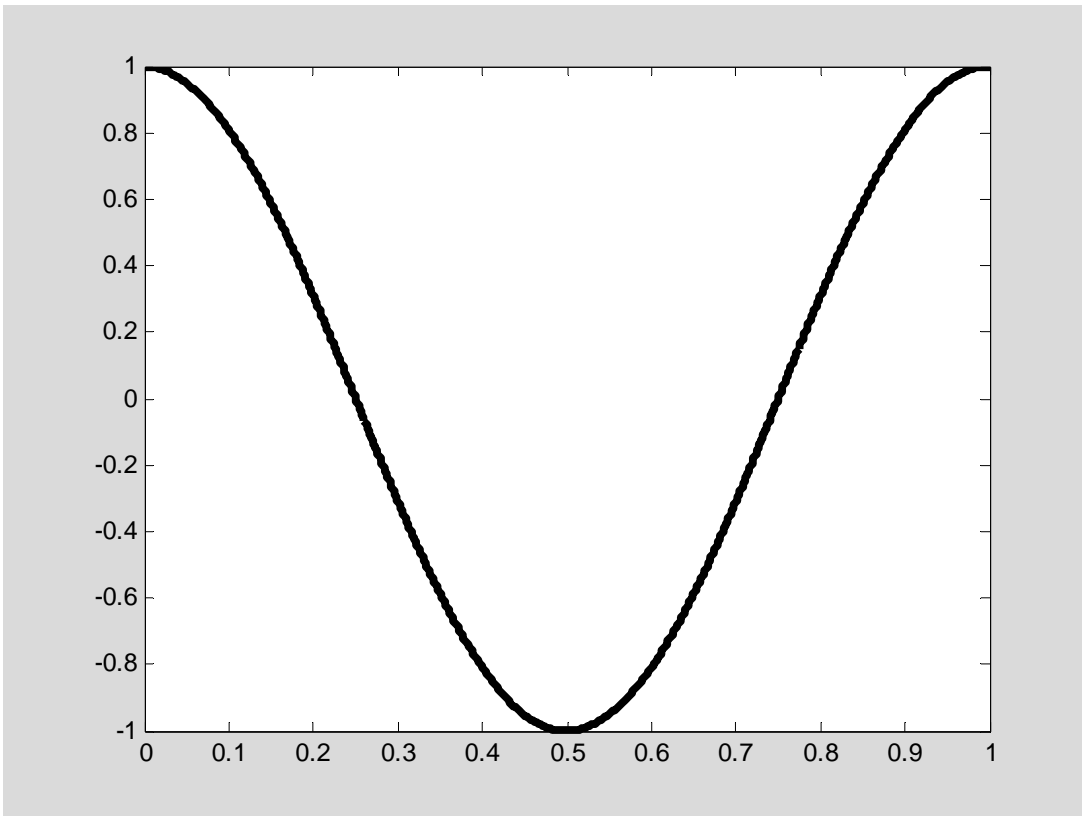


Am Ort des jeweiligen Atoms lokalisierte Wellenfunktion. Die gesamte Wellenfunktion ist als Summe der einzelnen Wellenfunktionen auch lokalisiert und kann **reell** gewählt werden.

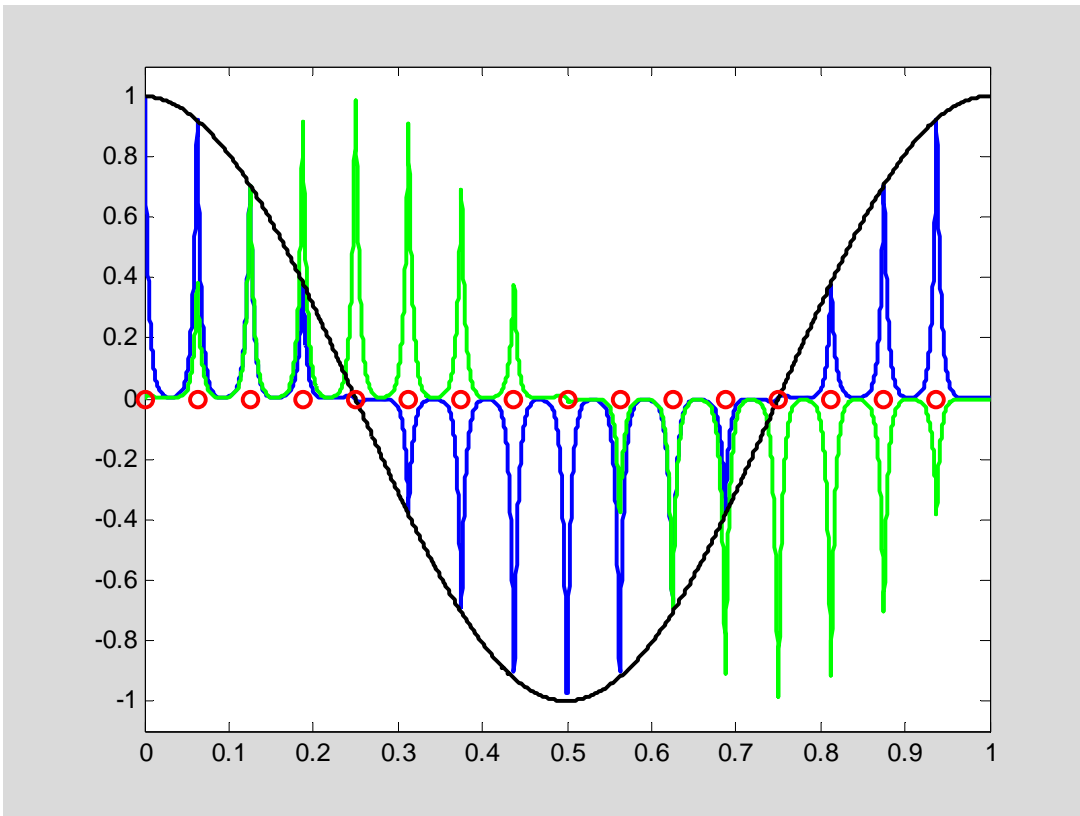
Aber: Es muss bei N Atomen insgesamt N verschiedene Wellenfunktionen geben, und all diese müssen als Bloch-Funktionen darstellbar sein:

$$\psi_{\underline{k}}(\underline{r}) = \exp(i\underline{k} \cdot \underline{r}) \cdot u_{\underline{k}}(\underline{r})$$

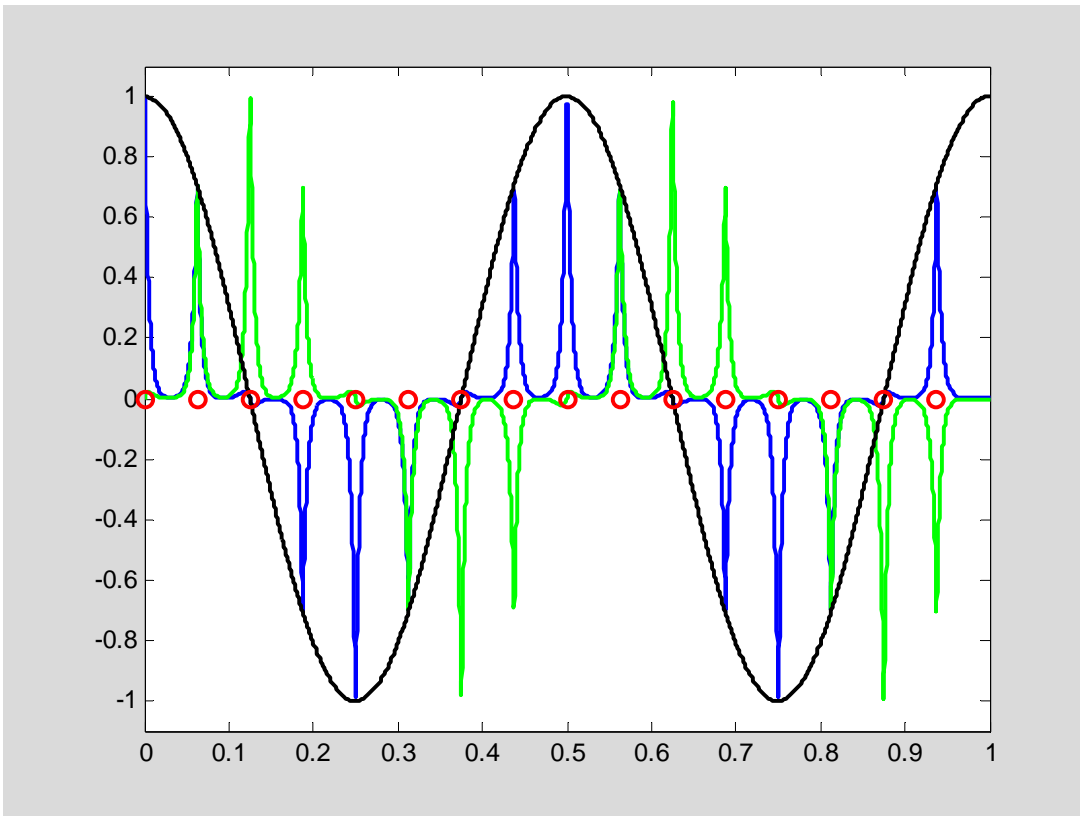
```
kBrill=pi/a;
k=kBrill/8;
envelop=cos(k*x);
plot(x,envelop,'k-','Linewidth',3);
```



```
realpart=wellenfunktion.*cos(k*x);  
imagpart=wellenfunktion.*sin(k*x);  
  
plot(x,realpart,'b-',x,imagpart,'g-',x,envelop,'k-'  
,xatom,yatom,'ro','Linewidth',2);axis([0 1 -1.1 1.1]);
```



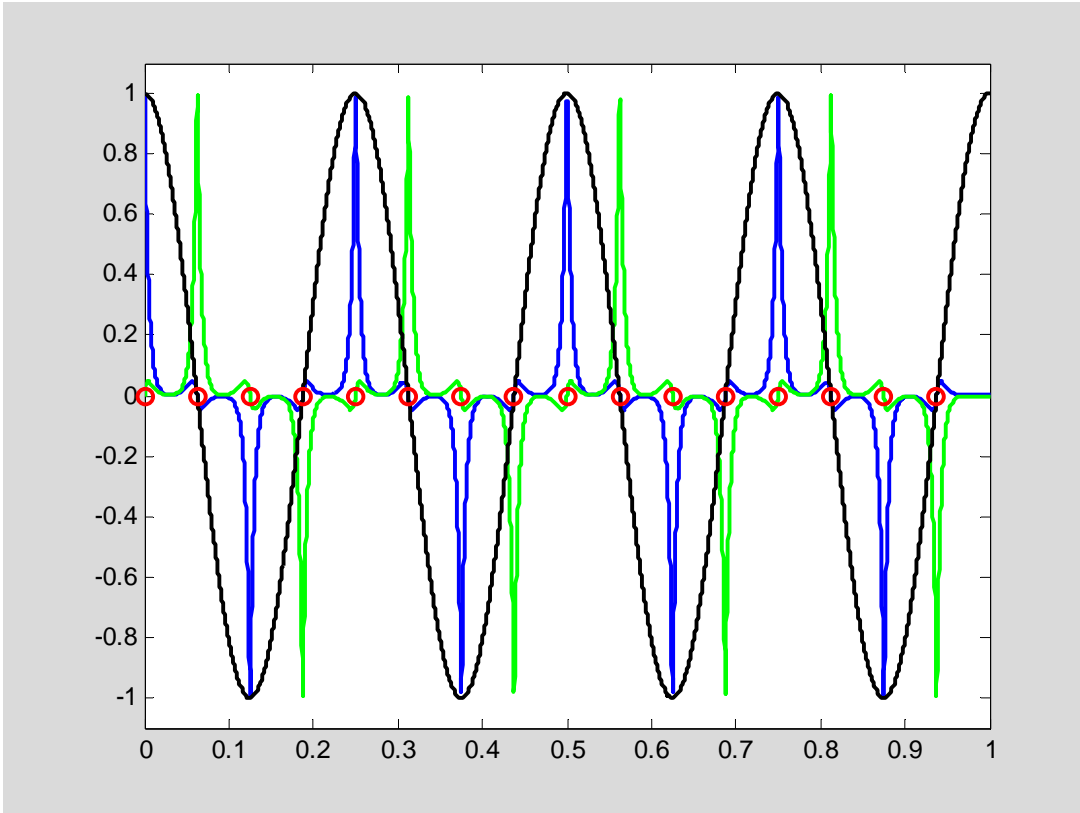
```
kBrill=pi/a;
k=kBrill/4;
envelop=cos(k*x);
realpart=wellenfunktion.*cos(k*x);
imagpart=wellenfunktion.*sin(k*x);
plot(x,realpart,'b-',x,imagpart,'g-',x,envelop,'k-
',xatom,yatom,'ro','Linewidth',2);axis([0 1 -1.1 1.1]);
```



```

kBrill=pi/a;
k=kBrill/2;
envelop=cos(k*x);
realpart=wellenfunktion.*cos(k*x);
imagpart=wellenfunktion.*sin(k*x);
plot(x,realpart,'b-',x,imagpart,'g-',x,envelop,'k-
',xatom,yatom,'ro','Linewidth',2);axis([0 1 -1.1 1.1]);

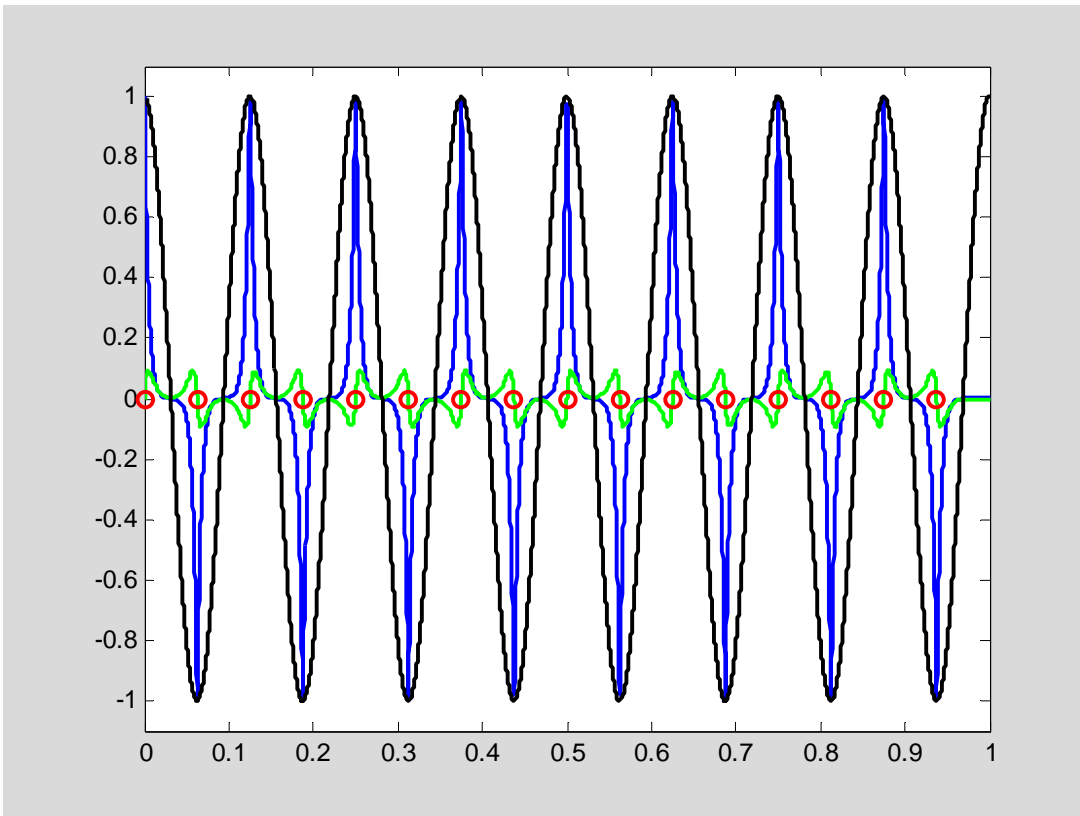
```



```

kBrill=pi/a;
k=kBrill;
envelop=cos(k*x);
realpart=wellenfunktion.*cos(k*x);
imagpart=wellenfunktion.*sin(k*x);
plot(x,realpart,'b-',x,imagpart,'g-',x,envelop,'k-
',xatom,yatom,'ro','Linewidth',2);axis([0 1 -1.1 1.1]);

```



Spin-orbit interaction

The spin-orbit interaction is basically a consequence of the relativistic transformation of the electromagnetic fields in a moving frame of reference.

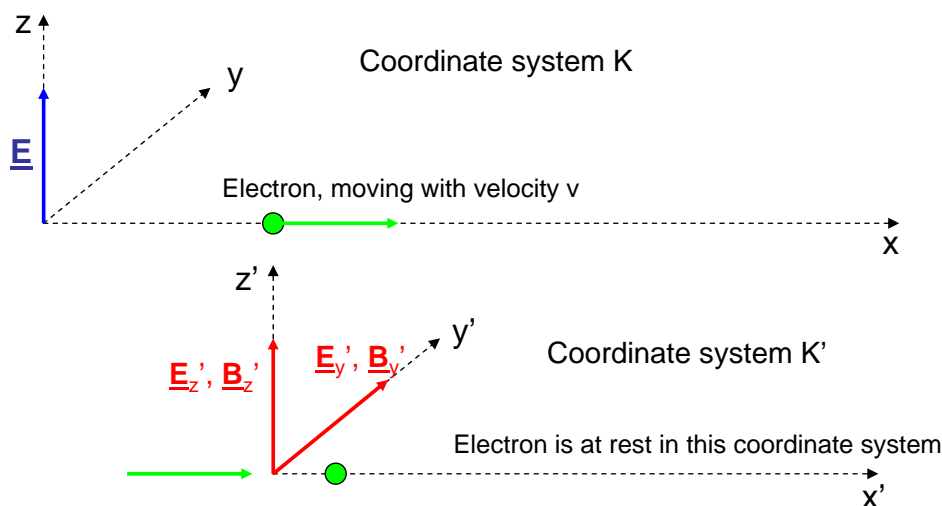
The following scenario explains the basic steps of the reasoning:

- ✳ Inside the material there exists an electric field $\underline{E}(\underline{r}) = -\underline{\nabla}\phi(\underline{r})$. This field is at rest in the laboratory frame of reference K.
- ✳ An electron moves with velocity \underline{v} through the material. In its own frame of reference K' it is at rest and "sees" transformed fields \underline{E}' and \underline{B}' .
- ✳ The interaction of the magnetic moment $\underline{\mu}$ of the electron with the field \underline{B}' is called "spin-orbit interaction": $-\underline{\mu} \cdot \underline{B}'$ is the relevant term in the Hamiltonian.

The reason why this interaction is called spin-orbit interaction is:

If the potential $\phi(\underline{r})$ is spherically symmetric (this situation is given in an atom with a central potential), the interaction term will be proportional to the product $(\underline{r} \times \underline{p}) \cdot \underline{\mu}$ and thus proportional to $\underline{L} \cdot \underline{S}$, where \underline{L} is the orbital angular momentum and \underline{S} is the spin angular momentum.

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If we have fields \underline{E} and \underline{B} in the coordinate system K, these fields are transformed into the moving frame of reference K'. We have to distinguish between the components parallel to the velocity \underline{v} and the components perpendicular to the velocity \underline{v} .

Parallel component:

$$\underline{E}'_{\parallel} = \underline{E}_{\parallel} \qquad \underline{B}'_{\parallel} = \underline{B}_{\parallel}$$

Perpendicular component:

$$\underline{E}'_{\perp} = \frac{(\underline{E} + \underline{v} \times \underline{B})_{\perp}}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad \underline{B}'_{\perp} = \frac{(\underline{B} - \frac{\underline{v} \times \underline{E}}{c^2})_{\perp}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

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These transformations are the **Lorentz transformations** from classical (relativistic) electrodynamics.

If there is only an electric field \underline{E} in the reference frame K, there will be a magnetic field \underline{B}' in the moving frame of reference K'.

We will consider the case $|\underline{v}| \ll c \implies \sqrt{1 - \frac{v^2}{c^2}} \approx 1$

$$\underline{B}' = \frac{-\underline{v} \times \underline{E}}{c^2}$$

This is the magnetic field acting on the electron magnetic moment $\underline{\mu}$. Note that this field has no influence on the electron charge $-e$, since the electron is at rest in its frame of reference K'!

The electron has a magnetic moment $\underline{\mu} = -g \cdot \mu_B \cdot \underline{S}$. The interaction term with the field \underline{B}' in the Hamiltonian is:

$$W = -\underline{\mu} \cdot \underline{B}' = -\frac{g \mu_B}{c^2} \cdot \underline{S} \cdot (\underline{v} \times \underline{E}) = \frac{g \mu_B}{c^2} \cdot (\underline{E} \times \underline{v}) \cdot \underline{S}$$

$$W = \frac{g \mu_B}{m c^2} \cdot (\underline{E} \times \underline{p}) \cdot \underline{S} \quad \text{We have used: } \underline{p} = m \cdot \underline{v} \text{ , } \underline{p} \text{ is the momentum}$$

We get the appropriate operator for this interaction by replacing $\underline{p} \rightarrow \hat{\underline{p}}$ and $\underline{S} \rightarrow \hat{\underline{S}}$

$$\hat{H}_{SO} = \frac{g \mu_B}{m c^2} \cdot (\underline{E} \times \hat{\underline{p}}) \cdot \hat{\underline{S}}$$

This is the spin-orbit interaction operator.

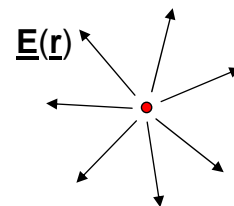
If we consider the field \underline{E} to be derived from a potential, $\underline{E}(\underline{r}) = -\nabla V(\underline{r})$, the Hamiltonian is:

$$\hat{H}_{SO} = \frac{g \mu_B}{m c^2} \cdot \hat{\underline{S}} \cdot (\nabla V(\underline{r}) \times \hat{\underline{p}})$$

This form is particularly suited to the situation in semiconductors (and metals).

The reason why this interaction is called the spin-orbit interaction comes from the particular situation in a central potential (e.g. in an atom). In an atom, the potential $V(\underline{r})$ is a central potential $V(\underline{r}) = V(r)$.

$$\underline{E}(\underline{r}) = -\nabla V(\underline{r}) = -\frac{dV(r)}{dr} \cdot \frac{\underline{r}}{|\underline{r}|} = \frac{1}{r} \cdot \frac{dV(r)}{dr} \cdot \underline{r}$$



This is only valid for a central potential.

$$\hat{H}_{SO} = -\frac{g \mu_B}{m c^2} \cdot \left(\frac{1}{r} \frac{dV(r)}{dr} \cdot \underline{r} \times \hat{\underline{p}} \right) \cdot \hat{\underline{S}} = -\frac{g \mu_B}{m c^2} \cdot \frac{1}{r} \frac{dV(r)}{dr} \cdot \hat{\underline{L}} \cdot \hat{\underline{S}}$$

$$\hat{\underline{L}} = \hat{\underline{r}} \times \hat{\underline{p}}$$

This operator is usually abbreviated as:

$$\hat{H}_{\text{SO}} = \xi_{\text{SO}} \cdot \hat{\underline{L}} \cdot \hat{\underline{S}} \quad \text{With the spin-orbit coupling "constant"} \quad \xi_{\text{SO}} = -\frac{g\mu_B}{mc^2} \cdot \frac{1}{r} \frac{dV(r)}{dr}$$

In an atom, the quantity ξ_{SO} has to be calculated by the expectation value:

$$\left\langle \frac{1}{r} \frac{dV(r)}{dr} \right\rangle \quad \text{with the appropriate spatial wave function of the electrons.}$$

For simple atoms (like H) this can be done, since both $V(r)$ and the wave functions are known precisely.

For more complicated atoms, for molecules and especially for the case of semiconductors (and metals), one has to take ξ_{SO} as a parameter from experiment.

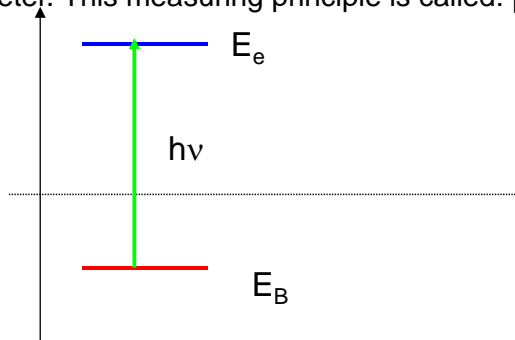
Photoemission Spectroscopy

Photoemission is one of the fundamental experimental techniques to determine the band structure of materials directly.

The basic process is the interaction of a photon, energy $h\nu$, with an electron, energy E_B in the material.

This electron is excited to an energy $E_e = E_B + h\nu$.

If this electron energy E_e is above the vacuum level of the material, and if the velocity component towards the surface is sufficiently large for the electron to leave the material, its energy E_e and the direction can be determined by an electron spectrometer. This measuring principle is called: **photoemission spectroscopy**

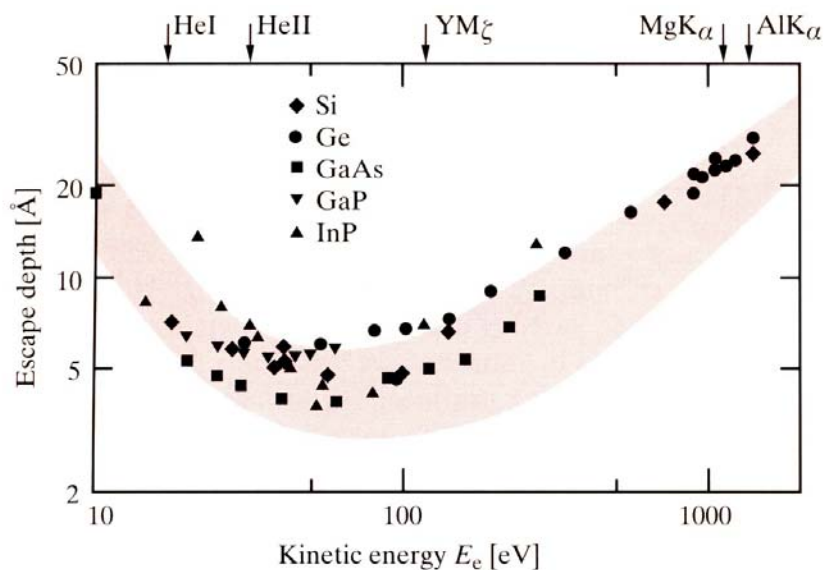


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For slow electrons with energies E_e in the 10eV to 100 eV range, the electron escape depth from the material is very small. Photoemission in this UV and soft X-ray regime is therefore a surface sensitive technique.

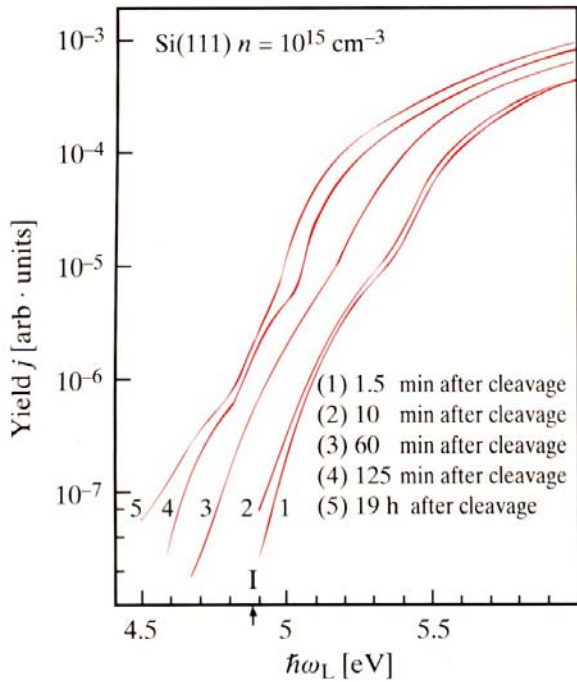


Escape depth of slow electrons in different materials

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Photocurrent (yield) near threshold for a Si(111) surface.

The effects of surface contaminations is clearly visible.

There is a photothreshold I (also called ionization energy I):

At this photothreshold the (kinetic) electron energy E_e (with respect to the vacuum level) is zero.

Electrons with lower energy cannot escape into the vacuum.

$$E_e = h\nu - I$$

For a metal, I would be the work function $e\Phi_m$

For a semiconductor, the definition of the relevant energy levels is slightly more involved.

The **yield** is the (angle integrated) photocurrent.

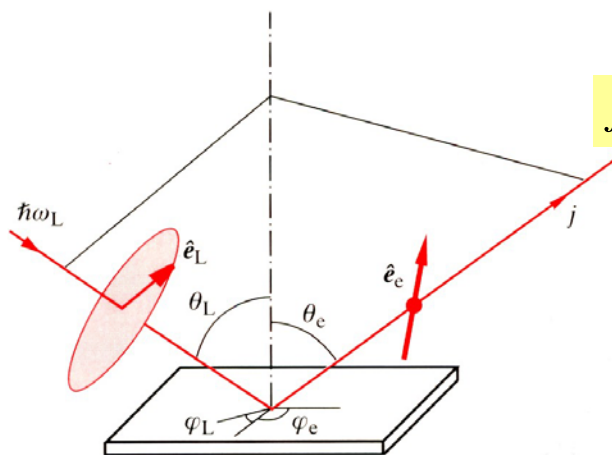
Near threshold, this yield is particularly sensitive to the surface conditions.

For a complete description of a photoemission experiments, one has to specify:

- i) Photon: Energy $h\nu$, polarization vector \hat{e}_L , directions θ_L, φ_L with respect to the surface.
- ii) Electron: Energy E_e , polarization vector \hat{e}_e , directions θ_e, φ_e with respect to the surface

A complete experiment would measure the photocurrent j (count the number of photoelectrons) as a function of all of these variables.

$$j = j(h\nu, \hat{e}_L, \theta_L, \varphi_L, E_e, \hat{e}_e, \theta_e, \varphi_e)$$



Definition of relevant angles for angle resolved photoemission.

Basic experiments:

$h\nu$ is fixed, the angles θ_L, φ_L are fixed.

The electrons are not analyzed with respect to the spin \hat{e}_e .

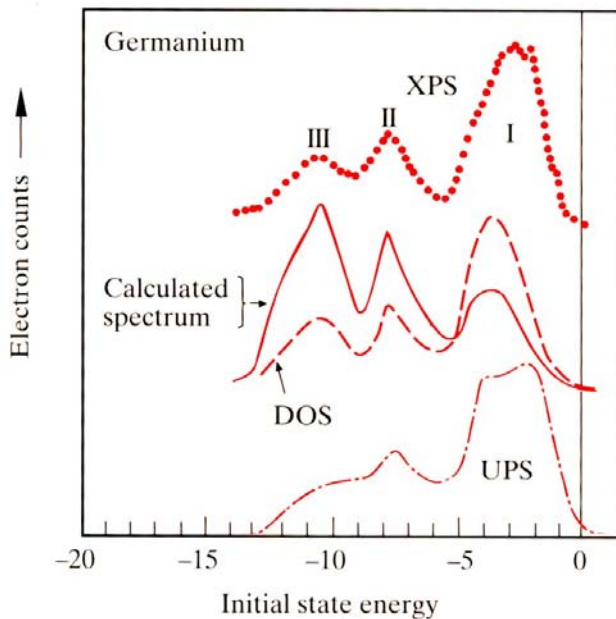
One measures the current with respect to E_e .

If the electron energy analyzer resolves the angles θ_e, φ_e , the experiment is called:

Angle Resolved PhotoElectron Spectroscopy : ARPES

If the electron energy analyzer integrates over the angles θ_e, φ_e , the experiment is called:

Angle Integrated Photoelectron Spectroscopy.



The direct result of a photoelectron spectroscopy experiment are:

Energy Distribution Curves: EDC

These measured EDCs have to be compared with band structure calculations in order to extract details of the band structure.

In angle integrated experiments, one measures something like the Density of States (DOS) of the various valence bands.

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There are three crucial parts in a photoemission setup:

- i) The photon source
- ii) The electron energy analyzer
- iii) The electron detector.

i) The ideal photon source should:

Produce an adjustable flux of photons with adjustable energy, adjustable energy resolution, and adjustable polarization.

The flux of photons should be as high as possible.

The source where most of these properties are realized:

Synchrotron radiation facility.

However:

Synchrotron light is very expensive (and is only available in dedicated synchrotron radiation facilities).

Laboratory light sources: UV: Helium I and Helium II gas discharge lamps.

X-rays: characteristic X-ray sources like Al K_α at 1486.6 eV.

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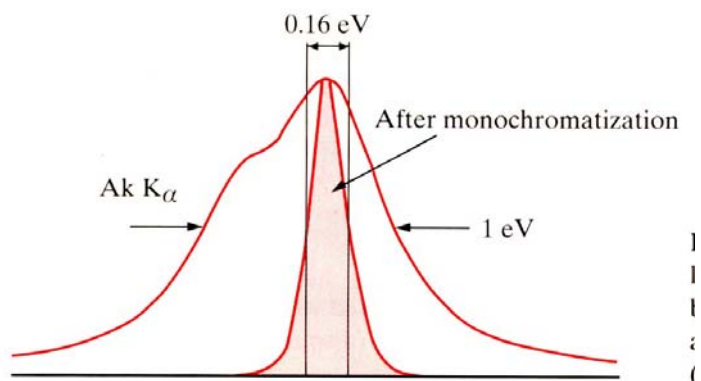
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Energy resolution of the photons:

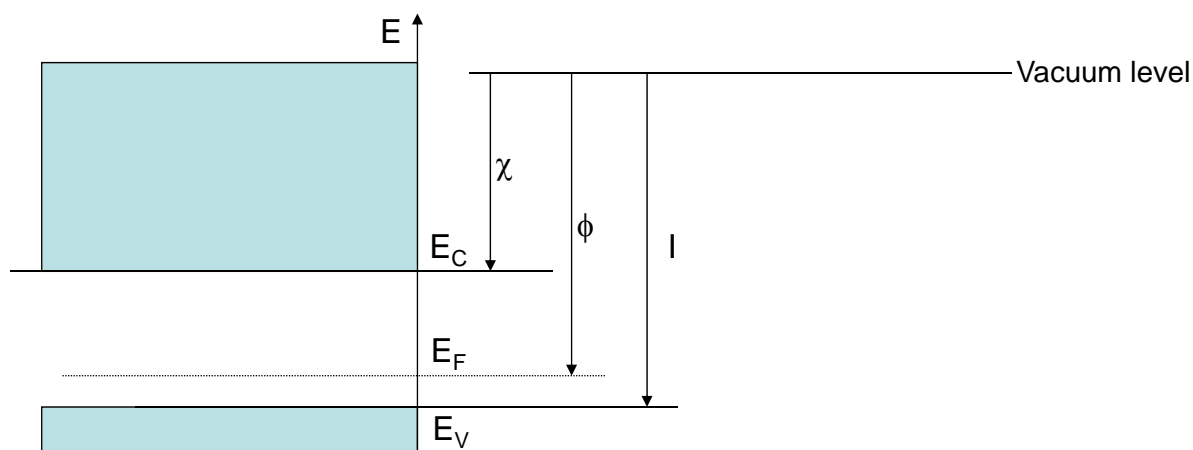
Gas discharge lamps like HeI and HeII: $\Delta(h\nu) \approx 1 \text{ meV}$

X-ray sources: have to be monochromatized!

This results in (severe) loss of intensity



Synchrotron radiation has to be monochromatized anyhow, because it is broadband.



Relevant energy definitions for a semiconductor:

E_V : valence band edge

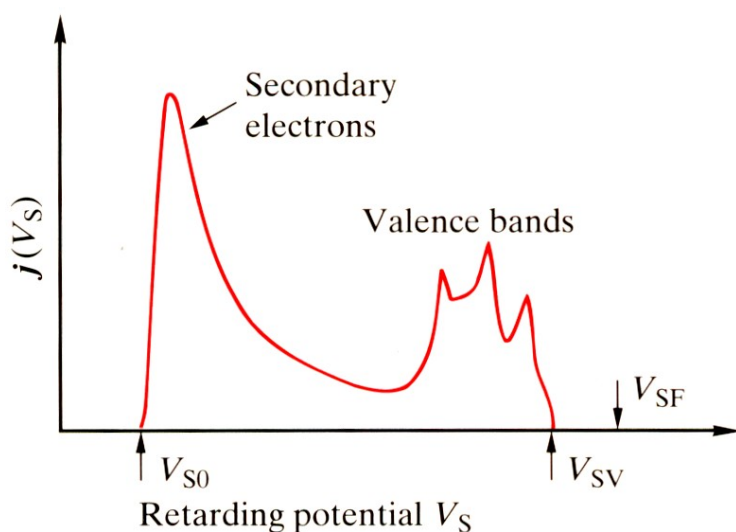
E_C : conduction band edge

χ : electron affinity

ϕ : electron work function

I : photothreshold energy

Experimental difficulty: How does one measure the kinetic energy of a charged particle like the electron?



V_{S0} : Vacuum level

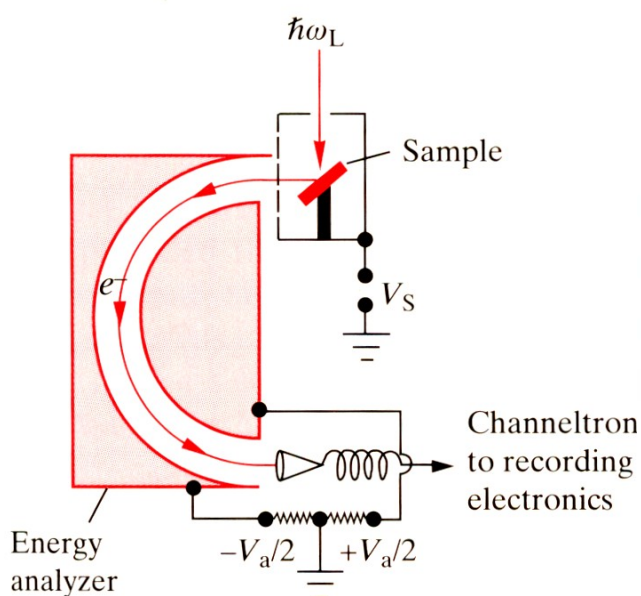
V_{SV} : Top of the valence bands

V_{SF} : Fermi level of the sample

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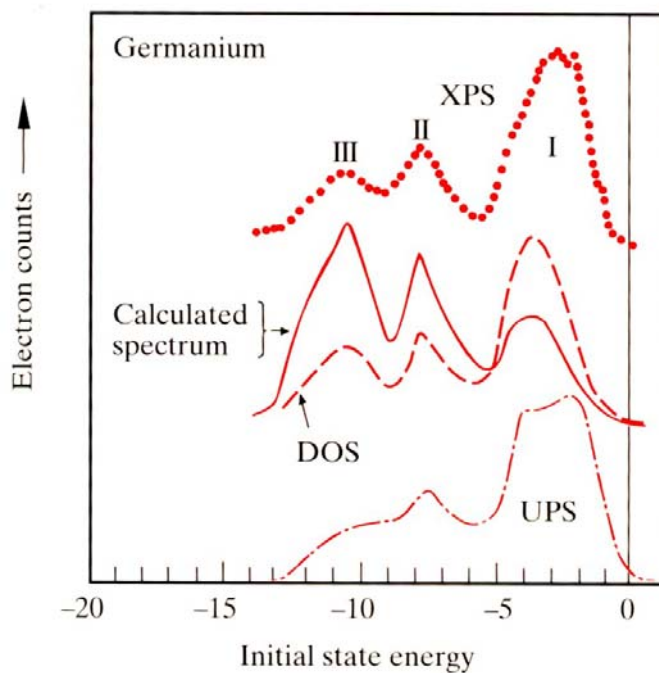
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Photoelectron spectrometer with hemispherical analyzer.

Detector: Channeltron.

V_s : Retarding Potential



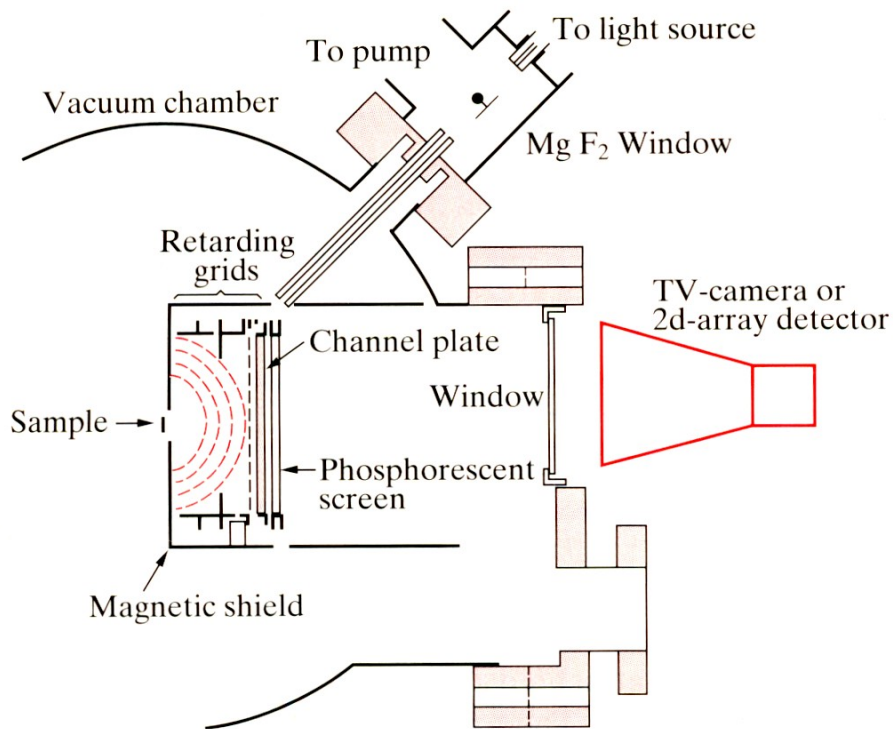
XPS and UPS spectra of the valence band of germanium.

Dashed line: Calculated density of states multiplied by the transition probability.

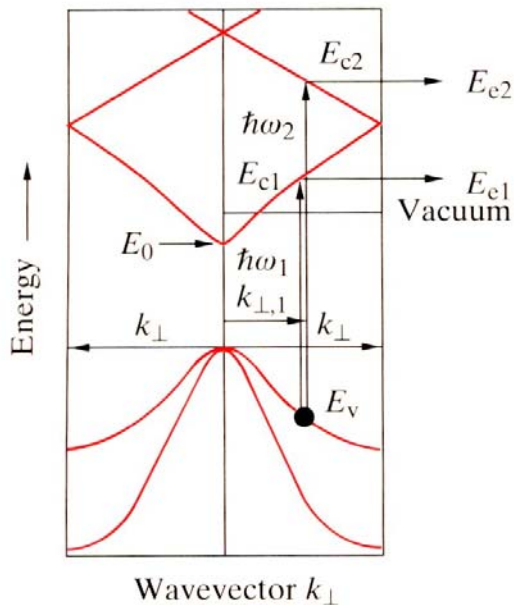
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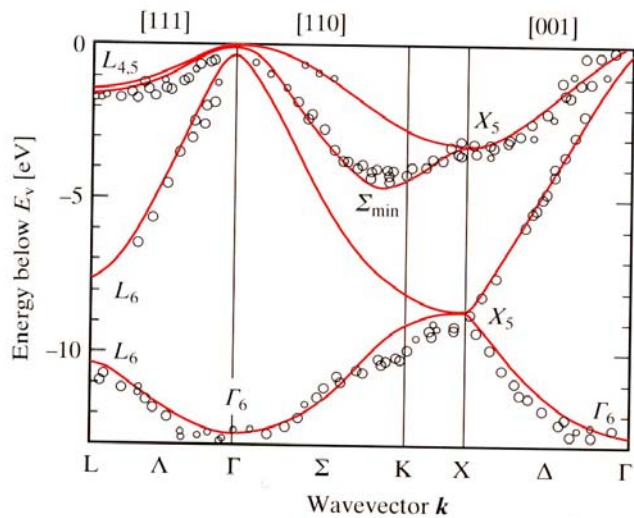
Angle resolved multi channel photoemission system. The electron energy analyzer is based on a retarding potential LEED system.



Method to determine k_{\perp} under the assumption of free electron like conduction bands.

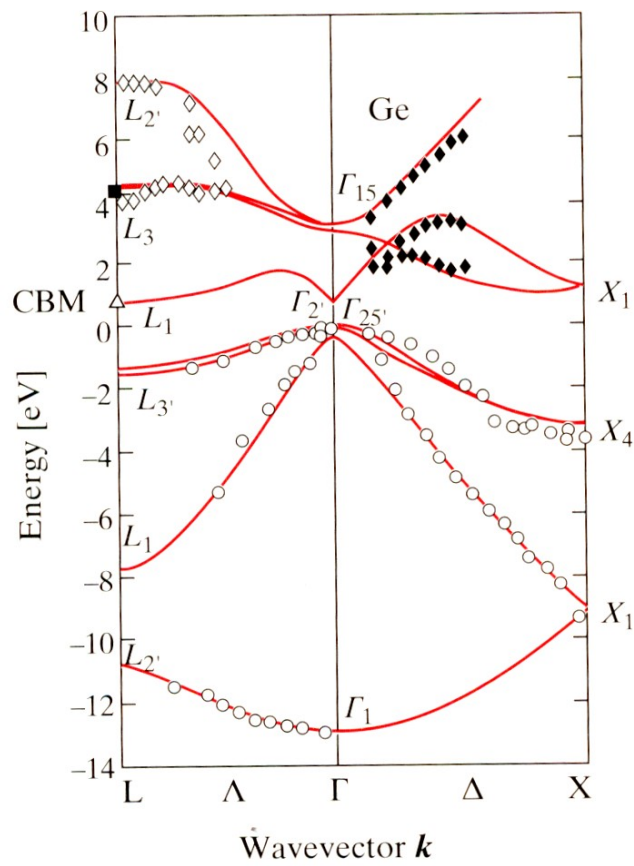
Two photon energies are used.

E_0 is adjusted.



Valence band structure of Ge by angle resolved UPS (circles).

Comparison to band structure calculation.



Germanium band structure.

Valence bands: UPS

Conduction bands:

Inverse Photoemission.

Inverse Photoemission can explore the unoccupied bands, particularly those between the Fermi level and the vacuum level.

Inverse Photoemission usually detects the photons at a fixed energy, e.g. at ≈ 10 eV by efficient energy selective photon detectors.