FY3464 Solid State Physics, Advanced Course

Problemset Numerical

NTNU

Institutt for fysikk

In this problem, you are expected to use a numerical programming tool of your choice (*e.g.* Python, MATLAB, Julia, Mathematica, or similar) to perform the calculations and produce the required plots.

You are free to use external resources, including AI tools, for assistance with coding and technical issues. However, the main purpose of this exercise is that you develop an understanding of the numerical methods and how they connect to the physics.

In particular, you should make sure that:

- You understand the code you use and are able to explain how it works.
- You should carry out the numerical analysis yourself, meaning that you make and justify choices of method, select suitable parameter values, and verify your results through convergence checks.
- You interpret the results in terms of the underlying physical concepts.

Simply generating code or plots without understanding the procedure and the results will not promote learning. This is a chance to improve both your numerical skills and your ability to interpret results physically.

Problem 1

Consider a one-dimensional tight-binding model with both nearest-neighbor and next-nearest-neighbor hopping for spinless fermions:

$$H = -t\sum_i (c^\dagger_{i+1}c_i + \text{h.c.}) - t'\sum_i (c^\dagger_{i+2}c_i + \text{h.c.}). \tag{1}$$

We will study this system numerically and extract physical properties from the resulting dispersion.

(a) Using periodic boundary conditions, compute numerically the dispersion relation $E(k)$ for the following parameter values:

$$t = 1, \quad t' = 0.0,\ 0.2,\ 0.4,\ 0.5. \tag{2}$$

Plot all dispersions on the same graph.

(b) The effective mass near $k = 0$ is defined as

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}. \tag{3}$$

Compute the second derivative numerically and extract the effective mass for each value of t'. Describe the numerical method you use.

(c) Inspect your results and determine whether the curvature at $k = 0$ changes sign within the given parameter range. What is the physical interpretation of a change in sign of the curvature?

(d) Derive analytically the dispersion relation $E(k)$ for this model and compute $\frac{d^2E}{dk^2}$ at $k = 0$. Compare your analytical result with your numerical data.

(e) Repeat the numerical calculation of the second derivative using at least three different k-grid resolutions. Discuss how your result depends on the grid spacing and comment on the convergence of your method.

(f) Briefly answer the following questions:

- What is a numerical challenge when computing second derivatives?
- What determines the accuracy of your result?
- Suggest one way to improve the numerical accuracy.

Problem 2

Consider the Landau free energy:

$$F(m) = a(T)m^2 + bm^4, \tag{4}$$

where $b > 0$ and $a(T)$ changes sign at a critical temperature T_c. To carry out the computation, one must specify the function $a(T)$. A common choice is to assume a linear dependence near the critical temperature:

$$a(T) = a_0(T - T_c), \tag{5}$$

where $a_0 > 0$.

(a) For several values of T, compute numerically the value of m that minimizes $F(m)$.

(b) From your numerical results, estimate the critical temperature T_c at which the position of the minimum changes qualitatively. Describe clearly how you identify this transition from your data.