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Quantum transport theory for semiconductor superlattices

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Abstract. The Kadanoff–Baym–Keldysh non-equilibrium Green's function technique is used to study quantum transport within the lowest miniband of semiconductor superlattices (SLs) under high-electric fields. Both intra-collisional field effects (ICFEs) and lifetime broadening are taken into account. An inevitable extension of the generalized Kadanoff–Baym ansatz is discussed. The collisional broadening of electro-phonon resonances due to scattering on impurities is calculated. Even if the mean impurity scattering strength is considerably smaller than the miniband width, the oscillatory current anomalies, which result from ICFEs, are completely smeared out.

1 Introduction

If the Bloch frequency $\Omega = eEd/\hbar$ (E is the electric field strength and d the SL period) is larger than some effective scattering rate, $1/\tau$, carriers confined to the lowest miniband are expected to be Bragg reflected before being scattered by phonons or imperfections in the crystal. This gives rise to Bloch oscillations and to the formation of a Wannier–Stark (WS) ladder. The electric field induced WS localization results in non-analytic resonant-type anomalies in the current-voltage characteristic (I–V), known as electro-phonon resonances [1]. Whereas these current anomalies have been observed in narrow band semiconductors, there are no experiments that clearly demonstrate such quantum effects in the SL transport. To resolve this puzzle we develop a quantum transport theory that treats simultaneously electro-phonon resonances as well as scattering induced lifetime broadening.

There is a fundamental problem that arises when the collisional broadening is taken into account within a consequent quantum-mechanical approach. As the eigenenergies of the system are no longer sharp, the electron distribution function depends explicitly on a time variable even for stationary transport problems. This expresses the non-Markovian character of the transport. For a non-degenerate electron gas a solution of the Dyson equation can be searched for by employing the following extended generalized Kadanoff–Baym (KB) ansatz

$$\widetilde{G}^{<}(\mathbf{k},t) = -\widetilde{G}^{>}(\mathbf{k},t)\, f\left(\mathbf{k} - \frac{e\mathbf{E}}{2\hbar}\,|\,t\,|, t\right), \tag{1}$$

where we introduced the notation

$$\widetilde{G}^{\gtrless}(\mathbf{k},t) \equiv G^{\gtrless}\left(\mathbf{k} - \frac{e\mathbf{E}}{2\hbar}t, t\right), \text{ with } \widetilde{G}^{\gtrless}(\mathbf{k},t)^{*} = -\widetilde{G}^{\gtrless}(\mathbf{k},-t). \tag{2}$$

$G^{\gtrless}$ are the closed-time path Green's functions. If the collisional broadening plays only a minor role, the explicit time dependence in the distribution function disappears ($f(\mathbf{k},t) \to f(\mathbf{k})$) and Eq. (1) becomes identical with the well known generalized KB ansatz [2], which has been used in the literature to study quantum transport in semiconductors. Unlike the early KB ansatz, which has fundamental limitations, the generalized KB ansatz is fully consistent with the dynamical structure of the theory and agrees exactly with results derived from the Liouville equation for the density matrix. This ansatz takes the causality for the time evolution of the particle propagator properly into account and follows unambiguously from the symmetry properties of the electron system in an external electric field. If, however, lifetime broadening becomes important, the generalized KB ansatz no longer solves the kinetic equation and one has to determine a distribution function $f^{\gtrless}(\boldsymbol{k} - e\boldsymbol{E} \mid t \mid /2\hbar, t)$ that depends explicitly on a time variable. This leads to additional complications because a closed equation cannot be derived for the distribution function $f^{\gtrless}(\boldsymbol{k}, t = 0)$ which is used to calculate the current density.

In this paper we will study the damping of electron-phonon resonances in the SL transport. We will show below that such resonances survive only when the lifetime broadening is extremely small. In this case $f(\boldsymbol{k}, t)$ is nearly independent of t and the kinetic equation simplifies accordingly.

2 Numerical results and discussion

We consider a simple tight-binding energy band of the SL

$$\varepsilon(\boldsymbol{k}) = \varepsilon(\boldsymbol{k}_\perp) + \varepsilon(k_z) = \frac{\hbar^2 \boldsymbol{k}_\perp^2}{2m^*} + \frac{\Delta}{2}(1 - \cos k_z d), \tag{3}$$

where m^* is the effective mass and Δ the miniband width. $\widetilde{G}^>$ is calculated from the Dyson equation under the condition $G^< \sim 0$, which holds true for a non-degenerate electron gas. In quasi-classical approximation and for elastic scattering on impurities we get

$$\widetilde{G}^>(\boldsymbol{k}, t) = -i \exp\left[\frac{i}{\hbar}\int_{-t/2}^{t/2} d\tau \varepsilon\left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{\hbar}\tau\right) - s(\varepsilon(\boldsymbol{k}_\perp)) \mid t \mid\right], \tag{4}$$

where the damping function $s(\varepsilon)$

$$s(\varepsilon) = \frac{m^* u^2}{\pi^2 \hbar \Delta d}\int_{\max(0,\varepsilon-\Delta)}^{\varepsilon+\Delta} d\varepsilon' K\left(\sqrt{1 - \left(\frac{\varepsilon - \varepsilon'}{\Delta}\right)^2}\right), \tag{5}$$

is proportional to the scattering strength u^2. K is the complete elliptic integral of the first kind. The current density is calculated from the stationary electron distribution function, which is the solution of a kinetic equation. Integrating by parts, we obtain

$$j_z = -\frac{e}{\hbar V}\sum_{\boldsymbol{k}} \varepsilon(k_z)\frac{\partial f(\boldsymbol{k}, t = 0)}{\partial k_z}, \tag{6}$$

where V is the volume of the crystal. The collision integral can be introduced in Eq. (6) when $\partial f(\boldsymbol{k}, 0)/\partial k_z$ is replaced by the right-hand side of the kinetic equation. In the case of high electric fields and weak scattering ($\Omega\tau > 1$) we get

$$j_z = \frac{em^* n_s \omega_0^2 \Gamma}{2\pi \hbar^4 k_B T d}\frac{1}{1 - e^{-\beta}}\sum_{l=-\infty}^{\infty}\frac{1}{\pi}\int_0^\pi dz\, l J_l^2\left(\frac{\Delta}{\hbar\Omega}\sin z\right)\int_0^\infty d\varepsilon d\varepsilon' e^{-\varepsilon'/k_B T}$$
$$\times\left\{\frac{s(\varepsilon, \varepsilon')}{(l\Omega + (\varepsilon' - \varepsilon)/\hbar - \omega_0)^2 + s(\varepsilon, \varepsilon')^2} + \frac{e^{-\beta} s(\varepsilon, \varepsilon')}{(l\Omega + (\varepsilon' - \varepsilon)/\hbar + \omega_0)^2 + s(\varepsilon, \varepsilon')^2}\right\}, \tag{7}$$

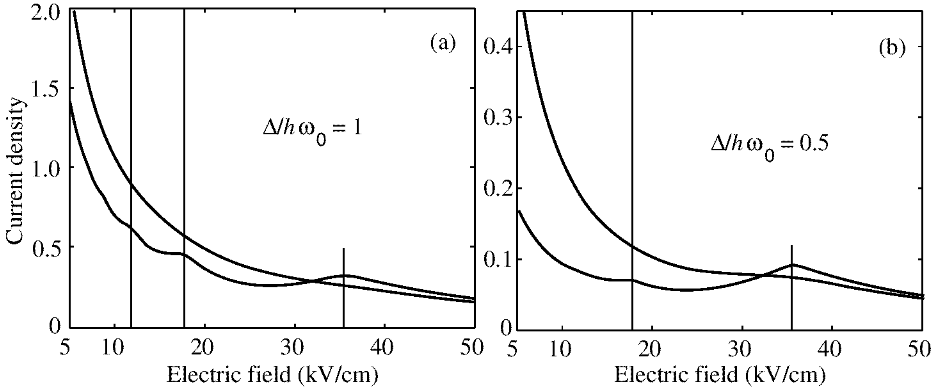

Fig. 1. (a) Field dependence of the dimensionless current density j_z/j_{z0} with $j_{z0} = em^* n_s \omega^2 \Gamma / 2\pi \hbar^3 d$ for $\Delta/\hbar\omega_0 = 1$ and $\hbar\omega_0/k_B T = 5$. The scattering strength parameter $m^* u^2/\pi^2 \Delta d$ is given by 0.005 and 0.05 for the solid and dashed line, respectively.
(b) The same as in (a) for $\Delta/\hbar\omega_0 = 0.5$.

where the lateral electron distribution function has been replaced by the Boltzmann distribution. n_s is the sheet density, Γ the coupling constant, ω_0 the phonon frequency, $\beta = \hbar\omega_0/k_B T$, and $s(\varepsilon, \varepsilon') = s(\varepsilon) + s(\varepsilon')$.
Within our approach we obtained a broadened Lorentzian energy conservation in Eq. (7). This approximation has the defect that higher and higher energy states become populated because the Lorentz curve falls off only gradually. To avoid this run-away effect the explicit time dependence of the distribution function has to be retained. In our present analytic study, however, we will not address the details of such an analysis, but present some numerical results that reveal already the main features of ICFEs and collisional broadening in the SL transport.

Numerical results calculated from Eq. (7) are shown in Figs. 1 (a) and (b) for $\Delta/\hbar\omega_0 =$ 1 and 0.5, respectively. Vertical lines mark the positions of electro-phonon resonances at $E = \hbar\omega_0/led$ with $l = 1, 2, 3$ (for d we used 10 nm). The solid lines have been calculated for the case when the impurity scattering strength is much smaller than the miniband width ($m^* u^2/\pi^2 \Delta d = 0.005$). In this case weak current oscillations appear, which, however, are rapidly smeared out, when the impurity strength becomes slightly larger. This is shown by the dashed lines, which have been calculated for $m^* u^2/\pi^2 \Delta d =$ 0.05. The lifetime broadening effect, obtained from the microscopic model, seems to be larger than phenomenological estimates suggest. This is due to the fact that in Eq. (7) both energy integrals are affected by the damping function $s(\varepsilon)$.
Our numerical results demonstrate that current oscillations, which are due to ICFEs, occur only, when the lifetime broadening is extremely small. This might be the reason, why quantum mechanical current oscillations have not been observed in high-field transport measurements in SLs until now.

In conclusion we believe that our quantum-mechanical approach, which accounts for both ICFEs and collision broadening, can be used to study the stationary transport in other nanostructure devices, too.

References

[1] V. V. Bryksin and Y. A. Firsov, *Sov. Phys. - JETP* **34**, 1272 (1971); [*JETP* **61**, 2373 (1971).]
[2] P. Lipavsky and V. Spicka and B. Velicky, *Phys. Rev. B* **34**, 6933 (1986).