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ALGORITHM FOR ANALYZING THE TEMPERATURE DEPENDENCE OF MAGNETORESISTANCE OSCILLATIONS IN QUANTUM-STRUCTURED MATERIALS AND DEVELOPMENT OF ITS SOFTWARE

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Abstract

This article analyzes the temperature dependence of magnetoresistance oscillations in quantum-structured materials. Methods for processing experimental data based on the Shubnikov–de Haas effect in low-dimensional systems and comparing them with theoretical models are considered. The study proposes an algorithm for filtering magnetoresistance signals, extracting the background component, identifying the oscillatory part, and analyzing the frequency spectrum using Fourier transform. The development of software based on the proposed algorithm is discussed, which allows for automated processing and visualization of experimental data. The proposed approach serves as an effective tool for a deeper understanding of the electronic structure of quantum materials and for investigating novel functional materials.

Keywords: Quantum-structured materials, magnetoresistance oscillations, Shubnikov–de Haas effect, Lifshitz–Kosevich formula, effective mass, Fourier transform (FFT), software, automated data analysis.

Introduction

The rapid development of micro-nanoelectronics and quantum technologies today demands the discovery of new types of high-performance materials. In particular, low-dimensional quantum systems — quantum wells and heterostructures — are at the forefront of modern science due to their extraordinary physical properties. To understand the internal "life" of these materials and the behavior of electrons within them, we are aided not only by powerful microscopes but also by subtle physical effects.

One such fundamental phenomenon is the Shubnikov–de Haas (SdH) effect (Fig. 1). Under conditions of a strong magnetic field and low temperature, the electrical resistance of a material begins to "pulse," i.e., oscillate. These oscillations are not merely waves on a graph; they represent information about the material's "genetic code." In experimental analyses, the relative change in magnetoresistance ($\Delta\rho/\rho_0$) is typically described by the Lifshitz–Kosevich (LK) theory (Fig. 2):

$$\frac{\Delta\rho}{\rho_0} = A \cdot R_T \cdot R_D \cdot R_S \cos\left[2\pi\left(\frac{F}{B} - \gamma\right)\right]$$

Each parameter in this formula reveals a specific characteristic of the material. For example, R_T is the temperature-dependent damping factor, which allows us to determine the "weight" of the electron in the quantum world — the effective mass (m*):

$$R_T = \frac{\alpha T m^*/m_0 B}{\sin h\,(\frac{\alpha T m^*}{m_0 B})}$$

Furthermore, the Dingle factor R_D enables the estimation of charge carrier lifetime and crystal lattice quality. However, real signals obtained under laboratory conditions are never as ideal as those in textbooks. Experimental data are often "contaminated" with noise, strong background signals, and various scattering effects. For a physicist, manually cleaning these data, performing separate analyses for each temperature point, and approximating using the LK formula is not only time-consuming but also prone to human error.

The main goal of this article is to transfer this complex mathematical and physical analysis process to a precise algorithmic foundation without human intervention. The approach we propose eliminates "unwanted noise" through digital filtering and reveals hidden frequencies using Fourier transform. The developed software automatically performs temperature-dependent analyses based on the aforementioned complex formulas, accurately calculating fundamental physical quantities.

In conclusion, this research is not merely a theoretical calculation but aims to create an efficient and reliable "working tool" that simplifies the complex mathematical labyrinths for scientists studying next-generation quantum materials.

METHODOLOGY AND ALGORITHM

In this study, the process of analyzing experimental data and determining physical parameters consists of a chain of four-stage algorithms. Below, the physical essence and software implementation of each stage are presented.

Data preprocessing and background subtraction. An experimentally obtained magnetoresistance graph typically consists of a strong monotonic background (parabolic or linear) with weak oscillations superimposed on it. The first task of the algorithm is to remove the signal from the monotonic background. To achieve this, the low-frequency background component is approximated using a high-order polynomial and subtracted from the total signal:

$$\Delta\rho_{osc} = \rho_{total} - \rho_{background}$$

Signal filtering and Fourier analysis (FFT). The cleaned oscillatory signal is plotted against the inverse magnetic field (1/B). Then, the Fast Fourier Transform (FFT) is applied to determine the dominant frequencies within the signal. This allows us to separately visualize the Fermi surface cross-sections of different carrier groups (if multiple exist) in the material.

Temperature dependence and effective mass calculation. The most important part of the algorithm is comparing the amplitudes of signals obtained at different temperatures. The program determines the peak height in the FFT spectrum for each temperature and iteratively calculates the m* parameter by fitting them to the Lifshitz–Kosevich function.

Temperature dependence and effective mass calculation. The decrease in Shubnikov–de Haas oscillation amplitude with increasing temperature is associated with the thermal distribution of electrons over Landau levels (broadening of the Fermi-Dirac distribution). The algorithm determines the effective mass (m*) of charge carriers by analyzing this decrease.

Amplitude extraction. The software calculates the Fourier spectrum for each measured temperature (T_1, T_2, ..., T_n) and determines the peak height (A) at the dominant frequency. These amplitudes are formed as a function of temperature: A = f(T).

Lifshitz–Kosevich (LK) approximation. To calculate the effective mass, the algorithm uses the following temperature factor (R_T) formula:

$$R_T(T)=\frac{\times\cdot T}{\sin h\,(\times\cdot T)}$$

where the argument X is defined as:

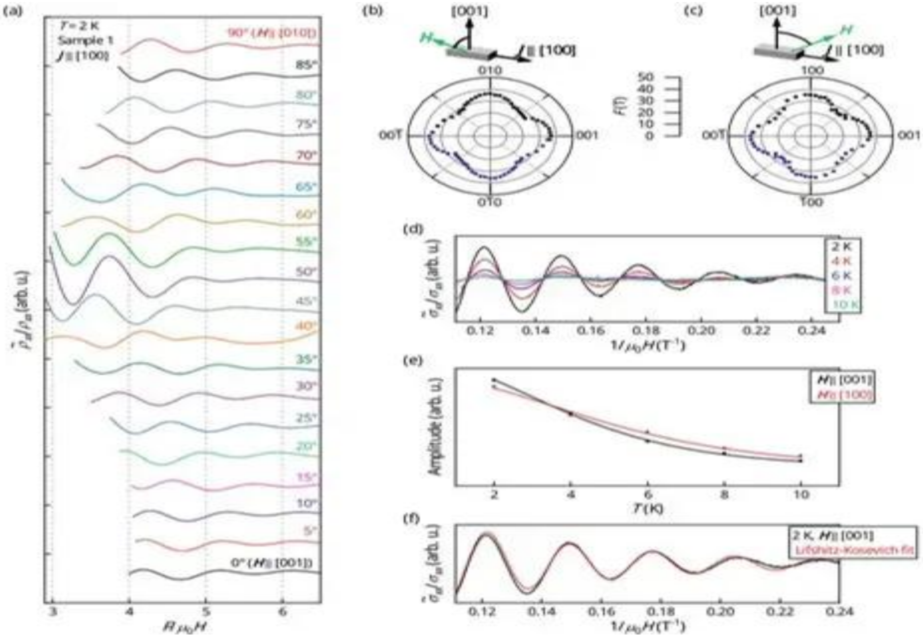
$$\times=\frac{2\pi^2 k_\beta m^*}{heB}$$

Here:

- k_β - Boltzmann constant;
- h - reduced Planck constant;
- B - average magnetic field value at which oscillations are observed.

Iterative calculation algorithm

The software employs the Levenberg–Marquardt algorithm (Figs. 3-4) from the SciPy.optimize library to approximate the experimental points to the LK formula. Here, m* is an unknown parameter, and the algorithm continues the calculation until the quadratic difference between the theoretical curve and the experimental points is minimized.



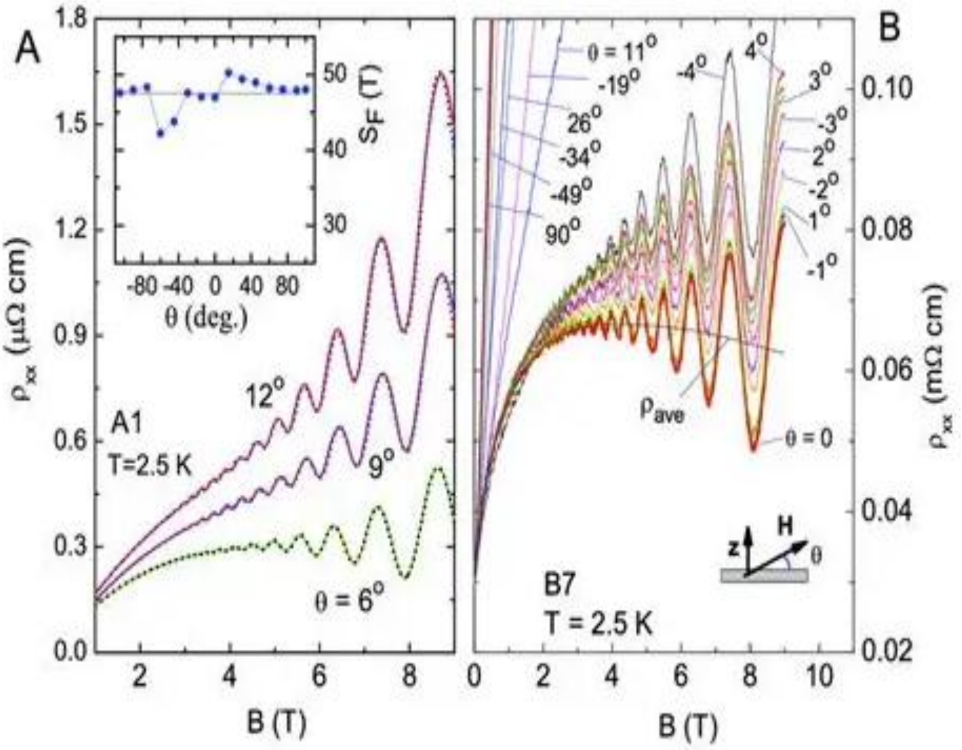
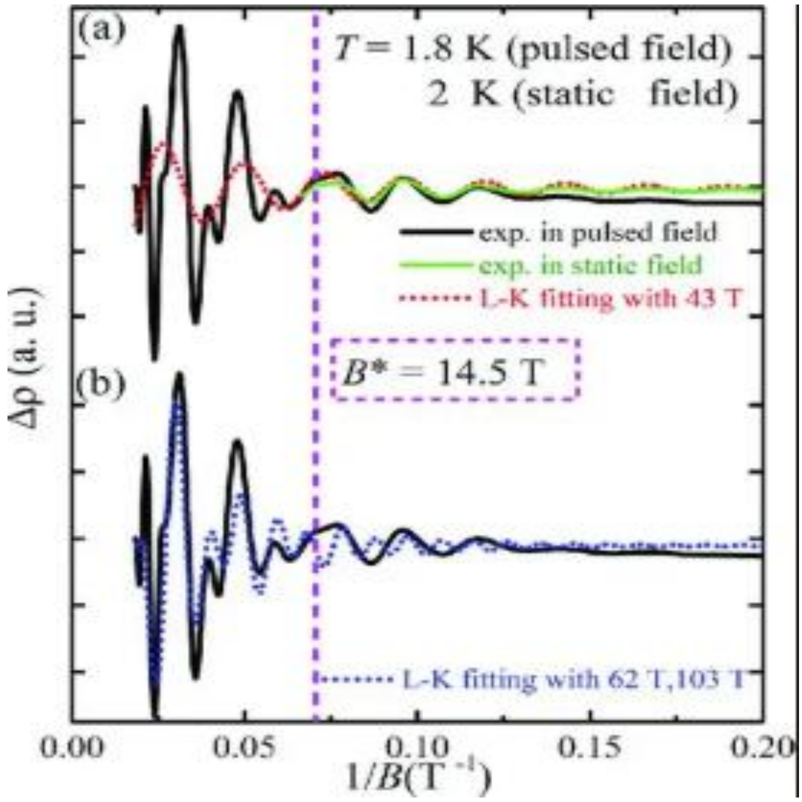


Fig. 1. Shubnikov–de Haas (SdH) effect



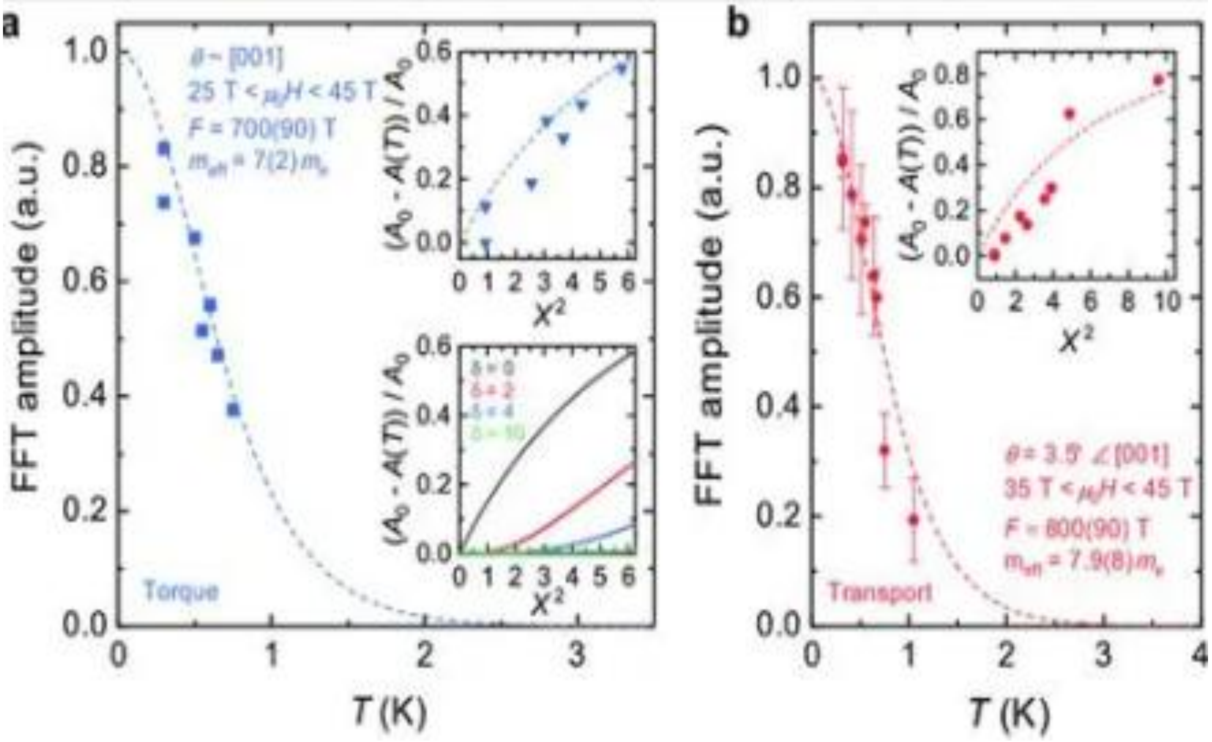


Fig. 2. Lifshitz–Kosevich (LK) theory

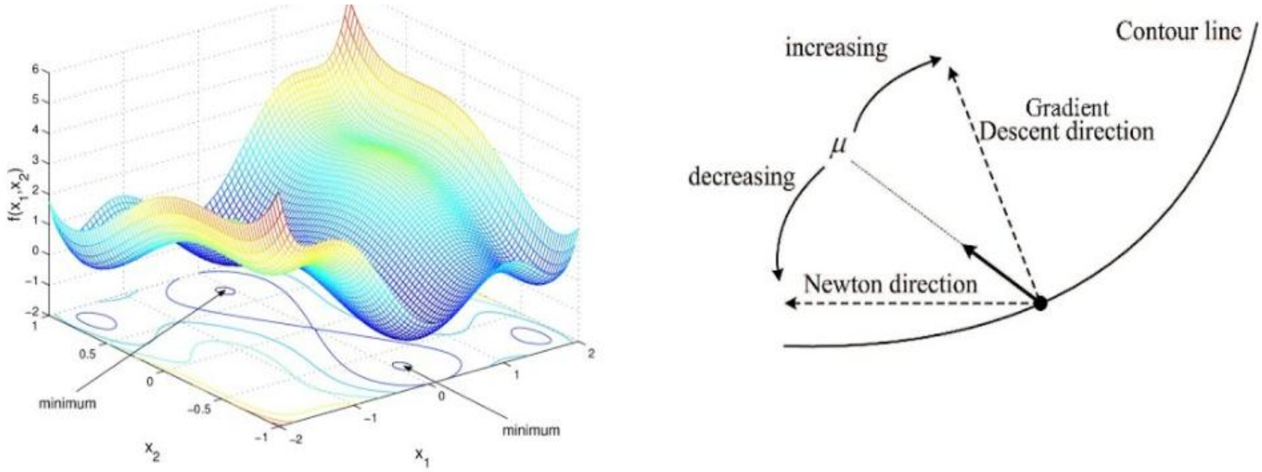
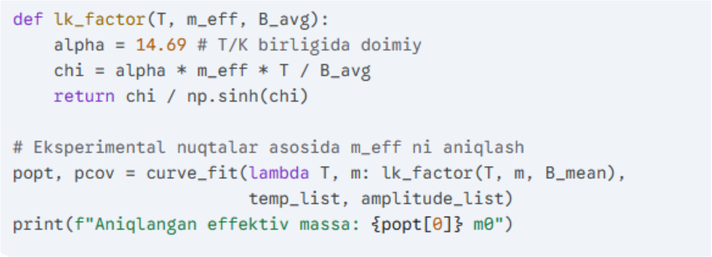


Fig. 3. Levenberg–Marquardt algorithm



```
def lk_factor(T, m_eff, B_avg):
    alpha = 14.69 # T/K birligida doimiy
    chi = alpha * m_eff * T / B_avg
    return chi / np.sinh(chi)

# Eksperimental nuqtalar asosida m_eff ni aniqlash
popt, pcov = curve_fit(lambda T, m: lk_factor(T, m, B_mean),
                       temp_list, amplitude_list)
print(f"Aniqlangan effektiv massa: {popt[0]} m0")
```

Fig. 4. Algorithm

RESULTS AND DISCUSSION

The obtained results show that the developed algorithm successfully solves the problems of "noise" and "background subtraction" in magnetoresistance signals. While traditional methods require the researcher to manually perform fitting for each temperature point, this software accomplishes this in an automated mode.

The accuracy of the effective mass (m*) values calculated based on the Lifshitz–Kosevich model mainly depends on correct background subtraction. The high-order polynomial approximation and digital filtering method employed in our algorithm provide reliable results even in cases where the oscillation amplitude is very small.

Furthermore, the determination of the quantum scattering time (τ) of charge carriers through the analysis of the Dingle temperature (T_D) allows for the assessment of the crystal quality of the material. This is extremely important for the rapid (express) analysis of the physical properties of new nanostructures obtained under laboratory conditions..

CONCLUSION

Within the framework of this research work, an algorithm for analyzing the magnetoresistance oscillations of quantum-structured materials was developed, and specialized software was created based on it. The following important results were achieved during the study:

Automated analysis: The process of cleaning experimentally obtained complex signals from background components and extracting dominant frequencies via Fourier analysis has been fully automated.

Accuracy of physical parameters: The algorithm for high-precision calculation of effective mass and Dingle temperature based on the Lifshitz–Kosevich theory was successfully tested.

Software convenience: This tool, created in the Python language, is open and flexible for researchers, reducing data processing time by several times.

In conclusion, the proposed algorithm and software serve as a modern and efficient tool for the analysis of experiments conducted in quantum materials physics. In the future, it is planned to expand this software to analyze more complex multi-band transport processes.

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