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"Electric-Field-Induced Hopping Transport in Superlattices"

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These are preliminary lecture notes, intended only for distribution to participants.

Electric-field-induced hopping transport in superlattices

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Introduction

Wannier-Stark localization

Hopping transport picture

Localization by parallel electric and magnetic fields

) Quantum transport due to dc and ac electric fields

Outlook



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Superlattices (SLs) are man-made layered semiconductor structures with a huge lattice period d along the growth direction.

d is much larger than the bulk lattice constant *a*.



This gives rise to pronounced electric field effects described by the Bloch frequency $\Omega = e \mathcal{E} d / \hbar$.

The lateral degrees of freedom are characterized by the lateral distribution function $n(\mathbf{k}_{\perp})$

1) FIELD-INDUCED LOCALIZATION

For a simple tight-binding model the dispersion relation is given by

$$\mathbf{\varepsilon}(\mathbf{k}) = \mathbf{\varepsilon}_{\perp}(\mathbf{k}_{\perp}) + \frac{\Delta}{2}(1 - \cos k_z d)$$

 $(\Delta \text{ miniband width})$. Due to scattering, the carrier momentum and energy are changed.



If $\Omega \tau \ll 1$ (τ scattering time, $\Omega = e \mathcal{E} d / \hbar$), the carrier energy remains restricted to the bottom of the subband $\varepsilon(k_z) \sim k_z^2 \rightarrow$ The states are spatially extended.

If $\Omega \tau \gg 1$ Bloch oscillations occur \rightarrow The states are spatially localized.

)) WANNIER-STARK LOCALIZATION

If $\mathcal{E} \neq 0$ all layers are equivalent but the subband energy shifts from layer to layer.

The wavefunction becomes localized around given quantum wells ($R_L = \Delta/e\mathcal{E}$) and the dispersion relation splits into a Wannier-Stark (WS) ladder.

Under the condition $\Omega \tau \gg 1$, the hopping regime is established.



1) TRANSPORT REGIMES

A clear physical picture arises from a 1D model.

If the collisional broadening is larger than the energy separation of the steps, the transport is carried by extended states. This is the Ohmic regime, where scattering hinders transport $j \sim 1/W$.



If the energy separation of the steps is larger than the collisional broadening, hopping transport occurs. The current is due to inelastic scattering $j \sim W$.

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2 HOPPING PICTURE

A unified description of both hopping and transport via extended states provides the quantum kinetics. The approach may start from low (extended states) or high (localized states) electric field strengths.

Let us start from the hopping regime (high fields, $\Omega \tau \gg 1$), where the drift velocity v_z is expressed by

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

md hopping length. \widetilde{W} field-dependent scattering probability [1/s]. $n(\mathbf{k}_{\perp})$ normalized lateral distribution function.

2 RATE EQUATION

The approach is based on the rate equation for the conditional probability function $P_{m'm}^{m'm}(\mathbf{k}_{\perp}', \mathbf{k}_{\perp} | t)$ (to find a particle with m', \mathbf{k}_{\perp}' at time t, provided it occupied the state m, \mathbf{k}_{\perp} at an earlier time t = 0). In the Laplace space, we obtain

$$sP_{m',m}^{m',m}(\mathbf{k}_{\perp}',\mathbf{k}_{\perp} \mid s) = \delta_{m,m'}\delta_{\mathbf{k}_{\perp},\mathbf{k}_{\perp}'} + \sum_{m''}\sum_{\mathbf{k}_{\perp}''}P_{m',m''}^{m',m''}(\mathbf{k}_{\perp}',\mathbf{k}_{\perp}' \mid s)\widetilde{W}_{m'',m}^{m'',m}(\mathbf{k}_{\perp}',\mathbf{k}_{\perp} \mid s)$$

The effective scattering probability is calculated from:

 $\widetilde{W}_{m_2,m_4}^{m_1,m_3}(\mathbf{k}_{\perp}',\mathbf{k}_{\perp}\mid s)=W_{m_2,m_4}^{m_1,m_3}(\mathbf{k}_{\perp}',\mathbf{k}_{\perp}\mid s)$

$$+\sum_{\mathbf{k}_{\perp}''}\sum_{m_{5}\neq m_{6}}\widetilde{W}_{m_{2},m_{6}}^{m_{1},m_{5}}(\mathbf{k}_{\perp}',\mathbf{k}_{\perp}''\mid s)\frac{\hbar}{ie\mathcal{E}d(m_{6}-m_{5})}W_{m_{6},m_{4}}^{m_{5},m_{3}}(\mathbf{k}_{\perp}'',\mathbf{k}_{\perp}\mid s)$$

In the ultra-quantum limit ($\Omega \tau \gg 1$), we have $\widetilde{W} \approx W$.

2 LATERAL DISTRIBUTION FUNCTION

The lateral distribution function $n(\mathbf{k}_{\perp})$ describes scattering mediated heating of the lateral electron motion (T_e). $n(\mathbf{k}_{\perp})$ is the solution of the kinetic equation

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

Under the condition $k_B T_e \approx \Delta$, the distribution function becomes independent of k_z (and the current approaches zero).

The lateral distribution function is given by its equilibrium expression $n(\mathbf{k}_{\perp}) \sim \exp[-\varepsilon(\mathbf{k}_{\perp}/k_BT)]$, when the miniband width is much smaller than the Bloch energy ($\Delta \ll \hbar \Omega$).

2 k REPRESENTATION

One may switch from the Houston representation (which diagonalizes H_0) to the k representation (which is more suitable for extended states) to derive other equivalent forms.

We obtain for the NDC regime

$$v_{z} = \frac{1}{e\mathcal{E}} \sum_{\mathbf{k},\mathbf{k}'} \left[\varepsilon(k_{z}') - \varepsilon(k_{z}) \right] n(\mathbf{k}_{\perp}') \widetilde{W}(\mathbf{k}',\mathbf{k})$$

Only inelastic scattering gives rise to current. Without intracollisional field effects $(\tilde{W} \text{ independent of } \mathcal{E}): v_z \sim 1/\mathcal{E}.$ We obtain for the Ohmic regime

$$v_{z} = \sum_{\mathbf{k}} \left[\frac{1}{\hbar} \frac{\partial \boldsymbol{\varepsilon}(\mathbf{k})}{\partial k_{z}} - i \sum_{\mathbf{k}'} \frac{\partial}{\partial \kappa_{z}} W(\mathbf{k}, \mathbf{k}', \kappa) \mid_{\kappa=0} \right] f(\mathbf{k})$$

where the distribution function $f(\mathbf{k})$ solves the quantum Boltzmann equation.

QUANTUM DIFFUSION

Similar results are obtained for the diffusion coefficient. Within the hopping picture, the general expression is given by

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

In the ultra-quantum limit ($\Omega \tau \gg 1$), the mobility is obtained from

$$\mu = \frac{eD_{zz}}{k_BT} \frac{\tanh(e\mathcal{E}d/2k_BT)}{e\mathcal{E}d/2k_BT},$$

which reproduces the Einstein relation for high temperatures.

For classically high electric fields ($D_{zz} \sim 1/\mathcal{E}^2$):

$$D_{zz} = \frac{1}{2} \frac{1}{(e\mathcal{E})^2} \sum_{\mathbf{k},\mathbf{k}'} [\varepsilon(k_z) - \varepsilon(k'_z)]^2 n(\mathbf{k}'_\perp) W(\mathbf{k}',\mathbf{k})$$

2) ELECTRO-PHONON RESONANCES

Two non-classical field effects:

1) NDC (negative differential conductivity) $j \sim 1/\mathcal{E}$. At the band edges the carriers experience a negative effective mass m^* ($\hbar^2/m^* = \partial^2 \varepsilon(\mathbf{k})/\partial k_z^2$). The degree of localization increases with increasing field strength.



2) Electro-phonon resonances appear whenever the multiple of the Bloch frequency matches the frequency of polar-optical phonons $l\Omega = \omega_0$. This is a pure quantum effect, which results from intra-collisional field effects $[W(\mathcal{E})]$.

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3 COMPLETE LOCALIZATION

□ The lateral carrier motion becomes quantized by a magnetic field applied perpendicular to the layers.

□ The extended states of the crystal are completely converted to localized states by external electric and magnetic fields.

□ Scattering plays a fundamental role because without any scattering transport phenomena does not occur.

□ There is a close relationship between the energy spectrum (density of states) and the statistical properties (distribution function). This retroaction depends on time even for the steady state.

3 COMPLETE LOCALIZATION

Applying strong parallel electric and magnetic fields, the energy spectrum becomes completely discrete. How do we describe this field-induced "metal-insulator transition"? An essential role plays the double-time character of the correlation functions (which emerge beyond the Kadanoff-Baym ansatz). The quantum kinetic equation is derived within the Keldysh formalism.

$$\widetilde{G}^{\gtrless}(\mathbf{k} \mid t, t') = \mp i \widehat{G}(\mathbf{k} \mid t, t') f^{\gtrless}\left(\mathbf{k} + \frac{[\mathbf{A}(t') - \mathbf{A}(t)]}{2} \mid t, t'\right)$$

$$\widehat{G}(\mathbf{k} \mid t, t') = \exp\left\{-\frac{i}{\hbar} \int_{t'}^{t} d\tau \varepsilon (\mathbf{k} + \mathbf{A}(i\nabla_k) + \mathbf{A}(\tau) - [\mathbf{A}(t) + \mathbf{A}(t')]/2)\right\}$$
$$d\mathbf{A}(t)/dt = e\mathcal{E}(t)/\hbar, \quad T = (t+t')/2, \quad t_- = t' - t$$

3) FIELD-INDUCED HOPPING

The stationary transport regime is usually assumed to be characterized by a time-independent distribution function $f^{<}(\mathbf{k})$. However, to describe field mediated localization correctly, it is necessary to determine a time dependent function $f^{<}(\mathbf{k} | t_{-})$. Three important features appear:



1) There are pronounced electro-phonon resonances.

2) Current gaps appear in the I-V characteristics.

3) There is a crossover from the quasi-classical $(j \sim 1/\mathcal{E})$ to the activated, hopping transport regime.

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4) **PHONONLESS QUANTUM TRANSPORT**

Stationary phononless quantum transport occurs in the hopping regime. A photon-induced current component appears beyond the Kadanoff-Baym ansatz. Let us treat the Fourier transformed Greens functions for a 1D model

$$g_{l,m}^{<}(\omega) = g_{l,m}^{>}(\omega)f_{l,m}(\omega)$$

l: k_z ; *m*: T = (t + t')/2, ω_{ac} ; ω : t_- .

Even for the stationary transport, a time (frequency) dependence has to be determined beyond the periodic response forced by the applied ac field.

$$j_{z} = \sum_{k} A_{k}(\omega_{ac}, \Omega_{ac}, \Omega_{dc}) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g_{00}^{>}(\omega) g_{00}^{>}(\omega + \omega_{ac}(k + \frac{\Omega_{dc}}{\omega_{ac}})) \times \left[f_{00}(\omega + \omega_{ac}(k + \frac{\Omega_{dc}}{\omega_{ac}})) - f_{00}(\omega) \right]$$

4 PHOTON INDUCED CURRENT

Photon-induced carrier transport is predicted to occur in 1D SLs at low lattice temperatures.

The collisional broadening of the WS ladder can be smaller than ħω_{ac}.
Current gaps appear whenever the joint density of states becomes zero.

3) The ac field induces a stationary current that may flow against the field direction. The energy provided by photon absorption is used by the carriers to travel the WS ladder upwards.

4) Electro-photon resonances exist.

□ Intersubband transitions: Population inversion may occur in biased multi-subband SLs. Unipolar mid-infra-red lasers have been fabricated (quantum cascade lasers).

□ Intersubband transitions: Calculation of the drift velocity and the diffusion coefficient. Study of spacecharge waves and electric-field domain formation. It can be used for more realistic device simulations.

□ Intrasubband and intersubband transitions: Study of noise phenomena in biased SLs.

□ A strong electric field applied parallel to the SL axis leads to Wannier-Stark localization of the eigenstates. There are two transport pictures that are quite different but nevertheless equivalent. One is most suitable for localized states, whereas the other one is applicable to extended states.

□ The hopping picture for the drift velocity and the diffusion coefficient has been developed.

□ **Complete localization** by electric and magnetic fields is described by the double-time approach.

□ A photon-induced phononless current component has been identified that has a quantum-mechanical origin.