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J. Phys. A: Math. Gen. **33** (2000) 233–246. Printed in the UK PII: S0305-4470(00)07718-0

High-electric-field quantum transport theory for semiconductor superlattices

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Received 13 September 1999

Abstract. Nonlinear quantum transport in semiconductor superlattices (SLs) is studied based on the Kadanoff–Baym–Keldysh non-equilibrium Green function technique. Emphasis is placed on quantum box SLs with a discrete energy spectrum. Special results are obtained for the high-field transport of a one-dimensional SL model. Both intra-collisional field effects and lifetime broadening are treated self-consistently on an equal footing. For narrow miniband SLs exact results are derived for the field and temperature dependence of the current density, which even differ qualitatively from those obtained by making use of the generalized Kadanoff–Baym ansatz. The rigorous quantum mechanical treatment reveals the hopping character of the transport in narrow miniband SLs. This is compared with results derived from the density-matrix approach.

1. Introduction

We will consider superlattice (SL) transport along the symmetry axis under the conditions of sufficiently low carrier concentration suppressing the field-domain formation, and a wide minigap to prevent Zener tunnelling in the electric field region of interest. The formation of electric field domains results in a number of interesting effects (see, e.g., [1]). In this paper, however, we assume that the field distribution is homogeneous. When the Bloch frequency of the SL $\Omega = eEd/\hbar$ (E is the electric field and d the SL period) exceeds some effective scattering rate $1/\tau$, the miniband of carrier states splits into a Wannier–Stark (WS) ladder, the energetic separation between the rungs of which is inversely proportional to the field strength. Electron transport results from phonon-induced hopping between localized oscillator-like states. Negative differential conductance is predicted to occur [2] with a characteristic $1/E$ dependence of the current due to Houston oscillations [3] of electrons confined to a region of the order of Δ/eE (Δ is the miniband width). When an integer multiple of the Bloch frequency Ω equals the frequency of polar-optical phonons ω_0, electrophonon resonances are expected to appear [3, 4] giving rise to a non-monotonic current–voltage dependence. Such resonant-type current anomalies around the electro-phonon resonances were observed in thin ZnS films many years ago [5, 6]. As the anisotropic band structure of a SL can easily be tuned over a wide parameter range, it seemed to be promising to investigate this interesting quantum interference phenomenon also in artificial SL systems. Recently, electrophonon resonances in SLs were theoretically studied [7, 8]. Their temperature dependence has been found to be much stronger than in narrow-band semiconducting films. Unfortunately, to our knowledge, in SL transport electro-phonon resonances have not been observed in experiment until now.

0305-4470/00/020233+14$30.00 © 2000 IOP Publishing Ltd

This could be due to strong elastic and inelastic scattering present in the studied SLs, which may mask the predicted current anomalies.

Electro-phonon resonances are strongly enhanced by a quantizing magnetic field, which is applied parallel to the electric field and perpendicular to the SL layers [10,11]. This pronounced enhancement of current resonances is due to the dimensionality reduction by the magnetic field, which leads essentially to one-dimensional (1D) transport within a quantum box superlattice (QBSL). The magnetic field gives rise to additional cyclotron-Stark resonances, which have been studied both theoretically [9–11] and experimentally [12, 13].

From a theoretical point of view the application of a quantizing magnetic field perpendicular to the SL layers poses some fundamental problems. Landau quantization of the in-plane motion and the WS localization of carriers moving along the field direction result in a completely discrete energy spectrum. As a consequence, the carrier transport becomes singular with δ-like peaks, when the scattering is treated only in lowest-order perturbation theory, which does not introduce any collisional broadening. To obtain meaningful physical results a phenomenological damping parameter has been used in recent theoretical studies [9–11]. From a microscopic quantum kinetic point of view this procedure is completely inadequate, when treating systems with discrete energy states. In this case, the finite lifetime of states is expected to depend non-analytically on the coupling constant of the respective scattering mechanism, which requires to sum up an appropriate infinite set of scattering diagrams. A non-equilibrium theory of the SL transport that accounts for finite-lifetime effects has been proposed recently [14–16] using the Kadanoff–Baym–Keldysh non-equilibrium Green function technique. In an earlier paper [16] we used the generalized Kadanoff–Baym (KB) ansatz [17, 18]. Even this sophisticated approach seems to be inadequate when considering quantum transport in systems, in which all eigenstates are completely discrete if scattering is absent. Under this circumstance the interaction can no longer be described by an instantaneous scattering process as the generalized KB ansatz suggests, because the neglect of the scattering duration is not in line with the non-perturbative character of the problem. When lifetime effects become essential, the electron distribution function depends explicitly on a time variable even for stationary carrier transport [16]. Otherwise, the distribution function does not solve the kinetic equation. This explicit time dependence, which is neglected when using the generalized KB ansatz, affects the energy-conserving delta function of the Fermi golden rule in the energy domain in a similar way as the lifetime broadening. When treating the QBSL transport, we are faced with the interesting quantum kinetic problem to take into account simultaneously both intra-collisional field effects, which give rise to WS localization, and a sizable lifetime broadening, which cannot be treated consistently within the framework of the generalized KB ansatz. The consideration of this general quantum kinetic task could, likewise, be useful for transport studies in other periodic arrays of nanostructures.

On the basis of the non-equilibrium Green function approach, we will calculate the current density for the Esaki–Tsu model in the high-field region, where the inequality $\Omega\tau > 1$ is satisfied. Both intra-collisional field effects and collisional broadening are consistently taken into account within this quantum kinetic approach, which does not rely on the generalized KB ansatz, but solves the kinetic equation exactly.

2. Basic theory

We focus on electron transport in the lowest narrow miniband of a SL at low carrier concentration, when the electron gas is considered to be non-degenerate. The starting point of the non-equilibrium Green function approach is the Dyson equation for the double-time Green functions $G^{\gtrless}$, which we prefer to present in the wavenumber representation [16]

$$\left[\mathrm{i}\hbar\frac{\partial}{\partial t} - \varepsilon(\boldsymbol{k}) + \mathrm{i}e\boldsymbol{E}\nabla_{\boldsymbol{k}}\right] G^{\gtrless}(\boldsymbol{k}t|\boldsymbol{k}'t')$$
$$= \pm\hbar\int \mathrm{d}\boldsymbol{k}_1\left\{\int_{t'}^{t}\mathrm{d}t_1\,\Sigma^{\gtrless}(\boldsymbol{k}t|\boldsymbol{k}_1t_1)G^{\gtrless}(\boldsymbol{k}_1t_1|\boldsymbol{k}'t') + \int_{-\infty}^{t'}\mathrm{d}t_1\,\Sigma^{\gtrless}(\boldsymbol{k}t|\boldsymbol{k}_1t_1)G^{\lessgtr}(\boldsymbol{k}_1t_1|\boldsymbol{k}'t') - \int_{-\infty}^{t}\mathrm{d}t_1\,\Sigma^{\lessgtr}(\boldsymbol{k}t|\boldsymbol{k}_1t_1)G^{\gtrless}(\boldsymbol{k}_1t_1|\boldsymbol{k}'t')\right\}. \tag{1}$$

The SL energy dispersion relation $\varepsilon(\boldsymbol{k})$ describes carrier propagation along the SL-axis by a tight-binding model and allows free electron motion with an effective mass m^* in all lateral directions:

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

where Δ is the miniband width and $\hbar\boldsymbol{k}_\perp$ the transverse quasi-momentum. The self-energy components $\Sigma^{\gtrless}$ will be calculated within the self-consistent Born approximation.

Crucial for possible simplifications of the Dyson equation are the symmetry properties of the Green functions. For the stationary carrier transport and in the scalar-potential gauge, the Green functions depend on two wavenumber vectors, but only on the time difference. In addition, there is a spatial symmetry property of the problem, which accounts for the fact that a carrier moving the distance $\boldsymbol{r}$ under the influence of the field $\boldsymbol{E}$ restores its quasi-momentum, when the energy is shifted by $e\boldsymbol{E}\boldsymbol{r}$. These symmetry properties of the Green functions are expressed by [16]

$$G^{\gtrless}(\boldsymbol{k}t|\boldsymbol{k}'t') = G^{\gtrless}(\boldsymbol{k}, t'-t)\,\delta\left(\boldsymbol{k}' - \boldsymbol{k} - \frac{e\boldsymbol{E}}{\hbar}(t'-t)\right). \tag{3}$$

In the absence of any electric field, equation (3) reconstitutes the symmetry of a homogeneous electron system. As the relationship (3) also applies to the self-energy components $\Sigma^{\gtrless}$, the Dyson equation (1) simplifies considerably. Another symmetry of the Green functions relates the upper and lower time branches to each other. This symmetry becomes particularly transparent for the Green functions defined by

$$\widetilde{G}^{\gtrless}(\boldsymbol{k}, t) \equiv G^{\gtrless}\left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar}t, t\right) \tag{4}$$

for which we get, according to equation (3) and the antisymmetry of $G^{\gtrless}$ [16],

$$\widetilde{G}^{\gtrless}(\boldsymbol{k}, t)^* = -\widetilde{G}^{\gtrless}(\boldsymbol{k}, -t). \tag{5}$$

The left-hand side of equation (1) simplifies by introducing new functions

$$\widetilde{G}^{\gtrless}(\boldsymbol{k}, t) = \mp\mathrm{i}g^{\gtrless}(\boldsymbol{k}, t)\exp\left[\frac{\mathrm{i}}{\hbar}\int_{-t/2}^{t/2}\mathrm{d}\tau\,\varepsilon\left(\boldsymbol{k} + \frac{e\boldsymbol{E}}{\hbar}\tau\right)\right] \tag{6}$$

which satisfy, according to equation (5), the symmetry relation

$$g^{\gtrless}(\boldsymbol{k}, t) = g^{\gtrless}(\boldsymbol{k}, -t)^*. \tag{7}$$

The self-energy, entering the Dyson equation (1), is calculated in the self-consistent Born approximation

$$\widetilde{\Sigma}^{\gtrless}_{ph}(\boldsymbol{k}, t) = \sum_{q\lambda} D^{\gtrless}_{q\lambda}(t)\,\widetilde{G}^{\gtrless}(\boldsymbol{k} + \boldsymbol{q}, t) \tag{8}$$

where scattering on polar-optical phonons is described by

$$D_{q\lambda}^{\gtrless}(t) = \frac{2\pi}{\hbar^2} \frac{|M_{q\lambda}|^2}{\sinh(\hbar\omega_{q\lambda}/2k_B T)} \cos\omega_{q\lambda}\left(t \mp \frac{\mathrm{i}\hbar}{2k_B T}\right). \tag{9}$$

$M_{q\lambda}$ is the electron–phonon coupling constant for phonons of wavevector $\boldsymbol{q}$ in branch λ, and $\omega_{q\lambda}$ is the phonon frequency. T denotes the temperature. In this paper, we will not consider the details of the electron–phonon interaction in a SL, but will restrict ourselves to the simple bulk-phonon model. For elastic scattering on isolated impurities, the phonon Green function $D_{q\lambda}^{\gtrless}(t)$ in equation (9) is replaced by a constant coupling parameter U measuring the scattering strength. Equation (8) for the self-energy closes the set of basic self-consistent equations, which allow a quantum kinetic treatment of the nonlinear SL transport. In the next section, we will derive an equation for $\widetilde{G}^{>}$, the solution of which enables the calculation of the field-dependent density of states (DOS).

3. Density of states

In this section, we consider the Keldysh Green function $\widetilde{G}^{>}$. On the right-hand side of the Dyson equation (1), we retain only the term $\Sigma^{>}G^{>}$, which is admissible for a non-degenerate electron gas, where $G^{<}$ introduces only small corrections, which can be neglected. Inserting equations (3) and (4) into the Dyson equation (1), we obtain

$$\left[-\mathrm{i}\hbar\frac{\partial}{\partial t} + \varepsilon\left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar}t\right) + \frac{\mathrm{i}}{2}e\boldsymbol{E}\nabla_{\boldsymbol{k}}\right]\widetilde{G}^{>}(\boldsymbol{k},t)$$
$$= -\hbar\int_0^t \mathrm{d}t_1 \widetilde{\Sigma}^{>}\left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar}(t-t_1), t_1\right)\widetilde{G}^{>}\left(\boldsymbol{k} + \frac{e\boldsymbol{E}}{2\hbar}t_1, t-t_1\right) \tag{10}$$

where the time t is an abbreviation for the time difference $t' - t$ resulting from equation (1). To proceed further, the expression for the self-energy (8) together with equation (6) is inserted into the Dyson equation. We obtain the integro-differential equation for the Green function

$$-\frac{\partial}{\partial t}\widetilde{g}^{>}(\boldsymbol{k},t) = \sum_{q\lambda}\int_0^t \mathrm{d}t_1 D_{q\lambda}^{>}(t_1)\widetilde{g}^{>}\left(\boldsymbol{k}+\boldsymbol{q} - \frac{e\boldsymbol{E}}{\hbar}(t-t_1), t_1\right)\widetilde{g}^{>}(\boldsymbol{k}, t-t_1)$$
$$\times \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^{t_1}\mathrm{d}\tau\left[\varepsilon\left(\boldsymbol{k}+\boldsymbol{q} - \frac{e\boldsymbol{E}}{\hbar}(t-\tau)\right) - \varepsilon\left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{\hbar}(t-\tau)\right)\right]\right\} \tag{11}$$

with

$$\widetilde{g}^{\gtrless}(\boldsymbol{k},t) = g^{\gtrless}\left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar}t, t\right). \tag{12}$$

An analytic solution of this equation is derived for weak scattering and high electric fields, for which negative differential conductivity may occur and the inequality $\Omega\tau \gg 1$ is valid. In this case, we will exploit a fundamental symmetry property of the problem, namely the invariance under the translation by a reciprocal lattice vector, valid even in the presence of a homogeneous electric field of any strength [3]. This symmetry is accounted for by a discrete Fourier transformation of the Green functions

$$\widetilde{g}^{\gtrless}(\boldsymbol{k},t) = \sum_{l=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}lk_z d}\widetilde{g}_l^{\gtrless}(\boldsymbol{k}_\perp, t). \tag{13}$$

In the limit of high electric fields ($\Omega\tau \gg 1$), the lowest-order Fourier coefficient $\widetilde{g}_0^{\gtrless}(\boldsymbol{k}_\perp, t)$ dominates the sum in equation (13), meaning that only this contribution can be retained on the right-hand side of the Dyson equation (11). Furthermore, we will treat a 1D transport model (in fact, the Esaki–Tsu model [2]) without any lateral degrees of freedom. It is expected that the essence of our results will not be strongly modified, when a more realistic SL model is studied, in which the confinement of the lateral electron motion is due to a strong magnetic field. With the restriction to the lowest-order Fourier coefficient, we obtain for the 1D transport model from equation (11):

$$\frac{\mathrm{d}}{\mathrm{d}t} g_0^>(t) = -\int_0^t \mathrm{d}t_1 D^>(t_1) g_0^>(t_1) g_0^>(t-t_1) J_0^2\left(\frac{\Delta}{\hbar\Omega}\sin\frac{\Omega t_1}{2}\right) \tag{14}$$

where in the derivation of this equation we used

$$\left|\sum_{k_z} \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^{t_1} \mathrm{d}\tau\, \varepsilon\left(k_z + \frac{e\boldsymbol{E}}{\hbar}\tau\right)\right\}\right|^2 = J_0^2\left(\frac{\Delta}{\hbar\Omega}\sin\frac{\Omega t_1}{2}\right) \tag{15}$$

and $\tilde{g}_0^>(t_1) = g_0^>(t_1)$. After a Laplace transformation of equation (14), we obtain the formal solution

$$g_0^>(s) = \frac{1}{s + H(s)} \tag{16}$$

where $H(s)$ itself depends on $g_0^>(t)$

$$H(s) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st} D^>(t) g_0^>(t) J_0^2\left(\frac{\Delta}{\hbar\Omega}\sin\frac{\Omega t}{2}\right). \tag{17}$$

The integral equation (16) can be solved by iteration, while in each step the inverse Laplace transform of $g_0^>(s)$ has to be calculated. We assume that the lifetime broadening is mainly governed by elastic impurity scattering. In this case, taking into account the Fourier representation

$$J_0^2\left(\frac{\Delta}{\hbar\Omega}\sin\frac{\Omega t}{2}\right) = \sum_{l=-\infty}^{\infty} F_l\left(\frac{\Delta}{\hbar\Omega}\right)\mathrm{e}^{-\mathrm{i}l\Omega t} \tag{18}$$

with

$$F_l\left(\frac{\Delta}{\hbar\Omega}\right) = \frac{1}{\pi}\int_0^\pi \mathrm{d}x\, J_l^2\left(\frac{\Delta}{\hbar\Omega}\sin x\right) \tag{19}$$

a difference equation for the Keldysh Green function is obtained

$$\left[s + U\sum_l F_l\left(\frac{\Delta}{\hbar\Omega}\right) g_0^>(s + \mathrm{i}l\Omega)\right] g_0^>(s) = 1 \tag{20}$$

which has to be solved under the constriction $g_0^>(t=0) = 1$. In the limit of narrow minibands ($\Delta \to 0$), only the term with $l = 0$ survives in the sum of equation (20), and we find the exact solution

$$g_0^>(s) = \frac{\sqrt{s^2 + 4U} - s}{2U} \tag{21}$$

which has a universal character, because it does not depend on the electric field. After an inverse Laplace transformation, we obtain

$$g_0^>(t) = \frac{1}{\sqrt{U}t} J_1(2\sqrt{U}t) \tag{22}$$

which oscillates in time and exhibits a power-law decay. This has to be contrasted with the pole approximation of equation (16) leading to an exponential dependence $g_0^>(t) = \exp(-H(s =$

$0)|t|)$, which allows the definition of a relaxation time according to $\tau = 1/H(s = 0)$. From $g_0^>(s)$ the DOS is obtained by an analytical continuation

$$g_0^>(\omega) = \frac{1}{\pi}\mathrm{Re}\, g_0^>(s)|_{s=\mathrm{i}\omega}. \tag{23}$$

Inserting into this equation the exact solution (21), we get

$$g_0^>(\omega) = \frac{1}{2\pi U}\mathrm{Re}\sqrt{4U - \omega^2}. \tag{24}$$

It is astonishing that this result completely agrees with the well known DOS calculated within the self-consistent Born approximation for electrons in an impurity band under the condition of low or zero electric fields. In our approach, we focus on the non-equilibrium situation caused by high electric fields ($\Omega\tau \gg 1$) and find in the ultra-quantum limit ($\Delta/\hbar\Omega \ll 1$) a universal field-independent expression for the DOS, which surprisingly reproduces the DOS obtained at $\boldsymbol{E} = 0$. This coincidence is due to the disappearance of the electric field in the sequential tunnelling regime ($\Delta/\hbar\Omega \ll 1$).

The non-analytic dependence of the DOS in equation (24) on the coupling constant U is characteristic for the scattering-induced decay of discrete eigenstates and cannot be reproduced by a simple perturbation approach. Essential is the appearance of band edges, which prevent run-away effects due to the strong electric field. The situation is completely different in the pole approximation, where the exponential decay of $g_0^>(t)$ leads to a Lorentzian DOS, which falls off only gradually and is, therefore, plagued by run-away effects. Any approximate treatment of scattering has to focus on the asymptotic regime of large s (or small t) in order to reproduce the expected band edges in the DOS.

For a finite miniband width Δ, equation (20) allows the calculation of the field-dependent DOS. The result is a slightly modified central peak around $\omega = 0$. In addition, for large ω (or small time t) sidebands appear at $\omega = l\Omega$, the width of which is of the order of $\sqrt{U}$. The height of these sidebands decreases with increasing l as $(\Delta/\hbar\Omega)^{2l}$. The numerical analysis of equation (20) showed that under the condition $\Omega\tau \gg 1$ the sidebands are so weak that they can always be neglected.

4. Distribution function

The kinetic equation for the Keldysh Green function $G^<$ is derived from equation (1), where for a non-degenerate electron gas the contribution $\Sigma^< G^<$ on the right-hand side of this equation is only of secondary importance and will be neglected. Equations (3), (4), (6) and (8) are inserted into the Dyson equation (1). Simple substitutions of time integrals lead to the result presented in the appendix. Once more, we exploit the Fourier transformation (13) with respect to the k_z dependence and retain in the limit $\Omega\tau \gg 1$, only the $l = 0$ Fourier coefficient. As a consequence, the left-hand side in equation (A1) vanishes and the kinetic equation can be cast into the form

$$\sum_{\boldsymbol{q}_\perp\lambda}\int_{-\infty}^{\infty}\mathrm{d}t_1[F_\lambda^<(\boldsymbol{q}_\perp,\boldsymbol{k}_\perp,t_1)g_0^<(\boldsymbol{k}_\perp+\boldsymbol{q}_\perp,t_1)g_0^>(\boldsymbol{k}_\perp,t-t_1)$$
$$-F_\lambda^>(\boldsymbol{q}_\perp,\boldsymbol{k}_\perp,t_1)g_0^>(\boldsymbol{k}_\perp+\boldsymbol{q}_\perp,t_1)g_0^<(\boldsymbol{k}_\perp,t-t_1)] = 0 \tag{25}$$

where the following kernels have been introduced:

$$F_\lambda^{\gtrless}(\boldsymbol{q}_\perp,\boldsymbol{k}_\perp,t_1) = \sum_{k_z q_z} D_{\boldsymbol{q}\lambda}^{\gtrless}(t_1)$$
$$\times\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^{t_1}\mathrm{d}\tau\left[\varepsilon\left(\boldsymbol{k}+\boldsymbol{q}+\frac{e\boldsymbol{E}}{\hbar}\tau\right)-\varepsilon\left(\boldsymbol{k}+\frac{e\boldsymbol{E}}{\hbar}\tau\right)\right]\right\}. \tag{26}$$

At this stage a lateral electron distribution function $f(\boldsymbol{k}_\perp, t)$ can be defined by

$$g_0^<(\boldsymbol{k}_\perp, t) = g_0^>(\boldsymbol{k}_\perp, t) f(\boldsymbol{k}_\perp, t). \tag{27}$$

Unlike the KB ansatz, equation (27) is not associated with any approximation. This equation is nothing but the definition of a time-dependent distribution function $f(\boldsymbol{k}_\perp, t)$, which is determined by a kinetic equation obtained from the integral equation (25). In general, even for stationary transport problems the explicit time dependence in $f(\boldsymbol{k}_\perp, t)$ must be preserved, as it accounts for a characteristic interaction time, which gives rise to non-perturbative scattering corrections similar to the lifetime broadening. When this time dependence is neglected, as it is proposed by the generalized KB ansatz, the Dyson equations for $g_0^>$ and $g_0^<$ can be solved only approximately in the limit of vanishing scattering. As scattering-induced lifetime broadening is crucial for systems, whose unperturbed eigenstates are discrete, the validity of such an approximation has to be strongly questioned.

For the 1D Esaki–Tsu model, we obtain the following homogeneous integral equation for $f(t)$:

$$\int_{-\infty}^{\infty} \mathrm{d}t_1 g_0^>(t_1) g_0^>(t - t_1)[F^<(t_1) f(t_1) - F^>(t_1) f(t - t_1)] = 0 \tag{28}$$

which has to be solved under the condition $f(0) = 1$. In deriving equation (28), we neglected the dispersion of optical phonons and replaced the screened electron–phonon coupling matrix element by a constant $\omega_0^2\Gamma$. The functions $F^{\gtrless}(t)$ are given by

$$F^{\gtrless}(t) = \frac{2\pi}{\hbar^2} \frac{\omega_0^2\Gamma}{\sinh(\hbar\omega_0/2k_B T)} J_0^2\left(\frac{\Delta}{\hbar\Omega}\sin\frac{\Omega t}{2}\right)\cos\omega_0\left(t \mp \frac{\mathrm{i}\hbar}{2k_B T}\right). \tag{29}$$

For elastic scattering, we have $F^>(t) = F^<(t)$, and equation (28) is solved by $f(t) = 1$, which is in accordance with the generalized KB ansatz. However, as we will show in the next section, without any inelastic scattering the current vanishes. When inelastic scattering is taken into account, equation (28) no longer admits the trivial solution $f(t) = 1$. To calculate the distribution function in the presence of inelastic scattering, we switch to Fourier space and obtain, from equation (28), for the 1D model

$$\int_{-\infty}^{\infty} \mathrm{d}\omega' [F^<(\omega') g_0^>(\omega) g_0^<(\omega - \omega') - F^>(\omega') g_0^<(\omega) g_0^>(\omega - \omega')] = 0. \tag{30}$$

In order to solve this equation, a distribution function $f(\omega)$ in Fourier space is introduced by

$$g_0^<(\omega) = g_0^>(\omega) f(\omega). \tag{31}$$

The generalized KB ansatz would require $f(\omega) = 1$. Here we proceed without using this approximation. With equation (31) the integral equation (30) is expressed in terms of the distribution function $f(\omega)$ without any loss of generality. Calculating $F^{\gtrless}(\omega)$ from equations (29) and (18), from equation (30) we obtain

$$\sum_{l=-\infty}^{\infty} F_l\left(\frac{\Delta}{\hbar\Omega}\right)\{g_0^>(\omega + \omega_0 - l\Omega)[f(\omega + \omega_0 - l\Omega) - \exp(\hbar\omega_0/k_B T) f(\omega)]$$
$$+ g_0^>(\omega - \omega_0 - l\Omega)[f(\omega - \omega_0 - l\Omega)\exp(\hbar\omega_0/k_B T) - f(\omega)]\} = 0 \tag{32}$$

which has to be solved under the condition

$$\int \frac{\mathrm{d}\omega}{2\pi} g_0^>(\omega) f(\omega) = 1. \tag{33}$$

The difference equation (32) for the distribution function $f(\omega)$ agrees with the kinetic equation for the lateral distribution function of a 3D SL derived some years ago (cf equation (18) in [7]).

This analogy is nearly perfect as in our earlier density-matrix approach the quantity $g_0^>$ is replaced by a theta function, which is nothing but the DOS of the lateral, 2D carrier motion. The agreement of both kinetic equations seems to be accidental in spite of the dissimilarity of the involved distributions. In our former approach, the lateral distribution function $n(\boldsymbol{k}_\perp)$ counted the field-dependent carrier population along directions perpendicular to the electric field, whereas $f(\omega)$ has a dynamical origin and is associated with the finite scattering duration. This frequency dependence of the distribution function has no counterpart in the density-matrix approach.

In the limit of vanishing miniband width ($\Delta \to 0$), equation (32) has an exact, field-independent solution

$$f(\omega) = \frac{2\hbar\sqrt{U}/k_B T}{I_1(2\hbar\sqrt{U}/k_B T)} \exp\left(\frac{\hbar\omega}{k_B T}\right) \tag{34}$$

where the normalization condition (33) has already been accounted for. It relates the distribution function to the parameters characterizing the main scattering events responsible for the lifetime broadening (in our case the coupling constant U of the impurity scattering). In equation (34), I_1 is the modified Bessel function. When a finite miniband width has to be considered, equation (32) can be solved as in our previous work [7], either numerically or analytically, by means of some asymptotic approximations.

From the distribution function $f(\omega)$ and equation (31), the time-dependent Keldysh Green function $g_0^<(t)$ is obtained by an inverse Fourier transformation

$$g_0^<(t) = \frac{1}{1 - \mathrm{i}tk_B T/\hbar} \frac{I_1((1 - \mathrm{i}tk_B T/\hbar)2\hbar\sqrt{U}/k_B T)}{I_1(2\hbar\sqrt{U}/k_B T)} \tag{35}$$

where $g_0^<(t)$ is complex and oscillates in time. Under the condition $2\hbar\sqrt{U}/k_B T \ll 1$, the difference between $g_0^<(t)$ and $g_0^>(t)$ becomes vanishingly small. The exact result (35) has to be compared with the solution of the problem derived within the pole approximation and by exploiting the generalized KB ansatz. As mentioned earlier, in this case we have $f(t) = 1$ or $g_0^<(t) = g_0^>(t)$. From equation (16), we get $g_0^>(t) = \exp(-H(s = 0)|t|)$, which is inserted into equation (17). For narrow minibands ($\Delta \to 0$) and dominant impurity scattering, we obtain for the scattering rate $H(s = 0) = \sqrt{U}$. The result $g_0^<(t) = g_0^>(t) = \exp(-\sqrt{U}|t|)$ has the typical form of a damping term that has often been used in transport studies. Its time dependence deviates even qualitatively from the exact solutions (22) and (35), which do not allow the definition of any relaxtion time. This underlines the importance of quantum corrections calculated beyond the generalized KB ansatz for the considered system, in which the energy spectrum is discrete, when scattering is absent.

5. Current density

The current density along the SL-axis is calculated from the stationary electron distribution function according to

$$j_z = -en \sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) \frac{\partial g^<(\boldsymbol{k}, t = 0)}{\partial k_z} \tag{36}$$

where n is the electron density. This equation has been derived by integration by parts and relates the current to the collision integral, when the quantity $\partial g^<(\boldsymbol{k}, t = 0)/\partial k_z$ is replaced by the right-hand side of the kinetic equation (A1). Under the condition $\Omega\tau \gg 1$, we will keep only the $l = 0$ Fourier coefficient in the collision integral. For the 1D model, it follows from equation (A1) that

$$eE\frac{\partial}{\partial k_z}g^{<}(k_z,t=0)=\hbar\sum_{q_z\lambda}\int_0^\infty \mathrm{d}t_1[R(k_z,q_z,t_1)-R(k_z,q_z,-t_1)]$$
$$\times[D^{<}_{q_z\lambda}(t_1)g_0^{<}(t_1)g_0^{>}(-t_1)-D^{>}_{q_z\lambda}(t_1)g_0^{>}(t_1)g_0^{<}(-t_1)] \tag{37}$$

with

$$R(k_z,q_z,t_1)=\exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^{t_1}\mathrm{d}\tau\left[\varepsilon\left(k_z+q_z+\frac{eE}{\hbar}\tau\right)-\varepsilon\left(k_z+\frac{eE}{\hbar}\tau\right)\right]\right\}. \tag{38}$$

If there was only elastic scattering, the current would vanish, because in this case $D^{>}_{q_z\lambda}(t_1)=D^{<}_{q_z\lambda}(t_1)$ and $g_0^{>}(t)=g_0^{<}(t)$. Inelastic scattering gives rise to a non-vanishing current contribution, which is mainly determined by the time dependence of the Keldysh Green functions $g_0^{>}(t)$ and $g_0^{<}(t)$.

To derive the final expression for the current density, the q_z and k_z integrals are calculated. Considering equation (38) and the periodicity of the k_z integral, we obtain the exact result

$$\sum_{q_zk_z}\varepsilon(k_z)[R(k_z,q_z,t)-R(k_z,q_z,-t)]=\sum_{l=-\infty}^{\infty}l\hbar\Omega F_l\left(\frac{\Delta}{\hbar\Omega}\right)\mathrm{e}^{\mathrm{i}l\Omega t} \tag{39}$$

where F_l is given by equation (19). In our previous paper [7] these quasi-momentum integrals were calculated within an approximation that only become exact in the limit of vanishing lifetime broadening.

From equations (36)–(39), we obtain our final result for the current density valid in the high-field region, when $\Omega\tau\gg 1$

$$j_z=\frac{4\pi en\omega_0^2\Gamma d}{\sinh(\hbar\omega_0/2k_BT)}\sum_{l=-\infty}^{\infty}lF_l\left(\frac{\Delta}{\hbar\Omega}\right)\mathrm{Re}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}l\Omega t}\cos\left(\omega_0t+\mathrm{i}\frac{\hbar\omega_0}{2k_BT}\right)g_0^{>}(t)g_0^{<}(t). \tag{40}$$

Another instructive form for the current density is derived from equation (40) by switching to the Fourier space and using (31)

$$\frac{j_z}{j_0}=\sum_{l=-\infty}^{\infty}lF_l\left(\frac{\Delta}{\hbar\Omega}\right)\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}g_0^{>}(\omega)g_0^{>}(\omega+\omega_0+l\Omega)[(N_0+1)f(\omega)-N_0f(\omega+\omega_0+l\Omega)] \tag{41}$$

where $j_0=4\pi en\omega_0\Gamma d$ is a field-independent reference current density and N_0 is the Bose–Einstein distribution function of optical phonons. This representation allows a clear physical interpretation within the hopping transport picture with the hopping length ld, the hopping probability $F_l(\Delta/\hbar\Omega)$ and the field-dependent combined DOS. The term $(N_0+1)f(\omega)$ describes the dominating hopping along the field direction due to phonon emission, whereas phonon absorption $[N_0f(\omega+\omega_0+l\Omega)]$ leads to a negative current contribution. The phonon-induced transport is governed by a thermal distribution function $f(\omega)$ given by equation (34). This refers to a transport regime, where the thermalization time is much shorter than a characteristic hopping time. In general, these two timescales determine the frequency dependence of the distribution function. For an arbitrary ratio of these two times, equation (32) allows the calculation of $f(\omega)$. When the characteristic hopping time is not sufficiently large (i.e., when Δ is not extremely small), the thermodynamic equilibrium distribution (34) is not a solution of the kinetic equation. In this case, the hopping transport becomes non-Markovian because the transition probability at a given time depends on former hops.

The representation (41) of the current density allows a clear discrimination between the hopping and band transport regime. At high electric fields, when $\Omega>\sqrt{U}$, the carrier transport proceeds by phonon-induced tunnelling transitions. Without any inelastic scattering, the carriers move back and forth, which does not result in any net current. In contrast, at low fields, when $\Omega < \sqrt{U}$, even elastic scattering leads to a delocalization of WS states and to the occurrence of a finite current. At these low-field strengths the hopping transport picture is not adequate and our approximation, to keep only the lowest $l = 0$ Fourier component in equation (13) is no longer valid.

It is interesting to compare equation (40) with an expression for the current obtained within the pole approximation and on the basis of the generalized KB ansatz. In this approximation, which corresponds to our former approach [7, 16], we have $g_0^<(t) = g_0^>(t) = \exp(-\sqrt{U}|t|)$ and obtain from equation (40) the temperature-independent result

$$\frac{j_z}{j_0} = \sum_{l=-\infty}^{\infty} lF\left(\frac{\Delta}{\hbar\Omega}\right)\frac{2\omega_0\sqrt{U}}{4U + (l\Omega - \omega_0)^2}. \tag{42}$$

Figure 1 shows the relative current density j_z/j_0 calculated from (40) (solid curves) and (42) (dashed curves), respectively. The miniband width for the upper curves is two times larger than for the lower ones. Pronounced electro-phonon resonances appear at field strengths $E = \hbar\omega_0/led$ denoted by thin vertical lines. Despite the simultaneous appearance of these interesting quantum transport resonances, which are rapidly smoothed out by collision broadening, the results calculated from (40) and (42) even differ qualitatively. The rigorous quantum kinetic approach leads to pronounced gaps, where the current exactly vanishes, unless scattering on acoustic phonons or the dispersion of optical phonons is considered. These windows of inhibited transport are due to the hopping character of carrier motion. In a real SL, Coulomb interaction and scattering on acoustic phonons smear out these gaps and one expects current minima instead. These minima have a complete other origin than the antiresonances studied by Lyanda–Geller and Leburton [19–21]. They showed that acoustic phonons with the wavelength nd (with n being an integer number) do not cause intersite transitions because the corresponding matrix element turns out to be zero. Consequently, the current vanishes at certain single field strengths as long as lifetime broadening is neglected and the hopping transitions are restricted to nearest neighbours. Antiresonances as predicted by Lyanda–Geller and Leburton [19, 20] have been studied experimentally in [22].

A second peculiarity exists in the current–voltage characteristic at field strengths below 10 kV cm^{-1}, when the miniband width becomes lower than the energy of optical phonons. The dashed curve calculated within the pole approximation and the KB ansatz still exhibits a $1/E$ dependence as expected from a quasi-classical picture. In contrast, the exact quantum kinetic current density (solid curve) approaches zero, as it is expected for phonon-induced hopping under the condition $\Delta/\hbar\omega_0 < 1$, when the quasi-classical transport model is not adequate. This expected crossover from quasi-classical to hopping transport with decreasing $\Delta/\hbar\omega_0$ is only satisfactorily described by our complete quantum kinetic approach leading to equation (40).

The temperature dependence of our exact solution (40) and the result (42), obtained by using the KB ansatz, also differ significantly from each other. Quite similar to narrow-band semiconductors [4], where the electron distribution function is constant, the current is independent of temperature, when in the 1D model the approximation $f(t) = 1$ is used leading to equation (42). The exact solution (40) behaves quite differently. Its temperature dependence is similar to ones of a 3D SL, where the lateral distribution function plays an essential role [7]. The function $f(\omega)$ introduces a strong dependence on temperature. For narrow minibands ($\Delta/\hbar\omega_0 \ll 1$) and weak scattering ($\sqrt{U}/\omega_0 \ll 1$), hopping transport prevails, giving rise to a phonon-induced increase of the current at low temperatures until it reaches saturation. The behaviour becomes more complex and strongly field dependent, when the scattering-induced

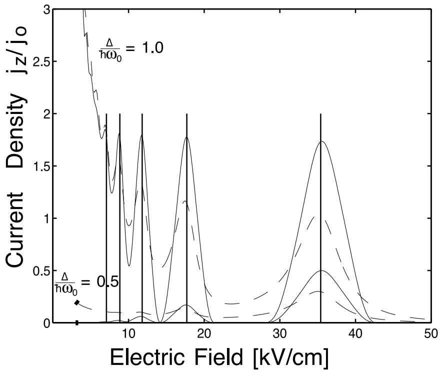

Figure 1. The field dependence of the relative current density j_z/j_0 for $\Delta/\hbar\omega_0 = 1$ (upper curves) and 0.5 (lower curves). The solid and dashed curves have been calculated from equations (40) and (42), respectively. Other parameters are $\sqrt{U}/\omega_0 = 0.05$, $\hbar\omega_0/k_BT = 5$, and $d = 10$ nm.

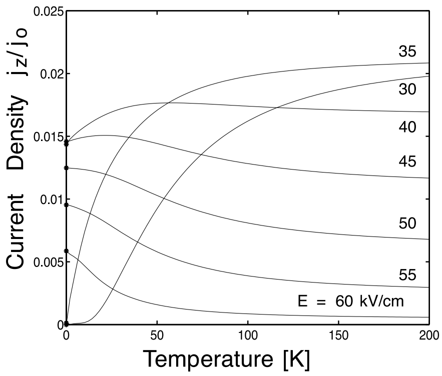

Figure 2. Temperature dependence of the relative current density j_z/j_0 for $\Delta/\hbar\omega_0 = 0.2$ and $\sqrt{U}/\omega_0 = 0.2$. The electric field strength is incremented by 5 kV cm^{-1} steps between 30 and 60 kV cm^{-1} as indicated.

bandwidth is not much smaller than the energy of optical phonons. An example shows figure 2 for $\sqrt{U}/\omega_0 = 0.2$ and $\Delta/\hbar\omega_0 = 0.2$. The curves are calculated from equation (40) for different electric field strengths. Interesting is the appearance of a crossover from an activated hopping-like transport at 30 and 35 kV cm^{-1} to a more band-like transport regime, where the current decreases with increasing temperature. The crossover appears at about $eEd = \hbar\omega_0$. Above this field strength the carrier transport loses its resonant character and becomes similar to band transport. Below the field strength $E = \hbar\omega_0/ed$, resonant phonon-induced transitions between neighbouring WS levels drive the current and lead to a hopping-like temperature characteristics. As in our previous approach [7], the current exhibits a non-analytic behaviour at $T = 0$. In this limit, we obtain from equation (35) $g_0^<(t) = \exp(-2\mathrm{i}\sqrt{U}t)$, and from (40)

$$\frac{j_z}{j_0} = \frac{\omega_0}{\sqrt{U}} \sum_{l=-\infty}^{\infty} l F_l\left(\frac{\Delta}{\hbar\Omega}\right) \Theta\left(1 - \left|\frac{2\sqrt{U} - l\Omega + \omega_0}{2\sqrt{U}}\right|\right) \sqrt{1 - \left(\frac{2\sqrt{U} - l\Omega + \omega_0}{2\sqrt{U}}\right)^2}. \tag{43}$$

Data calculated from this equation are shown in figure 2 by asterisks. According to equation (43), the current density calculated from equation (43) exhibits antisymmetric peaks around renormalized resonance positions located at $2\sqrt{U} - l\Omega + \omega_0 = 0$.

The current–voltage characteristic calculated with the same set of parameters as in figure 2 is shown in figure 3. Again the solid and dashed curves are calculated from equations (40) and (42), respectively. For the considered miniband width ($\Delta/\hbar\omega_0 = 0.2$) the $l = 1$ resonance dominates, whereas all other resonances at $leEd = \hbar\omega_0$ with $l > 1$ are strongly reduced by the factor $F_l(\Delta/\hbar\Omega)$. In contrast to the dashed curve calculated from equation (42), the exact result (40) accounts for the fact that hopping transport becomes impossible both at low electric fields and when E becomes larger than $(4\sqrt{U} + \hbar\omega_0)/ed$. The strong discrepancy between the dashed and solid curves in figure 3 again stresses our conclusion that a quantum mechanical treatment of transport in SLs with narrow minibands must go beyond the generalized KB ansatz.

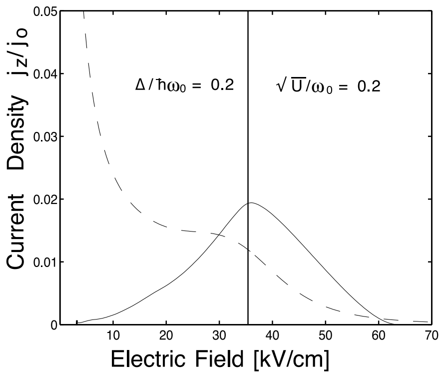

Figure 3. The field dependence of the relative current density j_z/j_0 calculated from equations (40) (solid curve) and (42) (dashed curve) for $\hbar\omega_0/k_BT = 5$, $\Delta/\hbar\omega_0 = 0.2$, and $\sqrt{U}/\omega_0 = 0.2$.

6. Summary

SL transport has been studied within a rigorous quantum kinetic approach on the basis of the Kadanoff–Baym–Keldysh non-equilibrium Green function theory. We focused on SLs, whose eigenstates are completely discrete when scattering is absent. Such QBSLs can be realized by a quantizing magnetic field aligned parallel to the SL-axis or by a periodic array of quantum dots. Starting from the Dyson equation and exploiting the symmetry properties of the correlation functions, equations for the Keldysh Green functions $G^{\gtrless}$ have been derived. Exact analytical solutions have been found for 1D SLs with a narrow miniband width, subject to a strong electric field ($\Omega\tau > 1$). These exact solutions differ even qualitatively from results, which are compatible with the density-matrix approach, and which are obtained by making use of the generalized KB ansatz and the pole approximation for $G^{>}$. This exciting finding stresses the importance of the double-time nature of correlation functions for the studied system. It provides an interesting example, which demonstrates that an unsophisticated usage of the density-matrix approach is not sufficient for describing the quantum transport physics. We arrived at the conclusion that it is absolutely necessary to go beyond the generalized KB ansatz within the double-time Green function approach when QBSL transport is treated.

The DOS depends non-analytically on the coupling constant and exhibits band edges, which prevent run-away effects. The scattering-induced energy band is slightly modified by an electric field, which gives rise to additional weak sidebands.

Essential for the carrier statistics is the fact that the distribution function depends explicitly on time even for the stationary transport. This time variable accounts for a finite duration of the interaction, describing the scattering-induced decay of the electronic states. Its influence on the distribution function is described by the non-equilibrium Green function approach beyond the generalized KB ansatz. In this paper, we demonstrated that quantum effects, which are traditionally not considered in the density-matrix approach, play an essential role in the transport of QBSLs. With respect to the time dependence of the Keldysh Green functions, we found that they do not fall off exponentially, as in former approaches, but oscillate accompanied by a power-law decrease of the amplitude.

The field-dependent transport in SLs with narrow minibands exhibits hopping character. Under the condition of small collisional broadening, real gaps are predicted to appear in the current–voltage characteristics, unless scattering on acoustic phonons or the phonon dispersion are taken into account. The appearance of these transport gaps are a manifestation of its hopping nature. Starting with SLs, whose miniband width Δ is larger than $\hbar\omega_0$, there is a crossover from a region, where the current decreases with increasing field as $1/E$, to hopping transport, when Δ becomes smaller than $\hbar\omega_0$. Hopping is not possible, when the energy gain of carriers in the electric field is not sufficient to permit phonon-induced transitions.

The hopping nature of the transport is also manifest by its temperature dependence, which is mainly governed by the non-equilibrium distribution function $f(\omega)$ calculated beyond the generalized KB ansatz. In dependence on the miniband width, the scattering strength, and the electric field, we found a complex temperature characteristics, which has no counterpart in results derived from the density-matrix approach.

Finally, let us point out that there are also other periodic nanostructures, whose bare energy spectrum is discrete. We can imagine that our approach is useful for studying quantum transport in such structures, too.

Acknowledgments

The authors acknowledge discussions with J P Leburton and Y Lyanda-Geller. This work was supported by the Deutsches Zentrum für Luft- und Raumfahrt.

Appendix

In this appendix, a kinetic equation for $g^<(\boldsymbol{k}, t)$ is derived from the Dyson equation (1). To this end equations (3), (4), (6) and (8) are inserted into (1) to get an equation for $g^<$. For the considered non-degenerate electron gas it is sufficient to retain only terms on the right-hand side of the resulting equation, which contain the product $g^<g^>$. Manipulations of the τ-integrals allow a simplification of the exponents introduced by equation (6). We obtain

$$
\begin{aligned}
&e\boldsymbol{E}\nabla_{\boldsymbol{k}} g^<(\boldsymbol{k}, t)\\
&\quad = \hbar \sum_{\boldsymbol{q}\lambda} \Bigg\{ \int_0^\infty \mathrm{d}t_1 \Bigg[P^<(\boldsymbol{kq}|t-t_1, t) g^< \left(\boldsymbol{k} + \boldsymbol{q} - \frac{e\boldsymbol{E}}{2\hbar} t_1, t - t_1 \right) \\
&\qquad \times g^> \left(\boldsymbol{k} + \frac{e\boldsymbol{E}}{2\hbar}(t - t_1), t_1 \right) - Q^>(\boldsymbol{kq}|t_1, t) g^> \left(\boldsymbol{k} + \boldsymbol{q} + \frac{e\boldsymbol{E}}{2\hbar}(t - t_1), t_1 \right) \\
&\qquad \times g^< \left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar} t_1, (t - t_1) \right) \Bigg] \\
&\qquad - \int_{-\infty}^0 \mathrm{d}t_1 \Bigg[P^>(\boldsymbol{kq}|t_1, t) g^> \left(\boldsymbol{k} + \boldsymbol{q} - \frac{e\boldsymbol{E}}{2\hbar}(t - t_1), t_1 \right) g^< \left(\boldsymbol{k} + \frac{e\boldsymbol{E}}{2\hbar} t_1, t - t_1 \right) \\
&\qquad - Q^<(\boldsymbol{kq}|t - t_1, t) g^< \left(\boldsymbol{k} + \boldsymbol{q} + \frac{e\boldsymbol{E}}{2\hbar} t_1, t - t_1 \right) g^> \left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar}(t - t_1), t_1 \right) \Bigg] \Bigg\}
\end{aligned}
\tag{A.1}
$$

with

$$
\begin{aligned}
P^{\gtrless}(\boldsymbol{kq}|t_1, t) = D^{\gtrless}_{\boldsymbol{q}\lambda}(t_1) \exp \Bigg\{ \frac{\mathrm{i}}{\hbar} \int_0^{t_1} \mathrm{d}\tau \Bigg[\varepsilon \left(\boldsymbol{k} + \boldsymbol{q} - \frac{e\boldsymbol{E}}{2\hbar} t + \frac{e\boldsymbol{E}}{\hbar} \tau \right) \\
- \varepsilon \left(\boldsymbol{k} - \frac{e\boldsymbol{E}}{2\hbar} t + \frac{e\boldsymbol{E}}{\hbar} \tau \right) \Bigg] \Bigg\}
\end{aligned}
\tag{A.2}
$$

and

$$
Q^{\gtrless}(\boldsymbol{kq}|t_1, t) = D^{\gtrless}_{\boldsymbol{q}\lambda}(t_1) \exp \Bigg\{ \frac{\mathrm{i}}{\hbar} \int_0^{t_1} \mathrm{d}\tau \Bigg[\varepsilon \left(\boldsymbol{k} + \boldsymbol{q} + \frac{e\boldsymbol{E}}{2\hbar} t - \frac{e\boldsymbol{E}}{\hbar} \tau \right)
$$

$$-\varepsilon\left(\boldsymbol{k}+\frac{e\boldsymbol{E}}{2\hbar}t-\frac{e\boldsymbol{E}}{\hbar}\tau\right)\Bigg]\Bigg\}. \tag{A.3}$$

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