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Condensed Matter Theory I — WS05/06

Numerical Exercise

N.1 Hartree-Fock Approximation

In one of the previous exercises we found an expression for the occupation number of spin-up and spin-down electrons in the presence of a local potential within a Hartree-Fock approximation:

$$\langle n_\sigma \rangle = \frac{1}{N} \sum_k \left\{ 1 + \exp\left(\frac{\varepsilon_k + U\langle n_{-\sigma}\rangle - \mu}{T} \right) \right\}^{-1} \tag{1}$$

The absolute value of the magnetization is then given by

$$m = |\langle n_\uparrow \rangle - \langle n_\downarrow \rangle|$$

Assume that the density of states has the shape of a half circle, i.e.

$$N(\varepsilon) = \frac{2N}{\pi} \cdot \sqrt{D^2 - \varepsilon^2}$$

and choose $D = 1$ and $U = 2$.

Solve then the two equations for $\langle n_\uparrow \rangle$ and $\langle n_\downarrow \rangle$ self consistently in the temperature interval $T \in [0, 1]$, i.e. start with non-symmetric distributions (for instance $\langle n_\uparrow \rangle = 0.55$ and $\langle n_\downarrow \rangle = 0.45$), calculate first with these distributions the chemical potential such that the condition

$$\langle n_\uparrow \rangle + \langle n_\downarrow \rangle = 1$$

is fulfilled and then calculate in a second step the right side of (1). The results will define new distributions. Now iterate this procedure until the results will be stable. Plot m as a function of T. (The result should look like the plot in Fig. 1)

Hint: The simplest way to calculate the integral numerically is to use an equidistant grid and to approximate the integral as a discrete sum over the gridpoints.

The chemical potential can be found by using a sequence of nested intervals.

N.2 Coupled Differential Equations

In this exercise we want to try to find numerical solutions for two different systems of coupled differential equations.

a) The first example is the following well-known system of two coupled differential equations

$$\begin{aligned} f'(x) &= g(x) \\ g'(x) &= -f(x) \end{aligned} \quad \text{with the boundary condition:} \quad \begin{aligned} f(0) &= 0 \\ g(0) &= 1 \end{aligned}$$

Rewrite these equations as integral equations and calculate the two functions in the interval $x \in [0, 2\pi]$ and compare the numerical result with the exact solution.

b) The second example is a typical example for a differential equation as it appears in *renormalization group* calculations.

$$f'(x) = -\frac{f^2(x)}{x} \quad \text{with:} \quad f(1) = f_0$$

Calculate f for $x \in [0, 1]$ for the two cases $f_0 = \pm 1$.

c) Consider now the more general case

$$\begin{aligned} f'(x) &= -\frac{g^2(x)}{x} & \qquad & f(1) &= f_0 \\ & & \text{with:} & & \\ g'(x) &= -\frac{f(x) \cdot g(x)}{x} & & g(1) &= g_0 \end{aligned}$$

Solve this system for different values of f_0 and g_0.

Physical background: These equations arise by studying the influence of a single magnetic impurity in a non-magnetic host ('Kondo model'). Its solution contains very important information about the low temperature behaviour of a spin-spin-coupling between the impurity and the band electrons.

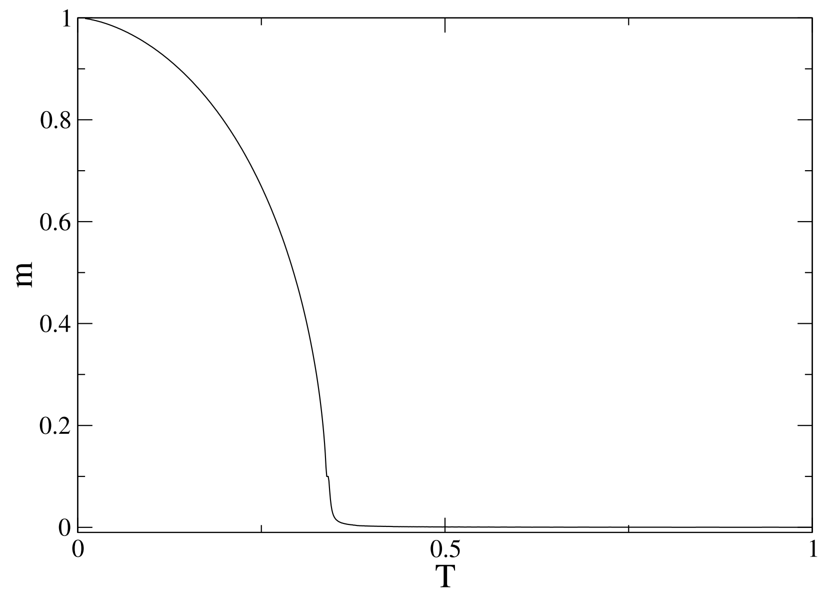

Figure 1: The magnetization as a function of temperature