Simulation of the effect of peculiarities of the energy spectrum structure on the Hall coefficient behaviour in high-temperature superconductors

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Abstract. In this paper, we have investigated the influence of peculiarities of the normal-state energy spectrum structure in high-temperature superconductors on the temperature dependences of the Hall coefficient, $R_H$. Methods for accounting different specific features of the charge-carrier system when approximating the differential Hall conductivity function were proposed and used for simulating the $R_H(T)$ dependences in the framework of a narrow-band model. Simulation results show the Hall coefficient to be most sensitive to the existence of an asymmetry of the dispersion law. Taking this property into account one can obtain the calculated $R_H(T)$ curves corresponding well to the experimental ones observed for samples of the Y-based system with different deviations from the stoichiometric composition. This finding corresponds well to results obtained previously when analyzing the Nernst coefficient behavior in the same system and should be used for a further development of the approach to the joint quantitative analysis of the normal-state electron transport in high-temperature superconductors.

1. Introduction

It is well known that along with high critical temperature values and a number of specific features of superconducting state properties (see, for example, [1-3]), high-temperature superconductors (HTSC) are characterized by an unusual nature of the normal state. One of the consequences of this is the peculiarities of the temperature and concentration dependences of the transport coefficients observed in HTSC of different systems [4-8] and requiring for their description and explanation the development of non-standard models or approaches. Such a situation is obviously caused by the absence of the reliable information on the general features and particular parameters of the energy spectrum structure in HTSC. While different and often mutually exclusive approaches have been proposed to address the above problem (see, e.g., their description in [7]) it can be stated that choosing the model to most adequately describe the electron transport phenomena in HTSC materials is still essential question of HTSC physics.

In this paper, we consider the normal-state Hall coefficient, $R_H$, behavior. The measurements of this transport coefficient in various materials is known to be used for the determination of the charge-carrier concentration. However, in case of HTSC we meet again unusual situation and according to different investigations the Hall concentration in these materials does not correspond to the real one...
[4, 7]. As a result, to interpret both the value and type of the temperature dependences of the Hall coefficient different models have been proposed [9-14]. Note that most of these models aim to describe only the Hall coefficient behavior regardless the results for other transport coefficients. Our approach (so-called narrow-band model) compares favorably with them due to the possibility to describe simultaneously the temperature dependences of the resistivity, thermopower, Hall and Nernst coefficients using the common set of the model parameters [7, 14]. However, contrary to the thermopower and Nernst coefficient whose experimental temperature dependences for HTSC samples of different compositions can be quantitatively described in all the details [7, 8], in case of the Hall coefficient we could only demonstrate a possibility to obtain the calculated curves corresponding qualitatively to the main peculiarities characteristic of the Hall coefficient behavior in HTSC [7, 14]. For a more accurate description of the experimental \( R_H(T) \) dependences including a character of their modification under different deviations from the stoichiometric sample composition it is necessary to answer two questions. First, which peculiarities of the energy spectrum structure have the strongest impact on the Hall coefficient and second, how to take these peculiarities into account when calculating the \( R_H(T) \) dependences within the narrow-band model.

For the above reasons, this paper aims to simulate the influence of possible features of the energy spectrum structure on the temperature dependence of the Hall coefficient, to analyze the calculated results with regard to peculiarities of the experimental \( R_H(T) \) dependences, and to choose the most suitable method for the further quantitative analysis of the Hall coefficient behavior in HTSC.

2. Peculiarities of the Hall coefficient behaviour in HTSC and approach to its temperature dependence calculation

Before modeling the temperatures dependences of the Hall coefficient let us point out the main peculiarities of this coefficient behavior in HTSC which should be taken into account when analyzing the validity of the calculation results. Although \( R_H(T) \) dependences are generally similar for different HTSC systems, we will consider doped YBa\(_2\)Cu\(_3\)O\(_y\) samples as a model object.

The Hall coefficient is always positive. For near-stoichiometric samples it is characterized by a strong temperature dependence closed to \( R_H \propto T^1 \) and a very small absolute value (of about \( 10^{-3}\text{cm}^2/\text{C} \)). Only selected impurities influencing directly the energy spectrum structure (such as calcium in the yttrium position or zinc in the plane cooper position) are characterized by an appearance of specific peculiarities on the \( R_H(T) \) dependence [4, 15, 16]. Mainly, impurities of different types as well as an oxygen deficit result in a strong but analogous modification of these dependences. With increasing doping level, the \( R_H \) value increases, the \( R_H \) dependence becomes weaker and there appears a maximum on this dependence at low temperatures. Note that the last property is of great importance in order to estimate the validity of any model proposed to describe the Hall coefficient in HTSC.

As already mentioned, our approach is based on the narrow-band model [7, 14]. The main assumption of this model is that the half-width of the band responsible for the conduction process, \( W/2 \), does not exceed the value of \( k_B T \) (where \( k_B \) is the Boltzmann constant) by more than an order of magnitude. If so, the Fermi smearing covers a considerable part of the band and such characteristics of the charge carrier as the relaxation time, velocity, and effective mass (disregarding the sign) can be averaged in the energy interval from \(-W/2\) to \( W/2 \) (i.e., over the band). This makes it possible to use the simplest rectangular approximations for the density-of-state, \( D(\varepsilon) \), differential conductivity, \( \sigma(\varepsilon) \), and Hall conductivity, \( \sigma_H(\varepsilon) \), functions:

\[
D(\varepsilon) = \begin{cases} < D > & \text{at } -W_D/2 < \varepsilon < W_D/2 \\ 0 & \text{at } \varepsilon < -W_D/2 \text{ and } \varepsilon > W_D/2 \end{cases},
\]

\[
\sigma(\varepsilon) = \begin{cases} < \sigma > & \text{at } -W_\sigma/2 < \varepsilon < W_\sigma/2 \\ 0 & \text{at } \varepsilon < -W_\sigma/2 \text{ and } \varepsilon > W_\sigma/2 \end{cases},
\]

\[
\sigma_H(\varepsilon) = \begin{cases} -< \sigma_H > & \text{at } -W_\sigma/2 < \varepsilon < 0 \\ < \sigma_H > & \text{at } 0 < \varepsilon < W_\sigma/2 \\ 0 & \text{at } \varepsilon < -W_\sigma/2 \text{ and } \varepsilon > W_\sigma/2 \end{cases}, \tag{1}
\]
where

\[
<D> = \frac{1}{W} \int_{-W/2}^{W/2} D(\varepsilon)d\varepsilon, \quad <\sigma> = \frac{1}{W} \int_{-W/2}^{W/2} \sigma(\varepsilon)d\varepsilon, \quad <\sigma_H> = -\frac{2}{W} \int_{-W/2}^{W} \sigma_H(\varepsilon)d\varepsilon
\]

\[
<\sigma_H> = \frac{2}{W} \int_{0}^{W/2} \sigma_H(\varepsilon)d\varepsilon,
\]

\[
W_D \quad \text{and} \quad W_\sigma \quad \text{are the model parameters corresponding to the total effective bandwidth and the effective width of the energy intervals, electrons from which give the main contributions to the conduction process. Besides, the model contains additional parameter, namely, the band filling degree with electrons, } F, \quad \text{which equals to the ratio of the number of electrons to the number of states in the band.}
\]

Substituting the above functions in the standard kinetic integrals by these approximations one can obtain analytical expressions describing the temperature dependences of the transport coefficients. Such an approach makes it possible to analyse quantitatively the temperature dependences of the thermopower in doped HTSC of different systems, to determine the values of the model parameters for samples of varied composition, and to analyse then mechanisms of the influence of different impurities on the normal-state energy spectrum structure [7, 14, 17]. As for the Hall coefficient, its temperature dependence can be calculated within a constant factor. But what is much more important is that the derived equations allow one to obtain the calculated \(R_H(T)\) curves corresponding only very qualitatively to the experimental ones. In particular, a maximum on the calculated \(R_H(T)\) dependence appears only when using rather high values of the \(F\) parameter not realizing for most of doped samples [7]. It is the main reason that gave rise to our attempts to modify the method of the Hall coefficient calculation within the narrow-band model. Note that we have studied possible ways of an approximation for the only \(\sigma_H(\varepsilon)\) function using the approximations for the \(D(\varepsilon)\) and \(\sigma(\varepsilon)\) functions presented above in order to keep the correct description of the thermopower temperature dependence in the framework of our approach. The only exclusion is the case of modelling the energy dependence of the relaxation time, \(\tau(\varepsilon)\), that requires to modify both the \(\sigma(\varepsilon)\) and \(\sigma_H(\varepsilon)\) functions.

The model-independent expression for the Hall coefficient can be presented as

\[
R_H = \frac{l_{\sigma_H}^2}{(l_\sigma)^2}, \quad l_\sigma = \int \left( -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \sigma(\varepsilon)d\varepsilon, \quad l_{\sigma_H} = \int \left( -\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right) \sigma_H(\varepsilon)d\varepsilon,
\]

where \(f(\varepsilon)\) is the Fermi-Dirac distribution function, the integration is taken over the entire band. Using rectangular approximations for the \(\sigma(\varepsilon)\) and \(\sigma_H(\varepsilon)\) functions one can obtain:

\[
R_H = const \frac{A}{B^2},
\]

where

\[
A = -v^2 \left( \frac{1}{e^{(\varepsilon_{max}/2k_BT-\mu')} + 1} - \frac{1}{e^{(\varepsilon_0'/2k_BT-\mu')} + 1} \right) + v^2 \left( \frac{1}{e^{(\varepsilon_0/2k_BT-\mu')} + 1} + \frac{1}{e^{(\varepsilon_0/2k_BT-\mu')} + 1} \right)
\]

\[
B = -v \left( \frac{1}{e^{(\varepsilon_{max}/2k_BT-\mu')} + 1} + \frac{1}{e^{(\varepsilon_{min}/2k_BT-\mu')} + 1} \right) + \frac{1}{e^{(-\mu')} + 1} + \frac{1}{e^{(-\mu')} + 1}.
\]

\(\text{const}\) is a positive multiplier depending on heights of rectangles approximating the \(\sigma(\varepsilon)\) and \(\sigma_H(\varepsilon)\) functions, \(\varepsilon_{\text{min}}, \varepsilon_{\text{max}}\) and \(\varepsilon_0', \varepsilon_{\text{max}}'\) are energies corresponding to the boundaries of these two rectangles, respectively, \(\varepsilon_0\) is the point where the \(\sigma(\varepsilon)\) function changes its sign, \(v\) is a parameter taking into account a possible difference in heights of the \(\sigma(\varepsilon)\) and \(\sigma_H(\varepsilon)\) rectangles in the lower and upper halves of the band, \(\mu' = \mu/k_BT\), \(\mu\) is the chemical potential. We will use below equation (3) for
the calculation of the temperature dependences of the Hall coefficient when taking into account different peculiarities of the energy spectrum structure.

3. Methods of simulating the \( R_H(T) \) dependences and results of calculations

To simulate the temperature dependences of the Hall coefficient we have used four methods of the \( \sigma_H(\varepsilon) \) approximation allowing to take into account different features of the energy spectrum structure and charge-carrier system properties that can potentially affect this coefficient behavior. These features are: i) the presence of the energy dependence of the relaxation time; ii) the difference in energy intervals electrons from which give the contributions to the conductivity and Hall conductivity correspondingly; iii) the presence of an asymmetry of the density-of-state function; iv) the presence of an asymmetry of the dispersion law. The approximations modelling these features and used in calculations are shown in figure 1 and will be explained below.

![Figure 1](image-url)

**Figure 1.** Different methods of approximations of the \( D(\varepsilon) \), \( \sigma(\varepsilon) \), and \( \sigma_H(\varepsilon) \) functions used for calculations of the \( R_H(T) \) dependences. See explanations in the text.
Let us consider the ways of taking into account the above features of the energy spectrum when calculating the Hall coefficient.

Simulating an energy dependence of the relaxation time. In this case, $\varepsilon_{\text{min}}, \varepsilon'_{\text{min}} = -W_D = -CW_D$; $\varepsilon_{\text{max}}, \varepsilon'_{\text{max}} = W_D = CW_D$, $\varepsilon_0 = 0$. As known, $\sigma(\varepsilon) = \frac{e^2}{3} v^2(\varepsilon) \tau(\varepsilon) D(\varepsilon)$ and $\sigma_H(\varepsilon) = -\left( \frac{e \tau(\varepsilon)}{m^*(\varepsilon)} \right) \sigma(\varepsilon)$, where $e$ is the elementary charge, $v$ is the electron velocity, $m^*$ is their effective mass. If so, keeping the rectangular approximations, the presence of the $\tau(\varepsilon)$ dependence can be simulated by introducing different heights of the $\sigma(\varepsilon)$ and $\sigma_H(\varepsilon)$ rectangles in the lower and upper halves of the band. Since $\sigma(\varepsilon) \propto \tau(\varepsilon)$ and $\sigma_H(\varepsilon) \propto \tau^2(\varepsilon)$, the first function in the upper band half should be multiplied by a factor $V$ while the second one should be multiplied by a factor $V^2$ (see figure 1(A)). The case of $V > 1$ corresponds to a $\tau$ increase with energy, the case of $V < 1$ corresponds to its decrease.

Simulating a difference in energy intervals corresponding to the main electron contribution to the conductivity and Hall conductivity. In other words, this case takes into account different degrees of the charge carrier and Hall carrier localization and can be modelled by changing the width of $\sigma_H(\varepsilon)$ rectangle, i.e., $\varepsilon_{\text{min}}, \varepsilon'_{\text{min}} = \mp W_D = \mp CW_D$; $\varepsilon_{\text{max}}, \varepsilon'_{\text{max}} = \mp W_H = \mp C_H W_D$ (see figure 1(B)).

Simulating an asymmetry of the $D(\varepsilon)$ function. In this case, all the three rectangles should be shifted on the energy scale but, in the first approximation, these shifts will be the same. If so, the only we should do is to shift the point where the $\sigma_H(\varepsilon)$ function changes its sign. Thus, $\varepsilon_{\text{min}}, \varepsilon'_{\text{min}} = -W_D = -CW_D$; $\varepsilon_{\text{max}}, \varepsilon'_{\text{max}} = W_D = CW_D$, $\varepsilon_0 = k W_D$ (see figure 1(C)), where $k$ is a parameter characterizing the degree of the $D(\varepsilon)$ asymmetry.

Simulating an asymmetry of the dispersion law. Because $\nu = \partial \varepsilon / \partial \kappa$ and $m^* = \hbar^2 / (\partial^2 \varepsilon / \partial \kappa^2)$, where $\kappa$ is the wave vector, an $\varepsilon(\kappa)$ asymmetry will result in shifting both the boundaries of the $\sigma_H(\varepsilon)$ rectangle and the point of changing $\sigma_H(\varepsilon)$ sign. Thus, in this case, $\varepsilon_{\text{min}}, \varepsilon_{\text{max}} = +W_D = +CW_D$; $\varepsilon'_{\text{min}} = -CW_D + k W_D$, $\varepsilon'_{\text{max}} = CW_D + k W_D$, $\varepsilon_0 = k W_D$, where where $k$ is a parameter characterizing the degree of the $\varepsilon(\kappa)$ asymmetry (see figure 1(D)).

In order to estimate the possibility of using these approximations for the correct description of the $R_H(T)$ dependences in samples of different compositions, for each of them the calculations were performed for two sets of the main model parameters ($F, W_D, C = W_d/W_D$): $F = 0.505$, $W_D = 100$ meV, $C = 0.4$ and $F = 0.533$, $W_D = 200$ meV, $C = 0.2$. According to the thermopower analysis within the narrow-band model [7, 14], the first of them corresponds to samples of near-stoichiometric compositions while the second one can be considered as being typical for heavily-doped samples.

![Figure 2](image-url.png)

**Figure 2.** Calculated $R_H(T)$ dependences in case of simulating an asymmetry of the dispersion law. The values of the main model parameters are $F = 0.505$, $W_D = 100$ meV, $C = 0.4$ (A) and $F = 0.533$, $W_D = 200$ meV, $C = 0.2$ (B).
The results of calculations within the approximations described above show the following. First three approximations give no possibility to describe all the features of the experimental \( R_H(T) \) dependences characteristic of samples with different degrees of deviation from the stoichiometry. The simulations of the existence of both a \( \tau(\varepsilon) \) dependence and an \( D(\varepsilon) \) asymmetry result in changing slope of the calculated \( R_H(T) \) curve from negative to positive or even lead to negative \( R_H \) values in the whole temperature range. The latter peculiarity is appeared if \( \tau \) decreases with increasing energy or the parameters of a \( D(\varepsilon) \) asymmetry is negative. Increasing degree of the Hall carrier localization (a decrease in the \( C_H \) parameter) relative to a fixed \( C \) value results in increasing a rise of the \( R_H \) values at low temperatures. Introducing \( C_H > C \) gives a possibility to obtain a weaker \( R_H(T) \) dependence that corresponds to the experimental results for heavily-doped samples. However, first, such a relation between \( C \) and \( C_H \) is difficult to explain for physical reasons (one can rather expect the opposite relation) and, second, a maximum on the \( R_H(T) \) dependences observed experimentally for heavily-doped samples does not appear on the calculated curves when using the second set of the main model parameters.

The results of calculations when simulating the presence of a dispersion law asymmetry are shown in figure 2. Let us first note that at \( k > 0 \) the \( R_H \) values become to be negative, so one should use only negative values of an asymmetry parameter that corresponds well to the results obtained earlier when analyzing the Nernst coefficient in the framework of the narrow-band model [18-21]. Calculated \( R_H(T) \) dependences in this case correspond qualitatively well to the experimental observations for both near-stoichiometric and heavily-doped samples. For the latter, increasing the negative \( k \) values results in smoothing of the \( R_H(T) \) curves, moreover, at some values of this parameter the calculated curves demonstrate a maximum at low temperatures that follows through with the experimental data (see figure 2(B)). Thus, it is the dispersion law asymmetry that should be taken into account for achieving a better agreement of the experimental and calculated \( R_H(T) \) dependences. Note additionally that this finding, together with the results of the Nernst coefficient analysis [18-21], gives grounds to speculate that the proposed approximation can be further used for the simultaneous quantitative description of the temperature dependences of the thermopower, Hall and Nernst coefficients in HTSC.

4. Conclusions

Thus, we have performed the simulation of the temperature dependences of the Hall coefficient in the framework of the narrow-band model with regard to different specific features of the energy spectrum structure. A qualitative comparison of the calculated results with the experimental data obtained for Y-based HTSC with different doping levels indicates that it is necessary to take into account the presence of a dispersion law asymmetry. Other possible peculiarities of the energy spectrum are not of importance and can be excluded from consideration when analyzing the results on the Hall coefficient.

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