Theoretical Materials Science

(Condensed Matter Theory I & II)

Wahlpflichtfach

Tue & Wed 10 – 12
exercises Wed 14 – 16

combine with
Quantenmechanik gebundene Atome (Udo Schatz)
Mo 12 – 14

or
Comp. aspects of Stat. phys. (Luca Ghiringhelli)
Mo 10 – 12

Who are we ?

Matthias Scheffler	Fritz-Haber-Institut of MPG
Alex Tkatchenko	
Patrick Rinke	
Volker Blum	

http://th.FHI-Berlin.MPG.de

Literature: see 1. exercise sheet

Script: 1) this handwritten material (available directly after the lecture)

2) A typed manuscript available "soon" after the lecture we try 1-2 days.

Chapter 0 A general intro

1) 10^{23} electrons & 10^{23} nuclei
   ⇒ basic theory: electronic structure theory (many-body)
   ⇒ interaction between atom
   ⇒ reaction to outside perturbation
   ⇒ properties
2) properties ⇒ function
3) predict improved functional material (photovoltaic, new catalyst (energy from sun, wind ...) ⇒ "fuel"

⇒ urgent need; to tackle with energy challenge.

≡ fundamental research

Many-body theory

⟹ novel phenomena

do this is only getting possible now

a) new concepts and methods

b) high-performance computers

Future (next 5+x years)

Building a library of hitherto unknown materials

so far experiment trial & error

Soon calculate > 10000 potential material

⟹ new level of understanding, trends & mechanism

The field is huge & important

one indicator for Nobel prizes: since 1980 33 Nobel prizes to materials science

units

SI ← will use this in the beginning

then "atomic units"

$\frac{e^2}{4\pi\varepsilon_0} = 2$

$\hbar = 1$

$m_e = 0.5$

} Rydberg atomic units

natural unit of energy = 1 Ryd = 13,606 eV
= binding energy of electron in H.

length unit: 1 bohr = 0.529 Å
0.0529 nm

nano = 10^{-9}

Chapter 1 Introduction

1.1 The many body hamiltonian

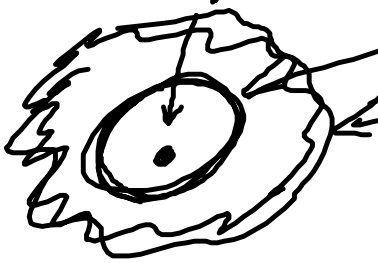
$$H\psi = E\psi$$

$\Updownarrow$

materials build from nuclei & electrons

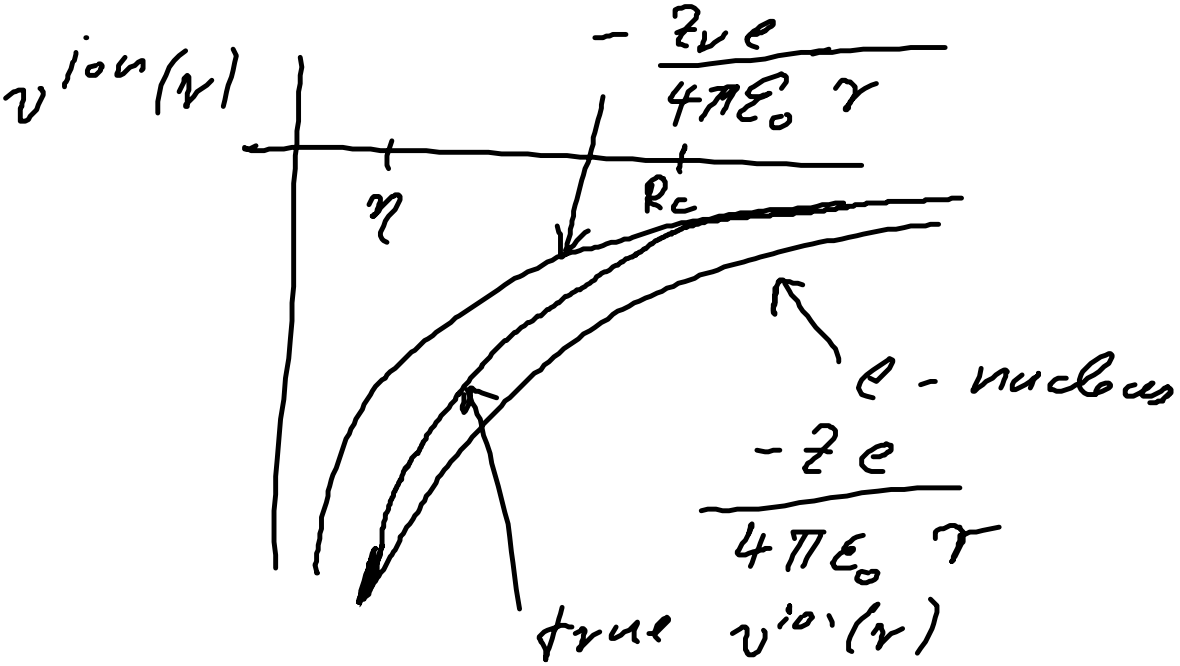
or

ions + all valence electrons



ions $\equiv$ core + valence elec

$\equiv$ fixed object



↑
frozen core approximation
not necessary
but good for talking.

number

atom	electronic configuration	Z	Z_V	R_c [bohr]	$v_{ion}(r)$ [Ryd]
H	$1s^1$	1	1	0	$-\frac{2}{r}$
He	$1s^2$	2	2	0	$-\frac{4}{r}$
C	$[1s^2]2s^2 2p^2$	6	4	0.7	$r \geq \eta$ $-\frac{8}{r}$ $\eta < r \leq R_c$ (?) $r \leq \eta = \frac{-12}{r}$
Si	$[1s^2 2s^2 2p^6]$ $3s^2 3p^2$	14	4	1.7	...

if interatomic distance $< 2R_c$
then frozen-core approach cannot be used.