Unified theory of quantum transport and quantum diffusion in semiconductors

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- Quantum diffusion is well established in the study of atomic migration in solids (tunneling)

Introduction

- The theory of hot-carrier quantum transport in semiconductors has a long history and reached a high level of sophistication
- **What is the quantity of main interest? The current density.**
- **But what about quantum diffusion?** The idea of diffusion has an even longer history. It dates back to Fourier and Laplace.
- Quantum diffusion is well established in the study of atomic migration in solids (tunneling)
- The Einstein relation does not help under nonequilibrium conditions. **A unified theory of quantum transport and quantum diffusion in semiconductors is needed.**

One-band theory: carrier drift

- **Starting point: Fokker-Planck equation for the probability density**

$$sP(r - r_0 \mid s) = \delta(r - r_0) + v_z(s)\frac{\partial}{\partial z}P(r - r_0 \mid s) + D_{zz}(s)\frac{\partial^2}{\partial z^2}P(r - r_0 \mid s)$$

where the transport coefficients

$$v_z(s) = -s^2 Z_1(s), \quad D_{zz}(s) = \frac{s^2}{2}Z_2(s) - \frac{v_z(s)}{s}$$

are calculated from the moments

$$Z_n(s) = \int \mathrm{d}^3 r (z - z_0)^n P(r - r_0 \mid s)$$

The main quantity is the probability propagator P.

One-band theory: carrier drift

- **The quantum mechanics comes in by identifying the probability P with a second-quantized expectation value.** [E. K. Kudinov, Y. A. Firsov Sov. Phys. JETP **22**, 603 (1966)]

$$P_{m_2 m_4}^{m_1 m_3}(s) = \frac{1}{Z}\int_0^\infty dt e^{-st}\mathrm{Tr}_{\mathrm{ph}}\left\{e^{-\beta H_{\mathrm{ph}}}\langle 0 \mid a_{m_2} e^{iHt/\hbar} a_{m_4}^\dagger a_{m_3} e^{-iHt/\hbar} a_{m_1}^\dagger \mid 0\rangle\right\}$$

All transport coefficients are simultaneously derived from the moments:

$$Z_n(s) = i^n \sum_{k,k'} \frac{\partial^n}{\partial \kappa_z^n} P(k,k',\kappa \mid s) \mid_{\kappa=0} \equiv i^n \sum_{k,k'} P_n(k,k' \mid s)$$

That's all! What remains are technical manipulations.

One-band theory: carrier drift

For the drift velocity, we obtain the final result:

$$v_z(s) = \sum_{k} v_{\text{eff}}(k, s) f(k, s)$$

with the quantum-kinetic Eq. for the distribution function:

$$f(k, s) = s \sum_{k'} P_0(k', k \mid s), \quad \left[s + \frac{eE}{\hbar} \nabla_k \right] f(k, s) = s + \sum_{k'} f(k', s) W(k', k \mid s)$$

and an effective spectral drift velocity:

$$v_{\text{eff}}(k, s) = v_z(k) - i \sum_{k'} W_1(k, k' \mid s)$$

Describe quantum transport via extended and localized states at the same footing.

One-band theory: quantum diffusion

The diffusion coefficient is calculated by the very same procedure:

$$D_{zz}(s) = \sum_{k} v_{\text{eff}}(k,s)\varphi(k,s) - \frac{1}{2}\sum_{k,k'} f(k,s)W_2(k,k' \mid s)$$

The main quantity cannot be a scalar distribution function (rather $\vec{\varphi} \sim \nabla_{\kappa} f(k,\kappa,t)|_{\kappa=0}$). The "quantum-Boltzmann" Eq. for diffusion phenomena is given by:

$$\left[s + \frac{eE}{\hbar}\frac{\partial}{\partial k_z}\right]\varphi(k,s) = \sum_{k'} \varphi(k',s)W(k',k \mid s) + v_z(k)f(k,s)$$
$$-\sum_{k'} v_{\text{eff}}(k',s)f(k',s) - i\sum_{k'} f(k',s)W_1(k',k \mid s)$$

One-band theory: limiting cases

- **Low field regime:**

$$v_z^{(1)} = \sum_k v_z(k) f^{(1)}(k),\ D_{zz}^{(0)} = \sum_k v_z(k)\varphi^{(0)}(k),\ f^{(1)}(k) = eE\varphi^{(0)}(k)/k_B T$$

The Einstein relation $\mu = eD_{zz}/k_BT$ is recovered (with $\mu = v_z^{(1)}/E$).

- **Wannier-Stark regime:**

$$v_z = -\frac{1}{eE}\sum_{k,k'}\left[\epsilon(k_z) - \epsilon(k'_z)\right] f(k')W(k',k) + \ldots$$

$$D_{zz} = \frac{1}{2}\frac{1}{(eE)^2}\sum_{k,k'}[\epsilon(k_z) - \epsilon(k'_z)]^2 f(k')W(k',k) + \ldots$$

Carriers execute Bloch oscillations, transport only due to inelastic scattering, negative differential conductivity.

One-band theory: hopping picture

- **Switching back to the real space by an exact transformation:**

$$v_z = \sum_{k_\perp, k'_\perp} \sum_{m=-\infty}^{\infty} (md) n(k'_\perp) \widetilde{W}^{0,m}_{0,m}(k'_\perp, k_\perp)$$

$$D_{zz} = \frac{1}{2} \sum_{k_\perp, k'_\perp} \sum_{m=-\infty}^{\infty} (md)^2 n(k'_\perp) \widetilde{W}^{0,m}_{0,m}(k'_\perp, k_\perp)$$

This is the hopping picture of transport, lateral distribution function:

$$\sum_{m=-\infty}^{\infty} \sum_{k'_\perp} n(k'_\perp) \widetilde{W}^{m,0}_{m,0}(k'_\perp, k_\perp) = 0, \quad \sum_{k_\perp} n(k_\perp) = 1$$

The field-dependent scattering probability $\widetilde{W}$ satisfies a nonlinear integral Eq. (intra-collisional field effects, electro-phonon resonances).

One-band theory: ultra-quantum limit

Under the condition $eEd\tau/\hbar \gg 1$, hopping is restricted to nearest neighbors. Principle of detailed balance:

$$W_{0,1}^{0,1}(k'_\perp, k_\perp)/W_{0,-1}^{0,-1}(k_\perp, k'_\perp) = \exp\left(\frac{eEd + \varepsilon(k'_\perp) - \varepsilon(k_\perp)}{k_B T}\right)$$

A "generalized Einstein relation" applies to this high-field regime:

$$D_{zz} = \frac{v_z d}{2}\coth\frac{eEd}{2k_B T}, \quad \mu = \frac{eD_{zz}}{k_B T}\frac{\tanh(eEd/2k_B T)}{eEd/2k_B T}$$

This simple result was confirmed by ensemble Monte Carlo simulations of hopping transport. [M. Rosini, L. Reggiani, Phys. Rev. B **72**, 195304 (2005)].

Two-band theory: basic equations

The main quantity is the conditional probability $P_{\nu\nu'}(r - r_0|t)$ to find an electron at a given time t and lattice site r in the νth band, provided it occupied r_0, ν' at an earlier time $t = 0$.

$$sP_{\nu\nu'}(r - r_0 \mid s) = \delta_{\nu\nu'}\delta(r - r_0) + \sum_{\mu} \frac{\partial}{\partial z} P_{\nu\mu}(r - r_0 \mid s) v_{\mu\nu'}(s)$$
$$+ \sum_{\mu} \frac{\partial^2}{\partial z^2} P_{\nu\mu}(r - r_0 \mid s) D_{\mu\nu'}(s) + \sum_{\mu} P_{\nu\mu}(r - r_0 \mid s) \omega_{\mu\nu'}(s)$$

The probability propagator is given by the vacuum expectation value:

$$P^{\alpha_1\alpha_3}_{\alpha_2\alpha_4}(s) = \frac{1}{Z}\int_0^\infty \mathrm{d}t e^{-st} \mathrm{Tr}_{\mathrm{ph}}\left\{ e^{-\beta H_{\mathrm{ph}}} \langle 0 \mid a_{\alpha_2} e^{\frac{i}{\hbar}Ht} a^\dagger_{\alpha_4} a_{\alpha_3} e^{-\frac{i}{\hbar}Ht} a^\dagger_{\alpha_1} \mid 0 \rangle \right\}$$

Procedure: formal solution of the equation of motion $\longrightarrow$ calculate moments and transport coefficients.

Two-band theory: kinetic equations

The carrier distribution function of the multiband system is defined by:

$$f_{\mu}^{\mu'}(k,s) = s \sum_{k'} \sum_{\nu} {}^{(0)}P_{\nu\mu}^{\nu\mu'}(k',k \mid s)$$

and satisfies the quantum-kinetic equation:

$$\left\{ s + \frac{eE}{\hbar} \cdot \nabla_k + \frac{i}{\hbar} \left[\varepsilon_{\nu'}(k) - \varepsilon_{\nu}(k) \right] \right\} f_{\nu}^{\nu'}(k,s)$$
$$+ \frac{i}{\hbar} eE \cdot \sum_{\mu} \left[Q_{\mu\nu}(k) f_{\mu}^{\nu'}(k,s) - Q_{\nu'\mu}(k) f_{\nu}^{\mu}(k,s) \right]$$
$$= s\delta_{\nu\nu'} + \sum_{k_1} \sum_{\mu,\mu'} f_{\mu}^{\mu'}(k_1,s) W_{\mu\nu}^{\mu'\nu'}(k_1,k' \mid s)$$

It is a generalization of the Boltzmann Eq. (intra-collisional field effects) and is also obtained by an alternative microscopic approach. [V.V. Bryksin et al. Sov. Phys. Solid State **22**, 1796 (1980)].

Two-band theory: drift velocity

The theory for the drift velocity is able to cope with transport via extended and localized states:

$$v_d(s) = \frac{1}{N_b} \sum_{k} \sum_{\nu,\nu'} v_{\nu}^{\nu'}(k \mid s) f_{\nu}^{\nu'}(k, s)$$

The effective drift-velocity tensor has diagonal and off-diagonal elements (tunneling):

$$v_{\nu}^{\nu'}(k \mid s) = v_{\nu}(k)\delta_{\nu\nu'} - \frac{eE}{\hbar} \cdot \nabla_k Q_{\nu\nu'}(k) - i \sum_{k'} \sum_{\mu} {}^{(1)}W_{\nu\mu}^{\nu'\mu}(k, k' \mid s)$$

Included is transport due to intersubband tunneling (Zener resonance).

The approach can be used to treat population inversion and gain in quantum-cascade lasers.

Two-band theory: diffusion coefficient

The basic result for $D_{zz}(s)$ is derived by applying the very same procedure.

$$D_{zz}(s) = \frac{1}{N_b}\sum_{k}\sum_{\nu,\nu'} v_{\nu}^{\nu'}(k \mid s)\varphi_{\nu}^{\nu'}(k \mid s) - \frac{1}{2N_b}\sum_{k}\sum_{\nu,\nu'} f_{\nu}^{\nu'}(k \mid s)\sum_{k'\mu} {}^{(2)}W_{\nu\mu}^{\nu'\mu}(k, k' \mid s)$$

The "quantum Boltzmann" Eq. for $\varphi_{\nu}^{\nu'}$ has the form:

$$\begin{aligned}
&\left\{ s + \frac{eE}{\hbar}\cdot\nabla_k + \frac{i}{\hbar}\left[\varepsilon_{\nu'}(k) - \varepsilon_{\nu}(k)\right]\right\}\varphi_{\nu}^{\nu'}(k \mid s) \\
&+\frac{i}{\hbar}eE\cdot\sum_{\mu}\left[Q_{\mu\nu}(k)\,\varphi_{\mu}^{\nu'}(k \mid s) - Q_{\nu'\mu}(k)\,\varphi_{\nu}^{\mu}(k \mid s)\right] \\
&=\sum_{k_1}\sum_{\mu,\mu'}\varphi_{\mu}^{\mu'}(k_1 \mid s)W_{\mu\nu}^{\mu'\nu'}(k_1, k' \mid s) \\
&+\sum_{k_1}\sum_{\mu,\mu'} f_{\mu}^{\mu'}(k_1 \mid s)v_{\mu\nu}^{\mu'\nu'}(k_1, k' \mid s) - v_d(s)\delta_{\nu\nu'}
\end{aligned}$$

Two-band theory: application

We treat a biased superlattice with two minibands in the high-field regime. Integration by parts:

$$v_d = -\frac{1}{\hbar N_b} \sum_{k} \sum_{\nu} \epsilon_\nu(k_z) \frac{\partial}{\partial k_z} f_\nu^\nu(k) = v_d^{(s)} + v_d^{(t)}$$

The drift velocity decomposes into a semiclassical scattering $v_d^{(s)}$ and quantum-mechanical tunneling $v_d^{(t)}$ contribution:

$$v_d^{(s)} = -\frac{1}{eE}\frac{1}{N_b} \sum_{k,k'} \sum_{\nu,\nu'} \sum_{\mu} \epsilon_\mu(k_z) f_\nu^{\nu'}(k') W_{\nu\mu}^{\nu'\mu}(k',k)$$

$$v_d^{(t)} = \frac{i}{\hbar}\frac{1}{N_b} \sum_{k} \sum_{\nu,\nu'} f_\nu^{\nu'}(k) Q_{\nu\nu'}(k) \left[\epsilon_{\nu'}(k_z) - \epsilon_\nu(k_z)\right]$$

The tunneling current is espressed by the off-diagonal elements of the density matrix.

Two-band theory: application

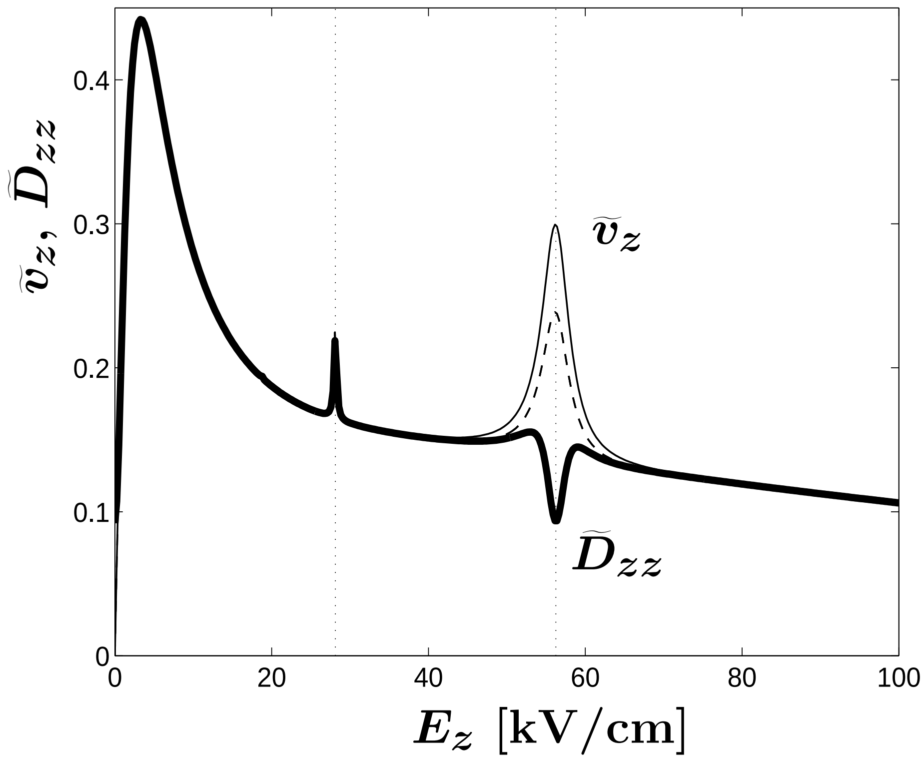
A similar decomposition applies to the diffusion coefficient:

$$D_{zz} = -\frac{1}{\hbar N_b} \sum_{k} \sum_{\nu} \epsilon_\nu(k_z) \frac{\partial}{\partial k_z} \varphi_\nu^\nu(k) = D_{zz}^{(s)} + D_{zz}^{(t)}$$

$D_{zz}^{(t)}$ depends on the difference of subband drift velocities, which changes its sign as a function of E and the superlattice parameters. $\longrightarrow$ Zener antiresonance possible in $D_{zz}^{(t)}$.

[At the tunneling resonance, the subband states are strongly mixed $\longrightarrow$ there is no additional spreading due to different subband velocities $\longrightarrow$ Minimum.]

Two-band theory: application



The dimensionless drift velocity $\tilde{v}_z = v_z/(2d/\tau)$ (thin solid line) and longitudinal diffusion coefficient $d^2\widetilde{D}_{zz}/\tau = D_{zz}$ (thick solid line) as a function of the electric field E_z. The dashed line shows the scattering induced contributions $\tilde{v}_z^{(s)}$ and $\widetilde{D}_{zz}^{(s)}$, which coalesce in this representation. The positions of tunneling resonances are indicated by vertical dotted lines. Parameters used in the calculation are: $T = 4$ K, $\tau_1 = 0.1$ ps, $\tau_2 = 0.05$ ps, $\tau_{21} = 2$ ps, $\tau = 1$ ps, and $d = 20$ nm, $\varepsilon_g = 100$ meV, $\Delta_1 = 5$ meV, $\Delta_2 = 20$ meV, $(Q_{12}/d)^2 = 0.1$.

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- We presented a rigorous theory of both transport coefficients that is applicable to transport both via extended and localized states as well as to the hopping regime.

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- The Einstein relation is not applicable under nonequilibrium conditions.
- There is a need to treat quantum diffusion in semiconductors.
- We presented a rigorous theory of both transport coefficients that is applicable to transport both via extended and localized states as well as to the hopping regime.
- To my knowledge: Our general results for the transport coefficients (beyond the Boltzmann approach) are not appreciated by the transport community.

The end

Thank you for your attention