
Theoretical Material Science

Prof. Scheffler, Dr. Alexandre Tkatchenko, Dr. Patrick Rinke
Theory Department
Fritz Haber Institute of the Max Planck Society
Faraday Weg 4-6
Berlin

Version: November 1, 2012

Table of Contents

0	Introductory Remarks	2
0.1	Introduction	2
0.2	Literature for this lecture	7
0.3	The following symbols and terms are used	10
0.4	Atomic Units	11
1	Introduction	12
1.1	The Many-Body Hamilton Operator	12
1.2	Separation of the Dynamics of Electrons and Ions	15
1.2.1	Adiabatic Approximation or Born-Oppenheimer Approximation	15
1.2.2	Static Approximation	19
1.2.3	Examples	20
1.2.3.1	Structure, Lattice Constant, and Elastic Properties of Perfect Crystals	21
1.2.3.2	Lattice Waves (Phonons)	22
1.3	The Ewald Method	23
2	Fermi Statistics of Electrons and Some Definitions	28
2.1	Statistical Mechanics	28
2.2	Fermi Statistics of the Electrons	29
2.3	Some Definitions	31
3	Electron-Electron Interaction	35
3.1	Electron-Electron Interaction	35
3.2	Hartree Approximation	36
3.3	Hartree-Fock Approximation	43
3.4	The Exchange Interaction	48
3.5	Koopmans' Theorem	54
3.6	The X_α Method	56
3.7	Thomas-Fermi Theory and the Concept of Screening	58
3.8	Density-Functional Theory	65
3.8.1	Meaning of the Kohn-Sham Single-Particle Energies ϵ_i	74
3.8.2	Spin Polarization	80
3.8.3	Two Examples	81
3.9	Summary (Electron-Electron Interaction)	84

4	Lattice Periodicity	88
4.1	Lattice Periodicity	88
4.2	The Bloch Theorem	104
4.3	The Reciprocal Lattice	106
5	The Band Structure of the Electrons	114
5.1	Introduction	114
5.1.1	What Can We Learn from a Band Structure?	117
5.2	General Properties of $\epsilon_n(\mathbf{k})$	121
5.2.1	Continuity of $\epsilon_n(\mathbf{k})$ and Meaning of the First and Second Derivatives of $\epsilon_n(\mathbf{k})$	121
5.2.2	Time Reversal Symmetry	125
5.2.3	The Fermi Surface	128
5.3	The LCAO (linear combination of atomic orbitals) Method	129
5.3.1	Band Structure and Analysis of the Contributions to Chemical Bonding	133
5.4	The Density of States, $N(\epsilon)$	135
5.5	Other Methods for Solving the Kohn-Sham Equations of Periodic Crystals	137
5.5.1	The Pseudopotential Method	137
5.5.2	APW and LAPW	138
5.5.3	KKR, LMTO, and ASW	138
5.6	Many-Body Perturbation Theory (beyond DFT)	138
6	Cohesion (Bonding) in Solids	139
6.1	Introduction	139
6.2	Van der Waals Bonding	142
6.3	Ionic bonding	150
6.4	Covalent bonding	156
6.4.1	Hybridization	158
6.5	Metallic bonding	162
6.6	Hydrogen bonding	172
6.6.1	Some Properties of Hydrogen bonds	173
6.6.2	Some Physics of Hydrogen bonds	174
6.7	Summary	176
7	Lattice vibrations	178
7.1	Introduction	178
7.2	Vibrations of a classical lattice	179
7.2.1	Adiabatic (Born-Oppenheimer) approximation	179
7.2.2	Harmonic approximation	180
7.2.3	Classical equations of motion	181
7.2.4	Comparison between $\epsilon_n(\mathbf{k})$ und $\omega_i(\mathbf{k})$	184
7.2.5	Simple one-dimensional examples	184
7.2.5.1	Linear chain with one atomic species	184
7.2.5.2	Linear chain with two atomic species	187
7.2.6	Phonon band structure	188
7.3	Quantum theory of the harmonic crystal	191

7.3.1	One-dimensional quantum harmonic oscillator	191
7.3.2	Three-dimensional quantum harmonic crystal	193
7.3.3	Lattice energy at finite temperatures	194
7.3.4	Phonon specific heat	196
7.3.4.1	High temperature limit (Dulong-Petit law)	197
7.3.4.2	Intermediate temperature range (Einstein approximation)	198
7.3.4.3	Low temperature limit (Debye approximation)	199
7.4	Anharmonic effects in crystals	201
7.4.1	Thermal expansion (and melting)	201
7.4.2	Heat transport	202
8	Magnetism	204
8.1	Introduction	204
8.2	Macroscopic Electrodynamics	206
8.3	Magnetism of atoms and free electrons	208
8.3.1	Total angular momentum of atoms	208
8.3.2	General derivation of atomic susceptibilities	209
8.3.2.1	Second term: Larmor/Langevin diamagnetism	212
8.3.2.2	Third term: Van Vleck paramagnetism	213
8.3.2.3	First term: Paramagnetism	213
8.3.2.4	Paramagnetic susceptibility: Curie's law	215
8.3.3	Susceptibility of the free electron gas	217
8.3.4	Atomic magnetism in solids	220
8.4	Magnetic order: Permanent magnets	223
8.4.1	Ferro-, antiferro- and ferrimagnetism	224
8.4.2	Interaction versus thermal disorder: Curie-Weiss law	226
8.4.3	Phenomenological theories of ferromagnetism	228
8.4.3.1	Molecular (mean) field theory	228
8.4.3.2	Heisenberg and Ising Hamiltonian	231
8.4.4	Microscopic origin of magnetic interaction	237
8.4.4.1	Exchange interaction between two localized moments	238
8.4.4.2	From the Schrödinger equation to the Heisenberg Hamiltonian	240
8.4.4.3	Exchange interaction in the homogeneous electron gas	242
8.4.5	Band consideration of ferromagnetism	244
8.4.5.1	Stoner model of itinerant ferromagnetism	246
8.5	Magnetic domain structure	250
9	Superconductivity	255
9.1	Introduction	255
9.2	Meissner effect	257
9.3	London theory	259
9.4	Flux quantization	261
9.5	Ogg's pairs	262
9.6	Microscopic theory - BCS theory	263
9.6.1	Cooper pairs	263
9.7	Bardeen-Cooper-Schrieffer (BCS) Theory	266

0 Introductory Remarks

0.1 Introduction

A solid or, more generally, condensed matter is a complex many-body-problem ($\sim 10^{23}$ electrons and nuclei per cm^3). The most important foundations of its theoretical description are electronic-structure theory and statistical mechanics. Due to the complexity of the many-body problem there is a large variety of phenomena and properties. Their description and understanding is the purpose of this lecture course on “condensed matter”. Keywords are e.g. crystal structure, hardness, magnetism, conductivity, superconductivity, etc.. The name of this lecture (*Theoretical Materials Science*) indicates that we intend to go a step further, i.e., “condensed matter” has been replaced by “materials”. This is a small, but nevertheless important generalization. When we talk about materials, then in addition to phenomena and properties we also think of potential applications, i.e., the possible function of materials, like in electronic, magnetic, and optical devices (solar cells or light emitters), sensor technology, catalysts, lubrication, and surface coatings (e.g. with respect to protection against corrosion and mechanical scratch-resistance). It is obvious that these functions, which are determined to a large extent by properties on a nanometer scale, play an important role in many technologies on which our lifestyle and also the wealth of our society are based. Also because of this (next to the fascination of the phenomena in fundamental research) today’s material science is playing a truly significant socio-economical role.

The field of electronic-structure theory, applied to problems from material science described above, is in an important, active phase with rapid developments in the underlying theory, new methods, new algorithms, and new computer codes. For several years now a theory is evolving that, taking advantage of high and highest performance computers, allows an atomistic modelling of complex systems with predictive power (starting from the fundamental equations of the interacting many-body problem). Two central ingredients of such *ab initio* theories are a reliable description of the underlying elementary processes (e.g. breaking and forming of chemical bonds), and a correct treatment of their statistical mechanics.

Because of the importance of many-body effects in the description of the interactions in poly-atomic systems up to now a systematic treatment was barely possible. The complexity of the quantum mechanical many-body problem required the introduction of approximations, which often were not obvious. “Only” since 1978 (or 1982)¹ have reliable

¹V.L. Moruzzi, J.F. Janak, and A.R. Williams, *Calculated Electronic Properties of Metals*, Pergamon Press (1978) ISBN 0-08-022705-8; and M.T. Yin and M.L. Cohen, *Theory of static structural properties*,

calculations for solids been carried out and only this allows to check the possibly reasonable (and often necessary) approximations and to give the reasons for their success; or it is demonstrated which approximations have to be abandoned. And the development of the underlying theory (density-functional theory, DFT) started only in 1964². Today this development has reached a feasible level for many types of problems, but it is not completed yet.

With these “new” developments the approximations, which in existing text books are introduced *ad hoc*, can be inspected. Further it is possible to make quantitative predictions, e.g. for the properties of new materials. But still *theoretical condensed matter physics* or *theoretical materials science*, is in an active state of development. Phenomena investigated or understood in a very incomplete way, include phase transitions, disorder, catalysis, defects (meta-, bistabilities), properties of heterostructures and quantum dots, crystal growth, systems containing *f*-electrons, high-temperature-superconductivity, electronic excitation, and transport.

For modern *theoretical material science* there are two main challenges:

1. To explain experimentally found properties and phenomena and to place them in a bigger context and order. This is done by developing models, i.e., by a reduction to the key physical processes, which enables a qualitative or semi-quantitative understanding. As mentioned before, there are examples for which these tasks are not accomplished yet.
2. To predict, independent of experiment, properties of systems that have not been investigated experimentally so far – or situations that cannot be investigated by experiments directly. The latter include conditions of very high pressures or conditions that of chemically or radioactively harsh. A recent development is concerned with building a “library of hitherto unknown materials”. We will get back to this project at the end of this lecture.

The latter point shall be illustrated by the following example:

Only today one starts to understand fundamental questions of condensed matter. Until recently it was not possible to show theoretically why diamond (carbon) is harder than Si. Further, properties can be calculated under conditions, which are inaccessible by experiment, e.g. the viscosity and the melting temperature of iron at pressures that exist at the earth core. These theoretical investigations have become possible only since 1978 (the example concerning the properties of iron can be investigated only since about 1999³).

The element carbon exists in three solid phases: *i*) as amorphous solid and in crystalline form *ii*) as graphite and *iii*) as diamond^{4,5}. Graphite is the most stable phase, i.e., the

crystal stability, and phase transformations: Application to Si and Ge, Phys. Rev. B **26**, 5668 (1982).

²To some extend earlier concepts by Thomas, Fermi, Hartree, and Slater may be considered as preparation for this route.

³D. Alfe, M.J. Gillan, and G.D. Price, NATURE **401**, 462 (1999).

⁴Diamond is the hardest known material, i.e., it has the highest bulk modulus. Diamonds without defects are most transparent to light. At room temperature their thermal conductivity is better than that of any other material.

⁵This statement is slightly simplified. More precisely (up to now) two types of graphite and two types

one with the lowest internal energy. Diamond is only a metastable state, but with a rather long lifetime. Usually when carbon atoms are brought together graphite or an amorphous phase is formed. Only under certain conditions (pressure, temperature) in the inner earth were diamonds formed. Therefore, in a certain sense, diamonds are known only accidentally. It cannot be excluded that also other elements (Si, Ge, Ag, Au) can exist in other yet unknown modifications. Examples for new, artificially created materials are semiconductor quantum dot or quantum wire systems, or epitaxial magnetic layers⁶. Once the interactions between atoms are understood, possibly materials with completely new physical properties could be predicted theoretically. A certain field of modern condensed matter physics is working on these questions. This field is called “materials science” or “materials engineering”. As an example, by the theoretical investigation of semiconductor heterostructures or of metal heterostructures it is actually attempted to predict new materials for light emitting diodes (LEDs) or new magnetic memory devices. By the theoretical investigation of alloys and surface alloys (for which no bulk-analogue exists) of new compositions the hope is to find new catalysts. This sounds like being very close to practical application. However, it should be noted that applications of such theoretical predictions cannot be expected in the too near future, because in industry many practical details (concerning the technical processes, cost optimization, etc.) are crucial for the decision if a physical effect will be used in real devices.

A theory is particularly useful, if it has predictive power. In these years there is a change in condensed matter theory. While previously the main focus was on the reproduction of experimental results and on the transfer to similar systems, nowadays theory is applied more and more independent of experiment, e.g. to predict new properties of solids and to stimulate new experiments.

In recent years, two phenomena have had a big impact on materials science and condensed matter physics: First, the potential technological importance of semiconductor physics, magnetism, surface physics (computer, communication and information technology, catalysis, lubrication, new materials). Second, since 1980 33 Nobel prizes have been awarded for work in the field of or related to material science. Just a short list is given here (see also: <http://www.nobelprize.org/>):

- 1981 Physics: Nicolaas Bloembergen and Arthur L. Schawlow “for their contribution to the development of laser spectroscopy”
Kai M. Siegbahn “for his contribution to the development of high-resolution electron spectroscopy”

of diamond are known. Additionally since 1968 and 1972, respectively, chaoit and carbon (VI), since 1985 fullerenes (e.g. C₆₀) and since 1991 carbon nanotubes are known. From the latter “soft matter” can be formed, and they can also be used directly as nano-materials (for example as nanotube transistors). These systems will be discussed in more detail later.

⁶In 1988, Albert Fert and Peter Grünberg independently discovered that an increased magnetoresistive effect (hence dubbed “giant magnetoresistance” or GMR) can be obtained in magnetic multilayers. These systems essentially consist of an alternate stack of ferromagnetic (e.g., Fe, Co, Ni, and their alloys) and non-ferromagnetic (e.g., Cr, Cu, Ru, etc.) metallic layers. It is unusual that a basic effect like GMR leads in less than a decade after discovery to commercial applications: Magnetic field sensors based on GMR were already introduced into the market as early as 1996, and by now e.g. all read heads for hard discs are built that way. In 2007 Albert Fert and Peter Grünberg were awarded the Nobel Prize in physics.

- 1981 Chemistry: Kenichi Fukui and Roald Hoffmann “for their theories, developed independently, concerning the course of chemical reactions”
- 1982 Physics: Kenneth G. Wilson “for his theory for critical phenomena in connection with phase transitions”
- 1982 Chemistry: Aaron Klug “for his development of crystallographic electron microscopy and his structural elucidation of biologically important nuclei acid-protein complexes”
- 1983 Chemistry: Henry Taube “for his work on the mechanisms of electron transfer reactions, especially in metal complexes”
- 1984 Chemistry: Robert Bruce Merrifield “for his development of methodology for chemical synthesis on a solid matrix”
- 1985 Physics: Klaus von Klitzing “for the discovery of the quantized Hall effect” (von Klitzing, Dorda, Pepper, *Phys. Rev. Lett.* **45**, 494 (1980); *Physics Today* **38**, 17 (1985))
- 1985 Chemistry: Herbert A. Hauptman and Jerome Karle “for their outstanding achievements in the development of direct methods for the determination of crystal structures”
- 1986 Physics: Ernst Ruska “for his fundamental work in electron optics and for the design of the first electron microscope”
Gerd Binnig and Heinrich Rohrer “for their design of the scanning tunneling microscope” (*Physics Today*, Jan. 1987, p. 17) and (Binnig, Rohrer, Gerber, Werbel, *Phys. Rev. Lett.* **49**, 57 (1982))
- 1986 Chemistry: Dudley R. Herschbach, Yuan T. Lee, and John C. Polanyi “for their contributions concerning the dynamics of chemical elementary processes”
- 1987 Physics: J. Georg Bednorz and K. Alexander Müller “for their important breakthrough in the discovery of superconductivity in ceramic materials”
- 1987 Chemistry: Donald J. Cram, Jean-Marie Lejn, and Charles J. Pedersen “for their development and use of molecules with structure-specific interactions of high selectivity”
- 1988 Chemistry: Johann Deisenhofer, Robert Huber, and Hartmut Michel, “for the determination of the three-dimensional structure of a photosynthetic reaction centre”
- 1991 Physics: Pierre-Gilles de Gennes “for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers”
- 1991 Chemistry: Richard R. Ernst “for his contributions to the development of the methodology of high resolution nuclear magnetic resonance (NMR) spectroscopy”
- 1992 Chemistry: Rudolph A. Marcus “for his contributions to the theory of electron transfer reactions in chemical systems”

- 1994 Physics: Bertram N. Brockhouse “for the development of neutron spectroscopy”, and Clifford G. Shull “for the development of the neutron diffraction technique”.
- 1996 Physics: David M. Lee, Douglas D. Osheroff, and Robert C. Richardson “for their discovery of superfluidity in helium-3”
- 1996 Chemistry: Robert F. Curl Jr., Sir Harold W. Kroto, Richard E. Smalley “for their discovery of fullerenes”
- 1997 Physics: Steven Chu, Claude Cohen-Tannoudji, and William D. Phillips “for development of methods to cool and trap atoms with laser light”
- 1998 Physics: Robert B. Laughlin, Horst L. Störmer, and Daniel C. Tsui “for their discovery of a new form of quantum fluid with fractionally charged excitations”
- 1998 Chemistry: Walter Kohn “for his development of the density-functional theory”
John A. Pople “for his development of computational methods in quantum chemistry”
- 1999 Chemistry: Ahmed H. Zewail “for his studies of the transition states of chemical reactions using femtosecond spectroscopy”
- 2000 Physics: Zhores I. Alferov and Herbert Kroemer “for developing semiconductor heterostructures used in high-speed- and opto-electronics”, and Jack S. Kilby “for his part in the invention of the integrated circuit”
- 2000 Chemistry: Alan J. Heeger, Alan G. MacDiarmid, and Hideki Shirakawa, “for the discovery and development of conductive polymers”
- 2001 Physics: Eric A. Cornell, Wolfgang Ketterle, and Carl E. Wieman “for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates”
- 2003 Physics: Alexei A. Abrikosov, Vitaly L. Ginzburg, and Anthony J. Leggett “for pioneering contributions to the theory of superconductors and superfluids”
- 2005 Physics: Roy J. Glauber “for his contribution to the quantum theory of optical coherence” and John L Hall and theodor Hänsch for their contributions to the development of laser-based precision spectroscopy, including the optical comb technique”
- 2007 Physics: Albert Fert and Peter Grünberg “for their discovery of Giant Magnetoresistance”
- 2007 Chemistry: Gerhard Ertl “for his studies of chemical processes on solid surfaces”
- 2009 Physics: Charles K. Kao “for groundbreaking achievements concerning the transmission of light in fibers for optical communication”
Willard S. Boyle and George E. Smith “for the invention of an imaging semiconductor circuit - the CCD sensor”
- 2010 Physics: Andre Geim and Konstantin Novoselov “for groundbreaking experiments regarding the two-dimensional material graphene”

2011 Chemistry: Dan Shechtman “for the discovery of quasicrystals”.

In the above list I ignored work on biophysics, though some developments in this area are now becoming also part of condensed matter physics.

The quantum-Hall-effect (Nobel prize 1985) is roughly understood these days, which is true only in a limited way for its “variant” the “fractional quantum-Hall-effect” (Nobel prize 1998). The latter is based on the strong correlation of the electrons and even these days unexpected results are found.

The theory of high- T_c superconductivity is still unclear (Nobel prize 1987). Here, the coupling seems to have a different symmetry than in conventional BCS-superconductors. These days high- T_c superconductors with critical temperatures close to 160 K are known. While high- T_c superconductors have a complex atomic structure and consist of at least 4 elements (z.B. La, Ba, Cu, O), recently a relatively simple material was found (MgB_2), which also has a high critical temperature ($T_c = 39$ K). In 2008, recently discovered iron compounds, called iron pnictides (the group VB element is often As), were found to exhibit unusual superconductivity. The critical temperature of SmFeAsO , for example, is 55K.

In this lecture:

1. Equations will not fall down from heaven, but we will derive them from first principles;
2. we will not only give the mathematical derivation, but also, and in particular, we will develop a physical feeling, i.e., we will spend a noticeable amount of time in interpreting equations;
3. we will give the reasons for approximations and clarify their physical meaning and the range of validity (as much as this is possible).

In contrast to most text books we will start with the “adiabatic principle” and subsequently discuss the quantum mechanical nature of the electron-electron interaction. In most text books both are introduced only in the middle or at the end.

In the first part of the lecture we will restrict ourselves – unless stated otherwise – to $T \approx 0$ K. Sometimes an extrapolation to $T \neq 0$ K is unproblematic. Still, one should keep in mind that for $T \neq 0$ K important changes and new effects can occur (e.g. due to the entropy).

0.2 Literature for this lecture

Author: Ashcroft, Neil W. and Mermin, N. David

Title: Solid state physics

Place: Philadelphia, PA

Year: 1981

Publisher: Saunders College Publishing

ISBN: 0-03-083993-9 = 0-03-049346-3

Author: Kittel, Charles
Title: Quantum theory of solids
Place: Hoboken, NJ
Year: 1963
Publisher: John Wiley & Sons, Inc.

Author: Ziman, John M.
Title: Principles of the theory of solids
Place: Cambridge
Year: 1964
Publisher: Cambridge University Press

Author: Ziman, John M.
Title: Models of disorder: the theoretical physics of homogeneously disordered systems
Place: Cambridge
Year: 1979
Publisher: Cambridge University Press
ISBN: 0-521-21784-9 = 0-521-29280-8

Author: Ibach, Harald and Lueth, Hans
Title: Solid-state physics: an introduction to principles of materials science
Edition: 2. Ed.
Place: Berlin
Year: 1995
Publisher: Springer
ISBN: 3-540-58573-7 = 0-387-58573-7

Author: Madelung, Otfried
Title: Festkörpertheorie, 3 Bände
Place: Berlin
Year: 1972
Publisher: Springer

Author: Scherz, Udo
Title: Quantenmechanik
Place: Stuttgart
Year: 1999
Publisher: Teubner
ISBN: 3519032465

Author: Dreizler, Reiner M. and Gross, Eberhard K. U.
Title: Density functional theory: an approach to the quantum many-body problem
Place: Berlin
Year: 1990
Publisher: Springer
ISBN: 3-540-51993-9 = 0-387-51993-9

Author: Parr, Robert G. and Yang, Weitao
Title: Density-functional theory of atoms and molecules
Place: Oxford
Year: 1994
Publisher: Oxford University Press
ISBN: 0-19-509276-7

Author: Anderson, Philip W.
Title: Basic notions of condensed matter physics
Place: London
Year: 1984
Publisher: Benjamin/Cummings
ISBN: 0-8053-0220-4 = 0-8053-0219-0

Author: Marder, Michael P.
Title: Condensed matter physics
Place: New York
Year: 2000
Publisher: John Wiley & Sons, Inc.
ISBN: 0-471-17779-2

Author: Martin, Richard M.
Title: Electronic Structure
Place: Cambridge
Year: 2004
Publisher: Cambridge University Press

0.3 The following symbols and terms are used

- $-e$ charge of the electron
- $+e$ charge of the proton
- m mass of the electron
- \mathbf{r}_k position of electron k
- σ_k spin of electron k
- Z_K nuclear charge of atom K
- Z_{v_K} valence of atom K
- M_K mass of nucleus K
- \mathbf{R}_K position of nucleus K
- ϕ electric field
- Ψ many body wave function of the electrons and nuclei
- Λ nuclear wave function
- Φ many body wave function of the electrons
- φ single particle wave function of the electrons
- χ spin wave function
- $\{\mathbf{R}_I\} \equiv \{\mathbf{R}_1, \dots, \mathbf{R}_M\}$ atomic positions
- $\{\mathbf{r}_i \sigma_i\} \equiv \{\mathbf{r}_1 \sigma_1, \dots, \mathbf{r}_N \sigma_N\}$ electron coordinates (position + spin)
- ε_0 dielectric constant of the vacuum
- ϵ_i single particle energy of electron i
- V_g volume of the base region
- Ω volume of a primitive cell
- $v_K^{\text{Ion}}(\mathbf{r})$ potential of ion K at position \mathbf{r}

0.4 Atomic Units

At least at the beginning of the lecture I will use SI-units (**S**ystème **I**nternational d'Unités).

However, in order to simplify the notation in quantum mechanics often the so-called atomic units (a.u.) are introduced. For historic reasons there are two, slightly different conventions. For both we have:

$$\text{length} : \frac{4\pi\epsilon_0\hbar^2}{me^2} = 1 \text{ bohr} = 0.529177 \text{ \AA} = 0.0529177 \text{ nm} \quad , \quad (0.1)$$

Further we have:

	$e^2/4\pi\epsilon_0$	\hbar	m	energy = $\frac{\hbar^2}{2ma_B^2}$	$\hbar^2/2m$	Hamilton operator of hydrogen atom
Rydberg a.u.	2	1	0.5	1 Ry = 13.606 (eV)	1	$-\nabla^2 + \frac{2}{r}$
Hartree a.u.	1	1	1	$\frac{1}{2}$ Ha; 1 Ha = 27.212 (eV)	0.5	$-\frac{1}{2}\nabla^2 + \frac{1}{r}$