

**A DRIFT-DIFFUSION EQUATION FOR CHARGE TRANSPORT IN
INHOMOGENEOUS MATERIALS**

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Abstract. From a hopping rate equation for disordered materials we derive a macroscopic drift–diffusion equation. For this purposes two space–time scales are simultaneously considered. The microscopic dynamics is characterized by the distribution of localized states and the hopping rate. On the macroscopic space scale both the hopping rate and the disordered material are allowed to be inhomogeneous.

1. INTRODUCTION

Transport of charge carriers in solids is frequently described at a *microscopic* level by a hopping model on a lattice of sites. When multiple occupations of sites are forbidden the time evolution of an ensemble of interacting charge carriers can be rigorously described by the dynamics of an exclusion process (cf.[7],[4]).

On much longer time and length scales a process of “averaging“ takes place so that the complicated microscopic structure of transport dynamics is replaced by a *macroscopic* drift–diffusion equation. But only if the material on the small microscopic scale will have some special, repetitive, structure and the range of hopping rate remains local the charge density will have a diffusion-drift behaviour on a large time–space scale. For example, when the lattice is periodic and the charge carriers only jump to neighbouring sites. In the periodic lattice case there are rigorous results. The diffusivity is a closed expression and it coincides with that given from the Green-Kubo formula. A review of stochastic dynamics of particle systems on a lattice is given by H.Spohn ([7]) , and the literature cited therein.

When the underlying lattice is disordered the situation is much more difficult. Disorder have to take into consideration if the sites of lattice are randomly distributed and if hopping rates depend on energy states on the sites. For disordered systems there are

substantial difficulties to overcome in order to be able to analyze rigorously a transition from microscopic to macroscopic level. In general, the large scale problem for disordered lattices cannot be solved by a closed formula for the macroscopic transport coefficients. Particular contributions have been given, for example, in the papers ([4],[8]). In ([6],[8]) Monte Carlo simulations have been performed in order to approximate the diffusivity for certain disordered systems.

In this paper we study a mean field transport dynamic based on a model which is intermediate between the microscopic and macroscopic scales. We assume a particular hopping rate equation describes the time evolution of the one-particle distribution function which depends on macroscopic position, localized energy state and the microscopic time. In this model both the disordered material and hopping rates are allowed to be spatially inhomogeneous at the large space scale. We shall be concerned with the derivation of a macroscopic drift-diffusion equation. The equation will have several drift terms caused by the spatially inhomogeneities. The assumption of the principle of a detailed balance for hops between the localized energy states will play a crucial role for the derivation of the transport equation.

2. TRANSPORT MODEL

2.1. The Hopping Rate. In this paper, a basic assumption for the microscopic charge transport is that carriers jump on a lattice of *localized energy states*. Arising from the Pauli principle, multiple occupancies of a state by charge carriers are excluded. A localized energy state $(\mathbf{x}, E_{\mathbf{x}})$, $\mathbf{x} \in \mathbb{R}^3$ and $E_{\mathbf{x}} \in \mathbb{R}$, is described by its spatial position \mathbf{x} on the lattice and the assigned energy value $E_{\mathbf{x}}$. Lattice is called a *disordered lattice* if $(\mathbf{x}, E_{\mathbf{x}})$ is randomly distributed. A jump of a carrier from state (\mathbf{x}, E) to a vacant state (\mathbf{y}, Q) occurs with a *hopping rate* $w(\mathbf{x}, E; \mathbf{y}, Q)$. In order to establish a hopping dynamics and to derive a macroscopic equation we need two space-time scales. Let t' , x' be the time, length parameters on the microscopic time-space scale and

$$t = \epsilon^2 t', \quad x = \epsilon x'$$

the time, length parameters on macroscopic time-space scale. Ratio ϵ of length parameters is chosen so that the average distance of sites \mathbf{x} of lattice on the macroscopic scale is of order ϵ .

We make the following fairly general ansatz for a hopping rate¹

$$w(\mathbf{x}, E; \mathbf{y}, Q) = r(|\mathbf{x}' - \mathbf{y}'|) s(\mathbf{x}, E; \mathbf{y}, Q) \quad (2.1)$$

with respect to time scale t' . The diffusive moment of transport is essentially characterized by the function r defined on the small scale and only depending on distance $|\mathbf{x}' - \mathbf{y}'|$. The second factor s describes the dependence of hopping rate on the energy levels E, Q

¹A typical example for a hopping rate is

$$w(\mathbf{x}, E; \mathbf{y}, Q) = \exp[e \mathbf{F} \cdot (\mathbf{x} - \mathbf{y})/2kT] \cdot \begin{cases} 1 & Q \leq E, |\mathbf{x} - \mathbf{y}| \leq a\epsilon \\ \exp[-(Q - E)/kT] & Q > E, |\mathbf{x} - \mathbf{y}| \leq a\epsilon \\ 0 & |\mathbf{x} - \mathbf{y}| > a\epsilon, \end{cases}$$

where e is the elementary charge, k the Boltzmann constant, T the absolute temperature, a a positive constant, and \mathbf{F} an electric field.

and on a possible drift caused by an external force or an other spatial inhomogeneity of hopping rate. We require they have to satisfy the following

Conditions:

Local interaction: $r(a)$ ($a \geq 0$) is a non-increasing function with the conditions

$$S'_0 := \int_{\mathbb{R}^3} r(|\mathbf{x}'|) d^3x' = 1 \quad (2.2)$$

and

$$S'_2 := \int_{\mathbb{R}^3} |\mathbf{x}'|^2 r(|\mathbf{x}'|) d^3x' < +\infty. \quad (2.3)$$

This condition for the first factor r of w guarantees that interaction only take place on microscopic distances and is necessary that the charge current will be finite.

Detailed balance: There is a sufficiently smooth "potential" function $\psi(\mathbf{x})$ so that the equation

$$\exp\left[-\frac{E + e\psi(\mathbf{x})}{kT}\right] s(\mathbf{x}, E; \mathbf{y}, Q) = \exp\left[-\frac{Q + e\psi(\mathbf{y})}{kT}\right] s(\mathbf{y}, Q; \mathbf{x}, E), \quad E, Q \in \mathbb{R}, \mathbf{x}, \mathbf{y} \in \mathbb{R}^3 \quad (2.4)$$

is fulfilled.

2.2. The Hopping Rate Equation. Given positive numbers $N(\mathbf{x})$ and a family of density functions $g(\mathbf{x}, E)$, $\mathbf{x} \in \mathbb{R}^3$ with

$$\int g(\mathbf{x}, E) dE = 1.$$

$N(\mathbf{x})$ describes the *concentration* of sites of lattice and $g(\mathbf{x}, E)$ is the *energy state density* of localized states at macroscopic position \mathbf{x} . If $N(\mathbf{x})$ and $g(\mathbf{x}, E)$ vary with \mathbf{x} then the disordered material is spatially inhomogeneous. The quantity

$$N'(\mathbf{x}) = \frac{N(\mathbf{x})}{\epsilon^{-3}} \quad (2.5)$$

is, roughly speaking², the *microscopic concentration* in surrounding of \mathbf{x} .

We still require

$$\iint \exp(-E/kT) s(\mathbf{x}, E; \mathbf{x}, Q) g(\mathbf{x}, E) g(\mathbf{x}, Q) dE dQ < +\infty, \quad \mathbf{x} \in \mathbb{R}^3. \quad (2.6)$$

When the conditions (2.3) and (2.6) hold the macroscopic diffusion and drift currents will be finite.

Let $f = f_t(\mathbf{x}, E)$ be the distribution function, depending on the position $\mathbf{x} \in \mathbb{R}^3$, the

²A more precise interpretation of spatial concentration $N'(\mathbf{x})$ and energy state density $g(\mathbf{x}, E)$ at the microscopic scale give the following approach. Given is a family \mathcal{P}^ϵ of distribution laws of disordered lattices depending on the parameter ϵ . Let $\sharp^\epsilon(\Delta, B)$ denotes the number of lattice points in the microscopic region Δ which have the energy state in $B \subseteq \mathbb{R}$. Further, let us choose a box $\Delta_\epsilon(\mathbf{x})$ centered at $\mathbf{x}' = \mathbf{x}/\epsilon$ and such that $|\Delta_\epsilon(\mathbf{x})| \rightarrow \infty$ but $\epsilon^3 |\Delta_\epsilon(\mathbf{x})| \rightarrow 0$ as $\epsilon \rightarrow 0$. The following ergodic property explains meaning of both $N'(\mathbf{x})$ and $g(\mathbf{x}, E)$.

$$\lim_{\epsilon \rightarrow 0} \frac{\sharp^\epsilon(\Delta_\epsilon(\mathbf{x}), B)}{|\Delta_\epsilon(\mathbf{x})|} = N'(\mathbf{x}) \int_B g(\mathbf{x}, E) dE$$

taking the limit in a suitable sense with respect to \mathcal{P}^ϵ

energy state $E \in \mathbb{R}$ and the time t . It is the probability of finding a charge carrier at position \mathbf{x} with energy state E at time t . One obtains the *relative concentration* of charge carriers

$$h_t(\mathbf{x}) = \int f_t(\mathbf{x}, E) g(\mathbf{x}, E) dE \quad (2.7)$$

and the *charge density*

$$\rho_t(\mathbf{x}) = e N'(\mathbf{x}) h_t(\mathbf{x}) \quad (2.8)$$

at \mathbf{x} and at time t .

Further, the distribution function $f_t(\mathbf{x}, E)$ is assumed to be a sufficiently smooth function of t , \mathbf{x} and E .

We assume the charge carriers motion is governed by the *hopping rate equation*

$$\begin{aligned} \frac{\partial f_{t'}(\mathbf{x}, E)}{\partial t'} = & - f_{t'}(\mathbf{x}, E) \int_{\mathbb{R}^3} \int (1 - f_{t'}(\mathbf{y}, Q)) s(\mathbf{x}, E; \mathbf{y}, Q) r(|\mathbf{x}' - \mathbf{y}'|) g(\mathbf{y}, Q) dQ N(\mathbf{y}) d^3 y \\ & + (1 - f_{t'}(\mathbf{x}, E)) \int_{\mathbb{R}^3} \int f_{t'}(\mathbf{y}, Q) s(\mathbf{y}, Q; \mathbf{x}, E) r(|\mathbf{x}' - \mathbf{y}'|) g(\mathbf{y}, Q) dQ N(\mathbf{y}) d^3 y. \end{aligned} \quad (2.9)$$

for all $\mathbf{x} \in \mathbb{R}^3, E \in \mathbb{R}$ and $t' \geq 0$.

The first term on the right-hand side describes the average current from “state” (\mathbf{x}, E) to other possible states. Analogously, the second term expresses the average current from outside to the given state.

This continuum model (2.9) does not take into account the complex microscopic structure of hopping transport. An interesting question is whether and under which conditions the hopping rate equation can be derived from a more basic level of microscopic dynamics.

Summarizing, in this paper hopping transport in disordered material is described by the *material parameters*

$$\{N'(\mathbf{x}), g(\mathbf{x}, E), w(\mathbf{x}, E; \mathbf{y}, Q)\}$$

at all the macroscopic positions \mathbf{x} and the hopping dynamics governed by a hopping rate equation (2.9). Here we assume in addition that the parameters are sufficiently smooth functions of \mathbf{x} and \mathbf{y} .

3. A DRIFT-DIFFUSION EQUATION

In order to derive from the hopping rate equation (2.9) a partial differential equation we need the following elementary proposition. Let $u(\mathbf{x})$ on \mathbb{R}^3 be a sufficiently smooth function. Generating the Taylor series expansion for $u(\mathbf{y})$ about the point $\mathbf{y}_0 = \mathbf{x}$ to order $|\mathbf{y} - \mathbf{x}|^2$, using (2.2) and (2.3), the following equation

$$\epsilon^{-3} \int r(|\mathbf{y}' - \mathbf{x}'|) u(\mathbf{y}) dy^3 = u(\mathbf{x}) + \epsilon^2 \frac{S'_2}{6} \Delta u(\mathbf{x}) + O(\epsilon^2) \quad (3.1)$$

holds.

After multiplying of equation (2.9) by $e N(\mathbf{x}) g(\mathbf{x}, E)$ and integrating with respect to energy E , the calculation of the integrals regarding the variable \mathbf{y} , using (2.5),(2.7),(2.8),

and (3.1), leads to a equation on the large time scale $t = \epsilon^2 t'$

$$\begin{aligned} \frac{\partial \rho_t(\mathbf{x}, E)}{\partial t} &= \int V[f_t](\mathbf{x}, \mathbf{y}) r(|\mathbf{x} - \mathbf{y}|/\epsilon) d^3 y \\ &= \frac{1}{\epsilon^2} e V[f_t](\mathbf{x}, \mathbf{x}) + \frac{1}{6} S'_2 e \Delta \mathbf{y} V[f_t](\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} \end{aligned} \quad (3.2)$$

with

$$\begin{aligned} V[f](\mathbf{x}, \mathbf{y}) &= \iint N'(\mathbf{x}) N'(\mathbf{y}) \left[-f(\mathbf{x}, E)(1 - f(\mathbf{y}, Q)) s(\mathbf{x}, E; \mathbf{y}, Q) \right. \\ &\quad \left. + (1 - f(\mathbf{x}, E)) f(\mathbf{y}, Q) s(\mathbf{y}, Q; \mathbf{x}, E) \right] g(\mathbf{y}, Q) g(\mathbf{x}, E) dQ dE. \end{aligned} \quad (3.3)$$

The evolution equation (3.2) can be interpreted as multiscale equation in time. First term $V[f](\mathbf{x}, \mathbf{x})$ works on the fast microscopic time scale and its stationary solution provides the *local equilibria*. Therefore, one can assume that local equilibria are achieved at all the macroscopic times t and all the macroscopic positions \mathbf{x} . Using detailed balance (2.4) the equation

$$V[f](\mathbf{x}, \mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^3 \quad (3.4)$$

is solved with f equal to the Fermi equilibrium

$$f_t(\mathbf{x}, E) = \frac{\exp(\zeta_t(\mathbf{x})/kT) \exp(-E/kT)}{1 + \exp(\zeta_t(\mathbf{x})/kT) \exp(-E/kT)}. \quad (3.5)$$

As usual, here $\zeta(\mathbf{x})$ denotes the *chemical potential* at spatial position \mathbf{x} . For a given relative concentration $h(\mathbf{x})$ at \mathbf{x} the chemical potential $\zeta = \zeta(\mathbf{x}, h(\mathbf{x}))$ which characterizes the local equilibrium can be calculated, using (2.7), from

$$h(\mathbf{x}) = \int \frac{\exp(\zeta/kT) \exp(-E/kT)}{1 + \exp(\zeta/kT) \exp(-E/kT)} g(\mathbf{x}, E) dE. \quad (3.6)$$

Now first “fast” term of the right-hand side of equation (3.2) can be canceled. Remaining expression produces a current what leads to new local equilibria. Next we will calculate the macroscopic current.

From (3.3) using (3.5) and the detailed balance (2.4) we obtain

$$\begin{aligned} V[f](\mathbf{x}, \mathbf{y}) &= \\ (b(\mathbf{y}) - b(\mathbf{x})) &\iint \frac{N'(\mathbf{x}) N'(\mathbf{y}) \exp[-(E + e\psi(\mathbf{x}))/kT] s(\mathbf{x}, E; \mathbf{y}, Q) g(\mathbf{x}, E) g(\mathbf{y}, Q) dE dQ}{(1 + b(\mathbf{x}) \exp[-(E + e\psi(\mathbf{x}))/kT]) (1 + b(\mathbf{y}) \exp[-(Q + e\psi(\mathbf{y}))/kT])} \\ &=: (b(\mathbf{y}) - b(\mathbf{x})) I(\mathbf{x}, \mathbf{y}) \end{aligned}$$

with

$$b(\mathbf{x}) = \exp \left[\frac{\zeta(\mathbf{x}, h(\mathbf{x})) + e\psi(\mathbf{x})}{kT} \right].$$

Due to the detailed balance relation (2.4) last duoble integral $I(\mathbf{x}, \mathbf{y})$ is a symmetrical function of \mathbf{x} and \mathbf{y} . Therefore the proposition

$$\nabla_{\mathbf{y}} I(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \frac{1}{2} \nabla_{\mathbf{x}} I(\mathbf{x}, \mathbf{x})$$

is valid. Hence we obtain

$$\Delta_{\mathbf{y}} V[f](\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{y}=\mathbf{x}} = \nabla_{\mathbf{x}} \cdot [I(\mathbf{x}, \mathbf{x}) \nabla_{\mathbf{x}} b(\mathbf{x})] = \nabla_{\mathbf{x}} \cdot [b(\mathbf{x}) I(\mathbf{x}, \mathbf{x}) \nabla_{\mathbf{x}} \log b(\mathbf{x})] \quad (3.7)$$

and finally the partial differential equation

$$\begin{aligned} \frac{\partial \rho_t(\mathbf{x})}{\partial t} &= \frac{S'_2}{6} e \nabla \cdot [b(\mathbf{x}) I(\mathbf{x}, \mathbf{x}) \nabla \log b(\mathbf{x})] \\ &= \nabla \cdot [\sigma(\mathbf{x}, h_t(\mathbf{x})) e^{-1} \nabla (\zeta_t(\mathbf{x}, h_t(\mathbf{x})) + e\psi(\mathbf{x}))] \end{aligned} \quad (3.8)$$

with a electric *conductivity*

$$\begin{aligned} \sigma(\mathbf{x}, h) &= \\ \frac{S'_2 (N'(\mathbf{x}))^2 e^2}{6 kT} &\iint \frac{\exp[(\zeta(\mathbf{x}, h) - E)/kT] s(\mathbf{x}, E; \mathbf{x}, Q) g(\mathbf{x}, E) g(\mathbf{x}, Q)}{(1 + \exp[(\zeta(\mathbf{x}, h) - E)/kT])(1 + \exp[(\zeta(\mathbf{x}, h) - Q)/kT])} dE dQ \end{aligned} \quad (3.9)$$

depending on \mathbf{x} and the relative concentration h . Because (2.3) and (2.6) the conductivity is finite.

If ψ is equal to an electric potential the quantity $\zeta + e\psi$ can be viewed as electrochemical potential. Then the transport equation (3.8) has a form well known from the phenomenological theory of charge transport where the current is proportional to gradient of electrochemical potential.

Assume $g(\mathbf{x}, E) = g_{\Theta}(\mathbf{x})(E)$, where $g_{\Theta}(E)$ is a one-parametric family of energy state densities. Equation (3.8) can be rewritten in a drift-diffusion equation for the charge density $\rho_t(\mathbf{x}) = e N'(\mathbf{x}) h_t(\mathbf{x})$ as following,

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D \nabla \rho - \mu^N \rho \nabla N' - \mu^{\ominus} \rho \nabla \Theta + \mu^{\psi} \rho \nabla e\psi). \quad (3.10)$$

The *diffusivity* D is calculated, from (3.8) and via (2.8), (3.6), by

$$\begin{aligned} D(\mathbf{x}, h) &= \frac{\sigma}{e} \left(\frac{\partial \rho}{\partial \zeta} \right)^{-1} \\ &= \frac{S'_2 N'(\mathbf{x})}{6} \iint \frac{\exp[(\zeta(\mathbf{x}, h) - E)/kT] s(\mathbf{x}, E; \mathbf{x}, Q) g_{\Theta}(\mathbf{x})(E) g_{\Theta}(\mathbf{x})(Q)}{(1 + \exp[(\zeta(\mathbf{x}, h) - E)/kT])(1 + \exp[(\zeta(\mathbf{x}, h) - Q)/kT])} dE dQ / \\ &\quad \int \frac{\exp[(\zeta(\mathbf{x}, h) - E)/kT] g_{\Theta}(\mathbf{x})(E)}{(1 + \exp[(\zeta(\mathbf{x}, h) - E)/kT])^2} dE \end{aligned} \quad (3.11)$$

It is easily to see that the *mobilities* μ^N , μ^{\ominus} and μ^{ψ} in (3.10) satisfy the relations

$$D : \mu^N : \mu^{\ominus} : \mu^{\psi} = \rho : \frac{\partial \rho}{\partial N} : \frac{\partial \rho}{\partial \Theta} : \frac{\partial \rho}{\partial \zeta}. \quad (3.12)$$

In case $\psi(\mathbf{x})$ is assumed to be equal to an electric potential $\varphi(\mathbf{x})$ from (3.12) we obtain a generalized Einstein relation (cf.[5])

$$\frac{\mu^{\varphi}(\rho)}{D(\rho)} = \frac{\partial \log \rho}{\partial \zeta}. \quad (3.13)$$

4. PARTICULAR CASES

In Sect.3 could be shown that a hopping model with the material parameters

$$\{N'(\mathbf{x}), g(\mathbf{x}, E), w(\mathbf{x}, E; \mathbf{y}, Q)\}, \quad \mathbf{x} \in \mathbb{R}^3$$

and a dynamics (2.9) leads, under certain assumptions, to a fairly general transport equation (3.10). In the following we investigate several particular situations.

4.1. Hopping Independent of Energy. If the dependence of hopping transport on anyone energy E can be neglected we set

$$w(\mathbf{x}, E; \mathbf{y}, Q) = r(|\mathbf{x}' - \mathbf{y}'|) s(\mathbf{x}, \mathbf{y})$$

with the local interaction condition (2.2, 2.3). As above, we assume the hopping rate factor $s(\mathbf{x}, \mathbf{y})$ obeys a

detailed balance: *There are a sufficiently smooth function $\psi(\mathbf{x}), \mathbf{x} \in \mathbb{R}^3$ so that the equation*

$$\exp[-e\psi(\mathbf{x})/kT] s(\mathbf{x}, \mathbf{y}) = \exp[-e\psi(\mathbf{y})/kT] s(\mathbf{y}, \mathbf{x}) \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3 \quad (4.1)$$

is fulfilled.

Following the derivation of drift-diffusion equation in Sect.3, $f(\mathbf{x}, E)$ in (3.5) is independent of E and coincides with the relative concentration

$$h(\mathbf{x}) = \frac{\exp[\zeta(\mathbf{x})/kT]}{1 + \exp[\zeta(\mathbf{x})/kT]}$$

where $\zeta(\mathbf{x})$ denotes the chemical potential. Finally one obtains a drift-diffusion equation

$$\frac{\partial \varrho}{\partial t} = \nabla \cdot (D \nabla \varrho - \mu^N \varrho \nabla N' + \mu^\psi \varrho \nabla e\psi) \quad (4.2)$$

with

$$\begin{aligned} D(\mathbf{x}, h) &= \frac{S'_2}{6} N'(\mathbf{x}) s(\mathbf{x}, \mathbf{x}), \\ \mu^N(\mathbf{x}, h) &= \frac{S'_2}{6} s(\mathbf{x}, \mathbf{x}), \\ \mu^\psi(\mathbf{x}, h) &= \frac{S'_2}{6 kT} N'(\mathbf{x}) s(\mathbf{x}, \mathbf{x}) (1 - h). \end{aligned}$$

Equation (4.2) is a generalized version of Burgers equation with viscosity (cf.[3]).

4.2. The Low Concentration Case. Interaction of carriers caused by the Pauli principle can be neglected at low concentration and the drift-diffusion equation (3.10)

$$\frac{\partial \varrho}{\partial t} = \nabla \cdot (D \nabla \varrho - \mu^N \varrho \nabla N' - \mu^\Theta \varrho \nabla \Theta + \mu^\psi \varrho \nabla e\psi) \quad (4.3)$$

becomes in limit a *linear* partial differential equation. In order to obtain a limit we have to require two conditions

$$\int \exp(-E/kT) g_\Theta(\mathbf{x})(E) dE < \infty, \quad \mathbf{x} \in \mathbb{R}^3$$

and

$$\int \exp(-E/kT) \frac{\partial g_{\Theta(\mathbf{x})}(E)}{\partial \Theta(\mathbf{x})} dE < \infty, \quad \mathbf{x} \in \mathbb{R}^3.$$

Then the limit $D(\mathbf{x}) = \lim_{h \rightarrow 0} D(\mathbf{x}, h)$ exists and is positive. One obtains the diffusivity

$$D(\mathbf{x}) = \frac{S'_2}{6} N'(\mathbf{x}) \frac{\iint s(\mathbf{x}, E; \mathbf{x}, Q) \exp(-E/kT) g_{\Theta(\mathbf{x})}(E) g_{\Theta(\mathbf{x})}(Q) dE dQ}{\int \exp(-E/kT) g_{\Theta(\mathbf{x})}(E) dE}$$

and the mobilities

$$\mu^N(\mathbf{x}) = \lim_{h \rightarrow 0} \mu^N(\mathbf{x}, h) = \frac{D(\mathbf{x})}{N'(\mathbf{x})}, \quad (4.4)$$

$$\mu^\Theta(\mathbf{x}) = \lim_{h \rightarrow 0} \mu^\Theta(\mathbf{x}, h) = D(\mathbf{x}) \frac{\int \exp(-E/kT) \frac{\partial g_{\Theta(\mathbf{x})}(E)}{\partial \Theta(\mathbf{x})} dE}{\int \exp(-E/kT) g_{\Theta(\mathbf{x})}(E) dE}, \quad (4.5)$$

$$\mu^\psi(\mathbf{x}) = \lim_{h \rightarrow 0} \mu^\psi(\mathbf{x}, h) = \frac{D(\mathbf{x})}{kT}. \quad (4.6)$$

When ψ is equal to an electric potential the last equation is the inhomogeneous version of the classical Einstein relation.

In the end we give

4.3. Two Examples for the Low Concentration Case.

4.3.1. *Example 1: Hopping Transport on Sites Having an Gaussian Distribution of Energie States.* We consider a modified Gaussian disorder model of H.Bässler and co-writer (cf.[1]). Given a concentration $N'(\mathbf{x})$ and assume the energy states at surrounding of \mathbf{x} are distributed according a Gaussian distribution

$$g(\mathbf{x}, E) = \frac{1}{\sqrt{2\pi}\Theta_2(\mathbf{x})} \exp\left[-\frac{(E - \Theta_1(\mathbf{x}))^2}{2\Theta_2(\mathbf{x})^2}\right] \quad -\infty < \Theta_1(\mathbf{x}) < \infty, \Theta_2(\mathbf{x}) > 0$$

with mean $\Theta_1(\mathbf{x})$ and standard deviation $\Theta_2(\mathbf{x})$. Assume $\Theta_1(\mathbf{x})$, $\Theta_2(\mathbf{x})$ are sufficiently smooth functions of \mathbf{x} . We choose a local interaction rate r holds (2.3) and a rate

$$s(\mathbf{x}, E; \mathbf{y}, Q) = \gamma(\mathbf{x}) \exp[-(Q - E + e(\varphi(\mathbf{y}) - \varphi(\mathbf{x}))) / 2kT],$$

where $\varphi(\mathbf{x})$ is an electric potential and $\gamma(\mathbf{x})$ a positive function. Then s obeys a detailed balance (2.4) with

$$\psi(\mathbf{x}) = \varphi(\mathbf{x}) + \frac{kT}{e} \log \gamma(\mathbf{x}).$$

According to (4.3), (4.4), (4.6) and (4.5) (here generalized for two parameters Θ_1, Θ_2) the charge transport is described by following drift-diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{S'_2}{6} \operatorname{div} \left[N' \gamma \exp\left(-\frac{\Theta_2^2}{4(kT)^2}\right) \left(\operatorname{grad} \rho - \rho \frac{1}{N'} \operatorname{grad} N' + \rho \frac{1}{\gamma} \operatorname{grad} \gamma + \rho \frac{e}{kT} \operatorname{grad} \varphi + \rho \frac{1}{kT} \operatorname{grad} \Theta_1 - \rho \frac{1}{(kT)^2} \Theta_2 \operatorname{grad} \Theta_2 \right) \right]. \quad (4.7)$$

The gradients of material parameters N' , γ , Θ_1 , Θ_2 produce drift currents analogously as an electric field $\mathbf{F} = -\text{grad}\varphi$.³

4.3.2. *Example 2.* The following example shows that two different microscopic structures can lead to the same transport law on a macroscopic scale. Assume we have two microscopic structures 1 and 2 without energy component with the characteristics

$$\begin{aligned} N'_1(\mathbf{x}) &= a(\mathbf{x}) & N'_2(\mathbf{x}) &\equiv 1 \\ w_1(\mathbf{x}, E; \mathbf{y}, Q) &= r(|\mathbf{x}' - \mathbf{y}'|) s_1(\mathbf{x}, \mathbf{y}) & w_2(\mathbf{x}, E; \mathbf{y}, Q) &= r(|\mathbf{x}' - \mathbf{y}'|) s_2(\mathbf{x}, \mathbf{y}) \\ s_1(\mathbf{x}, \mathbf{y}) &= a(\mathbf{x}) & s_2(\mathbf{x}, \mathbf{y}) &= a(\mathbf{x}) a(\mathbf{y}) \end{aligned}$$

The hopping rate s_1 and s_2 satisfy the detailed balance equation (4.1) with the functions

$$\psi_1(\mathbf{x}) = \frac{kT}{e} \log a(\mathbf{x}) \quad \psi_2(\mathbf{x}) \equiv \text{const.},$$

respectively.

According to 4.1 and 4.2, in the low concentration case the macroscopic transport equations for 1 and 2 coincide. The equation reads

$$\frac{\partial \rho_t(\mathbf{x})}{\partial t} = \text{div} \left[\frac{S'_2}{6} a^2(\mathbf{x}) \text{grad} \rho_t(\mathbf{x}) \right].$$

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³Obviously, several combinations of material parameters can lead to a pure diffusion equation. For example, under the assumption there are constants $c_1 > 0, c_2, c_3 > 0$ so that

$$\begin{aligned} N'(\mathbf{x}) &= c_1 \gamma(\mathbf{x}) \\ \Theta_1(\mathbf{x}) + e \varphi(\mathbf{x}) &= c_2 \\ \Theta_2(\mathbf{x}) &= c_3 \end{aligned}$$

hold then the sum of drift currents vanishes. It remains only a diffusion equation

$$\frac{\partial \rho}{\partial t} = \text{div}(D \text{grad} \rho)$$

with a spatially inhomogeneous diffusivity

$$D(\mathbf{x}) = \frac{S'_2}{6} N'(\mathbf{x}) \gamma(\mathbf{x}) \exp \left[-(c_3)^2 / 4(kT)^2 \right].$$