Definition of effective energy and distance of hopping electron transport

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Abstract

Hopping conductivity in crystalline semiconductors has been parameterized and there is an analytic expression for conductivity, suitable at very low temperatures. For the arbitrary temperatures, the analytic expression is not available. This work parameterizes the hopping conductivity using two parameters called the effective hopping energy and the effective hopping distance. This report presents a numerical method, which allows extraction of these parameters from a single temperature dependence of conductivity, simulated in a wide range of temperatures. An approximated method is proposed, which allows to extract the effective hopping energy from experimental temperature dependences of conductivity. The results agree qualitatively with the existing theories, created for the low and high-temperature limits, and bridge the gap between them by describing the behavior of effective parameters at moderate temperatures, where the transition from variable range hopping to nearest neighbor hopping occurs, accompanied by modifications of the energy-distribution of the density of localized states.

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The idea of this work was to parameterize the hopping conductivity using two effective parameters ϵ and r in a wide range of temperatures. These parameters will be called the effective hopping energy and effective hopping distance in this report.

These parameters are defined by simulating a macroscopic sample by a regular network (1, 2 or 3-dimensional) of identical resistances, each of which is characterized by and r instead of random values of ϵ_{ij} and r_{ij}.

This report presents how the effective parameters ϵ and r can be determined from the temperature dependence of resistivity and how they themselves depend on temperature.

Calculation is performed by numerically solving a system of two equations for t and g under condition that $\epsilon \approx 0$ and $r \approx 0$ for some relatively high temperature, at the border of the studied interval. Functions t and g represent the resistivity in hopping regime and its temperature derivative. These functions were simulated using mean field approach in this work.

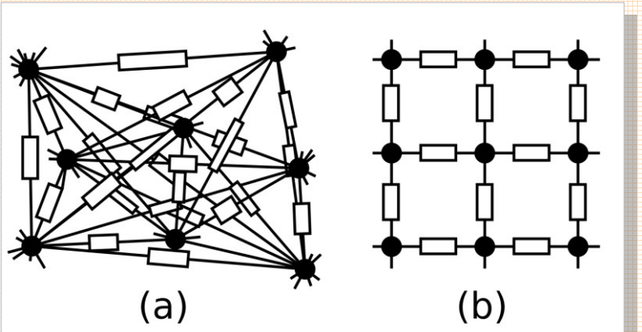

Fig. Schematic 2D models of the resistor networks used in this work to simulate the hopping electron transport. (a) Miller-Abrahams random resistor network, (b) a regular network of identical resistors arranged in a square lattice.

$$t = \frac{e^y (e^x - 1)}{xy},$$

$$g \equiv \frac{t'}{t} = y' \left(1 - \frac{1}{y}\right) + x' \left(\alpha - \frac{1}{x}\right),$$

$$t \equiv R_c/R_0,\ x \equiv \epsilon/T,\ \text{and}\ y \equiv 2r/a.$$

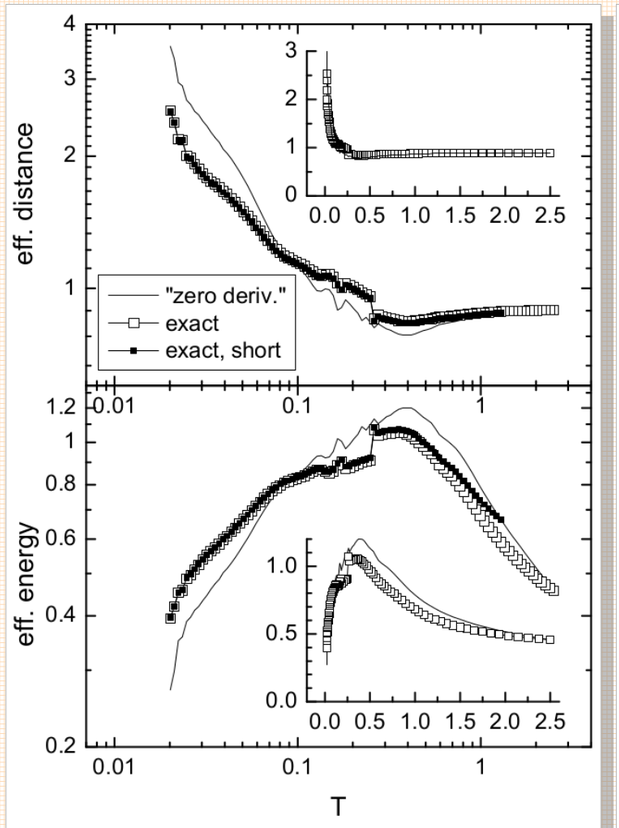

Fig. Dependencies of effective hopping energy and distance on temperature, calculated using realistic data obtained by mean-field simulations. Solid lines were obtained under approximation that $\epsilon' \approx 0$ and $r' \approx 0$. Open symbols and filled symbols show more precise dependencies calculated under assumption that $\epsilon' \approx 0$ and $r' \approx 0$ only at the highest considered temperature of T = 2.5 and T = 1.2, respectively. The insets show the same data in the linear scale, to emphasize that $\epsilon' \approx 0$ and $r' \approx 0$ at the upper boundary.

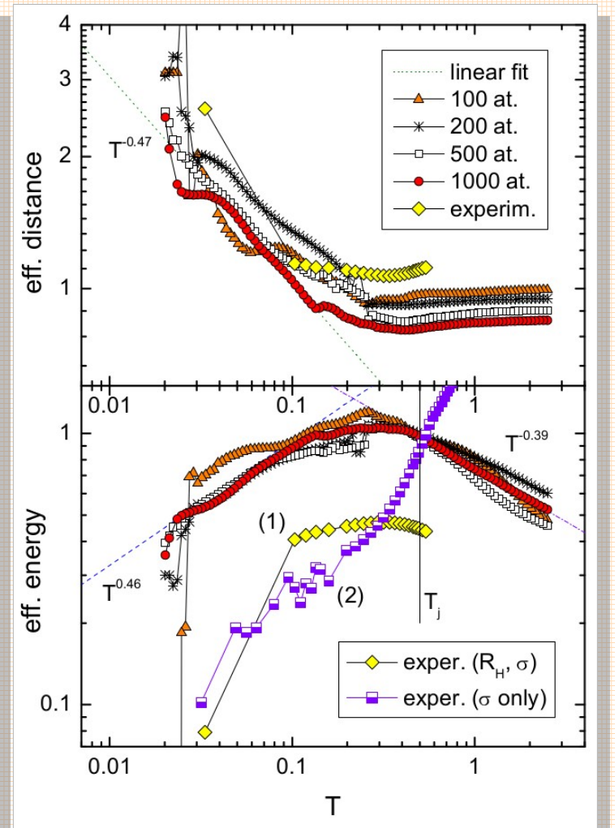

Fig. Dependencies of effective hoping energy and distance on temperature. Smaller symbols show simulated curves, calculated using cells with 100 (triangles), 200 (asterisks), 500 (white squares) and 1000 (circles) impurity atoms. Patterned lines show linear fits. Large symbols show curves calculated using experimental data for ZnO. Yellow diamonds were derived using the experimental conductivity and Hall effect data. Half-filled purple rectangles were derived using only the experimental conductivity data and the method proposed in this report.

Results:

In case of an electron system with a Coulomb gap in the density of states, this approach gives $\epsilon(T)$ and $r(T)$ dependencies which are qualitatively compatible with the Efros-Shklovskii law at low temperatures. At high temperatures, these dependencies show saturation, as expected in the constant activation energy regime. At intermediate temperatures ($T \sim 0.3$) the curves show an extremum. The most prominent is the maximum in the $\epsilon(T)$ curve, which is attributed to transition from variable range hopping to nearest neighbor hopping and to mixing of the energy bands of occupied and empty states.

An approximated method of extraction of effective hopping energy from a basic experimental temperature dependence of conductivity is also presented. This method does not require any parameters and does not require the extraction to be performed starting from temperatures where the activation energy is constant. Extraction can be performed independently, at any temperature.

Comparison of simulated and experimental $\epsilon(T)$ dependencies shows some qualitative agreement. The experimental values of effective activation energy are about three times smaller than the simulated ones. It seems that this difference cannot be explained using customary mechanisms of activation energy reduction. The magnitude of the r parameter can be determined from simulation with a much higher precision.

Comparison was also made with the independent experimental $\epsilon(T)$ and $r(T)$ dependencies obtained using data of conductivity and Hall effect measurements. There is a quite reasonable agreement between these experimental data.