On the structure of the energy distribution function in the hopping regime

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Abstract
The impact of the dispersion of the transport coefficients on the structure of the energy distribution function for charge carriers far from equilibrium has been investigated in the effective medium approximation for a model density of states. The investigations show that two regimes can be observed in energy relaxation processes. Below a characteristic temperature the structure of the energy distribution function is determined by the dispersion of the transport coefficients. Thermal energy diffusion is irrelevant in this regime. Above the characteristic temperature the structure of the energy distribution function is determined by energy diffusion. The characteristic temperature depends on the degree of disorder and increases with increasing disorder. Explicit expressions for the energy distribution function in both regimes are derived for a constant and an exponential density of states.

1. Introduction

A characteristic feature of many disordered materials is the strong dependence of their transport properties on the frequency of the applied external electric field for low frequencies. In that, disordered materials differ from ordered materials, which typically only show a pronounced frequency dependence at high frequencies. Also the character of the impact of an alternating electric field on the transport coefficients in disordered materials is different from that in ordered ones. Whereas in ordered materials an increase of the frequency is always reflected in a decrease of the conductivity, in disordered materials an increase of the frequency leads to an increase of the real part of the conductivity. The sensibility of the transport coefficients to a change of the frequency increases with increasing amount of disorder. Therefore, a particularly strong frequency dependence is observed in the strongly localized regime, in which transport proceeds by hopping between localized states, such as impurity bands, Anderson insulators, glasses, and polymers (see, e.g., [1–5]).

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The same frequency dependence, which governs the response to an alternating electric field, also determines the relaxation properties of the system. Accordingly, the dispersion of the dynamical conductivity in the hopping regime is also reflected in relaxation experiments close to equilibrium. It manifests itself, for example, in transient current experiments [1, 6], which test the diffusion properties of particle packets in a random environment. In such experiments the dispersion of the transport coefficients leads to dispersive transport; this is due to deviations from the conventional relationship $\langle R^2(t) \rangle \propto t$ for $t < t_{perc}$, where $\langle R^2 \rangle$ is the mean squared deviation of a particle packet at time t, which was a delta-pulse at time $t = 0$, and t_{perc} is the percolation time [2]. Accordingly, the diffusion process breaks up into two regimes: a regime of anomalous diffusion, which takes place for $t < t_{perc}$, and a regime of normal diffusion, which takes place for $t \gg t_{perc}$. Since the percolation time depends exponentially on the disorder parameter it depends strongly on the material in question, i.e. there is no typical timescale for it in the experiments. In practice, timescales between 10^{-8} and 5 s have been observed (see the discussion of experiments on p 216 of [1]).

Far from equilibrium, the effective rate analysis of [7] has mainly been applied to analytical investigations of relaxation phenomena. This method assumes that the relaxation process far from equilibrium is not affected by the dispersion of the transport coefficients, and that therefore the transport coefficients to be used in modelling the relaxation are the same as those at zero frequency. We would like to mention that despite this fact dispersive transport has also been discussed in applications of the effective rate analysis, but the nature of the dispersive transport discussed there, for example in [7], is very different from that in transient current experiments close to equilibrium. Whereas the dispersive relaxation close to equilibrium results from the frequency dependence of the transport coefficients, and thus reflects the peculiarity that the charge carriers in hopping systems try to optimize their jumps, the dispersion in the effective rate analysis results solely from the fact that the particles move in an inhomogeneous distribution of sites in the four-dimensional position–energy space. In this case dispersion arises since the transport coefficients depend on the instantaneous position of the particles in energy space, which changes with time. Therefore, similar dispersive contributions are also obtained for the relaxation of charge carriers in ordered systems. Clearly, they are much larger in the hopping regime than in ordered systems, since the transport coefficients depend much more strongly on the energy in the hopping regime than in ordered systems.

Given that the analytical results of the effective rate analysis correlate well with the results of numerical experiments for systems with strongly energy dependent density of states, the question arises whether the dispersion of the transport coefficients is important in relaxation processes far from equilibrium or not, and if so, which quantities are determined by it. To answer this question at zero temperature we have derived an equation for the energy distribution function in the hopping regime in [8] and investigated it further in [9] and [10]. The most important property of this equation is that the shape of the energy distribution function is entirely determined by the dispersion of the transport coefficients. The dispersion determines the first moment of the energy distribution function for systems with weakly energy dependent density of states and the second and higher moments both for systems with weakly energy dependent density of states and for systems with strongly energy dependent density of states. These moments can be investigated experimentally by line width measurements in time resolved photoluminescence spectroscopy experiments. In an exponential density of states the dispersive nature of the energy relaxation leads to a soliton-like motion of a particle packet in energy space at zero temperature.

It is natural to ask whether these results also apply to systems at finite temperatures or not. If so, these results would provide a further characteristic, which would set disordered hopping systems apart from other physical systems. The latter generally share the feature

that the structure of the energy distribution function is determined by energy diffusion processes [11, 12]. In the diffusion approximation, for example, this fact is reflected in the fact that the second derivatives with respect to the energy are as important as the first derivatives and therefore cannot be ignored [12]. Below we investigate this question analytically for charge carriers far from the Fermi energy in a constant density of states and charge carriers in an exponential density of states. For these model densities of states we show that there is a characteristic temperature, which sets two regimes apart: a regime where the structure of the energy distribution function is determined by the dispersion of the transport coefficients and a regime where the structure of the distribution function is governed by the energy diffusion current. The characteristic temperature discriminating these regimes is finite, depends on the amount of disorder, and increases with increasing disorder.

2. The model

We consider strongly localized non-equilibrium charge carriers far from the Fermi-energy. Such charge carriers can, for example, be produced by illumination. After their excitation the charge carriers relax by phonon-assisted hops. We assume that the number of charge carriers is small, so that we can neglect Fermi-correlation. In this case the transport can be described by the simple rate equation

$$\frac{dn_m}{dt} = \sum_n [n_n W_{nm} - n_m W_{mn}].\tag{1}$$

Here n_m is the probability to find a particle on the site m with site energy ϵ_m and position vector $\boldsymbol{R}_m$,

$$W_{nm} = \theta(\omega - |\epsilon_{nm}|)\nu \exp\left(-2\alpha|\boldsymbol{R}_{nm}| + \frac{\beta}{2}(\epsilon_{nm} - |\epsilon_{nm}|)\right),\tag{2}$$

$\epsilon_{nm} = \epsilon_n - \epsilon_m$, $\boldsymbol{R}_{nm} = \boldsymbol{R}_n - \boldsymbol{R}_m$, α^{-1} is the localization length, ν is the attempt-to-escape frequency, and β is the inverse temperature. Both the positions of the sites and the site energies are random quantities. We assume that the sites are distributed randomly in space and that the site energies are distributed according to a distribution function, which is proportional to the density of states $N(\epsilon)$ of the system.

In writing down equation (2) we have also assumed that there is a maximal amount of energy ω, which can be transferred from the electron to the phonon system, or vice versa, in one hop. The introduction of this energy scale is based on the observation that the electron–phonon coupling constant tends rapidly to zero for phonons with large momentum q. The electron–phonon coupling constant is a function which depends on both the overlap between the electron wavefunction and the phonon wavefunction and on the Fourier-transformed electromagnetic potential, which provides the coupling between the electron and the phonon wave. The overlap integral tends to zero for phonons with wavevector $q > 2\alpha$, and thus renders the modes with $q > 2\alpha$ ineffective. The Fourier-transformed potential is usually considered as a constant, in line with the deformation potential approximation. From the physical point of view this means that the electrons can move in such a way that they can keep the system neutral. In the strongly localized regime, however, there are no electrons which can move fast enough to screen out the alternations of the electric field produced by the phonon wave for most q. Accordingly, the Fourier-transformed Coulomb potential is a function which already drops rapidly to zero for tiny q. Due to these facts hops with large energy transfer can happen, but they are not characteristic. In our approximation we therefore ignore such jumps. Since at present there are no further investigations in the literature on the energy scale ω we take the point of view that ω is a phenomenological parameter, which can be determined by an experiment.

In our investigation we focus on energy relaxation processes. Quantities of interest are, for example, the mean energy

$$\langle \epsilon \rangle(t) = \left\langle \sum_n \epsilon_n n_n(t) \right\rangle, \tag{3}$$

and the mean squared deviation

$$\sigma^2(t) = \left\langle \sum_n \epsilon_n^2 n_n(t) \right\rangle - \langle \epsilon \rangle^2(t) \tag{4}$$

of a particle packet in energy space. Here the bracket symbolizes the configuration average. Both quantities can be measured in time-resolved photoluminescence experiments. In order to calculate these quantities we first assume that at time $t = 0$ there is a particle packet, characterized by $\{n_m(t = 0)\}$, and then use the function $P_{m'm}$ (see [1]), the Green function of equation (1), to calculate the electron distribution for $t > 0$ according to the equation

$$n_m(t) = \sum_n n_n(t = 0) P_{nm}(t). \tag{5}$$

3. The energy distribution function

In order to derive an equation for the energy distribution function we use the relationship

$$F(\epsilon', \epsilon | t) = \int \mathrm{d}\boldsymbol{R} \, F(\boldsymbol{R} | \epsilon', \epsilon, t) \tag{6}$$

between the energy distribution function $F(\epsilon', \epsilon | t)$ and the diffusion propagator $F(\boldsymbol{R} | \epsilon', \epsilon, t)$. The latter is calculated from the configuration average of the Green function P_{nm}. To calculate the average we first introduce continuous coordinates according to the definition

$$P(V'; V) = \sum_{nm} \delta(V' - V_n) P_{nm} \delta(V - V_m), \tag{7}$$

where $V = (\boldsymbol{R}, \epsilon)$ and $V_m = (\boldsymbol{R}_m, \epsilon_m)$. Thereafter, we apply the effective-medium approximation by Gouchanour *et al* [13]. Although this technique was developed originally for investigations of hopping systems with topological disorder it can be checked that the extension of this method to systems with both topological and energetic disorder only amounts to a change of notation. Accordingly, we can directly use the results of [13], as discussed also in [9].

The effective-medium approximation of [13] reduces the calculation of the diffusion propagator to the solution to the system of integral equations

$$\langle P(\boldsymbol{R}, \epsilon' | \boldsymbol{0}, \epsilon) \rangle = N(\epsilon') F(\boldsymbol{R} | \epsilon', \epsilon), \tag{8}$$

$$sF(\boldsymbol{R} | \epsilon', \epsilon) = \delta(\boldsymbol{R}' - \boldsymbol{R}) \delta(\epsilon' - \epsilon) + \int \mathrm{d}\rho_1 [F(|\boldsymbol{R} - \boldsymbol{R_1}| | \epsilon', \epsilon_1) \tilde{W}(R_1 | \epsilon_1, \epsilon) N(\epsilon)$$
$$- F(|\boldsymbol{R}| | \epsilon', \epsilon) \tilde{W}(R_1 | \epsilon', \epsilon_1) N(\epsilon_1)], \tag{9}$$

$$\tilde{W}(R | \epsilon', \epsilon) = \frac{W(R | \epsilon', \epsilon)}{1 + f(\epsilon) W(R | \epsilon, \epsilon') + f(\epsilon') W(R | \epsilon', \epsilon)}, \tag{10}$$

and

$$f^{-1}(\epsilon) = s + \int \mathrm{d}\epsilon_1 \, \mathrm{d}R \tilde{W}(R | \epsilon, \epsilon_1) N(\epsilon_1). \tag{11}$$

Here s is the Laplace frequency, which corresponds to a Laplace transformation with respect to time, $W(R | \epsilon', \epsilon) = W_{nm} |_{R_{nm} = R, \epsilon_n = \epsilon', \epsilon_m = \epsilon}$, and $\tilde{W}$ is the renormalized transition probability.

$f(\epsilon)$ is the effective-medium constant, which for the present system is strictly speaking not a constant, but a function of energy. According to these equations the functions F and $\tilde{W}$ also depend on s, but the dependence of F on s and the dependence of $\tilde{W}$ on s have been suppressed to simplify the notation.

Despite the effective-medium approximation the calculation of the diffusion propagator is still a difficult task, since it requires finding solutions of integral equations. Due to the lack of symmetry, however, it is impossible to solve these integral equations analytically if the density of states depends on energy, as is the case for most relevant physical systems. To simplify the equations we restrict the consideration to the limit $\beta\omega \ll 1$ and use the concept of quasi-elasticity. The introduction of this concept relies on the notion that the energy scale ω is small, so that

$$\frac{\omega}{f(\epsilon)} \frac{\mathrm{d}f(\epsilon)}{\mathrm{d}\epsilon} \ll 1. \tag{12}$$

Then the renormalized transition probability takes the form

$$\tilde{W}(R|\epsilon', \epsilon) = \theta(\epsilon' - \epsilon)\theta(\omega - \epsilon' + \epsilon)\tilde{W}(R|\epsilon') + \theta(\epsilon - \epsilon')\theta(\omega - \epsilon + \epsilon')\tilde{W}(R|\epsilon)\mathrm{e}^{-\beta(\epsilon-\epsilon')}, \tag{13}$$

where

$$\tilde{W}(R|\epsilon) = \frac{W(R)}{1 + 2f(\epsilon)W(R)}, \tag{14}$$

and $W(R) = \nu\exp(-2\alpha R)$. If we furthermore restrict the consideration to high temperatures, where $\beta\omega \ll 1$, and use the inequality (12) we find that the self-consistency equation (11) simplifies considerably. For $s = 0$ we find that the solution of this equation is given by

$$\rho_c(\epsilon, 0) = \frac{2\alpha}{(\omega N(\epsilon))^{1/d}}\left(\frac{d}{S_d}\right)^{1/d}, \tag{15}$$

and for small s, that is for s satisfying $|\rho_c(\epsilon, 0) - \rho_c(\epsilon, s)| \ll \rho_c(\epsilon, 0)$, we obtain the equation

$$(\rho_c(\epsilon, 0) - \rho_c(\epsilon, s))\exp(\rho_c(\epsilon, 0) - \rho_c(\epsilon, s)) = \frac{s}{\omega_0(\epsilon)}. \tag{16}$$

Here

$$\rho_c(\epsilon, s) = \ln(2f(\epsilon, s)\nu) \tag{17}$$

is the dimensionless characteristic hopping length,

$$\omega_0(\epsilon) = \frac{2d\nu}{\rho_c(\epsilon, 0)}\exp(-\rho_c(\epsilon, 0)), \tag{18}$$

and S_d is the solid angle in d dimensions ($S_2 = 2\pi$, $S_3 = 4\pi$). The dimensionless characteristic hopping length $\rho_c(\epsilon, s)$ and the characteristic hopping length $R_c(\epsilon, s)$ are connected by the relationship $\rho_c(\epsilon, s) = 2\alpha R_c(\epsilon, s)$.

In the same approximation the equation for the energy distribution function takes the form

$$sF(\epsilon', \epsilon) = \delta(\epsilon' - \epsilon) + \omega\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left[N(\epsilon)\nu(\epsilon, s)\left(\frac{\mathrm{d}}{\mathrm{d}\epsilon}\frac{F(\epsilon', \epsilon)}{N(\epsilon)} + \beta\frac{F(\epsilon', \epsilon)}{N(\epsilon)}\right)\right]. \tag{19}$$

Here

$$\nu(\epsilon, s) = \frac{\omega^2}{3}N(\epsilon)\int \mathrm{d}\boldsymbol{R}\,\tilde{W}(R|\epsilon) \tag{20}$$

is the spectral energy relaxation rate. Note that, due to equations (10) and (11), the effective transition probability depends on the Laplace frequency s. Therefore, the energy relaxation

rate is also frequency dependent, so that we can expect that dispersion of the energy relaxation rate manifests itself also in the moments of the energy distribution function.

In order to find a concrete expression for the spectral energy relaxation rate we use equation (13) and restrict the investigation to low frequencies. Doing so, we obtain

$$v(\epsilon, s) = \frac{\omega}{3} \nu \exp(-\rho_c(\epsilon, s)). \tag{21}$$

The equations (15), (16), (19) and (21) yield a closed set of equations for the calculation of the energy distribution function, which can be used for the investigation of energy relaxation processes in an arbitrary density of states, provided the inequalities (12) and $\beta\omega \ll 1$ are satisfied. Below we apply this set of equations to the investigation of energy relaxation processes in model densities of states.

4. Energy relaxation in a constant density of states

In this section we focus on energy relaxation processes in an unbounded constant density of states with $N\omega$ sites per volume. Investigations of energy relaxation processes in such densities of states should be relevant for charge carriers in certain types of Anderson-insulators above the glass temperature, as, for example, for those used in [14] and [15], for which field effect measurements indicate that the density of states varies only weakly with energy.

Since for a constant density of states the transport coefficients are independent of energy, the calculation simplifies considerably. In this case the differential equation (19) can be solved exactly. Its solution takes the form

$$F(\epsilon_0, \epsilon; s) = \frac{1}{2\omega v(s)} \frac{\exp\left(-\frac{\beta}{2}(\epsilon - \epsilon_0) - \sqrt{\frac{\beta^2}{4} + \frac{s}{\omega v(s)}} |\epsilon_0 - \epsilon|\right)}{\sqrt{\frac{\beta^2}{4} + \frac{s}{\omega v(s)}}}. \tag{22}$$

To find the dependence of the distribution function on time we have to perform an inverse Laplace transformation, according to

$$F(\epsilon_0, \epsilon; t) = \frac{1}{2\pi i} \int_c \mathrm{d}s \, \mathrm{e}^{st} F(\epsilon_0, \epsilon; s). \tag{23}$$

This integral yields the probability to find a particle on a site with site energy ϵ at time t, if it was on a site with site energy ϵ_0 at time $t = 0$. In calculating this integral we restrict the consideration to large times. For large times we expect that the particle packet has already moved down in energy space. It has somewhere in energy space a maximum and some width. The position of the maximum is characterized by the mean energy $\langle\epsilon\rangle(t)$ and the width by the dispersion $\sigma^2(t)$. We assume that t is so large that $\epsilon_0 > \langle\epsilon\rangle(t) - \sigma(t)$. In this case we can use the saddle point approximation. The saddle point satisfies the equation

$$t = \frac{\mathrm{d}}{\mathrm{d}s}(\epsilon_0 - \epsilon)\left(\frac{\beta}{2} - \sqrt{\frac{\beta^2}{4} + \frac{s}{\omega v(s)}}\right). \tag{24}$$

The solution of this equation is a function $s_0(\epsilon_0, \epsilon, t)$. If we assume that the integral is determined by the saddle point we deduce that

$$F(\epsilon_0, \epsilon, t) \propto \exp\left(\left(\frac{\beta}{2} - \sqrt{\frac{\beta^2}{4} + \frac{s_0(\epsilon_0, \epsilon, t)}{\omega v(s_0(\epsilon_0, \epsilon, t))}}\right)(\epsilon_0 - \epsilon)\right). \tag{25}$$

Accordingly, the maximum of the particle packet satisfies the equation

$$0 = \frac{d}{d\epsilon}\left[\left(\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} - \frac{s_0(\epsilon_0, \epsilon, t)}{\omega v(s_0(\epsilon_0, \epsilon, t))}}\right)(\epsilon_0 - \epsilon)\right]$$

$$= -\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} + \frac{s_0(\epsilon_0, \epsilon, t)}{\omega v(s_0(\epsilon_0, \epsilon, t))}}. \tag{26}$$

Here we have used the fact that s_0 satisfies equation (24). Thus, we know that the characteristic s_0 in the vicinity of the maximum is close to zero. Accordingly, in order to calculate the integral we can restrict the consideration to small s, and use this knowledge to expand the root in the exponent of equation (22). Doing so, we obtain

$$\sqrt{\frac{\beta^2}{4} + \frac{s}{\omega v(s)}} \approx \frac{\beta}{2}\left(1 + \frac{2s}{\beta^2\omega v(0)} - \frac{2s^2}{\beta^2\omega v(0)\omega_0} - \frac{2s^2}{(\beta^2\omega)^2 v^2(0)}\right). \tag{27}$$

Here it is important to realize that the third and fourth terms of this expansion are of different physical origin. Both terms, as can be seen further below, contribute to the mean squared deviation. However, while the third term results entirely from dispersion the fourth term results entirely from thermal energy diffusion. Thus the relationship between these two terms determines whether thermal activation affects the shape of the energy distribution function or not. If we use the expansion (27) the integrals become Gaussian. Doing the integrals we find that

$$F(\epsilon_0, \epsilon; t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}}\exp\left(-\frac{(\epsilon_0 - \epsilon - \beta\omega v(0)t)^2}{2\sigma^2(t)}\right), \tag{28}$$

where

$$\sigma^2(t) = 2\omega v(0)t\left(1 + \frac{\beta^2\omega v(0)}{\omega_0}\right). \tag{29}$$

Accordingly, at large times the particle packet moves with constant velocity. An increase of the temperature is reflected in a decrease of the energy relaxation rate. The shape of the packet is Gaussian, and its mean squared deviation is given by equation (29). In this equation the first term in the bracket on the right-hand side results entirely from thermal diffusion and the second entirely from dispersion. Remarkably, the thermal contribution to the packet's width is independent of temperature. Since

$$\frac{\beta^2\omega v(0)}{\omega_0} = \frac{(\beta\omega)^2\rho_c}{6d},$$

its contribution is only important if the temperature is large, that is, if $T \gg T_c$, where $kT_c = \omega\sqrt{\rho_c/(6d)}$. Accordingly, the second derivative in equation (19) is negligible for $T \ll T_c$. Consequently, the relaxation is determined by the first order differential equation

$$sF(\epsilon_0, \epsilon) = \delta(\epsilon_0 - \epsilon) + \frac{d}{d\epsilon}(F(\epsilon_0, \epsilon)\omega\beta v(s)), \tag{30}$$

for $T \ll T_c$. If the relaxation at zero temperature is also described percolation-like then this equation differs from the equation for the calculation of the energy distribution function at zero temperature (see [8]) only in that $v(0)$ is replaced by $\omega\beta v(0)$, so that all of the results derived in [8] are also valid in this regime, after a trivial change of parameters. Since $T_c \propto \sqrt{\rho_c}$, the range of applicability of these results increases with increasing disorder.

5. Energy relaxation in an exponential density of states

In this section we investigate the relaxation in an exponential density of states of the type

$$N(\epsilon) = N_0 \exp\left(\frac{\mathrm{d}\epsilon}{\Delta}\right). \tag{31}$$

Here N_0 and Δ are parameters characterizing the density of states. The consideration of the relaxation in such a density of states is relevant for investigations on relaxation phenomena in band tails of several amorphous semiconductors, as for example for the conduction band tail in amorphous hydrogenated silicon (see, for example, [7]).

Since the strong dependence of the density of states on energy manifests itself also in the transport coefficients, it turns out to be hard to find an analytical solution for the differential equation (19) in this case. Therefore, we focus at first on the solution for a particle which moves in a region with

$$kT \frac{\mathrm{d}\rho_c(\epsilon, 0)}{\mathrm{d}\epsilon} \ll 1. \tag{32}$$

That is, we first restrict the consideration to the shallow states in the tail. The lower limiting energy of this region agrees with the transport energy, as defined in [7, 16] and [17]. In the literature this region is also called the hopping down regime [7].

Within the range of the inequality (32) we can use the WKB approximation (see the details of the calculation in the appendix). Doing so, we find that the energy distribution function takes the form

$$F(\epsilon_0, \epsilon; t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} \exp\left(-\frac{(\epsilon - \langle\epsilon\rangle(t))^2}{2\sigma^2(t)}\right) \tag{33}$$

at large times, where the mean energy is given by

$$\langle\epsilon\rangle(t) \approx -\Delta \ln\left(\frac{1}{\rho_0} \ln\left(\frac{\beta\omega^2}{3\Delta}\nu t\right)\right) \tag{34}$$

(here $\rho_0 = \rho_c(\epsilon) \exp(\epsilon/\Delta)$) and the mean squared deviation by

$$\sigma^2(t) = \sigma_{\mathrm{therm}}^2(t) + \sigma_{\mathrm{disp}}^2(t). \tag{35}$$

Here

$$\sigma_{\mathrm{therm}}^2(t) \approx \frac{kT\Delta}{\rho_c(\langle\epsilon\rangle(t))}, \tag{36}$$

and

$$\sigma_{\mathrm{disp}}^2 \approx \frac{\Delta\beta\omega^2}{6d}. \tag{37}$$

Equation (33) differs from the predictions of the energy loss hopping model, which have been derived with the assumption that the relaxation at zero temperature is percolation-like, in two points. First, while in the energy loss hopping model the energy relaxation rate is independent of temperature [7, 8] the energy relaxation rate is determined by the parameter $\beta\omega^2\nu t/\Delta$ at finite temperatures in the limit $\beta\omega \ll 1$. Second, while the mean squared deviation of the particle packet in the energy loss hopping model is time independent, the dispersion becomes time dependent at finite temperatures. The time dependence results from the thermal contribution to the mean squared deviation. This contribution to the mean squared deviation is dominant if

$$kT \gg \omega\sqrt{\rho_c(\langle\epsilon\rangle(t))/(6d)}, \tag{38}$$

that is for high temperatures. In this temperature range the width of the energy distribution function increases with temperature. However, since the particle is sinking down, its hopping

length increases. From equation (36) we deduce that this increase tends to suppress the thermal contribution to the packet's width, and thus renders the disperse contribution more important. In contrast to the thermal contribution the disperse contribution is time independent, so that the packet moves in energy space without further distortion, once the thermal spreading of the packet has become insignificant. In this limit the motion of the packet in energy space is soliton-like. Here an increase of the temperature results in a decrease of the packet width.

The fact that the thermal spreading of the particle packet becomes unimportant outside the validity range of the inequality (38) indicates that in this region the second derivative with respect to the energy in equation (19) is negligible, so that instead of equation (19) the simple equation

$$sF(\epsilon_0, \epsilon) = \delta(\epsilon - \epsilon_0) + \frac{\mathrm{d}}{\mathrm{d}\epsilon}(F(\epsilon_0, \epsilon)\beta\omega v(\epsilon, s)) \tag{39}$$

can be used.

In the derivation of our results we have used the inequality (32), which controls the validity of the WKB approximation. However, the results of this calculation show that thermal spreading becomes unimportant when time goes by, that is when the hopping length becomes large. From our point of view this is intuitively clear, since the impact of the dispersion of the transport coefficients in the hopping regime increases strongly with disorder. This fact suggests that equation (39) also holds outside the validity range of the inequality (32), so that equation (39) can probably also be used for deep states in the tail, if only the condition (12), which governs the range of applicability of the quasi-elastic approximation, is met.

6. Conclusions

Our investigations show that the structure of the energy distribution function in the hopping regime is determined by the dispersion of the energy relaxation rate in a large temperature range. The characteristic temperature, governing the impact of the dispersion on the structure of the energy distribution function, depends on the strength of the disorder, and therefore on the details of the density of states. In both of the cases studied, the impact of energy diffusion processes on the structure of the energy distribution function were only significant for $kT \gg \omega\sqrt{\rho_c}(\epsilon, 0)$. This sets the situation in the hopping regime apart from that on the extended side of the metal–insulator transition, in which the structure of the energy distribution function is entirely determined by energy diffusion [11, 12].

In a constant density of states the parameter $\rho_c(\epsilon, 0)$ is independent of ϵ. Therefore, a global characteristic temperature exists, which governs the influence of the dispersion. Although in this case the mean squared deviation increases linearly with time for large times, the difference between the energy diffusion driven structuring of the energy diffusion function and a structuring due to the dispersion of the transport coefficients manifests itself in the temperature dependence of the second moment of the energy distribution function. The latter decreases quadratically with increasing temperature at large temperatures.

In an exponential density of states the situation is more intricate. In this case there is no globally defined characteristic temperature, since the criterion $kT \gg \omega\sqrt{\rho_c}(\epsilon, 0)$ depends on the instantaneous position of the packet in the tail. Since the particles are sinking down, their dimensionless hopping length $\rho_c(\epsilon, 0)$ increases when time elapses. Accordingly, the thermal spreading of the energy distribution function, which is important in the initial phase of the relaxation in the shallow states of the tail, becomes unimportant as time goes by. Deep in the tail the structure of the energy distribution function is entirely determined by the dispersion of the energy relaxation rate. Energy diffusion processes are negligible in this case. In this limit

the dispersive nature of relaxation process leads to a soliton-like motion of the particle packet in energy, i.e., the particle packet moves in energy space without distortion.

We would like to mention that in both cases studied an increase of the temperature results in a decrease of the energy relaxation rate. This result is in line with the results of the numerical simulations in [10] for a constant density of states, which have been performed in the same limit. It sets the situation in the limit of small energy transfer apart from that in conventional variable-range hopping systems, in which the relaxation rate usually speeds up with increasing temperature [7].

Appendix. Calculation of the inverse Laplace transform for the exponential density of states

Within the range of the inequality (32) we can use the WKB approximation. However, in applying the WKB approximation the following difficulty appears. To lowest order, that is within exponential accuracy, the WKB approximation immediately predicts

$$F(\epsilon_0, \epsilon) \propto \exp\left(-\frac{\beta}{2}(\epsilon - \epsilon_0) - \left|\int_\epsilon^{\epsilon_0} d\epsilon_1 \sqrt{\frac{\beta^2}{4} + \frac{s}{\omega v(\epsilon_1, s)}}\right|\right). \tag{A.1}$$

If we use the inequality (32) we can generate a systematic expansion of the preexponential factor of the diffusion propagator with respect to the parameter $kT\rho_c'(\epsilon)$, where the prime indicates the derivative with respect to energy. However, since the error estimate in the WKB approximation is of multiplicative type, none of the approximations can satisfy probability conservation exactly. Therefore, we only use the exponent, and determine the preexponential factor by normalization.

In investigating the energy distribution function further we again restrict the consideration to large times, where $\epsilon_0 \gg \langle\epsilon\rangle(t) - \sigma(t)$. In this case the calculation of the time dependence of the energy distribution function amounts to the calculation of the integral

$$I(t) = \frac{1}{2\pi i} \int_c ds \, \exp\left(st - \int_\epsilon^{\epsilon_0} d\epsilon_1 \left(\sqrt{\frac{\beta^2}{4} + \frac{s}{\omega v(\epsilon_1, s)}} - \frac{\beta}{2}\right)\right). \tag{A.2}$$

In order to calculate this integral we use the same method as for the constant density of states. Doing so, we find that

$$I(t) = \frac{1}{\sqrt{2\pi D^2(\epsilon)}} \exp\left(-\left(\frac{(t - t_\epsilon)^2}{2D^2(\epsilon)}\right)\right). \tag{A.3}$$

Here

$$t_\epsilon = \int_\epsilon^{\epsilon_0} d\epsilon_1 \frac{d\epsilon_1}{\beta \omega v(\epsilon_1, 0)}, \tag{A.4}$$

and

$$D^2(\epsilon) = D_{\text{therm}}^2(\epsilon) + D_{\text{disp}}^2(\epsilon), \tag{A.5}$$

where the thermal contribution is given by

$$D_{\text{therm}}^2(\epsilon) = 2 \int_\epsilon^{\epsilon_0} \frac{d\epsilon_1}{\beta^3 \omega^2 v^2(\epsilon_1, 0)}, \tag{A.6}$$

and the disperse contribution by

$$D_{\text{disp}}^2(\epsilon) = 2 \int_\epsilon^{\epsilon_0} \frac{d\epsilon_1}{\beta \omega v(\epsilon_1, 0) \omega_0(\epsilon_1)}. \tag{A.7}$$

Now we use the fact that our calculation of the inverse Laplace transformation is only correct in the vicinity of the peak. Since the peak is situated at $t = t_\epsilon$, the maximum of the packet in energy space $\langle\epsilon\rangle(t)$ is situated at $\epsilon = \langle\epsilon\rangle(t)$, where

$$t = t_{\langle\epsilon\rangle(t)}. \tag{A.8}$$

If we use equation (A.8) to calculate the mean energy at large times we obtain equation (34). Since our calculation of the inverse Laplace transformation is only correct in the vicinity of $\langle\epsilon\rangle(t)$, we now replace ϵ by $\langle\epsilon\rangle(t)$ in equation (A.3) and then adjust the preexponential factor, as discussed above. Doing so, we obtain equation (33), where

$$\begin{aligned}\sigma^2_{\text{therm}}(t) &= 2D_{\text{therm}}(\langle\epsilon\rangle(t))\beta^2\omega^2 v^2(\langle\epsilon\rangle(t), 0) \\ &\approx \frac{kT\Delta}{\rho_{\text{c}}(\langle\epsilon\rangle(t))},\end{aligned} \tag{A.9}$$

and

$$\sigma^2_{\text{disp}} = 2D_{\text{disp}}(\langle\epsilon\rangle(t))\beta^2\omega^2 v^2(\langle\epsilon\rangle(t), 0) \approx \frac{\Delta\beta\omega^2}{6d}. \tag{A.10}$$

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