Break-junction tunneling spectroscopy for doped semiconductors in the hopping regime

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We present a theory for tunneling spectroscopy in a break-junction semiconductor device for materials in which the electronic conduction mechanism is hopping transport. Starting from the conventional expression for the hopping current we develop an expression for the break-junction tunnel current for the case in which the tunnel resistance is much larger than the effective single-hop resistances. We argue that percolationlike methods are inadequate for this case and discuss in detail the interplay of the relevant scales that control the possibility to extract spectroscopic information from the characteristic of the device.

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I. INTRODUCTION

Tunneling spectroscopy is one of the most widely used tools for obtaining information on the electronic structure of solids.[1,2] If the tunneling takes place between electrons of the same energy (elastic or resonant tunneling) the tunneling current is a convolution of the densities of states (DOS) of the contact materials.[3] Thus the DOS of one material can be extracted if the DOS of the other material is known. In the case of inelastic tunneling the electronic transitions occur with emission or absorption of phonons. In this case the tunneling current becomes also sensitive to the phonon DOS.[4]

Applying tunneling spectroscopy to doped semiconductors in the hopping regime at low temperatures has proven to be very useful in revealing the influence of the electron–electron interaction on the DOS of the impurity band in the meV range. Such experiments have been performed with conventional metal-barrier-semiconductor contacts[5,6] as well as with mechanically controllable break junctions.[7] Both methods reveal the Coulomb gap in an impressive way.

The theoretical interpretation of break-junction experiments in which both contacts consist of a doped semiconductor[7] is more involved than that of a metal-insulator-semiconductor structure.[8] As the physical nature of the inelastic tunneling transitions between the contacts appears to be similar to those between the localized states in hopping transport the question could arise whether all transitions in question are a part of a global disordered resistor network which would have to be treated by conventional percolation methods. The assumption that this is indeed the case has, for example, been the basis of the arguments in Ref. 9.

At present it does not seem clear whether in the hopping regime the traditional method for the calculation of the tunneling current due to Bardeen[3] is applicable or has to be replaced by a more sophisticated version.

Even the question whether or not information on the electronic DOS *can* be extracted from break junction tunneling experiments is discussed controversially in the literature. In Ref. 9 it is claimed that the tunneling current should exhibit strong mesoscopic fluctuations as a function of the applied voltage. Indeed, if this would be true, little information on the global electronic DOS of the material could be obtained. On the other hand, other theoretical arguments[10] lead to the conclusion that, under certain conditions, information on the electronic DOS can be obtained. Furthermore, neither in experiments[7] nor in simulations of tunneling between materials with localized states[11] are strong fluctuations of the tunneling current as a function of the voltage observed.

Therefore we address this issue here from a fundamental point of view. We start from the rate equations for hopping transport and derive an expression for the tunneling current on the basis of these equations. The further development of the theory exploits the fact that the typical transition probabilities in hopping transport are orders of magnitude larger than those across the junction. This is due to the fact that the junction separation is large compared to the characteristic hopping length in the bulk and due to the fact that the inverse of the vacuum tunnel parameter κ is much smaller than the localization length α^{-1}, which is the tunnel parameter of the hopping transitions. Therefore a separate equilibrium is established in both contacts with two separate chemical potentials the difference of which is controlled by the bias voltage. The resulting expression for the current is similar to the conventional expression for tunneling spectroscopy. Using this expression we discuss under which conditions concerning the length scales and the electron-phonon coupling simplifications of the current formula occur.

II. THE TUNNELING CURRENT

In our derivation of an expression for the tunnel current in a break junction made of a lightly doped semiconductor we

first recapitulate the general theory of hopping transport in an impurity band of a bulk semiconductor, then we consider the case of two parts of a break junction separated very far from each other. These steps will then enable us to study the break junction under realistic conditions.

In the standard theory of hopping transport[12,13] the impurities are assumed to provide localized electronic states at sites $\mathbf{R}_m, \mathbf{R}_n$ with localization length α^{-1} and characteristic energies ϵ_m, ϵ_n. Charge carriers (electrons or holes, dependent on the type of doping) perform phonon-assisted tunneling transitions (hopping transitions) between these states under the influence of an externally applied electric field **E**. The interaction between the charge carriers is assumed to be Coulomb-like (Hubbard-interaction effects are ignored). For definiteness we assume the dopant to be *n* type, i.e., we consider electrons with charge $q=-e$ ($e=|q|$ is the elementary charge). If the interaction is treated in Hartree-Fock (HF) approximation (i.e., if many-particle jumps are ignored) the dynamics of the charge carriers can be described by the simple rate equation

$$\frac{\mathrm{d}\rho_m}{\mathrm{d}t} = \sum_n [\rho_n(1-\rho_m)W_{nm} - \rho_m(1-\rho_n)W_{mn}]. \tag{1}$$

Here ρ_m is the probability to find a charge carrier at site *m*,

$$W_{nm} = \nu(|V_{nm}|)\exp\left\{-2\alpha R_{nm} + \frac{\beta}{2}(V_{nm} - |V_{nm}|)\right\} \tag{2}$$

is the transition probability for a hop from the site *n* to the site *m*, $\beta = 1/kT$, $R_{nm} = |\mathbf{R}_{nm}|$ is the distance between the sites ($\mathbf{R}_{nm} = \mathbf{R}_n - \mathbf{R}_m$), and $V_{nm} = V_n - V_m$, where

$$V_m = \epsilon_m + e(\mathbf{E}R_m) + \sum_{m' \neq m} \frac{e^2\rho_{m'}}{4\pi\epsilon_0\epsilon R_{mm'}} \tag{3}$$

is the energy of a charge carrier at site *m* (ϵ is the dielectric constant of the host). $\nu(|V_{nm}|)$ is the spectral function which describes the influence of the electron-phonon coupling ("attempt-to-escape frequency"). The quantity $\nu(|V_{nm}|)$ characterizes the ability of the phonon to induce the transition. Since phonons with different energy can interact with localized electrons differently well, this frequency is a function of the energy transferred in one hop.

As a model for a break junction we now consider two samples made of a lightly doped semiconductor which are separated by a distance *l* (see Fig. 1). We distinguish between sites situated on the left and right with respect to the separation ("left sites" and "right sites") and denote the labels of the left sites with lower case letters m,n and those of the right sites with upper case ones M,N. Since the junction is a break junction both samples have the same densities of states in the absence of the electric field, that is $N_L(V)|_{\mathbf{E}=0} = N_R(V)|_{\mathbf{E}=0}$.

If both samples are separated very far from each other, there are no transitions between left sites and right sites. Therefore, Eq. (1) is valid for each of the samples separately. Since both samples are in equilibrium, the solutions to the transport equations are simply Fermi functions with two different chemical potentials μ_L and μ_R. For the left sample we have, for example

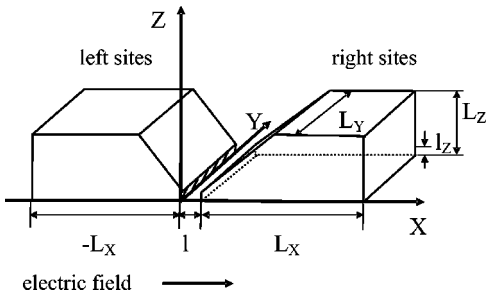

FIG. 1. Geometry of the break junction used in our theoretical treatment, which is schematically the sample geometry of the tunneling experiments in Ref. 7. The hatched area is the active tunneling region. The electric field is directed along the positive *x* axis. In the experiments of Ref. 7 $L_x \approx 3$ to 4 mm, $L_y = 0.8$ mm, $L_z = 1$ mm, and $l_z = 0.2-0.4$ mm. A first estimate for *l* is 10 nm.

$$\rho_{m|eq} = f_m = \frac{1}{1+\exp\{\beta(V_m - \mu_L)\}}. \tag{4}$$

If we now decrease the sample separation, tunneling transitions between the left and the right sample become possible with transition probabilities

$$W_{mM} = \nu(|V_{mM}|)\exp\left\{-2\kappa l_{mM} + \frac{\beta}{2}(V_{mM} - |V_{mM}|)\right\}. \tag{5}$$

The rate equations for the occupation probabilities $\rho_m(t)$ and $\rho_M(t)$ acquire additional terms of the form $\Sigma_M \rho_M(1-\rho_m)W_{Mm}$. It is important to note that the tunnel transitions between the left and the right sample do *not* contain the localization length α but the *vacuum tunneling parameter* κ between the two bulk samples. κ^{-1} is assumedly a few Angstroms, whereas α^{-1} typically takes values around 10 nm. Moreover, the site separation R_{mM} is replaced by the effective tunneling length $l_{mM} = l + \delta l_{mM}$. δl_{mM} is a small correction to the tunneling distance between the two samples taking into account the different wave function amplitudes for a given pair (m,M) of localized states.

If one knows the solution to the transport equations one can calculate the current from the formula

$$\mathbf{j} = -\frac{e}{\Omega}\left[\sum_m \mathbf{R}_m \frac{\mathrm{d}\rho_m}{\mathrm{d}t} + \sum_M \mathbf{R}_M \frac{\mathrm{d}\rho_M}{\mathrm{d}t}\right]. \tag{6}$$

Here Ω is the total volume which contains the sites contained in the summation in Eq. (6).

We now distinguish between two fundamentally different situations which can be controlled by the experimentally adjustable parameter *l*. If *l* is small enough, a common equilibrium between the two samples can be established. In this case the standard methods for solving the transport problem in a disordered hopping system, namely Mott's optimization,[17] percolation theory, [12,13] or the effective-medium approximation[12] can be applied. However, if $2\kappa l$ becomes appreciably larger than the exponents of the domi-

nant bulk transition probabilities (2) (which is already the case if l becomes larger than a few nm), a separate equilibrium is established in the two samples before a tunneling transition can take place. In this situation, which is the one we are interested in, the tunnel transitions are not a part of a percolating network because the charge carriers that cross the break junction cannot optimize their paths. In fact, the tunneling experiments reported in Ref. 7 are performed in such a way that the resistance of the tunneling contact R_{tu} is by orders of magnitudes larger than the equilibrium bulk resistance R_{eq}, so that the current is determined by jumps across the contact. Furthermore, care was taken to adjust the distance l in such a way to make sure that the resistance R_{tu} across the junction did not show the temperature dependence of the bulk resistance $R_{eq} \propto e^{(T_0/T)^x}$, $x \approx 0.5$ which would indicate that a common thermal equilibrium of the two contacts would exist. In the range $R_{tu} \gtrapprox 10^3 R_{eq}$ this regime was reached. It is this regime in which the Coulomb gap was observed. Accordingly, a charge carrier can hardly optimize its path by returning across the junction. We therefore make use of the separation of time scales in the present situation.

The time for a tunneling transition can be estimated as

$$t_{tu} \approx \frac{\exp\{2\kappa l\}}{\langle \nu \rangle}, \tag{7}$$

whereas the equilibration time is roughly

$$t_{eq} \approx \frac{\exp\{(T_0/T)^x\}}{\langle \nu \rangle}, \tag{8}$$

so that we have $R_{tu}/R_{eq} = t_{tu}/t_{eq}$. As mentioned above this ratio is of the order of 10^3 in the tunneling experiments, so that one can be sure that the two samples equilibrate separately before the tunnel transitions take place. In this situation the quantities ρ_m and ρ_M can be considered as Fermi functions as before, and we obtain for the tunneling current

$$\mathbf{j} = -\frac{e}{\Omega}(1 - e^{-\beta(\mu_R - \mu_L)}) \sum_{mM} \mathbf{R}_{mM}\, f_m(1 - f_M) W_{mM}. \tag{9}$$

Due to the disorder the expression (9) is unsuitable for practical analytical calculations. However, the experiments show that the disorder induced fluctuations of the tunneling current are small. In the experiments of Ref. 7, e.g., the disorder induced fluctuations were smaller than 10%. Thus the experiments indicate that the expression (9) can be simplified further by a suitable averaging procedure.

For calculating the configuration average we use the densities of states $N_{L/R}(V, \mathbf{R})$. In the presence of an electric field they are quantities which depend on the energy V and on the position vector $\mathbf{R}$. The latter dependence describes the space charge region. The space-charge region is the region in the sample, in which the charge carrier density in the presence of the field differs from that in the absence of the field. Such a region exists since the screening length in the hopping regime is a large length. Due to this fact the density of states in the vicinity of the boundary in the direction of the electric field is different from that in the sample. Accordingly, the density of states depends also on the position, that is $N_{L/R} = N_{L/R}(V, \mathbf{R})$. This dependence is only negligibly deep in the interior of the sample. There we have $N_{L/R} = N_{L/R}(V)$ independent of $\mathbf{R}$. Performing the configuration average by means of the densities of states we obtain the expression

$$\begin{aligned}\langle \mathbf{j} \rangle = -\frac{e}{\Omega}(1 - e^{-\beta(\mu_R - \mu_L)}) \int_{\Omega_L} d\mathbf{R} \int_{\Omega_R} d\mathbf{R}' \int \mathrm{d}V \mathrm{d}V' (\mathbf{R} - \mathbf{R}') \\ \times N_L(V, \mathbf{R}) N_R(V', \mathbf{R}') f_R(V')[1 - f_L(V)] \\ \times W(|\mathbf{R} - \mathbf{R}'|, V', V)\end{aligned} \tag{10}$$

for the configuration averaged current. Here the bracket $\langle \cdots \rangle$ symbolizes the configuration average.

To investigate the applicability of the averaging procedure we now investigate the disorder induced fluctuations of the tunneling current. Since the electric field is directed along the x direction we focus on j_x, the x component of the current ($\mathbf{j} = j_x \mathbf{e}_x$, $\mathbf{e}_x$ is the unit vector in x direction) and compare the standard deviation $\langle\langle j_x^2 \rangle\rangle = \langle j_x^2 \rangle - \langle j_x \rangle^2$ with the first moment $\langle j_x \rangle$. According to Eq. (9) the quantity j_x can be written in the form

$$j_x = \sum_{mM} j_{mM}. \tag{11}$$

Therefore we obtain

$$\langle\langle j_x^2 \rangle\rangle = \sum_{nN} \sum_{mM} \langle\langle j_{nN} j_{mM} \rangle\rangle. \tag{12}$$

Since the quantities j_{nN} depend only on the indices n and N the currents j_{nN} and j_{mM} in Eq. (12) are only correlated if either $n = m$ or $N = M$, or both equalities hold. Therefore

$$\begin{aligned}\langle\langle j_x^2 \rangle\rangle = \sum_{nN} \langle\langle (j_{nN})^2 \rangle\rangle + \sum_{n} \sum_{N \neq M} \langle\langle j_{nN} j_{nM} \rangle\rangle \\ + \sum_{M} \sum_{n \neq m} \langle\langle j_{nM} j_{mM} \rangle\rangle.\end{aligned} \tag{13}$$

In our averaging procedure the calculation of the configuration average amounts to an integration over the positions of the sites. Therefore the quantities $\langle\langle (j_{nM})^2 \rangle\rangle = \sigma_1^2$, $\langle\langle j_{nN} j_{nM} \rangle\rangle = \sigma_2^2$, and $\langle\langle j_{nN} j_{mN} \rangle\rangle = \sigma_3^2$ are independent of their indices. Consequently,

$$\langle\langle j_x^2 \rangle\rangle = N^2 \sigma_1^2 + N^2 (N - 1)(\sigma_2^2 + \sigma_3^2). \tag{14}$$

Here N is the number of initial sites, which is assumed to be the same as the number of final sites. In the same way we obtain $\langle j_x \rangle = N^2 \langle j \rangle$, where $\langle j \rangle = \langle j_{nm} \rangle$. Accordingly,

$$\frac{\langle\langle j_x^2 \rangle\rangle}{\langle j_x \rangle^2} = \frac{1}{N^2} \frac{\sigma_1^2}{\langle j \rangle^2} + \frac{1}{N} \frac{\sigma_2^2 + \sigma_3^2}{\langle j \rangle^2} \tag{15}$$

for a junction with $N \gg 1$. This argument shows that disorder induced fluctuations of the tunneling current are negligible in tunneling junctions of sufficiently large size.

While the calculation of the standard deviation indicates that the averaging procedure is applicable to tunneling junctions of sufficiently large size the experimental situation is often unclear. The situation for the experiments of Ref. 7 is depicted in Fig. 1. In this experiment the contact area is of macroscopic size ($L_y \approx 0.8$ mm, $l_z \approx 0.2$–0.4 mm). Therefore

we expect that N is a large number. The total number of initial sites in the contact area is of the order of 10^6. The number N, however, must be somewhat smaller, since only pairs in a strip of width $eU+kT$ in energy space contribute to the sum. The real number depends on the width and structure of the impurity band, which is not well known. Therefore the smallness of the fluctuations in the experimental situation remains the main indication which justifies the application of the averaging procedure.

We would like to emphasize that the same averaging procedure can also be applied to the conductivity of the bulk.[12] However, in this case a different expression for the current has to be used, which takes into account that the particle optimizes its path through the sample. Doing so, it often returns to its initial site. Therefore the distribution functions become functions of the transition probabilities, so that $f_m \rightarrow \rho_m(\{W_{mn}\})$. The latter quantities are calculated from the Miller-Abraham random resistor network. Percolative aspects of hopping transport are included if the statistical correlation between the transition probabilities in the distribution functions is taken into account, as it is done in the effective-medium theories. In a tunneling experiment, however, the situation is different. A particle, that has managed to cross the junction, never returns to its initial site to look for a better path, since every hop it can perform in its new surrounding is easier to perform than a hop across the junction. Accordingly, the particles equilibrate in their new surrounding on a time scale which is small compared to the tunneling time. Mathematically, this fact is expressed in that the occupation numbers are independent of the transition probabilities, so that the quantities j_{nm} in Eq. (11) depend only on n and on m, but not on any other site. The latter fact is a consequence of the separation of time scales.

Equation (10) is all what the kinetics tells us. If we want to simplify this equation further we have to use additional knowledge on the samples, that is, about the length scales present in the system. Such scales are the localization length α^{-1}, the tunneling distance l, the screening length l_e, and the sample length L_x. Different relationships between these length scales yield different expressions for the current, as discussed further below.

III. METAL-LIKE CONDITIONS

The expression (10) takes a particularly simple form in the case of metal-like conditions, i.e., $l_e \ll l$, $L_x \gg l_e$, and $l_e \ll \alpha^{-1}$. The first condition means that we can use the approximation $\mu_R - \mu_L = eEl = eU$. Here U is the voltage applied to the sample. If the second condition holds there is a region in the samples in which the densities of states are independent of $\mathbf{R}$. If the third condition applies mainly sites outside the space charge region contribute to the integral (10), so that the DOS measured is the densities of states in the bulk.

In the limit of strong disorder it is unlikely to find neighboring sites on opposite sides of the break junction with the same energy. Therefore mainly inelastic transitions are relevant in this limit. Furthermore, as mentioned before, jumps upwards in energy can be ignored at low temperatures since there are plenty of accessible sites, which can be reached by jumps down in energy space. Accordingly, we obtain[14] for $\beta eU > 1$

$$\langle j_x \rangle = e\tilde{W} \int \mathrm{d}V \mathrm{d}V' N_L(V) N_R(V') \times \theta(V' - V)\,\theta(\mu_R - V')\,\theta(V - \mu_L)\,\nu(|V - V'|), \quad (16)$$

where we have defined

$$\frac{1}{\Omega} \int_{\Omega_L} \mathrm{d}\mathbf{R}_m \int_{\Omega_R} \mathrm{d}\mathbf{R}_M (\mathbf{R}_m - \mathbf{R}_M) \exp\{-2\kappa l_{mM}\} \equiv -\tilde{W}\mathbf{e}_x. \quad (17)$$

Here Ω_L (Ω_R) is the volume of the left (right) sample, over which the integration takes place. Since the transition probabilities are exponentially small quantities with respect to the decay constant κ^{-1} the range of integration penetrates only over a distance of the order of a few times of κ^{-1} into the sample. Thus the relevant volume Ω is of the order of Al, where $A = L_y l_z$ is the area of the cross section of the break-junction.

Since the junction is a break-junction the densities of states N_L and N_R agree with each other if the electric field is switched off, as noted above. Therefore they differ only in the position of the zero point of the energy axis if the electric field is switched on. That is $N_R(V) = N_L(V - eU)$. Accordingly, we obtain

$$\langle j_x \rangle = e\tilde{W} \int_{\mu_L}^{\mu_L + eU} \mathrm{d}V' \int_{\mu_L}^{V'} \mathrm{d}V N_L(V) N_L(V' - eU)\,\nu(V' - V). \quad (18)$$

If it were not for the function $\nu(V' - V)$, which describes the energy dependence of the electron-phonon coupling, we would now have a tool for extracting information on the density of localized states. If this energy dependence is not known one might have difficulties in interpreting inelastic tunneling spectra.[10]

If we assume the deformation potential approximation to hold and that a Debye model for the phonons describes the situation adequately well, the energy dependence of ν is known and the integrals in Eq. (18) can be evaluated.

In deformation potential approximation the function $\nu(E)$ takes the form

$$\nu(E) = \nu_0 \frac{|E|}{\left[1 + \left(\frac{E}{2\hbar s \alpha}\right)^2\right]^4}, \quad (19)$$

where s is the velocity of sound, and ν_0 is a constant.[15] This approximation takes into account that the overlap between the phonon-wave function and the wave functions for localized electrons decreases rapidly if the phonon-wavelength becomes small compared to the localization length.

Of particular interest is the situation in which the DOS shows a pseudogap centered at the Fermi energy, as it is the case in the presence of a Coulomb gap at finite temperature. In this case the DOS has the structure

$$N_L(V) = N_0 + N_\gamma |V - \mu_L|^\gamma, \tag{20}$$

where $\gamma \approx 2$ for three-dimensional systems at zero temperature and N_0 vanishes at zero temperature.[13,16] Using (19) and (20) in Eq. (18) we obtain (see the Appendix)

$$\langle j_x \rangle \propto |U|^{3+\zeta} \tag{21}$$

for $e|U| \ll \hbar s\alpha$, where $\zeta \geqslant 0$ depends on the parameters appearing in Eqs. (19) and (20). Therefore the data for the tunneling conductance appear to scale to zero in an experiment, which is performed in the regime $\beta eU > 1$. Since the applied voltages are very small in the regime $\beta eU \ll 1$ we expect that this is also the behavior which would be observed in experiments. However, we would like to stress that the true value of the tunneling conductance at zero bias is nonzero. To calculate the derivative of the current at zero bias we use Eq. (10). Doing so, we obtain

$$\frac{\mathrm{d}\langle j_x \rangle}{\mathrm{d}U}_{U=0} = e^2 \nu_0 \tilde{W} (kT)^2 [N_0^2 J_{00} + 2N_0 N_\gamma (kT)^\gamma J_{0\gamma} + N_\gamma^2 (kT^{2\gamma}) J_{\gamma\gamma}], \tag{22}$$

where

$$J_{\gamma\lambda} = \frac{1}{4} \int \mathrm{d}x \mathrm{d}y x^\gamma y^\lambda \frac{|x-y| \exp(-|x-y|/2)}{\cosh(x/2)\cosh(y/2)}. \tag{23}$$

In the Appendix also results for $e|U| \gtrsim \hbar s\alpha$ are presented.

According to Eqs. (21) and (22) the tunneling conductance scales to zero with decreasing U for $\beta eU > 1$ and approaches a constant at $\beta eU \ll 1$. The zero bias tunneling conductance itself increases at least quadratically with increasing temperature. This strong temperature dependence is not observed in the experiments of Ref. 7. Therefore one has to ask whether Eq. (19) is really applicable to the materials of interest. This approximation is based on the notion that the charge carriers move to keep each part of the host lattice locally electrically neutral,[18] so that the Fourier transformed Coulomb potential, that provides the coupling between the electron and the phonon system, can be replaced by a constant, the deformation potential constant. However, in the systems of interest the mobile charge carriers are slow compared to the sound velocity and therefore the electromagnetic potential, which provides the electromagnetic coupling between the electron and the phonon system, is of very long range. Accordingly, the electron-phonon coupling constant already drops to zero for interaction events with very small energy transfer. To model this effect phenomenologically we use the approximation

$$\nu(|E|) = \nu_0 \theta(\omega - |E|) \tag{24}$$

which has already been applied successfully in other nonequilibrium hopping problems.[19] In this approximation the maximal amount of energy transferred in one hop is ω. If ω is small enough, we can expand $N_L(V)$ in Eq. (18) around $V = V'$ an retain only the first term. Then Eq. (18) takes the simple form

$$\langle j_x \rangle = e \nu_0 \tilde{W} \omega \int_{\mu_L}^{\mu_L + eU} \mathrm{d}V N_L(V) N_L(V - eU) \tag{25}$$

for $eU > \omega$. This equation has the same form as that which would be obtained for purely elastic transitions, although energy is exchanged with the phonon system. Therefore we call this approximation the quasielastic approximation. It is Eq. (25) which has been used in the interpretation of the experiments of Ref. 7.

For a DOS of the form (20) Eq. (25) yields

$$\langle j_x \rangle = e \nu_o \omega \tilde{W} eU \left[N_0^2 + \frac{2}{\gamma + 1} N_0 N_\gamma |eU|^\gamma + \frac{[\Gamma(1+\gamma)]^2}{\Gamma(2+2\gamma)} N_\gamma^2 |eU|^{2\gamma} \right]. \tag{26}$$

Here $\Gamma(x)$ is the Gamma function.[22] For large eU the asymptotic of this expression agrees with that of the conventional deformation potential approximation up to numbers. For small eU it differs appreciably from that. These differences manifest themselves in particular for small ω. In this case the tunneling conductance approaches the constant value

$$\frac{\mathrm{d}\langle j_x \rangle}{\mathrm{d}U} = e^2 \nu_0 \omega \tilde{W} N_0^2 \tag{27}$$

for $N_\gamma |eU|^\gamma / N_0 \ll 1$. The temperature dependence of the tunneling conductance is in this case governed by the temperature dependence of N_0^2, and thus weaker than that of Eq. (22). This sets the situation in the quasielastic approximation apart from that in the conventional deformation potential approximation and allows one to decide whether the hops in an experiment are quasielastic or inelastic. If ω is small but larger than kT Eq. (27) crosses over to Eq. (22) if eU becomes small compared to ω. If $\omega < kT$, the same dependence as in Eq. (27) is also observed at $U = 0$.

The data of Ref. 7 are not in line with the strong temperature dependence of Eq. (22) [see, e.g., Fig. 1 of Ref. 7 Sandow *et al.* (2001)]. They are, however, in line with Eqs. (25)–(27). Accordingly, the hops were quasielastic.

At this point it is tempting to use the experimental data to estimate ω. However, unfortunately the expression for the tunneling resistance depends too strongly on quantities which are not well known to yield a reliable estimate. According to Eq. (17) $\tilde{W}$ is of the order

$$\tilde{W} \approx \frac{l}{(2\kappa)^3} \exp(-2\kappa l). \tag{28}$$

While $l \approx 10$ nm the quantity κ^{-1} has not been determined so far. Its determination requires further experiments.

IV. INSULATORLIKE CONDITIONS

In this section we consider the case in which the localization length is the smallest length scale in the system (strongly localized regime). Accordingly, the inequality $l_e \gg \alpha^{-1}$ is not satisfied. There are not enough sites which can

be occupied by charge carriers to screen out the electric field on a distance of the order of the localization length. Therefore in the insulatorlike case one measures essentially the DOS in the space-charge region.

For lightly doped materials far from the metal–nonmetal transition the space-charge region can be quite large. Due to this fact there is also an electric field inside the sample. Therefore the simple approximation $eU=eEl$ does not hold. Instead of this relationship we have $eU=eU_L+eEl+eU_R$. Here U_L (U_R) is the potential difference across the left (right) sample. The charge carriers, which are important for the tunneling current, jump from the left surface of the right sample to the right surface of the left sample. Doing so, they have to change their energy by eEl. Accordingly, $\mu_R-\mu_L=eEl$. In order to relate the difference of the chemical potentials to the voltage applied to the sample we express the electric field by U. To this end we focus on the situation that the time for local equilibration in the right and in the left sample is the smallest time scale in the problem. This implies that also the resistance of the contacts is large compared to the resistance of the samples, but small compared to the tunneling resistance. In this case the impact of the space charge region on the tunneling experiment is largest. Furthermore, we assume that the screening of the external electric field can be described within the Debye approximation. In the context of hopping transport this approximation has been discussed, e.g., in Refs. 20 and 21. If we use this approximation we obtain $U=4l_eE+lE$. Accordingly, $eEl=e\tilde{U}$, where $\tilde{U}=Ul/(4l_e+l)$. Since in this case the DOS to the right is related to the DOS to the left by the relationship

$$N_R(V,\, x=l) = N_L(V-e\tilde{U},\, x=-L_x) \tag{29}$$

we obtain for the tunnel current the expression

$$\langle j_x\rangle = e\tilde{W}[1-\exp(-\beta e\tilde{U})]\int_{\mu_L}^{\mu_L+e\tilde{U}} \mathrm{d}V' \int_{\mu_L}^{V'} \mathrm{d}V \times N_L(V,x=0)N_L(V'-e\tilde{U},\, x=-L_x)\nu(|V-V'|). \tag{30}$$

From the practical point of view the most important difference between Eqs. (16) and (30) seems to be that the difference between the chemical potentials is reduced, and therefore U is replaced by $\tilde{U}$. Due to this replacement the range of integration in Eq. (30) is getting small if $l_e \gg l$. This fact renders measurements of tunneling currents more difficult. Moreover, the exponent $\exp(-\beta e\tilde{U})$, which turned out to be negligible in the metal-like situation, might prove to be essential in this case. Since the results of the experiments of Ref. 7 were independent of the tunneling distance l we conclude that in these experiments the condition $l>l_e$ was met. Accordingly, in these experiments l_e was at most of the order of a few times the average site spacing.

In the literature the order of magnitude of the screening length is a controversial point. In Refs. 16, 20, and 21 different expressions for the screening length have been obtained. The fact that the tunneling current depends on the screening length l_e raises the question whether this dependence can be used in order to obtain further information on l_e experimentally. We would like to mention that screening effects in tunneling experiments have been also discussed in Ref. 11.

V. CONCLUSIONS

Starting from the usual rate equations for hopping transport in the impurity band of a doped semiconductor we have derived an expression for the tunnel current across the gap of a break junction device in which the contact material is a doped semiconductor. The fact that the tunnel resistance in a break-junction tunneling experiment is much larger than the resistance of the material leads to a separation of time scales between the tunneling and the dynamics inside the contact. Therefore a separate equilibrium inside the contacts is established with different chemical potentials. This simplifies the resulting expression for the tunnel current as opposed to a situation in which the contacts would be in equilibrium with each other and in which the tunnel and sample dynamics would be part of a common optimization or percolation problem. Due to the separation of time scales the situation in break-junction tunneling experiments is not percolationlike. The resulting expressions for the tunnel current look very similar to those in conventional tunnel or point contact spectroscopy. They become equal to these expressions if metallic-like conditions apply, i.e., if the screening length is the smallest length scale in the problem. However, in the impurity band of lightly doped insulators the localization length is the smallest length scale. Therefore the relevant contact densities of states are those in the space charge region. An increasing extent of the space charge region leads to a reduction of the difference between the local chemical potentials, which affects the measurement if l is smaller or of the order of l_e. If the break junction separation l is larger than the screening length the influence of space charge effects become negligible.

We have investigated our expression for the tunneling current in two approximations, in the conventional deformation potential approximation and in an approximation which only takes into account hops with small energy transfer. The latter is called the quasielastic approximation. In the conventional deformation potential approximation the tunneling conductance has a powerlike current–voltage characteristic for $\beta eU>1$. Accordingly, the tunneling conductance scales to zero with decreasing voltage in this regime. At $\beta eU<1$ this trend is changed. The zero bias tunneling conductance is finite, even if the density of states vanishes at the Fermi energy. Its temperature dependence is governed by the temperature dependence of the density of states and by the temperature dependence of the width of the strip of accessible sites.

In the quasielastic approximation the expression for the tunneling current takes the same form as for a metal. For large voltages the current–voltage characteristic has the same asymptotic in this approximation as our expression for the conventional deformation potential approximation. For small voltages the quasielastic approximation reflects in an ohmic tunneling conductance, which only crosses over to the results

of the conventional deformation potential approximation if the characteristic inelastic energy is large compared to the thermal energy. In the opposite case it leads to a zero-bias tunneling conductivity which depends on temperature only via the density of states.

The characteristic features of the tunneling conductance in deformation potential approximation, in particular the strong temperature dependence of the zero bias tunneling conductance, are not observed in the experiments. The measurements are, however, in line with our results for the quasielastic approximation. Therefore, we conclude that only hops with very small energy transfer were important in the experiment. Additional data are available from further analysis of the tunneling conductance measurement and new experiments on the break junction in the next time.

Let us now discuss the previous theoretical work concerning break-junction tunneling between materials in the hopping regime. In our opinion the conclusions[9] that the tunneling current should be strongly fluctuating and strongly voltage dependent for large voltages have two reasons: First it has been assumed that the current limiting hop across the tunnel gap leads upwards in energy in contrast to our plausible reasoning. Second it was assumed that only a few tunneling events contribute to the current, whereas in a realistic situation the number N of "initial sites" for these events is very large. We have demonstrated that in this situation the fluctuations of the single current contributions do not significantly affect the measured current because of relation (15). Accordingly, we conclude, in contrast to Ref. 9, that statistical fluctuations of the tunneling current are negligible if the contact area of the break-junction is of macroscopic size, as it was, e.g., the case in Ref. 7. This conclusion is in line with the results of the experiments of Ref. 7, in which the current did not show measurable fluctuations.

Our expression for the tunneling current in deformation potential approximation agrees, however, with that of Ref. 10 for not too small U. For very small U the exponent of our result differs from that of Ref. 10 in two ways. First, the expression for the tunneling current in Ref. 10 yields zero for the tunneling conductance at zero bias. This is in contrast to Eq. (22) which is nonzero. The reason for this difference is that in Ref. 10 the occupation numbers have been replaced by step functions, and jumps upward have been ignored. These approximations become inapplicable at zero bias. They ignore that for $kT > eU$ the width of the strip of possible initial and final sites is not governed by eU but by kT, and that for $U \to 0$ upward hops with very small energy transfer are as likely and as frequent as downward hops. Second, the expression of Ref. 10 yields for small U a current-voltage characteristic that differs from our approach. The reason for the difference is that in our treatment we assume that charge carriers on the left side do not affect charge carriers on the right side. Accordingly, the common DOS can be replaced by a simple product of the DOS. In Ref. 10, however, it has been assumed that the Coulomb interaction between the left sites and the right sites is important, and that therefore also the common DOS cannot be replaced by a simple product. We expect that such correlation effects become unimportant with increasing sample separation. Tunneling experiments, however, are performed in such a way that the results are independent of the sample separation. Therefore these correlations should be not essential.

APPENDIX

Performing the integral (18) with the deformation-potential function (19) and the electronic DOS (20) we find that

$$\langle j_x \rangle = e\tilde{W}\nu_0(2\hbar s\alpha)^{3+2\gamma}N_\gamma^2\lambda^3[A^2 I_{00}(\lambda^2) + 2A\lambda^\gamma I_{0\gamma}(\lambda^2) + \lambda^{2\gamma} I_{\gamma\gamma}(\lambda^2)], \tag{A1}$$

where

$$I_{\alpha\beta}(\lambda^2) = \frac{\Gamma(1+\alpha)\Gamma(1+\beta)}{\Gamma(4+\alpha+\beta)} {}_3F_2[1, 3/2, 4; 2 + (\alpha+\beta)/2, 5/2 + (\alpha+\beta)/2; -\lambda^2], \tag{A2}$$

$\lambda = eU/(2\hbar s\alpha)$ and $A = N_0/[N_\gamma(2\hbar s\alpha)^\gamma]$ (${}_3F_2$ is the hypergeometric function). Accordingly, λ is determined by the voltage, and A is a measure for the depth of the dip of the density of states.

To get an expression for the tunneling current for small λ we expand Eq. (A2) with respect to λ. Doing so, we obtain

$$\langle j_x \rangle \propto C\lambda^{3+\zeta}[1 - B\lambda^2 + O(\lambda^4)]. \tag{A3}$$

Here $\zeta = 2\gamma$, $B = 12/[(2+\gamma)(5+2\gamma)]$, and

$$C = \frac{[\Gamma(1+\gamma)]^2}{\Gamma(4+2\gamma)} e\tilde{W}\nu_0(2\hbar s\alpha)^{3+2\gamma}N_\gamma^2 \tag{A4}$$

for $A/\lambda^\gamma \ll 1$, and $\zeta = 0$, $B = 6/5$, and

$$C = \frac{1}{9} e\tilde{W}\nu_0(2\hbar s\alpha)^{3+2\gamma}N_\gamma^2 A^2 \tag{A5}$$

for $A/\lambda^\gamma \gg 1$.

For large λ we obtain

$$\langle j_x \rangle \propto D\lambda^{1+2\gamma}[1 - E/\lambda + O(1/\lambda^2)], \tag{A6}$$

where $E = 1$ and

$$D = \frac{1}{6} e\tilde{W}\nu_0(2\hbar s\alpha)^{3+2\gamma}N_\gamma^2 A^2 \tag{A7}$$

for $A/\lambda^\gamma \gg 1$, and $E = 2\gamma + 1$ and

$$D = \frac{[\Gamma(1+\gamma)]^2}{6\Gamma(2+2\gamma)} e\tilde{W}\nu_0(2\hbar s\alpha)^{3+2\gamma}N_\gamma^2 \tag{A8}$$

for $A/\lambda^\gamma \ll 1$.

In order to get some feeling for typical values of the parameter λ we use the parameters of Ref. 7. In these experi-

ments voltages up to 8 mV have been used. If we use 2000 m/s as the estimate for the sound velocity and a value of $2\alpha \approx 10^8$ m^{-1} we find that in these experiments the parameter λ changed from 0 to 80. However, the data of Ref. 7 also show that in the most interesting region the parameter λ took on only values of the order of 10 and smaller. Accordingly, λ is probably neither small nor large in the most interesting region in an experiment, so that in many cases the expression (A2) has to be used for the interpretation of data.

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