Light-induced drift in semiconductor heterostructures: Microscopic theory

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We have developed a consistent microscopic theory of light-induced drift (LID) effect in semiconductor heterostructures. The strongly nonequilibrium nature of LID dictated our use of the Baym-Kadanoff-Keldysh's field-theoretical technique. We have found qualitative features of LID, including singularities in its spectrum and the reversal of current with temperature and light frequency associated with intersubband scattering. These effects should be experimentally observable. $[$0163-1829(99)03111-2]$

Effect of light-induced drift (LID) has been predicted for $gases¹$ as a physical implementation of an idea of Maxwell's demon, where a laser light selectively excites molecules within some velocity range and changes their translational motion, which results in a macroscopic motion of gas. The velocity-selective excitation is due to energy-momentum conservation (Doppler effect). The effect of the excitation on translational motion is due to collision-frequency (momentum-relaxation) dependence on an internal state of a molecule. One can think of LID as a result of extra friction introduced selectively for molecules moving at a given velocity. A close counterpart, LID of electrons in semiconductors in magnetic field, has been proposed² and observed.³ In that case the Landau-level state of an electron plays the role of an internal state of a molecule. A similar effect, called photon drug effect (PDE), has been suggested by Grinberg and Luryi 4.5 for electrons in semiconductor quantum structures and later observed. 6 For this type of PDE, statedependent relaxation of electrons is due to emission of optical phonons rather than elastic scattering. A closer counterpart of LID has been predicted for quantum wells^{7,8} based on *elastic* collisions of electrons with impurities, which depends on a state of electrons in the well. Elastic collisions have an advantage of causing less dephasing of internal states and, consequently, preserving a narrow line shape and high selectivity of excitation in velocity. We will arbitrarily use the term LID rather than PDE for the class of effects mentioned above.

By its mere physical nature, LID is based on the interdependence between the translational relaxation and excitation. Therefore it is very sensitive to relaxation processes, and their consistent description is required to obtain a qualitatively correct theory, not mentioning quantitative precision. A density-matrix technique with relaxation constants has been used in^{7,8} and in significant number of papers that followed (see, e.g., Refs. 9 and 10). However, that approach has an inherent drawback: while the electron confinement in a quantum structure and its interaction with light is taken into account microscopically, *via* a Hamiltonian, various relaxation and scattering processes are treated phenomenologically, *via* rate constants of the collision term.

In this paper we employ Baym-Kadanoff-Keldysh's nonequilibrium Green-function technique.^{12–17} This allows us to consistently treat collisions and relaxation microscopically and obtain a closed analytical result revealing new features of LID in quantum wells, which should be experimentally observable. These features are singularity in the spectrum associated with collision-induced transitions in the well and possible reversal of the LID current with temperature and photon energy. The Baym-Kadanoff-Keldysh's technique also solves a principal problem caused by time-dependence of the electromagnetic part of Hamiltonian. An oscillating optical field generates a strongly nonequilibrium state that renders equilibrium field-theoretical techniques¹¹ inapplicable.

A system under consideration consists of electrons confined in a 2D quantum well subjected to an external field **E** $\mathbf{E}_{\mathbf{q}}e^{i\mathbf{q}\mathbf{r}-i\omega_{q}t}$ + c.c. of an electromagnetic wave. Electrons interact with stationary impurities *via* a potential $U(\mathbf{r},z)$ $=\sum_{i}u(\mathbf{r}-\mathbf{r}_{i},z-z_{i})$, where (\mathbf{r}_{i},z_{i}) is a coordinate of a *j*th impurity, and $u(\mathbf{r},z)$ is a potential of one impurity. We set the quantum well to be in the *xy*-plane. All vectors (q, r, \ldots) are in this plane except for E_q that is normal to it. Given resonant nature of the effect, we will restrict our consideration to only two lowest states (subbands) in the well. We are using a system of units where $\hbar = c = 1$. The Hamiltonian of the system is

$$
H = \sum_{\mathbf{p}, \alpha} (\xi_{\mathbf{p}} + \varepsilon_{\alpha}) a_{\alpha, \mathbf{p}}^{\dagger} a_{\alpha, \mathbf{p}} + \sum_{\mathbf{p}, \alpha, \beta} (a_{\alpha, \mathbf{p}+\mathbf{q}}^{\dagger} a_{\beta, \mathbf{p}} V_{\alpha \beta}(t) + \text{H.c.})
$$

+
$$
\sum_{\alpha, \beta} \int \hat{\psi}_{\alpha}^{\dagger}(\mathbf{r}, z) U(\mathbf{r}, z) \hat{\psi}_{\beta}(\mathbf{r}, z) d^2 \mathbf{r} dz.
$$
 (1)

Here a^{\dagger} and *a* are electron creation and annihilation operators, $\alpha, \beta = 1,2$ denote subbands, ε_{α} are the energies of the levels in the well (subband offsets), **p** and **q** are 2d momenta of electron and photon, ξ_p is the kinetic energy of the electron measured from the Fermi energy, $\xi_p = \mathbf{p}^2/2m - \mu$, where *m* is the effective mass of the particle, $V_{\alpha\beta}(t) = Me^{i\omega_q t}$, where $M = -e z_{\alpha\beta} E_{\mathbf{q}}$, is the matrix element of the interaction with light, $z_{\alpha\beta} = \int \psi_{\alpha}^{*}(z)z\psi_{\beta}(z)dz$ is the dipole matrix element of the particle, and $\psi_{\alpha,\beta}(z)$ are the envelope wave functions for the well. The electron field operator is defined as $\hat{\psi}_{\alpha}(\mathbf{r},z) = \hat{\psi}_{\alpha}(\mathbf{r})\psi_{\alpha}(z)$, where $\hat{\psi}_{\alpha}(\mathbf{r}) \equiv \sum_{\mathbf{p}} a_{\alpha,\mathbf{p}} e^{i\mathbf{p}\mathbf{r}}/\sqrt{S}$ with *S* as the area of the well in the *xy* plane. To obtain closed analytical results, we will assume that the impurity potential is factorized $u(\mathbf{r},z) = v(\mathbf{r})f(z)$.

An important property (see, e.g., Refs. $14,15$) of the formal theory of nonequilibrium Green functions is that the perturbation expansion has the *same structure* as the $T=0$ equilibrium expansion. As a trade-off, instead of a single time-ordered Green function, one has to work with a matrix Green function that has four-components,

$$
\mathbf{G}_{\alpha\beta}^{<}(\mathbf{r},t) = i \langle \hat{\psi}_{\beta}^{\dagger}(0,0) \hat{\psi}_{\alpha}(\mathbf{r},t) \rangle,
$$

$$
\mathbf{G}_{\alpha\beta}^{>}(\mathbf{r},t) = -i \langle \hat{\psi}_{\alpha}(\mathbf{r},t) \hat{\psi}_{\beta}^{\dagger}(0,0) \rangle,
$$

$$
\mathbf{G}_{\alpha\beta}^{a,r}(\mathbf{r},t) = \mp \theta(\mp t) (\mathbf{G}_{\alpha\beta}^{>}(\mathbf{r},t) - \mathbf{G}_{\alpha\beta}^{<}(\mathbf{r},t)),
$$
 (2)

where $\langle \cdots \rangle$ denotes quantum averaging and statistical averaging over Gibbs ensemble with temperature *T* and over random positions of impurities (scatterers). Here and below, a bold-face notation is used for Green's functions that correspond to the full Hamiltonian (1), while $G^{a,r}, G^>$, and $G^<$ denote Green's functions in the zero order in electromagnetic field **Eq**, but completely taking into account scattering from impurities. The LID current in the second order in \mathbf{E}_{q} (the lowest order in which the effect appears) is expressed as

$$
\mathbf{j} = -i\frac{2e}{m}\sum_{\alpha} \int \frac{d\omega}{2\pi} \int \mathbf{p} \mathbf{G}_{\alpha\alpha}^{<(2)}(\mathbf{p}, \omega) \frac{d^2 \mathbf{p}}{(2\pi)^2},\qquad(3)
$$

where $\mathbf{G}^{<(2)}$ is the corresponding second-order lesser Green's function (exact with respect to the scattering).

The retarded, advanced, and lesser components of a product of two matrix Green functions is given by 14

$$
(\mathbf{G}_1\mathbf{G}_2)^{r,a} = \mathbf{G}_1^{r,a}\mathbf{G}_2^{r,a}, (\mathbf{G}_1\mathbf{G}_2)^{\leq} = \mathbf{G}_1^{r}\mathbf{G}_2^{\leq} + \mathbf{G}_1^{\leq}\mathbf{G}_2^{a}.
$$
 (4)

Products involving three or more matrix Green functions (or self-energies) can be expanded by recursion of these rules. A known procedure for averaging over positions of impurities¹¹ applied to a matrix Green function in non-equilibrium theory yields formally the same Dyson-type equation as in the *T* $=0$ theory,

$$
G_{\alpha\alpha}(\mathbf{p},\omega) = G_{\alpha\alpha}^{(0)}(\mathbf{p},\omega) + G_{\alpha\alpha}^{(0)}(\mathbf{p},\omega) \sum_{\beta} \int \frac{d^2 \mathbf{p}'}{(2\pi)^2} n
$$

$$
\times v |(\mathbf{p} - \mathbf{p}')|^2 f_{\alpha\beta,\beta\alpha} G_{\beta\beta}(\mathbf{p}',\omega) G_{\alpha\alpha}(\mathbf{p},\omega). \tag{5}
$$

Here $G^{(0)}$ is a matrix Green function without impurities, *n* is a 2*d* concentration of impurities, $v(\mathbf{p})$ is the Fourier transform of the impurity potential, and $f_{\alpha\beta,\sigma\delta}$ $\equiv \langle \int dz \psi_\alpha(z) \psi_\beta(z) f(z-z_i) \int dz' \psi_\sigma(z') \psi_\delta(z') f(z'-z_i) \rangle_{z_i},$ where $\langle \cdots \rangle_{z_i}$ is an average over distribution of the impurity atoms along the *z*-axis.

Equation (5) is obtained in the "ladder" approximation, 11 where we sum only those diagrams that do not contain intersecting impurity lines. The relative smallness of the neglected "intersecting" diagrams can be estimated 11 as $\sim 1/(\bar{\epsilon}\tau)$, where $\bar{\epsilon} \simeq \max(\mu, T)$ is a characteristic kinetic energy, and τ is the average time between collisions of an electron with impurities. Also we neglect the diagrams that contain $G_{\alpha\beta}$ with $\alpha \neq \beta$, which lack a resonant enhancement that $G_{\alpha\alpha}(p)$ has near the pole $\omega + \varepsilon_{\alpha} - \xi_p \sim 1/\tau$. Smallness

FIG. 1. Definition and diagrammatic equation for $\Gamma_{21}(p)$ $+q$,*q*). A solid line with indices α and *p* corresponds to a matrix Green function $G_{\alpha\alpha}(p)$, momentum-energy three-vectors p, p', and *q* denote $p = (\mathbf{p}, \omega), p' = (\mathbf{p}', \omega)$, and $q = (\mathbf{q}, \omega_q)$, a dotted impurity line corresponds to a constant $nv_0^2 f_{11,22}$, and a wave photon line corresponds to *M*.

of diagrams containing G_{12} or G_{21} with respect to those containing only G_{11} or G_{22} is also on order of $1/(\bar{\epsilon}\tau)$.

For the sake of simplicity, we assume that the impurity potential $v(\mathbf{r})$ has small characteristic width, $\delta r \ll 1/\sqrt{m\tilde{\epsilon}}$. Hence, we can consider the Fourier transform entering Eq. (5) to be a constant, $v(\mathbf{p}-\mathbf{p}')=v_0 \equiv \int d^2\mathbf{r}v(\mathbf{r})$. To obtain an equation for, e.g., advanced component of the matrix Green function, one needs to apply the Langreth's rules (4) to a product of three Green functions. Further solution of this equation is similar to the $T=0$ theory,¹¹ yielding

$$
G_{\alpha\alpha}^{a,r}(\mathbf{p},\omega) = \frac{1}{\omega - \varepsilon_{\alpha} - \xi_{\mathbf{p}} \mp i/2\tau_{\alpha}}.\tag{6}
$$

Here we neglected small corrections $\sim 1/\tau$ to the real part of the denominator. The times τ_{α} ($\alpha=1,2$) and τ_{e} (to be used later) are defined as

$$
\tau_2 = [nmv_0^2(f_{22,22} + f_{21,12})]^{-1}, \quad \tau_e = [nmv_0^2 f_{11,22}]^{-1},
$$

$$
\tau_1 = \tau_{10} + \theta(\omega + \mu - \varepsilon_2)(\tau_{11} - \tau_{10}),
$$
 (7)

where $\tau_{11} \equiv [nmv_0^2(f_{11,11} + f_{12,21})]^{-1}$, and τ_{10} $\equiv [nmv_0^2 f_{11,11}]^{-1}$. In what follows we assume for simplicity that all three times are the same order of magnitude, $\tau_1, \tau_2, \tau_e \sim \tau$. We will also set $\varepsilon_1 = 0$ and, correspondingly, $\varepsilon_2 = \varepsilon$, where ε is the intersubband excitation energy. Note that the time τ_1 depends on ω as given by the θ function in Eqs. (7) . This reflects the fact that an electron can be scattered by an impurity from the first to second well state only if it has enough energy. Such process becomes important at sufficiently large temperature, $T \gtrsim \varepsilon - \mu$. Similarly to Ref. 15, the lesser Green function can be obtained in the form

$$
G_{\alpha\alpha}^{<}(\mathbf{p},\omega) = \frac{n_{\omega}i/\tau_{\alpha}}{(\omega - \varepsilon_{\alpha} - \xi_{\mathbf{p}})^{2} + (1/2\tau_{\alpha})^{2}},
$$
(8)

where $n_{\omega} = (e^{\omega/T} + 1)^{-1}$ is the Fermi-Dirac distribution.

We define a matrix vertex function of an absorbed photon $\Gamma_{21}(p+q,p)$ by a diagrammatic equation shown in Fig. 1. Advanced, retarded and lesser components of $\Gamma_{21}(p+q,p)$ can be extracted by using the Langreth's rules (4) . An advanced (retarded) component of the vertex function $\Gamma_{21}(p)$ $+q$,*p*) is not renormalized by impurity scattering due to causality: all poles of G^a and Γ^a , or G^r and Γ^r in loops lie in the same lower, or upper half-plane of variable $\xi_{\bf p'}$. Specifically, $\Gamma_{21}^{a,r}(p+q,p) = MG_{22}^{a,r}(p+q)G_{11}^{a,r}(p)$.

The lesser component of $\Gamma_{21}(p+q,p)$ obeys an equation

FIG. 2. Diagrammatic expression for $\mathbf{G}^{<(2)}(p)$.

$$
\Gamma_{21}^{<}(p+q,p) = MG_{22}^{<}(p+q)G_{11}^{a}(p) + MG_{22}^{r}(p+q)
$$

× $G_{11}^{<}(p) + G_{22}^{r}(p+q)AG_{11}^{a}(p)$, (9)

where $A = \int d^2 \mathbf{p}'/(2\pi)^2 n v_0^2 f_{11,22} \Gamma_{21}^{\leq}(p' + q, p')$. Deriving Eq. (9) , we took into account that terms proportional to $\int d\mathbf{p}' \Gamma_{21}^{a,r}(p'+q,p')$ vanish due to causality. Equation (9) can be integrated yielding

$$
A = M(n_{\omega} - n_{\omega + \omega_q})/\tau_e D(\omega),
$$

$$
D(\omega) = \left[2(\omega + \mu)\frac{q^2}{m} - \left(\epsilon - \omega_q - \frac{i}{2\tau_1} - \frac{i}{2\tau_2}\right)^2\right]^{1/2} - \frac{1}{\tau_e},
$$

(10)

where τ_e is defined by Eq. (7). Similarly, for an emitted photon we have $\Gamma_{12}^{<}(p,p+q) = -(\Gamma_{21}^{<}(p+q,p))^{*}$, and $\Gamma_{12}^{a,r}(p,p+q) = MG_{11}^{a,r}(p)G_{22}^{a,r}(p+q).$

A diagrammatic expression for the matrix Green's function $\mathbf{G}^{(2)}$ (3) is given in Fig. 2. Deriving this, we neglect diagrams that have at least one impurity line connecting the two external electron lines. Contributions of such diagrams to $\mathbf{G}^{<(2)}$ depend only on $|\mathbf{p}|$ and vanish after integration over d^2 **p**. At the same time it is important to emphasize that sum of such diagrams diverges. One can convince himself that the resulting diverging contribution is proportional to the total time of the interaction with the electromagnetic field. This divergence would have cut off if one introduced an irreversible population-relaxation process from the excited state in the well that would lead to establishment of a stationary equilibrium state. We emphasize again that a specific form of diagrams in the diverging sum does not matter, because they do not contribute to the current.

The last diagram in Fig. 2 vanishes due to causality. For the same reason, the only terms to survive are those where the integral over \mathbf{p}' contains the lesser vertex function. Consequently, an expression for $\mathbf{G}_{11}^{<(2)}$ reduces to

$$
G_{11}^{<(2)}(p) = M^2(G_{11}(p)G_{22}(p+q)G_{11}(p))^{\leq} + G_{11}^r(p)
$$

× $G_{22}^r(p+q)AMG_{11}^a(p) - G_{11}^r(p)MA^*$
× $G_{22}^a(p+q)G_{11}^a(p)$. (11)

An expression for $\mathbf{G}_{22}^{<(2)}$ can be obtained similarly. Substituting $\mathbf{G}^{<(2)}$ into Eq. (3), we obtain a general expression for the LID current

$$
\mathbf{j} = \frac{\mathbf{q}}{\mathbf{q}^2} \frac{2 \, e \, m}{\pi} M^2 F(\omega_q),\tag{12}
$$

FIG. 3. Spectral contour $F(\omega_q)$ of the LID current as a function of light frequency ω_q for the case of small collision broadening (large Doppler shift), calculated from Eq. (13) . The values of collision times τ_{10}, τ_{11} , and τ_2 are shown in units of τ_0 $\equiv (m/2\mu_0\epsilon^2)^{1/2}$, where μ_0 is the Fermi energy at low temperature. We set $\tau_e = (1/\tau_{11} - 1/\tau_{10})^{-1}$, which is the case for $f(z) \propto \delta(z)$. We choose the following values of parameters realistic for a GaAs/ AlGaAs quantum well: $\mu_0 = 6$ meV corresponding to electron density 8.5×10^{10} cm⁻², $\varepsilon = 30$ meV, and $m = 0.07 m_e$.

where the dimensionless spectral contour of LID is

$$
F(\omega_q) \equiv \text{Im} \int_{-\mu}^{\infty} (n_{\omega} - n_{\omega + \omega_q}) (\tau_1 - \tau_2)
$$

$$
\times \left[\frac{1}{2\tau_1} + \frac{1}{2\tau_2} - \frac{1}{\tau_e} + i(\varepsilon - \omega_q) \right] \frac{1}{D(\omega)} d\omega.
$$
(13)

One can see that the LID contour $F(\omega_q)$ is an odd function of $\omega_a - \varepsilon$, which is a general signature of LID. We emphasize that the structure of current (13) differs dramatically from the corresponding result of the density matrix approach [cf. Eqs. (3) and (4) in Ref. 7].

For illustration we consider two limiting cases that differ by a value of Doppler shift $\Delta \omega_D = |\mathbf{q}| \sqrt{\frac{Z}{\epsilon}}/m$ with respect to the collision width τ^{-1} . First, in the limit $\Delta \omega_D \gg \tau^{-1}$, a large Doppler shift causes a highly selective excitation of a beam of electrons with a narrow spread of **p**. Features of LID in this limit are illustrated in Fig. 3. At zero temperature, the current vanishes for $|\omega_q - \epsilon| = |{\bf q}| \sqrt{2\mu/m}$ where only electrons at Fermi surface contribute. At finite temperatures, there is no edge and LID exists for any detuning. A singularity in the derivative of $F(\omega_a)$ occurs at a temperature-independent detuning $|\omega_q - \epsilon| = |\mathbf{q}| \sqrt{2 \varepsilon / m}$, where there is just enough kinetic energy of a Dopplerselected electron to open up a new channel of scattering that includes the transitions $|1\rangle \rightarrow |2\rangle \rightarrow |1\rangle$ in the well [cf. Eq. (7). This singularity has been missing in earlier theories.^{4,5,7–10} Another previously unknown qualitative feature of LID is that the effect may reverse its sign with increase of detuning or temperature. This is due to the fact that for the relation between relaxation times chosen ($\tau_{10} > \tau_2$) $>\tau_{11}$, the difference $\tau_1-\tau_2$ changes its sign with electron energy. Thus, the friction due to collisions for the electrons in the excited state $|2\rangle$ is greater than that in the ground state

FIG. 4. Same as in Fig. 3, but for the case of large collision broadening (small Doppler shift).

 $|1\rangle$ at low energies, but is smaller at higher energies. Such a relation between relaxation times may be tailored by properly chosen doping profile across the well.

The opposite case, where the Doppler shift is small compared to the collision broadening, $\Delta \omega_D \ll \tau^{-1}$, is illustrated

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in Fig. 4. We see that spectral contours of LID are significantly broadened and they have no singularities. The magnitude of the LID currents is much smaller than in Fig. 3. This implies that the scattering from impurities has an effect of the phase relaxation for the spectral contour. However, the analytical form of $F(\omega_a)$ is significantly different from that in the relaxation-constant model of Refs. 7–10.

In conclusion, we have developed a consistent microscopic theory of LID in semiconductor quantum wells. A strongly nonequilibrium nature of LID dictates our use of Baym-Kadanoff-Keldysh's field-theoretical technique. We have obtained a closed analytical expression for LID current that is significantly different from the previously-known results of the semi-phenomenological density-matrix theory based on relaxation-constant model. We have predicted new qualitative features of the LID effect that are experimentally verifiable. One of those is a singularity in its spectral contour related to the opening of a scattering channel with excitation into a higher subband. The other is a reversal of the LID current with light frequency and temperature also related to the intersubband scattering.

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