Computational Physics 2023

Sommersemester, 3th April, 2023 – 14th Juli, 2023

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3) Differentiation and integration
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5) Molecular dynamics simulations
6) Partial differential equations
7) **Iteration processes**
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9) Minimization
10) Random numbers
11) Monte Carlo (MC) Simulations
12) Perkolation
13) Stochastic Dynamics

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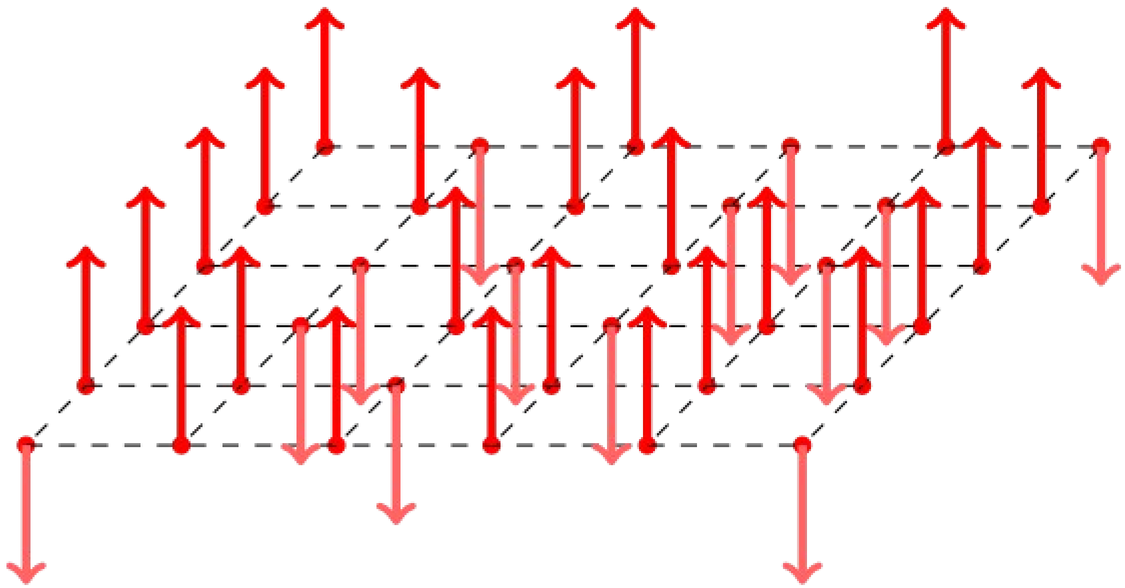
Ising model: mean field theory



Ising model: mean field theory

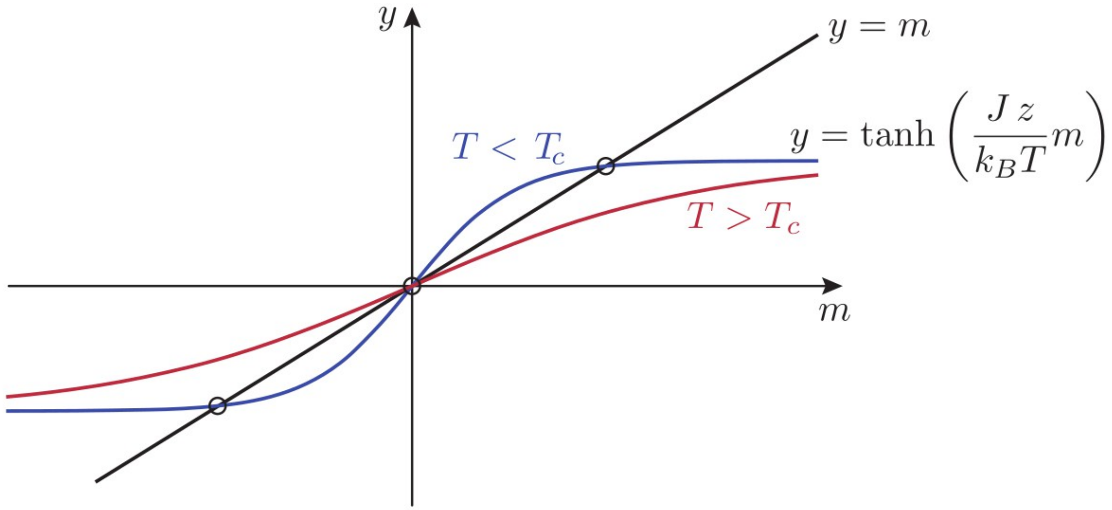


Abbildung 7.7: Grafische Lösung der Selbstkonsistenzgleichung ($\boxed{7.17}$) für $H = 0$. Die linke Seite $y = m$ und die rechte Seite $y = \tanh\left(\frac{1}{k_B T}(zJm)\right)$ der Gleichung werden in das gleiche Koordinatensystem eingetragen, Schnittpunkte der beiden Funktionen sind Lösungen der Gleichung.

Ising model: mean field theory

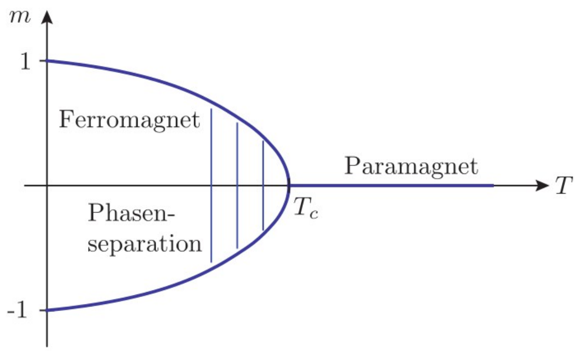


Abbildung 7.8: Phasendiagramm für $H=0$ in der m-T-Ebene. Am Punkt T_c steigt die Funktion $m(T)$ nach links mit dem kritischen Exponenten $\beta = 1/2$ an, also wie eine Wurzelfunktion.

2) Bei $T = T_c$ tritt eine **Bifurkation** auf. Der Fixpunkt $m = 0$ wird instabil und zwei weitere stabile Fixpunkte $\pm m(T)$ erscheinen.

$$\frac{Jzm}{k_B T} = \operatorname{arctan}(m) \approx m + \frac{m^3}{3} + \ldots$$

Es gilt

$$m^2(T) = \begin{cases} T > T_c : & 0 \\ T < T_c : & 3\left(\frac{T_c}{T} - 1\right), \end{cases}$$

also

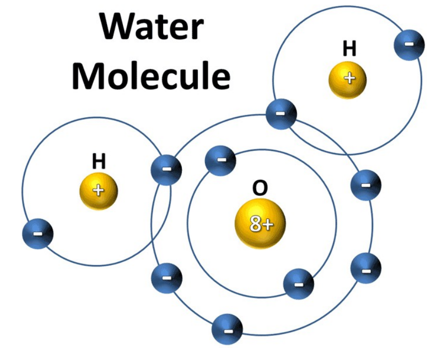
$$\boxed{m(T) \propto \left|\frac{T - T_c}{T_c}\right|^{\beta}}$$

mit einem **kritischen Exponenten**

$$\boxed{\beta_{\mathrm{MF}} = \frac{1}{2}}$$

Hatree-Fock

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$



electrons' kinetic energy

coulomb attraction between electrons and nuclei

repulsion between nuc

$$H = -\sum_{i=1}^{N}\frac{1}{2}\nabla_i^2 - \cancel{\sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2} - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \cancel{\sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}}$$

nuclei's kinetic energy

repulsion between electrons

The Born-Oppenheimer approximation states that, since nuclei are much heavier than electrons and move a lot slower, we can consider the electrons moving in the field of fixed nuclei. As a result, we can equate the second term in the above equation with zero and consider the last term as a constant, which can be neglected because adding any constant to an operator does not affect the operator eigenfunctions and only adds to operator eigenvalues

Hatree-Fock

The remaining terms are known as the electronic Hamiltonians, and they represent the motion of N electrons in the field of M fixed nuclei:

$$H_{elec} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}}$$

electron-electron interactions

Hatree (mean field)

Assume product state (electrons are uncorrelated):

$$\psi(\vec{r}_1 \ldots, \vec{r}_N) = \prod_{i=1}^{N} \phi_i(\vec{r}_i)$$

Solving a 1-electron Schroedinger equation (e.g., Hydrogen atom)

$$\boxed{\left(\frac{-\hbar^2}{2m}\vec{\nabla}_i^2 - \frac{Ze^2}{r_i} + V_i(\vec{r}_i)\right)\phi_i(\vec{r}_i) = \varepsilon_i\phi_i(\vec{r}_i) \quad \text{für} \quad i = 1, \ldots, N.}$$

The potential V(r) is an effective field depending on all the other electrons

$$\boxed{V_i(\vec{r}_i) = \sum_{j(\neq i)} \int d^3\vec{r}_i \; \frac{e^2}{|\vec{r}_i - \vec{r}_j|} |\phi_j(\vec{r}_j)|^2.}$$

Hatree

The total energy is given by:

$$E = \sum_i \varepsilon_i - \frac{1}{2} \sum_i \int d^3\vec{r}_i \; V_i(\vec{r}_i) |\phi_i(\vec{r}_i)^2| .$$

“Ionisation” energy

Hatree

These equations are coupled/dependent and have to be solved **self-consistently** (fixed point):

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}_i^2 - \frac{Ze^2}{r_i} + V_i(\vec{r}_i)\right)\phi_i(\vec{r}_i) = \varepsilon_i\phi_i(\vec{r}_i) \quad \text{für} \quad i = 1, \ldots, N.$$

$$V_i(\vec{r}_i) = \sum_{j(\neq i)} \int d^3\vec{r}_i \; \frac{e^2}{|\vec{r}_i - \vec{r}_j|} |\phi_j(\vec{r}_j)|^2.$$

Start here (Initial guess)

Hatree-Fock

Slater determinant (adding spin s=+/-1):

$$\psi(\vec{r}_1, s_1, \ldots, \vec{r}_N, s_N) = \begin{vmatrix} \phi_1(\vec{r}_1, s_1) & \cdots & \phi_1(\vec{r}_N, s_N) \\ \vdots & & \vdots \\ \phi_N(\vec{r}_1, s_1) & \cdots & \phi_N(\vec{r}_N, s_N) \end{vmatrix},$$

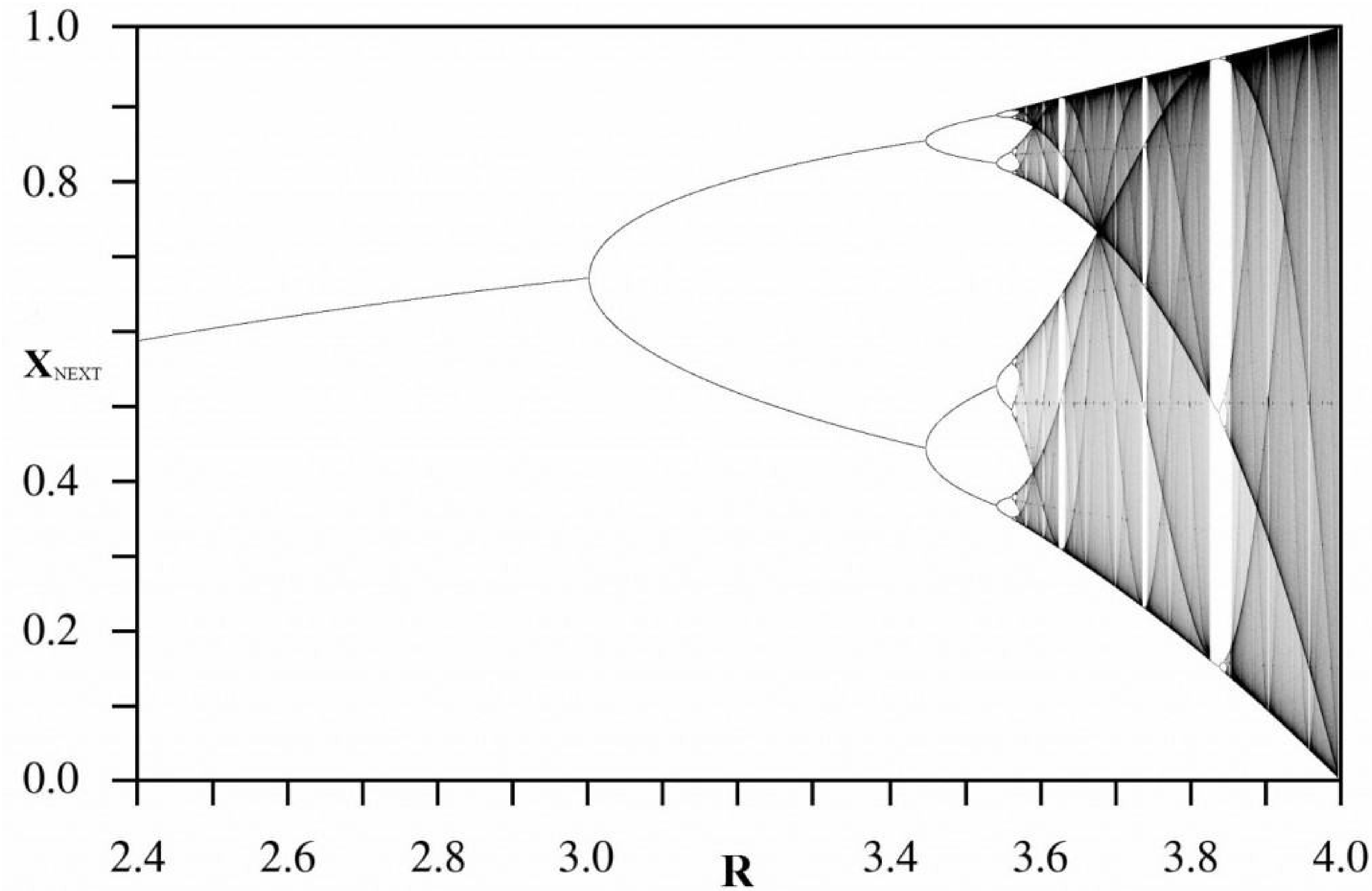
$$V_i(\vec{r}_i)\phi_i(\vec{r}_i) \to \sum_{j(\neq i)} \sum_{s_j} \int d^3\vec{r}_j \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \left[|\phi_j(\vec{r}_j, s_j)|^2 \phi_i(\vec{r}_i, s_i) - \underbrace{\phi_j^*(\vec{r}_j, s_j)\phi_j(\vec{r}_i, s_i)\phi_i(\vec{r}_j, s_j)\delta_{s_i s_j}} \right].$$

Pauli-principle

Compare with Hatree alone:

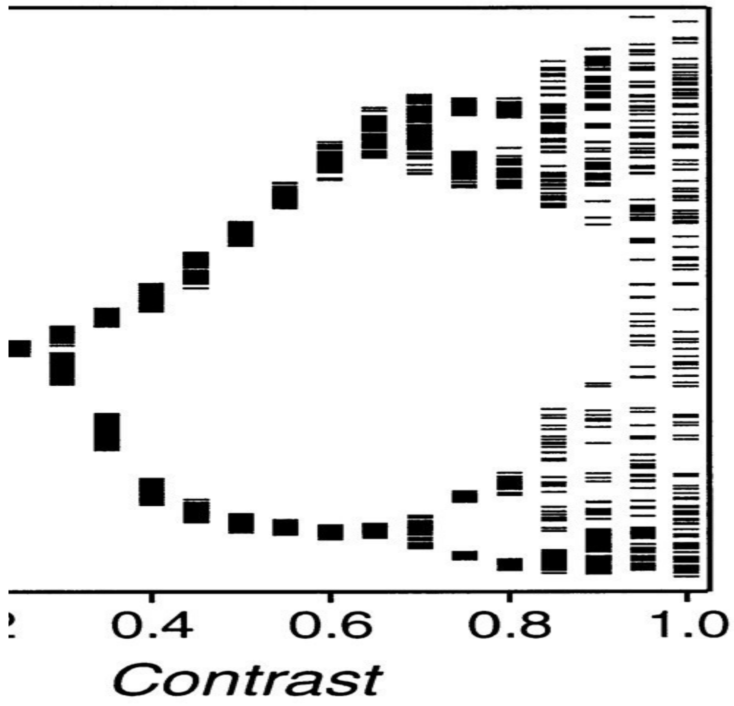
$$\boxed{V_i(\vec{r}_i) = \sum_{j(\neq i)} \int d^3\vec{r}_i \, \frac{e^2}{|\vec{r}_i - \vec{r}_j|} |\phi_j(\vec{r}_j)|^2.}$$

Logistic map



Logistic map

Crevier DW, Meister M. Synchronous period-doubling in flicker vision of salamander and man. J Neurophysiol. 1998 Apr;79(4):1869-78.



“Periodic flashes of light have long served to probe the temporal properties of the visual system. Here we show that during rapid flicker of high contrast and intensity the eye reports to the brain only every other flash of light.”