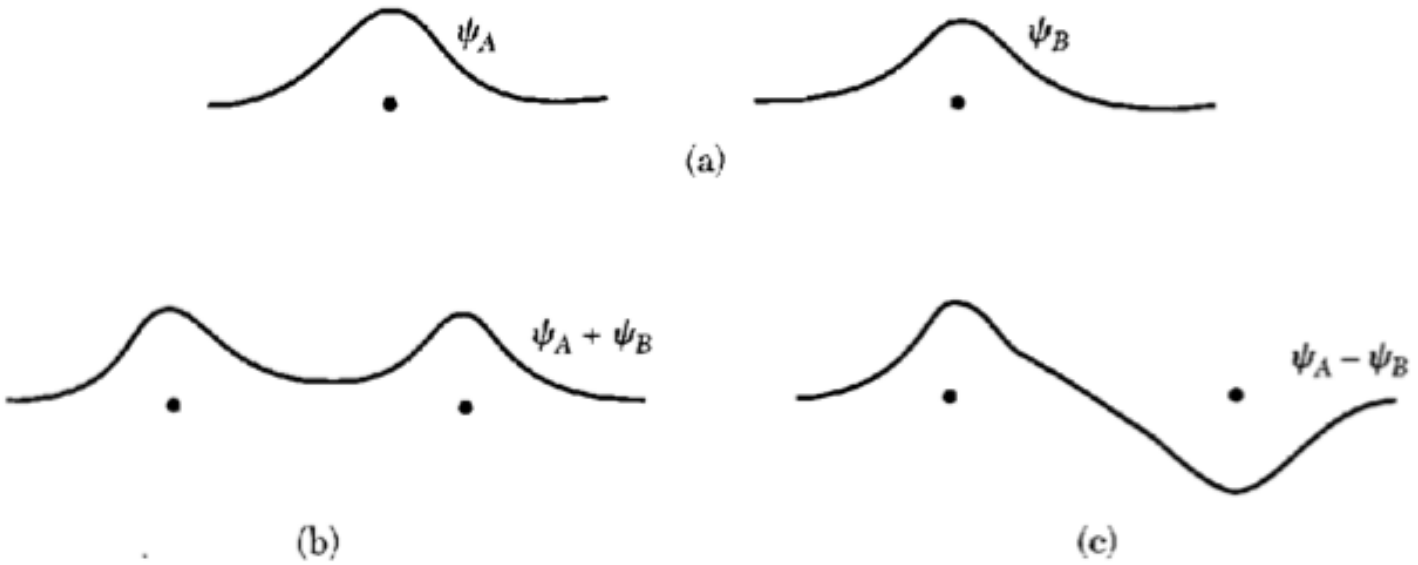
PHY404- Solid State Physics II

Assoc.Prof. Yeşim Moğulkoç

Calculation of Energy Bands

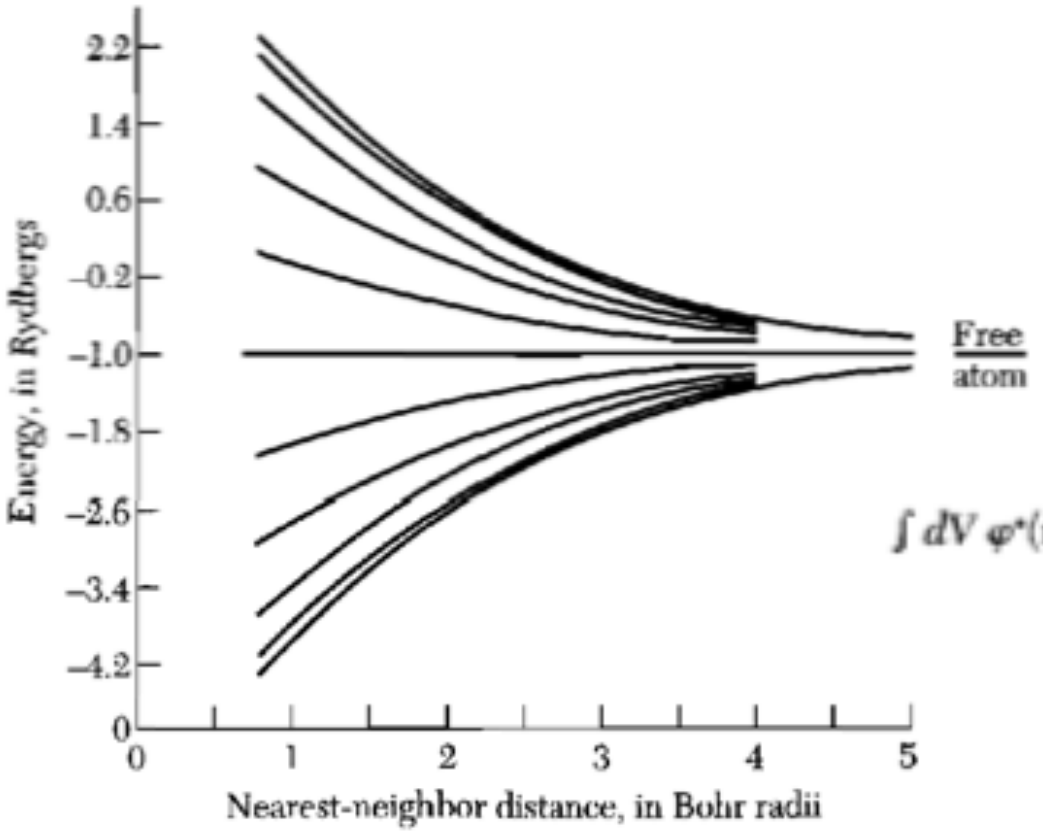
Tight Binding Method for Energy Bands

Consider two hydrogen atoms, each with an electron in the 1**s** ground state.



(The figure is used from Introduction to Solid State Physics, C. Kittel)

Calculation of Energy Bands



The 1s band of a ring of 20 atoms; the one-electron energies are calculated in the tight-binding approximation with the nearest-neighbor overlap integral with this eq:

$$\int dV\, \varphi^*(\mathbf{r}) H \varphi(\mathbf{r}) = -\alpha \;; \quad \int dV\, \varphi^*(\mathbf{r}-\boldsymbol{\rho}) H \varphi(\mathbf{r}) = -\gamma$$

(The figure is used from Introduction to Solid State Physics, C. Kittel)

Wigner-Seitz Method

Wigner and Seitz showed that for the alkali metals there is no inconsistency between the electron wavefunctions of free atoms and the nearly free electron model of the band structure of a crystal. Over most of a band the energy may depend on the wavevector nearly as for a free electron. However the Bloch wavefunction, unlike a plane wave, will pile up charge on the positive ion cores as in the atomic wavefunction.

A Bloch function satisfies the wave equation

$$\left(\frac{1}{2m}\mathbf{p}^2 + U(\mathbf{r})\right) e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) \quad .$$

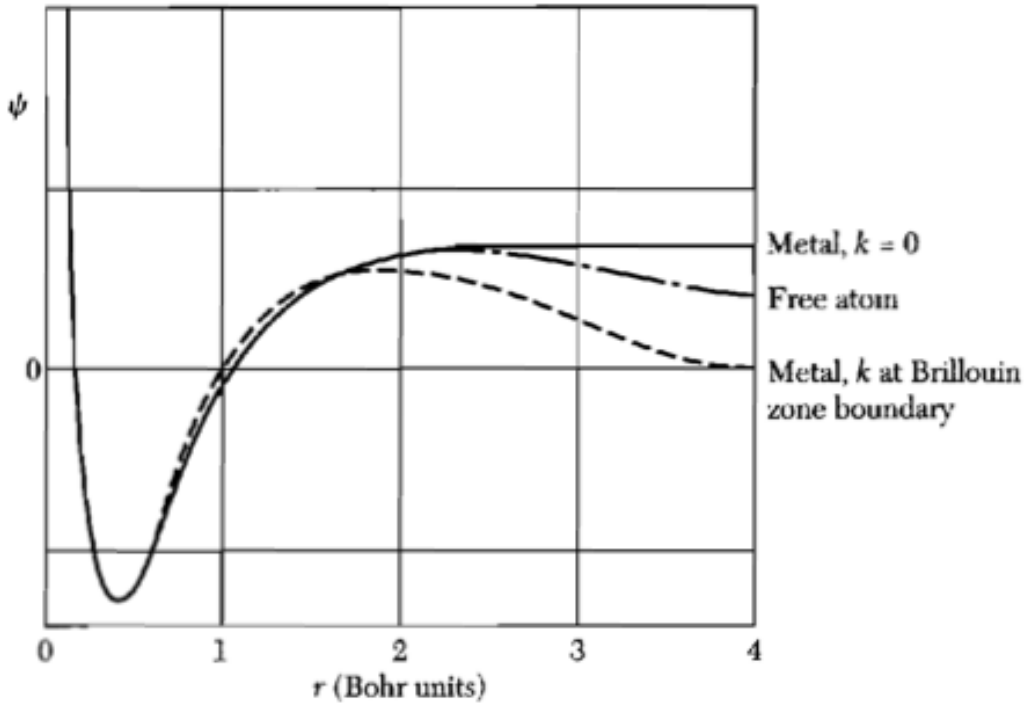
With $\mathbf{p} \equiv -i\hbar$ grad, we have

$$\mathbf{p}\, e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) = \hbar\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) + e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{p} u_{\mathbf{k}}(\mathbf{r}) \;;$$

$$\mathbf{p}^2 e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) = (\hbar k)^2 e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) + e^{i\mathbf{k}\cdot\mathbf{r}} (2\hbar\mathbf{k}\cdot\mathbf{p}) u_{\mathbf{k}}(\mathbf{r}) + e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{p}^2 u_{\mathbf{k}}(\mathbf{r})$$

(The figure is used from Introduction to Solid State Physics, C. Kittel)

Wigner-Seitz Method

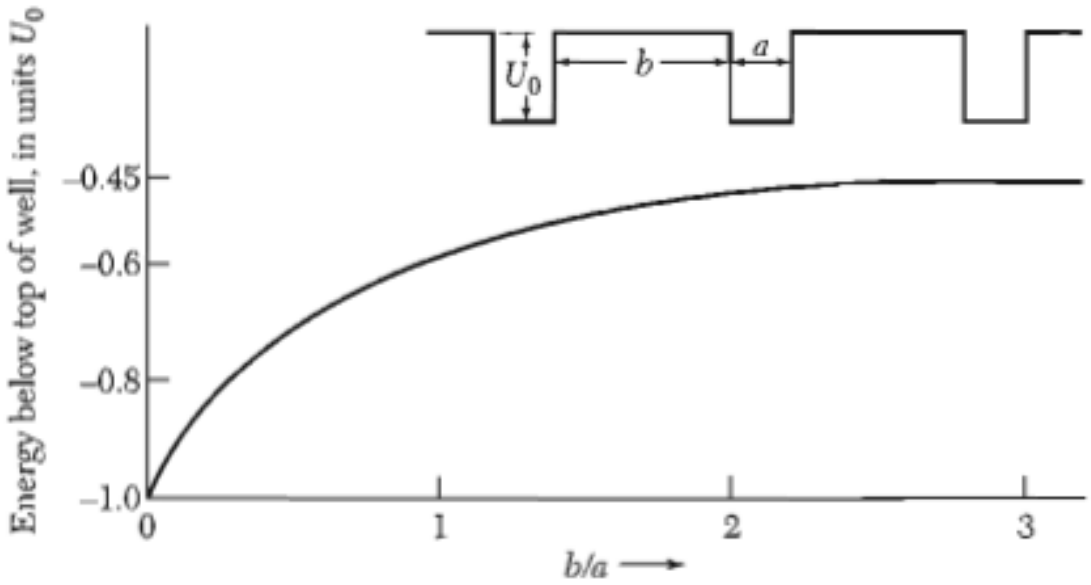


Radial wavefunctions for the **3s** orbital of free sodium atom and for the 3s conduction band in sodium metal.

(The figure is used from Introduction to Solid State Physics, C. Kittel)

Cohesive energy

The stability of the simple metals with respect to free atoms is caused by the lowering of the energy of the Bloch orbital with **k** = **0** in the crystal compared to the ground valence orbital of the free atom.



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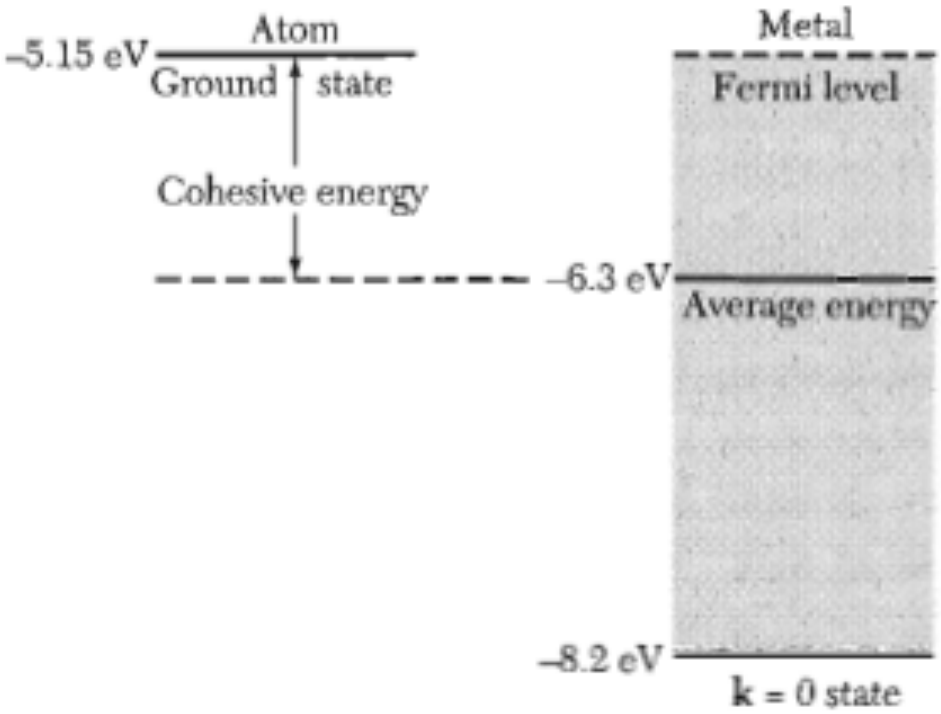
Cohesive energy



Cohesive energy of sodium metal is the difference between the average energy of an electron in the metal (-6.3 eV) and the ground state energy (-5.15 eV)

(The figure is used from Introduction to Solid State Physics, C. Kittel)