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Appendix A

Variable Range Hopping

In disordered lattices, the energies of the localized states are spread over a wide range. Adjacent localized states can have widely different energies. In any transition the energy difference must be supplied by a phonon. The transition probability can become so small that transition to further removed states, which involves the expenditure of a lesser amount of energy, becomes more likely. Thus we have a new hopping possibility to add to the *nearest-neighbour hopping*, namely, *variable-range hopping*.

We consider such process in the following, with the assumptions that polaron effects can be neglected and only *one* phonon takes part in the transition. This is simplification which is not necessarily realized in practice.

Fig. A.1 illustrates hopping processes between states with statistical distributions in space and energy. Let us look in particular at two states at locations R_i and R_j . Let them have energies E_i , E_j ($E_j > E_i$). The dominant terms in



Figure A.1: Hopping processes between localized states with statistically distributed position and energy. The hopping probability is determined by the spatial distance and the energy difference between the two states.

the transition probability $w_i j$ can be readily deduced. The electron crossed the distance $R = |\mathbf{R}_j - \mathbf{R}_i|$ by tunneling. The factor which determines the tunneling probability is the overlap in the wave functions of the two states. The simplest ansatz for the wave function of a localized state is an exponential decay from the center $\psi \propto \exp(-|\mathbf{r} - \mathbf{R}_i|/\lambda)$, where λ is a measure of the extent of the state(localization length). If λ is the same for the two states, the tunneling probability is proportional to $\exp(-\frac{2R}{\lambda})$.

The energy difference $W = E_j - E_i$ must (for positive W) be provided by a phonon. W cannot therefore be greater than the maximum energy in the phonon spectrum. The second factor for hopping comes from thermal equilibrium.

The numbers of phonons of energy W in thermal equilibrium goes into the

transition probability. For sufficiently low temperature $(k_B T \ll W)$ it is given by Boltzmann factor $\exp(-\frac{W}{k_B T})$. Altogether we thus have for the transition probability

$$W_{ij} = W_0 \exp\left(-\frac{2R}{\lambda} - \frac{W}{k_B T}\right) \quad \text{for} \quad W > 0.$$
 (A.1)

The factor W_0 can only be calculated when we make further assumptions about the localized states and the electron-phonon interaction.

We have only looked at the transition probability into a state of higher energy. For the reverse case, a jump from E_j back to E_i , corresponding equations are found for w_{ij} in which only the factor $\exp(-W/k_BT)$ is missing. One sees this most simply from the requirement that, in equilibrium, the transition rates in the two directions must be the same. The transition rate are defined as the product of transition probability, occupation probability of the initial state, and nonoccupation probability of the final state. In equilibrium

$$\Gamma_{ij}^{0} \equiv f_{i}(1 - f_{j})w_{ij} = f_{j}(1 - f_{i})w_{ji} \equiv \Gamma_{ji}^{0}$$
(A.2)

from which, with $f_i^{-1} = 1 + \exp[(E_i - E_F)/k_B T]$, it immediately follows that

$$w_{ji} = w_{ij} \exp\left(\frac{E_j - E_i}{k_B T}\right) = w_{ij} \exp\left(\frac{W}{k_B T}\right).$$
(A.3)

Eq.(A.2) can be simplified if we take all energies to be large compared with $k_B T$. The occupation probability $f_i = [1 + \exp\left(\frac{x}{k_B T}\right)]^{-1}$ is then 1 for negative x, and equal to $\exp(-x/k_B T)$ for positive x. We find

$$\Gamma_{ij}^{0} = \gamma_0 \exp[-2R/\lambda - (|E_i - E_F| + |E_j - E_F| + |E_i - E_j|)/2k_BT]$$
(A.4)

The factor γ_0 here is only weakly dependent on W.

For an estimate of the temperature dependence of the hopping cndutivity. we consider a model of the type illustrated in Fig. A.1. Let the energies of statistically destributed localized states be distributed over a finite energy range. We are thus concerned with an impurity band, which has been broadened by the potential flutuations of compensated impurities. Hopping process between adjacent states require greater energy than between more distant states. We inquire about the most probable jump distance \overline{R} , and the associated energy diffrence \overline{W} . We obtain the temperature dependence of the hopping conductivity.

At high temperatures there are enough phonons of energy W^0 (mean energy difference between adjacent states) available to allow hopping processes between nearest neighbours to occur. In the transition rate, \overline{R} becomes equal to R^0 (mean separation of nearest neighbours). Two possibilities have to be considered for the temperature-dependent factor in the transition rate: If the transitions occur at the Fermi energy, i.e., from a state $E_i < E_F$ in to a state $E_j > E_F$, eq.(A.4) leads to the factor $\exp[-(E_j - E_i)/k_BT] = \exp(-W^0/k_BT)$. If the transitions occurs between two E_i , E_j which both lie above E_F , factor $\exp[-(E_i - E_F + W^0)/k_BT]$ follows.

At low temperature no phonons are available with energy W^0 . The electron has to tunnel to reach more destant states $(R > R^0, \text{ but } W < W^0$. The most likely jump distance \overline{R} , and energy difference \overline{W} , can be readily evaluated. To do this we consider a state (R_i, E_i) at the Fermi energy and ask what radius R a sphere around R_i must have in order to find one state with $E_j = E_i + W$ within it. If we assume the dinsity of states g to be constant over the range of energies considered, the number of states with energies between E_i and $E_i + W$ in a sphere of radius R is equal to $(4\pi/3)R^3gW$. One finds one state for $W = 3/4\pi R^3 g$. One can use this dependence W(R) to determine the extremum of the exponent $-2R_{ij}/\lambda - W_{ij}/k_BT$ in the transition probability. It occurs at $\overline{R} = (\frac{g\lambda}{8\pi k_B T g})^{\frac{1}{4}}$, $\overline{W} = \frac{3}{4\pi R^3 g}$. If one inserts these values into the transition probability, one finds for W_{ij} and hence for the conductivity σ the temperature dependence

$$\sigma \propto \exp(-[\frac{T_0}{T}]^{\frac{1}{4}}), T_0 = \frac{512}{9\pi\lambda^3 k_B g}$$
 (A.5)

This is Mott's $T^{\frac{1}{4}}$ law.

The assumption that all jumps are over a fixed distance \overline{R} (fixed range hopping) is only justified for hops between nearest neighbours. For $\overline{R} > R^0$, hops of different distances will follow one another (variable range hopping).

Curriculum Vitae



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